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Cédric Bernardin · François Golse · Patrícia Gonçalves · Valeria Ricci · Ana Jacinta Soares *Editors*

From Particle Systems to Partial Differential Equations

International Conference, Particle Systems and PDEs VI, VII and VIII, 2017–2019

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Preface

This volume gathers the proceedings of the last three editions of the international conference on Particle Systems and Partial Differential Equations (PSPDE), namely the edition of 2017 at the University of Nice Sophia Antipolis, Nice, France, from 27th November to 1st December; the edition of 2018, at the University of Palermo, Italy, from 19th to 23rd November and, finally, the edition of 2019, at IST, University of Lisbon, from 2nd to 6th December.

These meetings were intended to bring together distinguished active researchers working in the areas of probability and partial differential equations, in view of presenting and discussing their latest scientific results in both areas. Many young researchers from different countries attended the meetings and had the opportunity to interact with other participants and follow the mini-courses included in the conference programme.

This volume includes eighteen contributed papers authored by conference participants on interesting and valuable topics in the fields of probability theory, partial differential equations and kinetic theory.

We believe that this volume will be of great interest to probabilists, analysts and also to those mathematicians with a general interest in mathematical physics, stochastic processes and differential equations, as well as those physicists whose work intersects with statistical mechanics, statistical physics and kinetic theory.

We would like to take this opportunity to extend our thanks to all the speakers, and to the participants, for contributing to the success of this series of meetings.

Lastly, we wish to gratefully acknowledge the financial support provided by the following sponsors:

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We really hope that you enjoy reading this book!

Nice, France — Cédric Bernardin
Palaiseau, France — François Golse
Lisbon, Portugal — Patrícia Gonçalves
Palermo, Italy — Valeria Ricci
Braga, Portugal — Ana Jacinta Soares
November 2020

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Brief Discussion of the L^r-Theory for the Boltzmann Equation: Cutoff and Non-cutoff

Ricardo J. Alonso

Abstract In this manuscript we go over the main ideas of the L^r-theory, with $r \in [1, \infty]$, for the homogeneous Boltzmann equation with Maxwell and hard potential kernels. A discussion for the cutoff and non-cutoff cases is presented in a concise manner. In the non-cutoff case the whole range of singularity is addressed.

Keywords Boltzmann equation · Propagation of norms · Regularity · Fractional diffusion

1 Introduction

We briefly discuss the main ideas around the L^r-theory of the Boltzmann equation in the so-called cutoff and non-cutoff cases. We restrict ourselves to the Maxwell and hard potential kernels.

Let us recall that the homogeneous Boltzmann equation is given by

$$\partial_t f(v) = Q_{\gamma,b}(f, f)(v)\,, \quad (t, v) \in \mathbb{R}^+ \times \mathbb{R}^d\,, \quad d \geq 2 \text{ is the dimension.} \tag{1}$$

The nature of the particle interaction is described in the collision operator $Q_{\gamma,b}$ and, more specifically, in its collision kernel

$$B(x, y) = x^\gamma\, b(y)\,, \quad \text{with } x \geq 0, \quad y \in [0, 1], \quad \gamma \in (-d, 1]\,.$$

The parameter $\gamma \in (-d, 1]$ is related to the nature of the kinetic potential. The potential is soft if $\gamma \in (-d, 0)$ and hard if $\gamma \in (0, 1]$. The case $\gamma = 0$ is addressed as Maxwell molecules. This parameter is in charge of the tail's behaviour of the solutions to the equation. In particular, the so-called generation of exponential tails

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for solutions to Eq. (1) happens when $\gamma > 0$. In this discussion we only consider the case $\gamma \in [0, 1]$ since the soft potential case requires a different approach.

The function $b(\cdot) > 0$ is called angular kernel and it is in charge of modelling the angular scattering properties of the particle interaction. In fact, the singular nature of this function divides the analysis into cutoff and non-cutoff cases. More precisely, we have that

$$\begin{aligned} &b \in L^1(\mathbb{S}^{d-1}) \ \text{ for the cutoff case, and} \\ &\sin^{d-2}\theta\, b(\cos\theta) \approx \frac{D}{\theta^{1+2s}}\,, \quad \theta \approx 0\,, \quad s \in (0,1) \quad \text{for the non-cutoff case}\,. \end{aligned} \tag{2}$$

The support of b is assumed in $[0, 1]$ thanks to a symmetrisation argument. The explicit expression of the collision operator is given by

$$\begin{aligned} Q_{\gamma,b}(f,g)(v) &= Q^+_{\gamma,b}(f,g) - Q^-_{\gamma,b}(f,g) \\ &:= \int_{\mathbb{R}^d}\int_{\mathbb{S}^{d-1}} f(v')g(v'_*)B(|u|,\hat{u}\cdot w)\mathrm{d}w\mathrm{d}v_* \\ &\qquad - f(v)\int_{\mathbb{R}^d}\int_{\mathbb{S}^{d-1}} g(v_*)B(|u|,\hat{u}\cdot w)\mathrm{d}w\mathrm{d}v_*\,, \end{aligned}$$

where the collisional variables are defined as

$$v' := v - u^-, \qquad v'_* := v_* + u^-, \qquad u := v - v_*, \qquad u^\pm := \frac{u \pm |u|w}{2}\,.$$

The scattering angle θ is defined as $\cos\theta := \hat{u}\cdot w$ with the understanding that unitary vectors are denoted as $\hat{u} := u/|u|$. The relevant initial data is assumed to be *nonnegative* and with finite mass and energy,

$$\int_{\mathbb{R}^d} f_0\langle v\rangle^2 \mathrm{d}v < \infty, \quad \text{where} \quad \langle v\rangle := \sqrt{1+|v|^2}. \tag{3}$$

It is well known that, under these conditions, the Boltzmann equation (1) has a unique weak solution $f(t, v) \geq 0$ that conserves mass, momentum and energy, see for instance [11, 15, 38, 43].

An important remark is that for the non-cutoff case $b \notin L^1(\mathbb{S}^{d-1})$, as a consequence $Q^\pm_{\gamma,b}$ are not finite quantities. In this way, the collision operator cannot be written separately as gain minus loss operators, that is, it must be kept as a whole

$$\begin{aligned} &Q_{\gamma,b}(f,g)(v) := \\ &\qquad \int_{\mathbb{R}^d}\int_{\mathbb{S}^{d-1}} \Big(f(v')g(v'_*) - f(v)f(v_*)\Big)B(|u|,\hat{u}\cdot w)\mathrm{d}w\mathrm{d}v_*\,. \end{aligned}$$

Such operator is well defined for sufficiently smooth functions f and g even for a singular b as described previously in (2) for the non-cutoff case. The techniques

presented here, cutoff and non-cutoff, are based on energy methods, thus, they exploit the weak formulation of the collision operator, namely, for any suitable test function $\psi := \psi(v)$

$$\begin{aligned}\int_{\mathbb{R}^d} Q_{\gamma,b}(f,g)(v)\psi(v)\mathrm{d}v = \int_{\mathbb{R}^d}\int_{\mathbb{R}^d}\int_{\mathbb{S}^{d-1}} f(v)g(v_*) \\ \times\Big(\psi(v')+\psi(v'_*)-\psi(v)-\psi(v_*)\Big)B(|u|,\hat{u}\cdot w)\mathrm{d}w\mathrm{d}v_*\mathrm{d}v\,.\end{aligned} \tag{4}$$

In the non-cutoff case, the weak formulation of the collision operator can be interpreted, to some extend, as an integration by parts of a fractional Laplacian operator.

2 The Cutoff Case

Propagation of L^r-norms for the Boltzmann equation with different degrees of cutoff in the scattering kernel b and weights in the norms has been of central interest to the community. Some papers dealing with such topic for the hard potential model $\gamma > 0$ are [5, 11, 13, 25, 39, 45, 47] for $r \in (1,\infty)$, [5, 11, 16, 19, 22, 28, 29] for $r = \infty$, and [45] with $r \in [1,\infty]$ for the Maxwell molecules model $\gamma = 0$. Propagation of exponentially weighted norms is more rare in the literature but can be found in [5, 11, 19, 28, 29]. See also [5, 10, 39] for similar results for propagation of Sobolev norms in the hard potential case.

2.1 Propagation of the L^r-Norm for the Cutoff Case

There are mainly three ingredients on which the propagation of Lebesgue norms in the cutoff case is based on. First, the gain part $Q^+_{\gamma,b}(f,g)$ of the collision operator enjoys compactness properties under cutting conditions on the collision kernel B. This observation has been used since the early stages of the development of the mathematical theory for the Boltzmann equation [22, 30, 31] and, in particular, in a series of influential papers [21, 27, 37, 39, 46]. This type of result is known in this context of Lebesgue norm propagation as *gain of integrability* for the gain collision operator. The following version of this result can be found in [9, 11].

Proposition 1 (Gain of integrability in L^r) *Let $r \geq 1$ and $d \geq 3$*

$$\begin{cases}\tilde{r} = \frac{d\,r}{r(d-1)+1}\,, \quad \theta = \frac{2}{r'} & \text{if } r \in [1,2]\,,\\ \tilde{r} = \frac{d\,r}{2d-1}\,, \quad \theta = \frac{2}{r} & \text{if } r \in [2,\infty)\,.\end{cases}$$

Fix $h \in L^{\tilde{r}}(\mathbb{R}^d)$, $\varepsilon > 0$, and assume a cutoff Maxwell potential

$$B(|u|, \hat{u} \cdot w) = \mathbf{1}_{|u| \geq \varepsilon}\, b(\hat{u} \cdot w)$$

with scattering kernel $b \in L^\infty(S^{d-1})$. *Then,*

$$||Q_B^+(g,h)||_{L^r} \leq \frac{C_d}{\varepsilon^{\frac{d-1}{2}\theta}} \|b\|_\infty \|g\|_{L^1} \left\|h\right\|_{L^{\tilde{r}}}. \tag{5}$$

Proposition 1 simply states that the L^r-norm of the gain operator can be controlled by a lower norm, since $\tilde{r} < r$, for particular cutoff kernels B.

Second, an idea inspired on the first, the decomposition of a general angular scattering kernel $b \in L^1(\mathbb{S}^{d-1})$ as

$$b = b^\infty + b_{res}\,, \qquad b^\infty\,,\ b_{res} \geq 0\,, \quad b^\infty \in L^\infty, \quad \|b_{res}\|_{L^1} \leq \varepsilon^\gamma\,,$$

and the decomposition of the kinetic part as

$$|u|^\gamma = |u|^\gamma \left(\mathbf{1}_{|u|<\varepsilon} + \mathbf{1}_{|u|\geq\varepsilon}\right).$$

Using such splitting on a general cutoff kernel B and some classical convolution-type estimates for the gain collision operator, see for instance [7, 8, 34], it is not difficult to arrive to an estimate of the following form.

Proposition 2 *Let* $\gamma > 0, b \in L^1(\mathbb{S}^{d-1})$, *and* $r \in (1, \infty)$. *For any* $\varepsilon > 0$ *the collision operator satisfies the following estimate*

$$\begin{aligned}\int_{\mathbb{R}^d} Q_\gamma^+(g,h)(v) h(v)^{r-1} \mathrm{d}v \leq\ & \varepsilon^\gamma\, C_d(b)\, \|\langle\cdot\rangle^{\gamma(1+1/r)} g\|_{L^1} \|\langle\cdot\rangle^{\gamma/r} h\|_{L^r}^r \\ & + C_d(b,\varepsilon) \|\langle\cdot\rangle^{\gamma(1+1/r)} g\|_{L^1} \|\langle\cdot\rangle^{\gamma/r} h\|_{L^1}^{1-\delta} \|\langle\cdot\rangle^{\gamma/r} h\|_{L^r}^{r-1+\delta},\end{aligned} \tag{6}$$

where $\delta = \frac{r}{r-1}\frac{\tilde{r}-1}{\tilde{r}} = \frac{r'}{\tilde{r}'} \in (0,1)$.

In other words, the gain collision operator for general B has two components, one that is large but compact related to the kernel parts b^∞ and $|u|^\gamma \mathbf{1}_{|u|\geq\varepsilon}$ controlled by the latter right term in (6), and a second that is singular but small related to b_{res} and $|u|^\gamma \mathbf{1}_{|u|<\varepsilon}$ controlled by the former right term. This idea of decomposing the collision operator in compact-singular parts has been very successful for the spectral analysis of the linearised collision operator as well, see [33] and references therein. Also, observe that the L^1-norms in (6) are controlled by conservation of mass and energy for $\gamma \in [0,1]$. Now that Proposition 2 has provided a suitable upper bound for the gain collision operator, the last ingredient is a suitable lower bound for the loss part of the collision operator. Indeed, it is possible to control from below the loss collisional operator using only the physical properties of conservation of mass and energy, and propagation of a higher-than-energy moment for solutions. For the cutoff hard potential and Maxwell cases, both cutoff and non-cutoff, the propagation of higher moments is a well known fact, see for instance [6, 17, 18, 20, 40, 42, 44]. The explicit control that one can show is given by the inequality

$$\big(f(t,\cdot) * |\cdot|^\gamma\big)(v) \geq c(f_0)\langle v\rangle^\gamma\,, \qquad \gamma \in [0,1]\,, \tag{7}$$

for an explicit constant $c(f_0) > 0$ depending on mass, energy, and a higher-than-energy moment of f_0. An elementary proof of this estimate can be found in [11, 12]. Proposition 2 and the lower bound (7) can then be used in an energy estimate type of argument that leads to the following theorem. Details of this discussion, including the Maxwell case, can be found in [11, 13].

Theorem 1 (Propagation of Lebesgue norms cutoff case) *Fix $r \in (1,\infty)$ and assume that the initial data satisfies $f_0 \in L^1_2 \cap L^r$. Let f be a solution to (1) with $\gamma \in [0,1]$ and $b \in L^1(S^{d-1})$. Then,*

$$\frac{1}{r}\frac{\mathrm{d}}{\mathrm{d}t}\|f\|_{L^r}^r \leq C(b,\,f_0) - c(f_0)\|f\|_{L^r}^r.$$

As a consequence, it follows that

$$\sup_{t\geq 0}\|f(t)\|_{L^r} \leq \max\left\{\|f_0\|_{L^r}, \left(\frac{C(b,\,f_0)}{c(f_0)}\right)^{1/r}\right\}.$$

We observe here that Theorem 1 can not be applied to $r = \infty$. The reason is that the constant $C(b,\,f_0)$ degenerates as $r \to \infty$ because $\delta \to 1$ in (6). The case $r = \infty$ is treated separately.

2.2 Propagation of the L^∞-Norm for the Cutoff Case

Propagation of the L^∞-norm is a byproduct of the L^2-norm propagation. We will see in the next section that this is the case for the non-cutoff case as well. A first proof of an estimation on the essential supremum for solutions was given in [16] under more stringent cutoff on b, say bounded. The approach that we present here here can be found in [11].

A key observation is to invoke classical convolution-type inequalities for the Boltzmann equation using the idea of the decomposition $b = b^\infty + b_{res}$. More specifically one has the estimates

$$\begin{aligned} \|Q^+_{|\cdot|^\gamma,b^\infty}(f,g)\|_{L^\infty(\mathbb{R}^d)} &\leq C_{b^\infty}\|\langle\cdot\rangle^\gamma f\|_{L^2(\mathbb{R}^d)}\|\langle\cdot\rangle^\gamma g\|_{L^2(\mathbb{R}^d)}\,, \qquad \text{and} \\ Q^+_{|\cdot|^\gamma,b_{res}}(f,g)(v) &\leq C\|b_{res}\|_{L^1(\mathbb{S}^{d-1})}\|f\|_{L^\infty(\mathbb{R}^d)}\|\langle\cdot\rangle^\gamma g\|_{L^1(\mathbb{R}^d)}\,\langle v\rangle^\gamma\,, \end{aligned} \tag{8}$$

which are particular applications of the so-called Young inequality for the gain collision operator [7, 8, 34]. With estimates (8) at hand, let us now implement an energy estimate argument to control such L^∞-norm for solutions to the Boltzmann equation (1). Considering a initial datum such that $\|\langle\cdot\rangle^\gamma f_0\|_{L^2(\mathbb{R}^d)} < \infty$, propagation of L^2-norms implies that

$$\sup_{t\geq 0}\|\langle\cdot\rangle^{\gamma} f(t,\cdot)\|_{L^2(\mathbb{R}^d)} < C(f_0)\,.$$

The upper bound (8) and lower bound (7) give us that

$$\begin{aligned}\partial_t f(v) &= Q^+_{|\cdot|^\gamma,b}(f,f)(v) - f(v)\big(f * |\cdot|^\gamma\big)(v)\\ &= Q^+_{|\cdot|^\gamma,b^\infty}(f,f)(v) + Q^+_{|\cdot|^\gamma,b_{res}}(f,f)(v) - f(v)\big(f * |\cdot|^\gamma\big)(v)\\ &\leq C_{b^\infty}\|\langle\cdot\rangle^{\gamma} f\|^2_{L^2(\mathbb{R}^d)}\\ &\quad + C\|b_{res}\|_{L^1(\mathbb{S}^{d-1})}\|f\|_{L^\infty(\mathbb{R}^d)}\|\langle\cdot\rangle^{\gamma} f\|_{L^1(\mathbb{R}^d)}\langle v\rangle^{\gamma} - c(f_0)f(v)\langle v\rangle^{\gamma}\,.\end{aligned} \tag{9}$$

Recall that one can take $\|b_{res}\|_{L^1(\mathbb{S}^{d-1})}$ in (9) sufficiently small. Thus, choosing b_{res} such that

$$C\|b_{res}\|_{L^1(\mathbb{S}^{d-1})}\|f\|_{L^1_2(\mathbb{R}^d)}\langle v\rangle^{\gamma} \leq \frac{c(f_0)}{2}\,,$$

it follows that

$$\partial_t f(t,v) \leq C(f_0) + \tfrac{c(f_0)}{2}\|f(t)\|_{L^\infty(\mathbb{R}^d)}\langle v\rangle^{\gamma} - c(f_0)f(t,v)\langle v\rangle^{\gamma}\,. \tag{10}$$

Now, integrate estimate (10) in $t \geq 0$ to obtain that

$$\begin{aligned} f(t,v) &\leq f_0(v)e^{-c_o\langle v\rangle^{\gamma} t}\\ &\qquad + \int_0^\infty e^{-c(f_0)\langle v\rangle^{\gamma}(t-s)}\Big(C(f_0) + \tfrac{c(f_0)}{2}\|f(s)\|_{L^\infty(\mathbb{R}^d)}\Big)\langle v\rangle^{\gamma}\mathrm{d}s\\ &\leq \|f_0\|_{L^\infty(\mathbb{R}^d)}\\ &\qquad + \Big(C(f_0) + \tfrac{c(f_0)}{2}\sup_{t\geq 0}\|f(t)\|_{L^\infty(\mathbb{R}^d)}\Big)\langle v\rangle^{\gamma}\int_0^\infty e^{-c(f_0)\langle v\rangle^{\gamma}(t-s)}\mathrm{d}s\\ &\leq \|f_0\|_{L^\infty(\mathbb{R}^d)} + C(f_0) + \tfrac{1}{2}\sup_{t\geq 0}\|f(s)\|_{L^\infty(\mathbb{R}^d)}\,, \quad \text{a.e. in } v\in\mathbb{R}^d\,.\end{aligned}$$

We can compute the essential supremum in $v \in \mathbb{R}^d$ and, then, the supremum in time of $f(t,v)$ to conclude that

$$\sup_{t\geq 0}\|f(t,\cdot)\|_{L^\infty(\mathbb{R}^d)} \leq 2\|f_0\|_{L^\infty(\mathbb{R}^d)} + C(f_0)\,.$$

Finally, one notices that if $f_0 \in L^1_2 \cap L^\infty$, then $f_0 \in L^2_\gamma$ which completes the argument.

3 The Non-cutoff Case

Arguments related to integrability properties of solutions for the non-cutoff Boltzmann equation have a different angle with respect to that of the cutoff case and it is inspired by arguments from parabolic PDE's. The approach that we present here, based in [5], is also of the type of energy estimate which exploit the weak formulation of the equation. Some papers treating well-posedness for the equation and estimates involving L^r-norm and Sobolev analysis for the homogeneous equation are [1, 2, 5, 25, 29, 41, 43]. The theory for the equation in the non-cutoff context has been developed through a mix of papers involving analysis of the collision operator [1, 18, 25, 26, 41, 43] and its application to estimates for solutions [2–4, 14, 23, 32, 35]. In particular, [1] was seminal after interpreting quantitatively the collision operator in the Maxwell case as a fractional diffusion

$$Q(g, f) \sim c(g)(-\Delta)^s f + \text{lower order terms.}$$

Indeed, it was in [1] and later refined in [2] where the key coercivity estimate

$$\begin{aligned} \mathscr{D}(g, F) := \int_{\mathbb{R}^d}\int_{\mathbb{R}^d}\int_{\mathbb{S}^{d-1}} g(v_*)\big(F(v') - F(v)\big)^2 |u|^\gamma b(\hat{u}\cdot\sigma)\mathrm{d}\sigma\,\mathrm{d}v_*\mathrm{d}v \\ \geq c_g \|\langle\cdot\rangle^{\gamma/2} F\|_{H^s}^2 - C_g \|\langle\cdot\rangle^{\gamma/2} F\|_2^2 \end{aligned} \tag{11}$$

was proven. Here the constants C_g, c_g depend only on the physical quantities mass, energy and entropy of g. We also note that a sophisticate approach related to the treatment of general fractional nonlinear parabolic equations has been successfully used recently in the non-cutoff Boltzmann context in [29, 36, 41] to find various regularity estimates for solutions of the inhomogeneous and homogeneous Boltzmann equations.

Since the constants in (11) depend also on the entropy of g, it will be handy for this section to define the space

$$\begin{aligned} \mathscr{U}(D_0, E_0) = \Big\{ g \ \text{ measurable } : \ g \geq 0\,, \ \int_{\mathbb{R}^d} g\,\mathrm{d}v \geq D_0\,, \\ \int_{\mathbb{R}^d} g\,(1 + |v|^2 + \ln g)\,\mathrm{d}v \leq E_0 \Big\}\,, \end{aligned}$$

and to assume that $f_0 \in \mathscr{U}(D_0, E_0)$. Conservation of mass and energy and dissipation of entropy implies that the solution to the Boltzmann equation $f(t) \in \mathscr{U}(D_0, E_0)$ at all times.

3.1 The L^r-Theory for the Non-cutoff Case

The idea that is considered here is explained easily noting the standard heat equation's L^r-energy estimate

$$\partial_t \| f \|_r^r + \tfrac{4}{r'} \| \nabla f^{r/2} \|_2^2 = 0 \,, \qquad r > 1 \,.$$

This estimate gives directly a L^r-theory for the equation even though it is in nature a L^2-estimate: the secret is, after integration by parts, to understand the Dirichlet product $\langle \nabla f, \nabla f^{r-1} \rangle_{L^2}$. The link between the L^2 and L^r versions of such Dirichlet product for the collision operator is the following simple lemma.

Lemma 1 *For any* $\theta \geq 0$

$$\theta^{2/r'} - 1 \leq \frac{1}{r'} (\theta^2 - 1) - \frac{1}{\max\{r, r'\}} \big(\theta - 1\big)^2 \,, \qquad r \in (1, \infty] \,.$$

Equality is achieved in such estimate for the case $r = 2$.

With Lemma 1 at hand one can compute and estimate

$$\begin{aligned} F(v) \Big(F(v')^{r-1} - F(v)^{r-1} \Big) &= F(v)^r \left(\Big(\frac{F(v')^{r/2}}{F(v)^{r/2}} \Big)^{2/r'} - 1 \right) \\ &\leq F(v)^r \left(\frac{1}{r'} \Big(\frac{F(v')^r}{F(v)^r} - 1 \Big) - \frac{1}{\max\{r, r'\}} \Big(\frac{F(v')^{r/2}}{F(v)^{r/2}} - 1 \Big)^2 \right) \\ &= \frac{1}{r'} \Big(F(v')^r - F(v)^r \Big) - \frac{1}{\max\{r, r'\}} \Big(F(v')^{r/2} - F(v)^{r/2} \Big)^2 . \end{aligned}$$

Using the weak formulation of the collision operator (4) and the coercivity estimate (11) one proves the following estimate suited for the L^r-norm.

Proposition 3 *Let* $g \in \mathscr{U}(D_0, E_0)$, *F be sufficiently smooth,* $\gamma \in [0, 1]$, $s \in (0, 1)$, *and* $r \in (1, \infty)$. *Then,*

$$\begin{aligned} &\int_{\mathbb{R}^d} Q(g, F)(v) F^{r-1}(v) \mathrm{d}v \\ &\qquad \leq - \frac{c_g}{\max\{r, r'\}} \| \langle \cdot \rangle^{\gamma/2} F^{r/2} \|_{H^s}^2 + \frac{C_g}{r'} \| \langle \cdot \rangle^{\gamma/2} F^{r/2} \|_2^2 \,, \end{aligned}$$

where the constants c_g *and* C_g *depend on* D_0 *and* E_0.

Using Proposition 3 in an energy estimate type of argument for the Boltzmann equation (1) proves the differential inequality

$$X_r'(t) + c_r \, X_r^{\frac{1}{\theta}}(t) \leq C_r \,, \qquad r \in (1, \infty) \,, \quad \theta \in (0, 1) \,,$$

where $X_r(t) := \|f(t)\|_r^r$ with $f := f(t,\cdot)$ solution to (1). The constants C_r, c_r depend on D_0 and E_0, thus, conservation is essential in the whole argument. Such differential inequality proves the following result.

Theorem 2 (Generation/propagation Lebesgue's norms) *Let $\gamma \in [0,1]$ and $s \in (0,1)$, and assume $f_0 \in \mathscr{U}(D_0, E_0)$. Then,*

$$\|f(t)\|_r \le C_r\left(\frac{1}{t^{\frac{d}{2sr'}}} + 1\right), \quad r \in (1,\infty).$$

Here C_r depends on the physical quantities D_0 and E_0. Furthermore, if additionally $f_0 \in L^r(\mathbb{R}^d)$, then

$$\sup_{t\ge 0}\|f(t)\|_r \le \max\left\{\|f_0\|_r,\, C_r\right\}, \qquad r \in (1,\infty).$$

The reader observes that, in contrast to the cutoff case, the non-cutoff Boltzmann equation instantaneously generates the L^r-integrability for solutions due to the strong diffusion nature of the scatter.

3.2 The L^∞-Theory for the Non-cutoff Case

A classical approach in parabolic theory for finding regularity estimates is the level set method. In particular, it is possible to prove L^∞-norm appearance and/or propagation invoking an argument by De Giorgi [24]. Let us explain how this argument works in the context of the Boltzmann equation. Fix a level $K > 0$ and define

$$F_K(v) := F(v) - K, \quad \text{and} \quad F_K^+(v) := F_K(v)1_{\{F_K\ge 0\}}.$$

Note that

$$\begin{aligned}
&F(v)\Big(F_K(v')1_{\{F_K'\ge 0\}} - F_K(v)1_{\{F_K\ge 0\}}\Big)\\
&\quad = F_K(v)\Big(F_K(v')1_{\{F_K'\ge 0\}} - F_K(v)1_{\{F_K\ge 0\}}\Big)\\
&\qquad + K\Big(F_K(v')1_{\{F_K'\ge 0\}} - F_K(v)1_{\{F_K\ge 0\}}\Big)\\
&\quad = F_K(v)\Big(1_{\{F_K\ge 0\}} + 1_{\{F_K<0\}}\Big)\Big(F_K(v')1_{\{F_K'\ge 0\}} - F_K(v)1_{\{F_K\ge 0\}}\Big)\\
&\qquad + K\Big(F_K(v')1_{\{F_K'\ge 0\}} - F_K(v)1_{\{F_K\ge 0\}}\Big).
\end{aligned}$$

Using that

$$F_K(v)1_{\{F_K<0\}}\Big(F_K(v')1_{\{F'_K\geq 0\}}-F_K(v)1_{\{F_K\geq 0\}}\Big)$$
$$= F_K(v)1_{\{F_K<0\}}F_K(v')1_{\{F'_K\geq 0\}}\leq 0\,,$$

we conclude that

$$\begin{aligned}
&F(v)\Big(F_K(v')1_{\{F'_K\geq 0\}}-F_K(v)1_{\{F_K\geq 0\}}\Big)\\
&\quad\leq F_K(v)1_{\{F_K\geq 0\}}\Big(F_K(v')1_{\{F'_K\geq 0\}}-F_K(v)1_{\{F_K\geq 0\}}\Big)\\
&\qquad\qquad + K\Big(F_K(v')1_{\{F'_K\geq 0\}}-F_K(v)1_{\{F_K\geq 0\}}\Big)\\
&\quad=\tfrac{1}{2}\Big(F_K^+(v')^2-F_K^+(v)^2\Big)-\tfrac{1}{2}\Big(F_K^+(v')-F_K^+(v)\Big)^2+K\Big(F_K^+(v')-F_K^+(v)\Big)\,.
\end{aligned}$$

Consequently, using the weak formulation we deduce that

$$\begin{aligned}
&\int_{\mathbb{R}^d}Q(g,F)(v)F_K(v)1_{\{F_K\geq 0\}}\mathrm{d}v\\
&=\int_{\mathbb{R}^{2d}}\int_{\mathbb{S}^{d-1}}g(v_*)F(v)\Big(F_K(v')1_{\{F'_K\geq 0\}}-F_K(v)1_{\{F_K\geq 0\}}\Big)|u|^\gamma b(\hat{u}\cdot\sigma)\mathrm{d}\sigma\,\mathrm{d}v_*\mathrm{d}v\\
&\qquad\qquad\leq -\mathscr{D}(g,F_K^+)+\mathscr{J}_1(g,F_K^+)+\mathscr{J}_2(g,F_K^+)\,,
\end{aligned}$$

where

$$\begin{aligned}
\mathscr{D}(g,F_K^+)&:=\tfrac{1}{2}\int_{\mathbb{R}^{2d}}\int_{\mathbb{S}^{d-1}}g(v_*)\Big(F_K^+(v')-F_K^+(v)\Big)^2|u|^\gamma b(\hat{u}\cdot\sigma)\mathrm{d}\sigma\,\mathrm{d}v_*\mathrm{d}v\,,\\
J_1(g,F_K^+)&:=\tfrac{1}{2}\int_{\mathbb{R}^{2d}}\int_{\mathbb{S}^{d-1}}g(v_*)\Big(F_K^+(v')^2-F_K^+(v)^2\Big)|u|^\gamma b(\hat{u}\cdot\sigma)\mathrm{d}\sigma\,\mathrm{d}v_*\mathrm{d}v\,,\\
J_2(g,F_K^+)&:=K\int_{\mathbb{R}^{2d}}\int_{\mathbb{S}^{d-1}}g(v_*)\Big(F_K^+(v')-F_K^+(v)\Big)|u|^\gamma b(\hat{u}\cdot\sigma)\mathrm{d}\sigma\,\mathrm{d}v_*\mathrm{d}v\,.
\end{aligned}\tag{12}$$

Using the Cancellation Lemma introduced in [1, Sect. 3], it follows that

$$\begin{aligned}
&\mathscr{J}_1(g,F_K^+)\leq C\|b\|_1\|\langle\cdot\rangle^\gamma g\|_1\|\langle\cdot\rangle^{\gamma/2}F_K^+\|_2^2\,,\quad\text{and}\\
&\mathscr{J}_2(g,F_K^+)\leq C\|b\|_1\,K\,\|\langle\cdot\rangle^\gamma g\|_1\|\langle\cdot\rangle^\gamma F_K^+\|_1\,.
\end{aligned}$$

For the diffusive term $\mathscr{D}(g,F_K^+)$ we use, again, the coercivity estimate (11) to obtain that

$$D(g,F_K^+)\geq c_g\|\langle\cdot\rangle^{\gamma/2}F_K^+\|_{H^s}^2-C_g\|\langle\cdot\rangle^{\gamma/2}F_K^+\|_2^2\,,$$

for constants C_g, c_g depending only on D_0 and E_0. This proves the following estimate.

Proposition 4 *Take $g\in\mathscr{U}(D_0,E_0)$, F sufficiently smooth, $\gamma\in[0,1]$, and $s\in(0,1)$. Then,*

$$\int_{\mathbb{R}^d} Q(g,F)(v)F_K^+(v)dv \le -c_g\|\langle\cdot\rangle^{\gamma/2}F_K^+\|_{H^s}^2 + C_g\|\langle\cdot\rangle^{\gamma/2}F_K^+\|_2^2 + C_g\,K\,\|\langle\cdot\rangle^{\gamma}F_K^+\|_1\,,$$

where the constants c_g and C_g depends on D_0 and E_0.

Once a coercive estimate on level sets has been stablished, such as the one of Proposition 4, one can follow a classical argument defining an energy functional of the form

$$W_k := \tfrac{1}{2}\sup_{t\in[t_k,T]}\|f_k(t)\|_2^2 + c_0\int_{t_k}^{T}\|\langle\cdot\rangle^{\gamma/2}f_k(s)\|_{H^s}^2\mathrm{d}s\,,\qquad 0<t_*<T\,,$$

for fixed $t_* > 0$ and suitable increasing times $t_k > 0$ and levels $K_k > 0$

$$K_k := K\big(1-1/2^k\big)\,,\quad t_k := t_*\big(1-1/2^{k+1}\big)\,,\quad k=1,2,\dots\,,$$

and where $f_k := f_{K_k}^+$. Proposition 4 together with Sobolev embedding and interpolation[1] lead to an estimate of the form

$$\tfrac{1}{2}W_k \le \frac{2^{\frac{d+4s}{d}k}\,C}{K^{\frac{4s}{d}}}\Big(\frac{1}{t_*}+1\Big)W_{k-1}^{\frac{d+2s}{d}}\,. \tag{13}$$

The fact that the exponent in the right side is bigger that one (that is $\frac{d+2s}{d} > 1$) is essential to conclude that

$$W_k \to 0 \quad \text{as} \quad k\to\infty\,,$$

provided W_0 is finite and $K > 0$ is sufficiently large. An estimation of such K is given by

$$K \le C\Big(t_*^{-\frac{d}{2s}} + \sqrt{T}\Big)\,,\qquad 0<t_*<T\,.$$

Since $K_k \nearrow K$ and $t_k \nearrow t_*$ as $k\to\infty$, the fact that W_k vanishes in the limit imply that

$$\sup_{t\in[t_*,T]}\|f_K^+(t)\|_2 = 0\,,\quad \text{that is}\,,\quad f(t)\le K\quad\text{for}\quad t\in[t_*,T]\,. \tag{14}$$

This argument proves the appearance of the L^∞-norm based on the L^2-theory. The reader should notice that the fact that $s > 0$ is important and such a procedure would not work in the cutoff case. Setting $t_* = 0$ in previous argument also proves propagation of the L^∞-norm provided the initial datum is essentially bounded.

[1] Again, conservation plays an important role, in particular, the constant C depends on D_0 and E_0 in the recurrence (13).

Theorem 3 (Generation/propagation of L^∞-norm) *Let $\gamma \in [0,1]$ and $s \in (0,1)$, and assume $f_0 \in \mathscr{U}(D_0, E_0)$. Then,*

$$\|f(t)\|_\infty \le C\left(t^{-\frac{d}{2s}} + 1\right), \qquad t > 0\,, \tag{15}$$

where C depends on D_0, E_0. Furthermore, if additionally $f_0 \in L^\infty(\mathbb{R}^d)$ then,

$$\sup_{t\ge 0} \|f(t)\|_\infty \le \max\left\{2\|f_0\|_\infty,\ C\|\langle\cdot\rangle^2 f_0\|_1\right\}, \tag{16}$$

where C depends also on $\|f_0\|_2$.

Details of the proof can be found in [5].

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References

1. R. Alexandre, L. Desvillettes, C. Villani, B. Wennberg, Entropy dissipation and long-range interactions. Arch. Rational Mech. Anal. **152**, 327–355 (2000)
2. R. Alexandre, Y. Morimoto, S. Ukai, C.-J. Xu, T. Yang, Smoothing effect of weak solutions for the spatially homogeneous Boltzmann equation without angular cutoff. Kyoto J. Math. **52**(3), 433–463 (2012)
3. R. Alexandre, Y. Morimoto, S. Ukai, C.-J. Xu, T. Yang, The Boltzmann equation without angular cutoff in the whole space: qualitative properties of solutions. Arch. Rational Mech. Anal. **202**(2), 599–661 (2011)
4. R. Alexandre, Y. Morimoto, S. Ukai, C.-J. Xu, T. Yang, Regularizing effect and local existence for non-cutoff Boltzmann equation. Arch. Rational Mech. Anal. **198**, 39–123 (2010)
5. R. Alonso, Emergence of exponentially weighted L^p-norms and Sobolev regularity for the Boltzmann equation. Commun. Part. Differ. Equ. **44**(5), 416–446 (2019)
6. R. Alonso, J.A. Canizo, I. Gamba, C. Mouhot, A new approach to the creation and propagation of exponential moments in the Boltzmann equation. Commun. Part. Differ. Equ. **38**(1), 155–169 (2013)
7. R. Alonso, E. Carneiro, Estimates for the Boltzmann collision operator via radial symmetry and Fourier transform. Adv. Math. **223**(2), 511–528 (2010)
8. R. Alonso, E. Carneiro, I. Gamba, Convolution inequalities for the Boltzmann collision operator. Commun. Math. Phys. **298**, 293–322 (2010)
9. R. Alonso, I. Gamba, Gain of integrability for the Boltzmann collisional operator. Kinet. Relat. Model. **4**(1), 41–51 (2011)
10. R. Alonso, I.M. Gamba, Propagation of L^1 and L^∞ Maxwellian weighted bounds for derivatives of solutions to the homogeneous elastic Boltzmann equation. J. Math. Pures Appl. **89**, 575–595 (2008)
11. Alonso, R., Gamba, I., Revisiting the Cauchy problem for the Boltzmann equation for hard potentials with integrable cross section: from generation of moments to propagation of L^p-bounds. *In preparation.* (2019)
12. R. Alonso, I.M. Gamba, S.H. Tharkabhushaman, Convergence and error estimates for the Lagrangian based conservative spectral method for Boltzmann equations. SIAM J. Numer. Anal. **56**(6), 3534–3579 (2018)

13. R. Alonso, I.M. Gamba, M. Tasković, Exponentially-tailed regularity and decay rate to equilibrium for the Boltzmann equation. https://arxiv.org/abs/1711.06596
14. R. Alonso, Y. Morimoto, W. Sun, T. Yang, Non-cutoff Boltzmann equation with polynomial decay perturbations. Rev. Mat. Iberoamericana **37**(1) (2021)
15. L. Arkeryd, Stability in L^1 for the spatially homogeneous Boltzmann equation. Arch. Rational Mech. Anal. **103**, 151–167 (1988)
16. L. Arkeryd, L^∞-estimates for the space-homogeneous Boltzmann equation. J. Statist. Phys. **31**, 347–361 (1982)
17. A. Bobylev, Moment inequalities for the Boltzmann equations and application to spatially homogeneous problems. J. Statist. Phys. **88**(5–6), 1183–1214 (1997)
18. A. Bobylev, The theory of the nonlinear, spatially uniform Boltzmann equation for Maxwellian molecules. Sov. Sci. Rev. C. Math. Phys. **7**, 111–233 (1988)
19. A. Bobylev, I. Gamba, Upper Maxwellian bounds for the Boltzmann equation with pseudo-maxwell molecules. Kinet. Relat. Model. (2016)
20. A. Bobylev, I. Gamba, V. Panferov, Moment inequalities and high-energy tails for Boltzmann equations with inelastic interactions. J. Statist. Phys. **116**(5–6), 1651–1682 (2004)
21. F. Bouchut, L. Desvillettes, A proof of the smoothing properties of the positive part of Boltzmann's kernel. Rev. Mat. Iberoamericana **14**, 47–61 (1998)
22. T. Carleman, Problèmes mathématiques dans la théorie cinétique des gaz, Publ. Sci. Inst. Mittag-Leer. 2. Almqvist & Wiksells Boktryckeri Ab, Uppsala (1957)
23. Y. Chen, L. He, Smoothing estimates for Boltzmann equation with full-range interactions: spatially homogeneous case. Arch. Rational Mech. Anal. **201**(2), 501–548 (2011)
24. E. De Giorgi, Sulla differenziabilità e l'analiticità delle estremali degli integrali multipli regolari. Mem. Accad. Sci. Torino. Cl. Sci. Fis. Mat. Nat. **3**(3), 25–43 (1957)
25. L. Desvillettes, C. Mouhot, About L^p estimates for the spatially homogeneous Boltzmann equation. Ann. Inst. H. Poincaré Anal. Non Linéaire. **22**(2), 127–142 (2005)
26. L. Desvillettes, B. Wennberg, Smoothness of the solution of the spatially homogeneous Boltzmann equation without cutoff. Comm. Part. Diff. Equ. 29-1-2, 133–155 (2004)
27. R.J. DiPerna, P.L. Lions, On the Cauchy problem for Boltzmann equations: global existence and weak stability. Ann. Math. **130**, 321–366 (1989)
28. I.M. Gamba, V. Panferov, C. Villani, Upper Maxwellians bounds for the spatially homogeneous Boltzmann equation. Arch. Rat. Mech. Anal **194**, 253–282 (2009)
29. I.M. Gamba, N. Pavlović, M. Tasković, On pointwise exponentially weighted estimates for the Boltzmann equation. SIAM J. Math. Anal. **51**(5), 3921–3955 (2019)
30. H. Grad, Asymptotic theory of the Boltzmann equation. II, in *Rarefied Gas Dynamics* (Proc. 3rd Internat. Sympos., Palais de l'UNESCO, Paris, 1962), vol. I. Academic Press, New York, 26–59 (1963)
31. H. Grad, Principles of the kinetic theory of gases, in *Handbuch der Physik* (herausgegeben von S. Flügge), Bd. 12, Thermodynamik der Gase. Springer, Berlin, 205–294 (1958)
32. P. Gressman, R. Strain, Global classical solutions of the Boltzmann equation without angular cut-off. J. AMS **24**(3), 771–847 (2011)
33. M.P. Gualdani, S. Mischler, C. Mouhot, Factorization of non-symmetric operators and exponential H-theorem. Memoires de la Société Mathématique de France, 153, 137 pp (2018)
34. T. Gustafsson, Global L^p-properties for the spatially homogeneous Boltzmann equation. Arch. Rational Mech. Anal. **103**, 1–38 (1988)
35. F. Hérau, D. Tonon, I. Tristani, Regularization estimates and Cauchy theory for inhomogeneous Boltzmann equation for hard potentials without cut-off. Commun. Math. Phys. **377**, 697–771 (2020)
36. C. Imbert, L. Silvestre, The weak Harnack inequality for the Boltzmann equation without cut-off. J. Eur. Math. Soc. **22**, 507–592 (2020)
37. P.-L. Lions, Compactness in Boltzmann's equation via Fourier integral operators and applications I. J. Math. Kyoto Univ. **34**, 391–427 (1994)
38. S. Mischler, B. Wennberg, On the spatially homogeneous Boltzmann equation. Ann. Inst. H. Poincaré Anal. Non Linéaire. **16**(4), 467–501 (1999)

39. C. Mouhot, C. Villani, Regularity theory for the spatially homogeneous Boltzmann equation with cut-off. Arch. Rational Mech. Anal. **173**, 169–212 (2004)
40. M. Pavić-Čolić, M. Tasković, Propagation of exponential moments for the Kac equation and the Boltzmann equation for Maxwell molecules. Kinet. Relat. Models **11**(3), 597–613 (2018)
41. L. Silvestre, A new regularization mechanism for the Boltzmann equation without cut-off. Comm. Math. Phys. **348**(1), 69–100 (2016)
42. M. Tasković, R. Alonso, I.M. Gamba, N. Pavlović, On Mittag-Leffler moments for the Boltzmann equation for hard potentials without cutoff. SIAM J. Math. Anal. **50**(1), 834–869 (2018)
43. C. Villani, On a new class of weak solutions for the spatially homogeneous Boltzmann and Landau equations. Arch. Rat. Mech. Anal. **143**, 273–307 (1998)
44. B. Wennberg, Entropy dissipation and moment production for the Boltzmann equation. Jour. Stat. Phys. **86**(5/6), 1053–1066 (1997)
45. B. Wennberg, Stability and exponential convergence for the Boltzmann equation. Arch. Rational Mech. Anal. **130**, 103–144 (1995)
46. B. Wennberg, Regularity in the Boltzmann equation and the Radon transform. Comm. Part. Differ. Equ. **19**, 2057–2074 (1994)
47. B. Wennberg, Stability and exponential convergence in L^p for the spatially homogeneous Boltzmann equation. Nonlinear Anal. **20**, 935–964 (1993)

The Maxwell–Stefan Diffusion Limit of a Hard-Sphere Kinetic Model for Mixtures

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Abstract We study a kinetic model for non-reactive mixtures of monatomic gases with hard-sphere cross-sections under isothermal condition. By considering a diffusive scaling of the kinetic model and using the method of moments, we formally obtain from the continuity and momentum balance equations of the species, in the limit as the scaling parameter goes to zero, the Maxwell–Stefan diffusion equations, with explicit expressions for the diffusion coefficients.

Keywords Kinetic theory of gases · Maxwell–Stefan equations · Diffusion

1 Introduction

The study of diffusion phenomena is very important due to its varied uses in many fields, such as engineering, physics, biology, chemistry, etc. The most classical constitutive law used to describe diffusive transport was given by Fick in [9, 10]. Fick postulated that flux goes from higher concentration regions to lower concentration regions with a magnitude that is proportional to the concentration gradient. This proportionality relation between flux and concentration gradient postulated by Fick is predominantly used to model diffusion. In many situations, it provides accurate description of diffusive transport, while in others, it seems to be too simplistic (as in the case of multispecies/multicomponent mixtures) and hence cannot be used to describe diffusion in these cases.

The limitations of using Fick's constitutive relation to describe diffusion in multicomponent gaseous mixtures and some other situations have been shown experimentally, see for example [8, 14]. In the case of multicomponent gaseous mixtures, three distinct diffusion phenomena, referred to as osmotic diffusion, uphill or reverse diffusion and diffusion barrier were observed. These three types of diffusion phenomena cannot be described by the Fickian approach. More precisely, osmotic diffusion corresponds to a situation of diffusion without a gradient. Uphill or reverse diffusion

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refers to a situation in which flux goes from lower concentration regions to higher concentration regions. Diffusion barrier is a situation of diffusion in which flux is zero.

Due to the shortcomings of the Fick's constitutive relation in describing diffusion in multicomponent mixtures, a more general constitutive relation known as the Maxwell–Stefan (MS) equations [15, 18] is often used instead. The MS equations rely on the fact that the driving force of the species in a multicomponent mixture is in local equilibrium with the total inter-species drag/friction force. For a continuum physics approach to modeling diffusion using the MS equations, see, [20, 21].

In spite of the importance of the MS equations in describing diffusion in multi-species mixtures, its mathematical study is relatively new. In particular, [4, 6, 11] dealt with the formal derivation of diffusion models of MS type from a diffusive scaling of Boltzmann type equations for non-reactive multi-species mixtures, under isothermal condition (i.e. uniform in space and constant in time mixture temperature). The existence and uniqueness issues, as well as the long-time behaviour of solutions of the MS diffusion systems have been considered in [3, 5, 13]. The numerical study of MS equations has been considered in [16]. The derivation of a non-isothermal diffusion model of MS type from a kinetic model for non-reactive mixtures has been considered in [12]. The derivation of an isothermal reaction diffusion model of MS type from the simple reacting sphere (SRS) kinetic model has been considered in [1]. More precisely, from a scaling of the SRS kinetic model which corresponds to a situation where the dominant role in the evolution of the species is played by mechanical interaction, while chemical reactions are assumed to be slow enough to allow the surroundings to continually compensate for the difference in heat between the reactants and products. Here explicit expressions for the MS diffusion coefficients were obtained. The derivation of non-isothermal diffusion model of MS type from a kinetic model for a reactive mixture of polyatomic gases with a continuous structure of internal energy has been considered in [2]. More precisely, from a scaling where mechanical collisions are dominant while chemical reactions are slow. Here the MS diffusion coefficients are not explicit because a general cross-sections was considered.

The goal of this work is to follow the formal method of deriving macroscopic equations from the Boltzmann equation, presented in [19] and derive an isothermal diffusion model of MS type, with explicit expressions for the MS diffusion coefficients, as a hydrodynamic limit of a Boltzmann type model for non-reactive mixtures, with hard-sphere cross-sections. Also, the computations are given in detail in order to show some particular aspects and technicalities involved in the derivation. The main differences between this work and [4, 6, 11] are the kinetic models studied and the cross-sections considered. More precisely, [4, 11] considered general and analytic cross-sections, respectively, while [6] dealt with the case of Maxwellian molecules. These cross-sections present different levels of difficulty, particularly in the computation of the diffusion coefficients. Therefore, in each case, different strategies and techniques were adopted to help compute the diffusion coefficients. In the case of general cross-sections, in order to compute the diffusion coefficients, one has to use the weak form of the collision operator together with an expansion of the distribution

function with respect to the scaling parameter. In the end, the expression obtained for the diffusion coefficients is not explicit as it contains the integral over the sphere and the six-fold integrals with respect to the velocity variables. In the case of analytic cross-sections and Maxwellian molecules, only the weak form of the collision operator was used. In the end, explicit expressions for the diffusion coefficients were obtained. In the present work, a different strategy from those used in [4, 6, 11] was employed. More precisely, a property of the collision operators which is a consequence of the form of the distribution functions considered was used. In addition, the diffusion coefficients obtained in this work is different from those obtain in [4, 6, 11] because we have studied a different kinetic model and a different cross-section.

The rest of this work is organized as follows. In Sect. 2, we introduce the kinetic model for a non-reactive mixture with hard-sphere cross-sections. In Sect. 3, we introduce the scaled kinetic equation, its properties and the assumptions that will be needed in our analysis. In Sect. 4, we present the MS diffusion limit of the scaled kinetic equations. More precisely, we obtain the species continuity equations and the momentum balance equations for the species from the scaled kinetic equations. Finally, we present the asymptotic analysis of the species continuity and momentum balance equations towards the diffusion model of MS type. Section 5 is dedicated to our conclusions.

2 Kinetic Model

The starting point of our analysis is a system of Boltzmann-type equations that describe the evolution of a non-reactive mixture of N monatomic inert gases, A_i with $i = 1, 2, \ldots, N$. Particles in the mixture undergo elastic collisions of hard-sphere type. These elastic collisions occur between particles of the same species and between particles of different species. More precisely, in the absence of external forces, let $f_i := f(t, \boldsymbol{x}, \boldsymbol{v}_i) \geq 0$ be the unknown probability distribution function, representing the density of particles of species A_i which at time t are located at position $\boldsymbol{x}$ and have velocity $\boldsymbol{v}_i$, we will study the following Cauchy problem:

$$\begin{aligned} &\frac{\partial f_i}{\partial t} + \boldsymbol{v}_i \cdot \frac{\partial f_i}{\partial \boldsymbol{x}} = J_i + \sum_{\substack{s=1 \\ s \neq i}}^{N} J_{is}, \quad (t, \boldsymbol{x}, \boldsymbol{v}_i) \in \mathbb{R}_+ \times \mathbb{R}^3 \times \mathbb{R}^3, \ i = 1, 2, \ldots, N, \\ &f_i(0, \boldsymbol{x}, \boldsymbol{v}_i) = (f_i^{\text{in}})(\boldsymbol{x}, \boldsymbol{v}_i), \quad (\boldsymbol{x}, \boldsymbol{v}_i) \in \mathbb{R}^3 \times \mathbb{R}^3, \end{aligned} \tag{1}$$

where

$$J_i = \sigma_{ii}^2 \int_{\mathbb{R}^3} \int_{\mathbb{S}_+^2} \left[f_i' f_{i_*}' - f_i f_{i_*} \right] \left\langle \epsilon, \boldsymbol{v}_i - \boldsymbol{v}_{i_*} \right\rangle d\epsilon \, d\boldsymbol{v}_{i_*} \tag{2}$$

is the mono-species collision operator and it represents collisions between particles of the same species,

$$J_{is} = \sigma_{is}^2 \int_{\mathbb{R}^3} \int_{\mathbb{S}_+^2} \left[f_i' f_s' - f_i f_s \right] \langle \epsilon, \boldsymbol{v}_i - \boldsymbol{v}_s \rangle \, d\epsilon \, d\boldsymbol{v}_s \tag{3}$$

is the bi-species collision operator and it represents collisions between particles of different species.

The functions f_i are not directly observable, however, they allow one to compute measurable macroscopic quantities like : the species concentrations c_i and the macroscopic velocities for the species $\boldsymbol{u}_i$, which can be expressed in terms of microscopic averages as given below:

$$\begin{aligned} c_i(t, \boldsymbol{x}) &= \int_{\mathbb{R}^3} f(t, \boldsymbol{x}, \boldsymbol{v}_i) \, d\boldsymbol{v}_i, \\ \boldsymbol{u}_i(t, \boldsymbol{x}) &= \frac{1}{c_i(t, \boldsymbol{x})} \int_{\mathbb{R}^3} \boldsymbol{v}_i f(t, \boldsymbol{x}, \boldsymbol{v}_i) \, d\boldsymbol{v}_i. \end{aligned} \tag{4}$$

In Eqs. (2) and (3) for the mono-species and bi-species collision operators, $f_i' = f(t, \boldsymbol{x}, \boldsymbol{v}_i')$, $f_{i*}' = f(t, \boldsymbol{x}, \boldsymbol{v}_{i*}')$, $f_s' = f(t, \boldsymbol{x}, \boldsymbol{v}_s')$, ϵ is a unit vector directed along the line joining the centre of the two spheres at the moment of impact (i.e. $\epsilon \in \mathbb{S}_+^2 = \left\{ \overline{\epsilon} \in \mathbb{R}^3 : \ \|\overline{\epsilon}\| = 1, \ \langle \overline{\epsilon}, \boldsymbol{v}_i - \boldsymbol{v}_s \rangle > 0 \right\}$), $\langle \cdot, \cdot \rangle$ represents the inner product in $\mathbb{R}^3$ and $\| \cdot \|$ is the norm induced by this inner product. Furthermore, $\boldsymbol{v}_i$, $\boldsymbol{v}_{i*}$, $\boldsymbol{v}_s$ are the pre-collisional velocities, $\boldsymbol{v}_i'$, $\boldsymbol{v}_{i_*}'$, $\boldsymbol{v}_s'$ are the post-collisional velocities, σ_{ii}^2 and σ_{is}^2 are the mono-species and the bi-species collision cross-sections defined respectively as

$$\sigma_{ii}^2 = d_i^2, \qquad \sigma_{is}^2 = \frac{1}{4}(d_i + d_s)^2, \qquad i, s = 1, 2, \ldots, N, \quad i \neq s,$$

where d_i and d_s are the diameters of particles of species A_i and A_s.

Since the collisions are elastic, both momentum and kinetic energy are conserved. Therefore, the conservation laws of linear momentum and kinetic energy for bi-species collisions are given by:

$$m_i \boldsymbol{v}_i + m_s \boldsymbol{v}_s = m_i \boldsymbol{v}_i' + m_s \boldsymbol{v}_s', \tag{5}$$

$$\frac{1}{2} m_i (\boldsymbol{v}_i)^2 + \frac{1}{2} m_s (\boldsymbol{v}_s)^2 = \frac{1}{2} m_i (\boldsymbol{v}_i')^2 + \frac{1}{2} m_s (\boldsymbol{v}_s')^2, \tag{6}$$

respectively. The post-collisional velocities can be written in terms of the pre-collisional velocities as

$$\boldsymbol{v}_i' = \boldsymbol{v}_i - 2\frac{\mu_{is}}{m_i} \epsilon \, \langle \epsilon, \boldsymbol{v}_i - \boldsymbol{v}_s \rangle \quad \text{and} \quad \boldsymbol{v}_s' = \boldsymbol{v}_s + 2\frac{\mu_{is}}{m_s} \epsilon \, \langle \epsilon, \boldsymbol{v}_i - \boldsymbol{v}_s \rangle, \tag{7}$$

where $\mu_{is} = \dfrac{m_i m_s}{m_i + m_s}$ is the reduced mass.

Remark 2.1 For same species collisions, the indices i and $i*$ are used to distinguish their velocities. Also, the conservation of linear momentum and kinetic energy for mono-species collisions are respectively, given by:

$$\boldsymbol{v}_i + \boldsymbol{v}_{i*} = \boldsymbol{v}_i' + \boldsymbol{v}_{i*}', \tag{8}$$

$$\frac{1}{2}(\boldsymbol{v}_i)^2 + \frac{1}{2}(\boldsymbol{v}_{i*})^2 = \frac{1}{2}(\boldsymbol{v}_i')^2 + \frac{1}{2}(\boldsymbol{v}_{i*}')^2. \tag{9}$$

Furthermore, the post-collisional velocities can be written in terms of the pre-collisional velocities as given below:

$$\boldsymbol{v}_i' = \boldsymbol{v}_i - \epsilon \langle \epsilon, \boldsymbol{v}_i - \boldsymbol{v}_{i*} \rangle \quad \text{and} \quad \boldsymbol{v}_{i*}' = \boldsymbol{v}_{i*} + \epsilon \langle \epsilon, \boldsymbol{v}_i - \boldsymbol{v}_{i*} \rangle . \tag{10}$$

Remark 2.2 The kinetic equations given in the first row of (1) with J_i and J_{is} defined in (2) and (3), respectively, can be obtained from the simple reacting sphere kinetic model studied in [17] when the chemical reaction is turned off.

3 Scaled Kinetic Equations, Properties and Assumptions

In this section, we first present the scaled version of the kinetic equations given in the first row of (1). Then we present some of its properties and the assumptions that will be used to obtain the desired diffusion model.

3.1 Scaled Kinetic Equations

Introducing a reference length and time scales together with a reference temperature, one can define the dimensionless time, space, velocities (obtained using the speed of sound in a monatomic gas), cross-sections and number densities. Thus the kinetic equations given in the first row of (1), where J_i and J_{is} are as defined in (2) and (3), respectively, can be written in the following dimensionless/scaled form

$$\begin{aligned} \alpha \frac{\partial f_i^\alpha}{\partial t} + \boldsymbol{v}_i \cdot \frac{\partial f_i^\alpha}{\partial \boldsymbol{x}} = & \underbrace{\frac{1}{\alpha} \sigma_{ii}^2 \int_{\mathbb{R}^3} \int_{\mathbb{S}_+^2} \left[f_i^{\alpha'} f_{i_*}^{\alpha'} - f_i^\alpha f_{i_*}^\alpha \right] \langle \epsilon, \boldsymbol{v}_i - \boldsymbol{v}_{i_*} \rangle \, d\epsilon \, d\boldsymbol{v}_{i_*}}_{J_i^\alpha} \\ & + \frac{1}{\alpha} \sum_{\substack{s=1 \\ s \neq i}}^{N} \underbrace{\sigma_{is}^2 \int_{\mathbb{R}^3} \int_{\mathbb{S}_+^2} \left[f_i^{\alpha'} f_s^{\alpha'} - f_i^\alpha f_s^\alpha \right] \langle \epsilon, \boldsymbol{v}_i - \boldsymbol{v}_s \rangle \, d\epsilon \, d\boldsymbol{v}_s}_{J_{is}^\alpha}, \end{aligned} \tag{11}$$

for $(t, \boldsymbol{x}, \boldsymbol{v}_i) \in \mathbb{R}_+ \times \mathbb{R}^3 \times \mathbb{R}^3$, $i = 1, 2, \ldots, N$ where α which is such that $0 < \alpha \ll 1$ is the formal scaling parameter representing the Knudsen number, f_i^α, $f_i^{\alpha'}$, f_{i*}^α, $f_{i*}^{\alpha'}$, f_s^α and $f_s^{\alpha'}$ are the scaled distribution function, J_i^α is the scaled mono-species collision operator and J_{is}^α is the scaled bi-species collision operator. We have also assumed that the Mach number is of the same order of magnitude as the Knudsen number.

In what follows, the evolution domain of the mixture is represented by an open bounded domain $\Omega \subset \mathbb{R}^3$, with regular boundary and we will consider the following Cauchy problem:

$$\begin{aligned} &\alpha \frac{\partial f_i^\alpha}{\partial t} + \boldsymbol{v}_i \cdot \frac{\partial f_i^\alpha}{\partial \boldsymbol{x}} = \frac{1}{\alpha}\left(J_i^\alpha + \sum_{\substack{s=1 \\ s\neq i}}^{N} J_{is}^\alpha\right), \quad (t, \boldsymbol{x}, \boldsymbol{v}_i) \in \mathbb{R}_+ \times \mathbb{R}^3 \times \mathbb{R}^3,\ i = 1, 2, \ldots, N, \\ &f_i^\alpha(0, \boldsymbol{x}, \boldsymbol{v}) = (f_i^{\text{in}})^\alpha(\boldsymbol{x}, \boldsymbol{v}), \quad (\boldsymbol{x}, \boldsymbol{v}) \in \mathbb{R}^3 \times \mathbb{R}^3. \end{aligned} \tag{12}$$

To ensure that the non-reactive mixture is considered in a closed domain Ω, without being precise, the boundary conditions which describe the interaction of the particles and the boundary of the evolution domain $\partial\Omega$, is assumed to be of specular reflection type.

3.2 Properties of the Collision Operators

Here we will present some properties of the mono-species and bi-species collision operators that will be needed in our analysis.

Lemma 3.1 *Let $\varphi(\boldsymbol{v}_i)$ be a sufficiently smooth test function. Then, the weak form of the mono-species collision operator J_i^α is given by*

$$\begin{aligned} \int_{\mathbb{R}^3} J_i^\alpha \varphi(\boldsymbol{v}_i)\, d\boldsymbol{v}_i = \frac{1}{4}\sigma_{ii}^2 \int_{\mathbb{R}^3}\int_{\mathbb{R}^3}\int_{\mathbb{S}_+^2} \left[f_i^{\alpha'} f_{i*}^{\alpha'} - f_i^\alpha f_{i*}^\alpha\right] \langle \epsilon, \boldsymbol{v}_i - \boldsymbol{v}_{i*}\rangle \\ \times \left[\varphi(\boldsymbol{v}_i) + \varphi(\boldsymbol{v}_{i*}) - \varphi(\boldsymbol{v}_i') - \varphi(\boldsymbol{v}_{i*}')\right] d\epsilon\, d\boldsymbol{v}_{i*} d\boldsymbol{v}_i. \end{aligned} \tag{13}$$

Lemma 3.2 *let $\varphi(\boldsymbol{v}_i)$ be a sufficiently smooth test function. Then, the weak form of the bi-species collision operator J_{is}^α is given by*

$$\int_{\mathbb{R}^3} J_{is}^\alpha \varphi(\boldsymbol{v}_i) d\boldsymbol{v}_i = \sigma_{is}^2 \int_{\mathbb{R}^3}\int_{\mathbb{R}^3}\int_{\mathbb{S}_+^2} \left[\varphi(\boldsymbol{v}_i') - \varphi(\boldsymbol{v}_i)\right] f_i^\alpha f_s^\alpha \, \langle \epsilon, \boldsymbol{v}_i - \boldsymbol{v}_s\rangle \, d\epsilon d\boldsymbol{v}_s d\boldsymbol{v}_i, \tag{14}$$

for each $i, s = 1, 2, \ldots, N$, with $i \neq s$.

The proofs of Lemmas 3.1 and 3.2 follow from standard arguments, see for example [6, 7].

Corollary 3.1 *The mono-species collision operator J_i^α is such that, for $i = 1, 2, \ldots, N$,*

$$\int_{\mathbb{R}^3} J_i^\alpha \begin{pmatrix} 1 \\ m_i \boldsymbol{v}_i \\ \frac{1}{2} m_i (\boldsymbol{v}_i)^2 \end{pmatrix} d\boldsymbol{v}_i = 0. \tag{15}$$

Proof The proof follows from Lemma 3.1 by setting $\varphi(\boldsymbol{v}_i) = 1$, $\varphi(\boldsymbol{v}_i) = m_i \boldsymbol{v}_i$ and using the mono-species conservation of momentum (8), $\varphi(\boldsymbol{v}_i) = \frac{1}{2} m_i (\boldsymbol{v}_i)^2$ and using the mono-species conservation of energy (9), respectively. □

Corollary 3.2 *The bi-species collision operator J_{is}^{α} is such that, for $i, s = 1, 2, \ldots, N$, with $i \neq s$,*

$$\begin{aligned} &\int_{\mathbb{R}^3} J_{is}^{\alpha} \, d\boldsymbol{v}_i = 0, \\ &\int_{\mathbb{R}^3} J_{is}^{\alpha} \begin{pmatrix} m_i \boldsymbol{v}_i \\ \frac{1}{2} m_i (\boldsymbol{v}_i)^2 \end{pmatrix} d\boldsymbol{v}_i + \int_{\mathbb{R}^3} J_{si}^{\alpha} \begin{pmatrix} m_s \boldsymbol{v}_s \\ \frac{1}{2} m_s (\boldsymbol{v}_s)^2 \end{pmatrix} d\boldsymbol{v}_s = 0. \end{aligned} \tag{16}$$

Proof The proof follows from Lemma 3.2 by setting $\varphi(\boldsymbol{v}_i) = 1$, $\varphi(\boldsymbol{v}_i) = m_i \boldsymbol{v}_i$ and using the bi-species conservation of momentum (5), $\varphi(\boldsymbol{v}_i) = \frac{1}{2} m_i (\boldsymbol{v}_i)^2$ and using the bi-species conservation of energy (6), respectively. □

Remark 3.1 The properties of the scaled collision operators given in Lemmas 3.1 and 3.2, Corollaries 3.1 and 3.2 are also valid for the non-scaled collision operators.

3.3 Assumptions

In order to derive the target equations (that is a purely diffusion model where the diffusion process is governed by the MS equations), we will assume that

(a) The temperature of the mixture T is uniform in space and constant in time.
(b) The bulk velocity of the mixture $\boldsymbol{u}^{\alpha}$ is small and goes to zero as $\alpha \to 0$.
(c) The initial conditions are local Maxwellians centered at the average velocity of the species $\boldsymbol{u}_i^{\alpha}$. More precisely the distribution functions at time $t = 0$ are of the form

$$f^{\alpha(in)}(\boldsymbol{x}, \boldsymbol{v}_i) = c_i^{\alpha(in)}(\boldsymbol{x}) \left(\frac{m_i}{2\pi k_B T} \right)^{\frac{3}{2}} \exp\left[- \frac{m_i \left(\boldsymbol{v}_i - \alpha \boldsymbol{u}_i^{\alpha(in)}(\boldsymbol{x}) \right)^2}{2 k_B T} \right], \ \boldsymbol{x} \in \Omega, \ \boldsymbol{v}_i \in \mathbb{R}^3,$$

where k_B is the Boltzmann's constant, c_i^{α} is the concentration of the species which is such that $c_i^{\alpha(in)} : \Omega \to \mathbb{R}_+$ and $\boldsymbol{u}_i^{\alpha(in)} : \Omega \to \mathbb{R}^3$, for $i = 1, 2, \ldots, N$.
(d) The evolution of the system leaves the distribution functions in the local Maxwellian state. More precisely, the distribution functions at time $t > 0$ are of the form

$$f^{\alpha}(t, \boldsymbol{x}, \boldsymbol{v}_i) = c_i^{\alpha}(t, \boldsymbol{x}) \left(\frac{m_i}{2\pi k_B T} \right)^{\frac{3}{2}} \exp\left[- \frac{m_i \left(\boldsymbol{v}_i - \alpha \boldsymbol{u}_i^{\alpha}(t, \boldsymbol{x}) \right)^2}{2 k_B T} \right], \boldsymbol{x} \in \Omega, \ \boldsymbol{v}_i \in \mathbb{R}^3 \tag{17}$$

where $c_i^{\alpha} : \mathbb{R}_+ \times \Omega \to \mathbb{R}_+$ and $\boldsymbol{u}_i^{\alpha} : \mathbb{R}_+ \times \Omega \to \mathbb{R}^3$, for $i = 1, 2, \ldots, N$.

Assumption (a) is the isothermal condition and it allows us to neglect effects due to temperature gradient. Assumption (b) allows us to neglect convective effects. Assumptions (c) and (d) represent a physical situation in which the system evolves not far away from the local Maxwellian equilibrium.

Lemma 3.3 *As a consequence of* (17)*, we have that*

$$f_i^{\alpha'} f_s^{\alpha'} - f_i^{\alpha} f_s^{\alpha} = M_i^{\alpha} M_s^{\alpha} \big(\alpha \boldsymbol{a}_{is} \cdot (\boldsymbol{v}_i' - \boldsymbol{v}_i) + \alpha^2 \boldsymbol{a}_{is} \cdot (\boldsymbol{v}_i' - \boldsymbol{v}_i)(\boldsymbol{a}_i \cdot \boldsymbol{v}_i) + \alpha^2 \boldsymbol{a}_{is} \cdot (\boldsymbol{v}_i' - \boldsymbol{v}_i)(\boldsymbol{a}_s \cdot \boldsymbol{v}_s) + \frac{\alpha^2}{2} \big(\boldsymbol{a}_{is} \cdot (\boldsymbol{v}_i' - \boldsymbol{v}_i)\big)^2 + O(\alpha^3)\big), \tag{18}$$

where

$$\begin{aligned} &\boldsymbol{a}_i = \frac{m_i \boldsymbol{u}_i^{\alpha}}{k_B T}, \quad \boldsymbol{a}_s = \frac{m_s \boldsymbol{u}_s^{\alpha}}{k_B T}, \quad \boldsymbol{a}_{is} = \frac{m_i (\boldsymbol{u}_i^{\alpha} - \boldsymbol{u}_s^{\alpha})}{k_B T}, \\ &M_i^{\alpha} = c_i^{\alpha} \left(\frac{m_i}{2\pi k_B T}\right)^{\frac{3}{2}} \exp\left(-\frac{m_i (\boldsymbol{v}_i)^2}{2k_B T}\right), \quad M_s^{\alpha} = c_s^{\alpha} \left(\frac{m_s}{2\pi k_B T}\right)^{\frac{3}{2}} \exp\left(-\frac{m_s (\boldsymbol{v}_s)^2}{2k_B T}\right). \end{aligned} \tag{19}$$

Proof Using Eq. (17), we can write

$$\begin{aligned} f_i^{\alpha'} f_s^{\alpha'} &= c_i^{\alpha} \left(\frac{m_i}{2\pi k_B T}\right)^{\frac{3}{2}} \exp\left[-\frac{m_i \left(\boldsymbol{v}_i' - \alpha \boldsymbol{u}_i^{\alpha}\right)^2}{2k_B T}\right] c_s^{\alpha} \left(\frac{m_s}{2\pi k_B T}\right)^{\frac{3}{2}} \exp\left[-\frac{m_s \left(\boldsymbol{v}_s' - \alpha \boldsymbol{u}_s^{\alpha}\right)^2}{2k_B T}\right] \\ &= c_i^{\alpha} c_s^{\alpha} \frac{(m_i m_s)^{\frac{3}{2}}}{(2\pi k_B T)^3} \exp\left[-\left(\frac{m_i \left(\boldsymbol{v}_i' - \alpha \boldsymbol{u}_i^{\alpha}\right)^2 + m_s \left(\boldsymbol{v}_s' - \alpha \boldsymbol{u}_s^{\alpha}\right)^2}{2k_B T}\right)\right]. \end{aligned} \tag{20}$$

Observe that

$$\begin{aligned} m_i \left(\boldsymbol{v}_i' - \alpha \boldsymbol{u}_i^{\alpha}\right)^2 + m_s \left(\boldsymbol{v}_s' - \alpha \boldsymbol{u}_s^{\alpha}\right)^2 &= m_i (\boldsymbol{v}_i')^2 + m_s (\boldsymbol{v}_s')^2 + m_i (\alpha \boldsymbol{u}_i^{\alpha})^2 \\ &\quad + m_s (\alpha \boldsymbol{u}_s^{\alpha})^2 - 2\alpha m_i \boldsymbol{u}_i^{\alpha} \cdot \boldsymbol{v}_i' - 2\alpha m_s \boldsymbol{u}_s^{\alpha} \cdot \boldsymbol{v}_s'. \end{aligned}$$

Using the bi-species conservation of kinetic energy (6), we obtain

$$\begin{aligned} m_i \left(\boldsymbol{v}_i' - \alpha \boldsymbol{u}_i^{\alpha}\right)^2 + m_s \left(\boldsymbol{v}_s' - \alpha \boldsymbol{u}_s^{\alpha}\right)^2 &= m_i \left(\boldsymbol{v}_i - \alpha \boldsymbol{u}_i^{\alpha}\right)^2 + m_s \left(\boldsymbol{v}_s - \alpha \boldsymbol{u}_s^{\alpha}\right)^2 \\ &\quad - 2\alpha m_i \boldsymbol{u}_i^{\alpha} \cdot (\boldsymbol{v}_i' - \boldsymbol{v}_i) - 2\alpha m_s \boldsymbol{u}_s^{\alpha} \cdot (\boldsymbol{v}_s' - \boldsymbol{v}_s). \end{aligned}$$

Using the bi-species conservation of momentum (5) rewritten as

$$m_i (\boldsymbol{v}_i' - \boldsymbol{v}_i) = -m_s (\boldsymbol{v}_s' - \boldsymbol{v}_s),$$

we obtain

$$m_i\left(\boldsymbol{v}_i' - \alpha \boldsymbol{u}_i^\alpha\right)^2 + m_s\left(\boldsymbol{v}_s' - \alpha \boldsymbol{u}_s^\alpha\right)^2 = m_i\left(\boldsymbol{v}_i - \alpha \boldsymbol{u}_i^\alpha\right)^2 + m_s\left(\boldsymbol{v}_s - \alpha \boldsymbol{u}_s^\alpha\right)^2 - 2\alpha m_i(\boldsymbol{v}_i' - \boldsymbol{v}_i)\cdot(\boldsymbol{u}_i^\alpha - \boldsymbol{u}_s^\alpha). \tag{21}$$

Substituting (21) into (20), we obtain

$$f_i^{\alpha'} f_s^{\alpha'} = c_i^\alpha c_s^\alpha \frac{(m_i m_s)^{\frac{3}{2}}}{(2\pi k_B T)^3} \times \exp\left[-\left(\frac{m_i\left(\boldsymbol{v}_i - \alpha \boldsymbol{u}_i^\alpha\right)^2 + m_s\left(\boldsymbol{v}_s - \alpha \boldsymbol{u}_s^\alpha\right)^2 - 2\alpha m_i(\boldsymbol{v}_i' - \boldsymbol{v}_i)\cdot(\boldsymbol{u}_i^\alpha - \boldsymbol{u}_s^\alpha)}{2k_B T}\right)\right].$$

Using the distribution function (17), we obtain

$$f_i^{\alpha'} f_s^{\alpha'} = f_i^\alpha f_s^\alpha \exp\left[\frac{\alpha m_i(\boldsymbol{v}_i' - \boldsymbol{v}_i)\cdot(\boldsymbol{u}_i^\alpha - \boldsymbol{u}_s^\alpha)}{k_B T}\right]. \tag{22}$$

Now, using (22), we can write

$$f_i^{\alpha'} f_s^{\alpha'} - f_i^\alpha f_s^\alpha = f_i^\alpha f_s^\alpha\left(\exp\left[\frac{\alpha m_i(\boldsymbol{v}_i' - \boldsymbol{v}_i)\cdot(\boldsymbol{u}_i^\alpha - \boldsymbol{u}_s^\alpha)}{k_B T}\right] - 1\right). \tag{23}$$

Taylor expanding the exponential term in (23) above with respect to α gives

$$\exp\left[\frac{\alpha m_i(\boldsymbol{v}_i' - \boldsymbol{v}_i)\cdot(\boldsymbol{u}_i^\alpha - \boldsymbol{u}_s^\alpha)}{k_B T}\right] = 1 + \frac{\alpha m_i(\boldsymbol{v}_i' - \boldsymbol{v}_i)\cdot(\boldsymbol{u}_i^\alpha - \boldsymbol{u}_s^\alpha)}{k_B T} + \frac{1}{2}\left(\frac{\alpha m_i(\boldsymbol{v}_i' - \boldsymbol{v}_i)\cdot(\boldsymbol{u}_i^\alpha - \boldsymbol{u}_s^\alpha)}{k_B T}\right)^2 + O(\alpha^3). \tag{24}$$

Substituting (24) into (23) gives

$$f_i^{\alpha'} f_s^{\alpha'} - f_i^\alpha f_s^\alpha = f_i^\alpha f_s^\alpha\left(\frac{\alpha m_i(\boldsymbol{v}_i' - \boldsymbol{v}_i)\cdot(\boldsymbol{u}_i^\alpha - \boldsymbol{u}_s^\alpha)}{k_B T} + \frac{1}{2}\left(\frac{\alpha m_i(\boldsymbol{v}_i' - \boldsymbol{v}_i)\cdot(\boldsymbol{u}_i^\alpha - \boldsymbol{u}_s^\alpha)}{k_B T}\right)^2 + O(\alpha^3)\right). \tag{25}$$

Observe that

$$\exp\left[-\frac{m_i(\boldsymbol{v}_i - \alpha \boldsymbol{u}_i^\alpha)^2}{2k_B T}\right] = \exp\left[-\frac{m_i(\boldsymbol{v}_i)^2}{2k_B T}\right]\exp\left[\frac{m_i \alpha \boldsymbol{u}_i^\alpha \cdot \boldsymbol{v}_i}{k_B T}\right]\exp\left[-\frac{m_i(\alpha \boldsymbol{u}_i^\alpha)^2}{2k_B T}\right].$$

The Taylor expansion of the last two terms on the right-hand side of the previous equation with respect to α is

$$\exp\left[\frac{m_i\alpha \boldsymbol{u}_i^\alpha \cdot \boldsymbol{v}_i}{k_B T}\right] = 1 + \alpha\frac{m_i \boldsymbol{u}_i^\alpha \cdot \boldsymbol{v}_i}{k_B T} + O(\alpha^2),$$
$$\exp\left[-\frac{m_i(\alpha \boldsymbol{u}_i^\alpha)^2}{2k_B T}\right] = 1 + O(\alpha^2).$$

Therefore,

$$\exp\left[-\frac{m_i(\boldsymbol{v}_i - \alpha\boldsymbol{u}_i^\alpha)^2}{2k_B T}\right] = \exp\left[-\frac{m_i(\boldsymbol{v}_i)^2}{2k_B T}\right]\left(1 + \alpha\frac{m_i \boldsymbol{u}_i^\alpha \cdot \boldsymbol{v}_i}{k_B T} + O(\alpha^2)\right)(1 + O(\alpha^2))$$
$$= \exp\left[-\frac{m_i(\boldsymbol{v}_i)^2}{2k_B T}\right]\left(1 + \alpha\frac{m_i \boldsymbol{u}_i^\alpha \cdot \boldsymbol{v}_i}{k_B T} + O(\alpha^2)\right).$$

Thus,

$$f_i^\alpha = c_i^\alpha\left(\frac{m_i}{2\pi k_B T}\right)^{\frac{3}{2}} \exp\left[-\frac{m_i(\boldsymbol{v}_i)^2}{2k_B T}\right]\left(1 + \alpha\frac{m_i \boldsymbol{u}_i^\alpha \cdot \boldsymbol{v}_i}{k_B T} + O(\alpha^2)\right).$$

Similarly,

$$f_s^\alpha = c_s^\alpha\left(\frac{m_s}{2\pi k_B T}\right)^{\frac{3}{2}} \exp\left[-\frac{m_s(\boldsymbol{v}_s)^2}{2k_B T}\right]\left(1 + \alpha\frac{m_s \boldsymbol{u}_s^\alpha \cdot \boldsymbol{v}_s}{k_B T} + O(\alpha^2)\right).$$

Taking the product of f_i^α and f_s^α, we obtain

$$f_i^\alpha f_s^\alpha = c_i^\alpha\left(\frac{m_s}{2\pi k_B T}\right)^{\frac{3}{2}} c_s^\alpha\left(\frac{m_i}{2\pi k_B T}\right)^{\frac{3}{2}} \exp\left[-\frac{m_i(\boldsymbol{v}_i)^2}{2k_B T}\right]$$
$$\times \exp\left[-\frac{m_s(\boldsymbol{v}_s)^2}{2k_B T}\right]\left(1 + \alpha\frac{m_i \boldsymbol{u}_i^\alpha \cdot \boldsymbol{v}_i}{k_B T} + \alpha\frac{m_s \boldsymbol{u}_s^\alpha \cdot \boldsymbol{v}_s}{k_B T} + O(\alpha^2)\right). \quad (26)$$

Substituting (26) into (25), expanding and using the definitions given in (19) gives the desired result □

4 The Maxwell–Stefan Diffusion Limit

In this section, we obtain the continuity equations, the momentum balance equations for the species and perform a formal asymptotic analysis of the continuity and momentum balance equations toward a diffusion model of MS type.

4.1 Continuity Equations for the Species

The continuity equations for the species can formally be derived from the scaled kinetic equations (11), by integrating over $\boldsymbol{v}_i \in \mathbb{R}^3$ as shown in the following lemma.

Lemma 4.1 *The continuity equations for the species in the non-reactive mixture are given by*

$$\frac{\partial c_i^\alpha}{\partial t} + \frac{\partial}{\partial \boldsymbol{x}}(c_i^\alpha \boldsymbol{u}_i^\alpha) = 0, \quad i = 1, 2, \ldots, N. \tag{27}$$

Proof Integrating both sides of (11) with respect to $\boldsymbol{v}_i \in \mathbb{R}^3$, we obtain for $i = 1, 2, \ldots, N$

$$\alpha \underbrace{\frac{\partial}{\partial t}\int_{\mathbb{R}^3} f_i^\alpha d\boldsymbol{v}_i}_{c_i^\alpha} + \underbrace{\frac{\partial}{\partial \boldsymbol{x}}\int_{\mathbb{R}^3} \boldsymbol{v}_i f_i^\alpha d\boldsymbol{v}_i}_{\alpha c_i^\alpha \boldsymbol{u}_i^\alpha} = \frac{1}{\alpha}\underbrace{\int_{\mathbb{R}^3} J_i^\alpha d\boldsymbol{v}_i}_{0} + \frac{1}{\alpha}\sum_{\substack{s=1\\ s\neq i}}^{N} \underbrace{\int_{\mathbb{R}^3} J_{is}^\alpha d\boldsymbol{v}_i}_{0}. \tag{28}$$

To show that the first term on the right-hand side of (28) vanishes, we use the weak form of the mono-species collision operator (13) with $\varphi(\boldsymbol{v}_i) = 1$, see Corollary 3.1 in Sect. 3.2. Similarly, using the weak form of the bi-species collision operator (14) with $\varphi(\boldsymbol{v}_i) = 1$, see Corollary 3.2 in Sect. 3.2, we obtain that the second term on the right-hand side of (28) vanishes. Finally, dividing both sides of (28) by α gives the desired result. □

4.2 Momentum Balance Equations for the Species

To derive the momentum balance equations for the species from the scaled kinetic equations (11), we multiply it by $m_i \boldsymbol{v}_i$ and integrating over $\boldsymbol{v}_i \in \mathbb{R}^3$ as shown in the following lemma.

Lemma 4.2 *The momentum balance equations for the species in the non-reactive mixture is given by*

$$\begin{aligned} &\alpha^2 m_i \frac{\partial}{\partial t}\left(c_i^\alpha \boldsymbol{u}_i^\alpha\right) + k_B T \frac{\partial c_i^\alpha}{\partial \boldsymbol{x}} + \alpha^2 m_i \frac{\partial}{\partial \boldsymbol{x}}\left(c_i^\alpha \boldsymbol{u}_i^\alpha \otimes \boldsymbol{u}_i^\alpha\right) \\ &\quad = \frac{32}{9}\sum_{\substack{s=1\\ s\neq i}}^{N} \sigma_{is}^2 (2\pi \mu_{is} k_B T)^{\frac{1}{2}} c_i^\alpha c_s^\alpha \left(\boldsymbol{u}_i^\alpha - \boldsymbol{u}_s^\alpha\right) + O(\alpha), \end{aligned} \tag{29}$$

for $i = 1, 2, \ldots, N$.

Proof Multiplying both sides of the scaled kinetic equations (11) by $m_i \boldsymbol{v}_i$ and integrating with respect to $\boldsymbol{v}_i \in \mathbb{R}^3$, we obtain for $i = 1, 2, \ldots, N$,

$$\alpha \frac{\partial}{\partial t} \underbrace{\left(\int_{\mathbb{R}^3} m_i \boldsymbol{v}_i f_i^\alpha d\boldsymbol{v}_i \right)}_{\alpha m_i c_i^\alpha \boldsymbol{u}_i^\alpha} + \frac{\partial}{\partial \boldsymbol{x}} \underbrace{\left(\int_{\mathbb{R}^3} m_i (\boldsymbol{v}_i \otimes \boldsymbol{v}_i) f_i^\alpha d\boldsymbol{v}_i \right)}_{c_i^\alpha k_B T + \alpha^2 m_i \left(c_i^\alpha \boldsymbol{u}_i^\alpha \otimes \boldsymbol{u}_i^\alpha \right)}$$
$$= \frac{1}{\alpha} \underbrace{\int_{\mathbb{R}^3} m_i \boldsymbol{v}_i J_i^\alpha d\boldsymbol{v}_i}_{0} + \frac{1}{\alpha} \underbrace{\sum_{\substack{s=1 \\ s \neq i}}^{N} \int_{\mathbb{R}^3} m_i \boldsymbol{v}_i J_{is}^\alpha d\boldsymbol{v}_i}_{\mathscr{O}_i}. \tag{30}$$

To show that the first term on the right-hand side of (30) vanishes, we use the weak form (13) with $\varphi(\boldsymbol{v}_i) = m_i \boldsymbol{v}_i$ together with the mono-species conservation of momentum given in (5), see Corollary 3.1 in Sect. 3.2. Concerning the second term on the right-hand side of (30), using the definition of J_{is}^α given in (11), we obtain

$$\mathscr{O}_i = \sum_{\substack{s=1 \\ s \neq i}}^{N} \sigma_{is}^2 \int_{\mathbb{R}^3} \int_{\mathbb{R}^3} \int_{\mathbb{S}_+^2} m_i \boldsymbol{v}_i \left[f_i^{\alpha'} f_s^{\alpha'} - f_i^\alpha f_s^\alpha \right] \langle \epsilon, \boldsymbol{v}_i - \boldsymbol{v}_s \rangle \, d\epsilon \, d\boldsymbol{v}_s \, d\boldsymbol{v}_i$$
$$= \alpha \sum_{\substack{s=1 \\ s \neq i}}^{N} \sigma_{is}^2 \int_{\mathbb{R}^3} \int_{\mathbb{R}^3} \int_{\mathbb{S}_+^2} m_i \boldsymbol{v}_i M_i^\alpha M_s^\alpha \boldsymbol{a}_{is} \cdot (\boldsymbol{v}_i' - \boldsymbol{v}_i) \langle \epsilon, \boldsymbol{v}_i - \boldsymbol{v}_s \rangle \, d\epsilon \, d\boldsymbol{v}_s d\boldsymbol{v}_i + O(\alpha^2),$$

where we have used (18) to obtain the previous equation. From the definition of post-collisional velocity (7), we can write

$$\begin{aligned} \boldsymbol{v}_i' - \boldsymbol{v}_i &= -\frac{2\mu_{is}}{m_i} \langle \epsilon, \boldsymbol{v}_i - \boldsymbol{v}_s \rangle \epsilon \\ &= -\frac{2 m_i m_s}{(m_i + m_s) m_i} \| \boldsymbol{v}_i - \boldsymbol{v}_s \| \cos\theta \frac{(\boldsymbol{v}_i - \boldsymbol{v}_s)}{\| \boldsymbol{v}_i - \boldsymbol{v}_s \|} \\ &= -\frac{2 m_s}{(m_i + m_s)} (\boldsymbol{v}_i - \boldsymbol{v}_s) \cos\theta. \end{aligned}$$

Setting $\boldsymbol{V} = \boldsymbol{v}_i - \boldsymbol{v}_s$, we obtain

$$\boldsymbol{v}_i' - \boldsymbol{v}_i = -\frac{2 m_s}{m_i + m_s} \boldsymbol{V} \cos\theta. \tag{31}$$

Therefore,

$$\mathscr{O}_i = -\alpha \sum_{\substack{s=1 \\ s\neq i}}^{N} \sigma_{is}^2 2\mu_{is} \int_{\mathbb{R}^3}\int_{\mathbb{R}^3}\int_{\mathbb{S}^2_+} \boldsymbol{v}_i M_i^\alpha M_s^\alpha \Big(\boldsymbol{a}_{is}\cdot \boldsymbol{V}\Big) \cos\theta \,\langle \epsilon, \boldsymbol{v}_i - \boldsymbol{v}_s\rangle \, d\epsilon d\boldsymbol{v}_s d\boldsymbol{v}_i + O(\alpha^2)$$

$$= -\alpha \sum_{\substack{s=1 \\ s\neq i}}^{N} \sigma_{is}^2 2\mu_{is} \int_{\mathbb{R}^3}\int_{\mathbb{R}^3}\int_{\mathbb{S}^2_+} \boldsymbol{v}_i M_i^\alpha M_s^\alpha \Big(\boldsymbol{a}_{is}\cdot \boldsymbol{V}\Big) \|\boldsymbol{v}_i - \boldsymbol{v}_s\| \cos^2\theta \, d\epsilon d\boldsymbol{v}_s d\boldsymbol{v}_i + O(\alpha^2)$$

$$= -\alpha \sum_{\substack{s=1 \\ s\neq i}}^{N} \sigma_{is}^2 2\mu_{is} \int_{\mathbb{R}^3}\int_{\mathbb{R}^3}\int_0^{\frac{\pi}{2}}\int_0^{2\pi} \boldsymbol{v}_i M_i^\alpha M_s^\alpha \Big(\boldsymbol{a}_{is}\cdot \boldsymbol{V}\Big) V \cos^2\theta \sin\theta d\phi d\theta d\boldsymbol{v}_s \, d\boldsymbol{v}_i + O(\alpha^2)$$

$$= -\alpha \sum_{\substack{s=1 \\ s\neq i}}^{N} \sigma_{is}^2 2\mu_{is} \int_{\mathbb{R}^3}\int_{\mathbb{R}^3} \boldsymbol{v}_i M_i^\alpha M_s^\alpha \Big(\boldsymbol{a}_{is}\cdot \boldsymbol{V}\Big) V d\boldsymbol{v}_s d\boldsymbol{v}_i \underbrace{\int_0^{\frac{\pi}{2}} \cos^2\theta \sin\theta d\theta}_{\frac{1}{3}} \underbrace{\int_0^{2\pi} d\phi}_{2\pi} + O(\alpha^2)$$

$$= -\alpha \sum_{\substack{s=1 \\ s\neq i}}^{N} \sigma_{is}^2 \frac{4\pi\mu_{is}}{3} \int_{\mathbb{R}^3}\int_{\mathbb{R}^3} \boldsymbol{v}_i M_i^\alpha M_s^\alpha \Big(\boldsymbol{a}_{is}\cdot \boldsymbol{V}\Big) V \, d\boldsymbol{v}_s \, d\boldsymbol{v}_i + O(\alpha^2)$$

$$= -\alpha \sum_{\substack{s=1 \\ s\neq i}}^{N} \sigma_{is}^2 \frac{4\pi\mu_{is}}{3} \frac{(m_i m_s)^{\frac{3}{2}}}{(2\pi k_B T)^3} c_i^\alpha c_s^\alpha \int_{\mathbb{R}^3}\int_{\mathbb{R}^3} \boldsymbol{v}_i \exp\left(-\frac{m_i(\boldsymbol{v}_i)^2 + m_s(\boldsymbol{v}_s)^2}{2k_B T}\right) \times \Big(\boldsymbol{a}_{is}\cdot \boldsymbol{V}\Big) V d\boldsymbol{v}_s d\boldsymbol{v}_i + O(\alpha^2).$$

It will be convenient to transform the above six fold integral from $\boldsymbol{v}_i$ and $\boldsymbol{v}_s$ to the center of mass velocity

$$\boldsymbol{X} = \frac{(m_i\boldsymbol{v}_i + m_s\boldsymbol{v}_s)}{m_i + m_s} \quad \Longleftrightarrow \quad (m_i + m_s)\boldsymbol{X} = m_i\boldsymbol{v}_i + m_s\boldsymbol{v}_s, \tag{32}$$

and relative velocity

$$\boldsymbol{V} = \boldsymbol{v}_i - \boldsymbol{v}_s \quad \Longleftrightarrow \quad \boldsymbol{v}_i = \boldsymbol{V} + \boldsymbol{v}_s. \tag{33}$$

Observe that by substituting (33) into (32), we obtain

$$(m_i + m_s)\boldsymbol{X} = m_i\boldsymbol{V} + (m_i + m_s)\boldsymbol{v}_s.$$

Dividing both sides by $m_i + m_s$, we obtain

$$\boldsymbol{X} = \boldsymbol{v}_s + \frac{m_i\boldsymbol{V}}{m_i + m_s} \quad \Longleftrightarrow \quad \boldsymbol{v}_s = \boldsymbol{X} - \frac{m_i\boldsymbol{V}}{m_i + m_s}. \tag{34}$$

Also, substituting (34) into (33), we obtain

$$\begin{aligned}\boldsymbol{v}_i &= \boldsymbol{V} + \boldsymbol{X} - \frac{m_i \boldsymbol{V}}{m_i + m_s} \\ &= \boldsymbol{X} + \frac{m_s \boldsymbol{V}}{m_i + m_s}. \end{aligned} \tag{35}$$

Furthermore, using (35), we obtain

$$\begin{aligned} m_i(\boldsymbol{v}_i)^2 &= m_i \left(\boldsymbol{X} + \frac{m_s \boldsymbol{V}}{m_i + m_s} \right)^2 \\ &= m_i \left\{ \boldsymbol{X} \left(\boldsymbol{X} + \frac{m_s \boldsymbol{V}}{m_i + m_s} \right) + \frac{m_s \boldsymbol{V}}{m_i + m_s} \left(\boldsymbol{X} + \frac{m_s \boldsymbol{V}}{m_i + m_s} \right) \right\} \\ &= m_i \left\{ X^2 + 2 \frac{m_s}{m_i + m_s} (\boldsymbol{V} \cdot \boldsymbol{X}) + \frac{m_s^2}{(m_i + m_s)^2} V^2 \right\}, \end{aligned}$$

where $X = \|\boldsymbol{X}\|$ and $V = \|\boldsymbol{V}\|$. Similarly, using (34), we obtain

$$m_s(\boldsymbol{v}_s)^2 = m_s \left\{ X^2 - 2 \frac{m_i}{m_i + m_s} (\boldsymbol{V} \cdot \boldsymbol{X}) + \frac{m_i^2}{(m_i + m_s)^2} V^2 \right\}.$$

Thus,

$$\begin{aligned} m_i(\boldsymbol{v}_i)^2 + m_s(\boldsymbol{v}_s)^2 &= (m_i + m_s) X^2 + \frac{\mu_{is} m_s}{m_i + m_s} V^2 + \frac{\mu_{is} m_i}{m_i + m_s} V^2 \\ &= (m_i + m_s) X^2 + \frac{\mu_{is}}{m_i + m_s} V^2 (m_i + m_s) \\ &= (m_i + m_s) X^2 + \mu_{is} V^2. \end{aligned} \tag{36}$$

Therefore, using the fact that the Jacobian of the transformation $(\boldsymbol{v}_i, \boldsymbol{v}_s) \mapsto (\boldsymbol{V}, \boldsymbol{X})$ has absolute value 1, we obtain

$$\begin{aligned} \mathscr{O}_i = -\alpha \sum_{\substack{s=1 \\ s \neq i}}^{N} \sigma_{is}^2 \frac{4\pi \mu_{is}}{3} \frac{(m_i m_s)^{\frac{3}{2}}}{(2\pi k_B T)^3} c_i^\alpha c_s^\alpha \int_{\mathbb{R}^3} \int_{\mathbb{R}^3} \left(\boldsymbol{X} + \frac{m_s \boldsymbol{V}}{m_i + m_s} \right) \\ \times \exp\left(- \frac{(m_i + m_s) X^2 + \mu_{is} V^2}{2 k_B T} \right) (\boldsymbol{a}_{is} \cdot \boldsymbol{V}) V d\boldsymbol{X} d\boldsymbol{V} + O(\alpha^2) \\ = -\alpha \sum_{\substack{s=1 \\ s \neq i}}^{N} \sigma_{is}^2 \frac{4\pi \mu_{is}}{3} \frac{(m_i m_s)^{\frac{3}{2}}}{(2\pi k_B T)^3} c_i^\alpha c_s^\alpha \int_{\mathbb{R}^3} \int_{\mathbb{R}^3} \boldsymbol{X} \exp\left(- \frac{(m_i + m_s) X^2 + \mu_{is} V^2}{2 k_B T} \right) \\ \times \left(\boldsymbol{a}_{is} \cdot \boldsymbol{V} \right) V d\boldsymbol{X} d\boldsymbol{V} \\ - \alpha \sum_{\substack{s=1 \\ s \neq i}}^{N} \sigma_{is}^2 \frac{4\pi \mu_{is} m_s}{3(m_i + m_s)} \frac{(m_i m_s)^{\frac{3}{2}}}{(2\pi k_B T)^3} c_i^\alpha c_s^\alpha \int_{\mathbb{R}^3} \int_{\mathbb{R}^3} \boldsymbol{V} \exp\left(- \frac{(m_i + m_s) X^2 + \mu_{is} V^2}{2 k_B T} \right) \\ \times \left(\boldsymbol{a}_{is} \cdot \boldsymbol{V} \right) V d\boldsymbol{X} d\boldsymbol{V} + O(\alpha^2) \end{aligned}$$

$$= -\alpha \sum_{\substack{s=1 \\ s\neq i}}^{N} \sigma_{is}^2 \frac{4\pi\mu_{is}}{3} \frac{(m_i m_s)^{\frac{3}{2}}}{(2\pi k_B T)^3} c_i^\alpha c_s^\alpha \underbrace{\int_{\mathbb{R}^3} \boldsymbol{X} \exp\left(-\frac{(m_i+m_s)X^2}{2k_B T}\right) d\boldsymbol{X}}_{\mathscr{A}}$$
$$\times \underbrace{\int_{\mathbb{R}^3} \exp\left(-\frac{\mu_{is}V^2}{2k_B T}\right) V\left(\boldsymbol{a}_{is}\cdot \boldsymbol{V}\right) d\boldsymbol{V}}_{\mathscr{B}}$$
$$-\alpha \sum_{\substack{s=1 \\ s\neq i}}^{N} \sigma_{is}^2 \frac{4\pi\mu_{is} m_s}{3(m_i+m_s)} \frac{(m_i m_s)^{\frac{3}{2}}}{(2\pi k_B T)^3} c_i^\alpha c_s^\alpha \underbrace{\int_{\mathbb{R}^3} \exp\left(-\frac{(m_i+m_s)X^2}{2k_B T}\right) d\boldsymbol{X}}_{\mathscr{C}}$$
$$\times \underbrace{\int_{\mathbb{R}^3} \boldsymbol{V} \exp\left(-\frac{\mu_{is}V^2}{2k_B T}\right) V\left(\boldsymbol{a}_{is}\cdot \boldsymbol{V}\right) d\boldsymbol{V}}_{\mathscr{D}} + O(\alpha^2).$$

Now let us evaluate the integrals $\mathscr{A}$, $\mathscr{B}$, $\mathscr{C}$ and $\mathscr{D}$. To do this, in the sequel we will use the integral representation of gamma function defined as given below:

$$\int_0^\infty x^n e^{-\eta x^2} dx = \frac{1}{2}\Gamma\left(\frac{n+1}{2}\right)\left(\frac{1}{\eta}\right)^{\frac{n+1}{2}}. \tag{37}$$

Using the fact that any vector $\boldsymbol{X}$ can be written in terms of a unit vector as $\boldsymbol{X} = X\mathbf{x}$, with $X = \|\boldsymbol{X}\|$ and $\mathbf{x}$ a unit vector, we can rewrite the integral $\mathscr{A}$ as given below

$$\mathscr{A} = \int_{\mathbb{R}^3} X\mathbf{x} \exp\left(-\frac{(m_i+m_s)X^2}{2k_B T}\right) d\boldsymbol{X}. \tag{38}$$

Writing (38) in spherical coordinates, we obtain

$$\mathscr{A} = \int_0^\infty \int_0^\pi \int_0^{2\pi} X(\hat{\mathbf{x}}\sin\theta\cos\phi + \hat{\mathbf{y}}\sin\theta\sin\phi + \hat{\mathbf{z}}\cos\theta) \exp\left(-\frac{(m_i+m_s)X^2}{2k_B T}\right)$$
$$\times X^2 \sin\theta d\phi d\theta dX$$
$$= \int_0^\infty X^3 \exp\left(-\frac{(m_i+m_s)X^2}{2k_B T}\right) dX \Bigg(\hat{\mathbf{x}} \underbrace{\int_0^\pi \sin^2\theta d\theta}_{\frac{\pi}{2}} \underbrace{\int_0^{2\pi} \cos\phi d\phi}_{0}$$
$$+ \hat{\mathbf{y}} \underbrace{\int_0^\pi \sin^2\theta d\theta}_{\frac{\pi}{2}} \underbrace{\int_0^{2\pi} \sin\phi}_{0} + \hat{\mathbf{z}} \underbrace{\int_0^\pi \cos\theta\sin\theta d\theta}_{0} \underbrace{\int_0^{2\pi} d\phi}_{2\pi}\Bigg),$$

where $\hat{\mathbf{x}}, \hat{\mathbf{y}}, \hat{\mathbf{z}}$ are the Cartesian unit vectors in $\mathbb{R}^3$. The integral in X can be evaluated using the integral representation of gamma function given in Eq. (37). More specifically,

$$\int_0^\infty X^3 \exp\left(-\frac{(m_i+m_s)X^2}{2k_BT}\right)dX = \frac{1}{2}\Gamma(2)\left(\frac{2k_BT}{m_i+m_s}\right)^2 = \frac{1}{2}\left(\frac{2k_BT}{m_i+m_s}\right)^2.$$

Thus,

$$\mathscr{A} = \frac{1}{2}\left(\frac{2k_BT}{(m_i+m_s)}\right)^2\left[\hat{\mathbf{x}}\left(\frac{\pi}{2}\times 0\right)+\hat{\mathbf{y}}\left(\frac{\pi}{2}\times 0\right)+\hat{\mathbf{z}}(0\times 2\pi)\right] = 0. \tag{39}$$

Now, using the fact that any vector $\boldsymbol{V}$ can be written in terms of a unit vector as $\boldsymbol{V} = V\mathbf{v}$, with $V = \|\boldsymbol{V}\|$ and $\mathbf{v}$ a unit vector, we obtain that the integral $\mathscr{B}$ can be rewritten as

$$\mathscr{B} = \boldsymbol{a}_{is}\cdot\int_{\mathbb{R}^3}\exp\left(-\frac{\mu_{is}V^2}{2k_BT}\right)V\mathbf{v}V\,d\boldsymbol{V}.$$

Transforming to spherical coordinates and integrating, we obtain

$$\begin{aligned}
&\boldsymbol{a}_{is}\cdot\int_{\mathbb{R}^3}\exp\left(-\frac{\mu_{is}V^2}{2k_BT}\right)V\mathbf{v}V\,d\boldsymbol{V}\\
&\quad=\boldsymbol{a}_{is}\cdot\int_0^\infty\int_0^\pi\int_0^{2\pi}\exp\left(-\frac{\mu_{is}V^2}{2k_BT}\right)V(\hat{\mathbf{x}}\sin\theta\cos\phi+\hat{\mathbf{y}}\sin\theta\sin\phi+\hat{\mathbf{z}}\cos\theta)\\
&\quad\times V^3\sin\theta d\phi d\theta dV\\
&\quad=\boldsymbol{a}_{is}\cdot\int_0^\infty V^4\exp\left(-\frac{\mu_{is}V^2}{2k_BT}\right)dV\Bigg(\hat{\mathbf{x}}\underbrace{\int_0^\pi\sin^2\theta d\theta}_{\frac{\pi}{2}}\underbrace{\int_0^{2\pi}\cos\phi d\phi}_{0}\\
&\quad+\hat{\mathbf{y}}\underbrace{\int_0^\pi\sin^2\theta d\theta}_{\frac{\pi}{2}}\underbrace{\int_0^{2\pi}\sin\phi d\phi}_{0}+\hat{\mathbf{z}}\underbrace{\int_0^\pi\sin\theta\cos\theta d\theta}_{0}\underbrace{\int_0^{2\pi}d\phi}_{2\pi}\Bigg),
\end{aligned}$$

where $\hat{\mathbf{x}}$, $\hat{\mathbf{y}}$, $\hat{\mathbf{z}}$ are the Cartesian unit vectors in $\mathbb{R}^3$. Evaluating the integral with respect to V using (37), we obtain

$$\int_0^\infty V^4\exp\left(-\frac{\mu_{is}V^2}{2k_BT}\right)dV = \frac{1}{2}\Gamma\left(\frac{5}{2}\right)\left(\frac{2k_BT}{\mu_{is}}\right)^{\frac{5}{2}} = \frac{1}{2}\frac{3}{4}\sqrt{\pi}\left(\frac{2k_BT}{\mu_{is}}\right)^{\frac{5}{2}}.$$

Therefore,

$$\mathscr{B} = \boldsymbol{a}_{is}\frac{3\sqrt{\pi}}{8}\left(\frac{2k_BT}{\mu_{is}}\right)^{\frac{5}{2}}\cdot\left[\hat{\mathbf{x}}\left(\frac{\pi}{2}\times 0\right)+\hat{\mathbf{y}}\left(\frac{\pi}{2}\times 0\right)+\hat{\mathbf{z}}(0\times 2\pi)\right] = 0. \tag{40}$$

Transforming the integral $\mathscr{C}$ to spherical coordinates and integrating, we obtain

$$\begin{aligned}\mathscr{C} &= \int_0^\infty \int_0^\pi \int_0^{2\pi} \exp\left(-\frac{(m_i+m_s)X^2}{2k_BT}\right) X^2 \sin\theta d\phi d\theta dX \\ &= \int_0^\infty X^2 \exp\left(-\frac{(m_i+m_s)X^2}{2k_BT}\right) dX \underbrace{\int_0^\pi \sin\theta d\theta}_{2} \underbrace{\int_0^{2\pi} d\phi}_{2\pi} \\ &= 4\pi \int_0^\infty X^2 \exp\left(-\frac{(m_i+m_s)X^2}{2k_BT}\right) dX.\end{aligned}$$

Evaluating the previous integral using the integral representation of gamma (37), we obtain

$$\begin{aligned}\mathscr{C} &= 4\pi \frac{1}{2}\Gamma\left(\frac{3}{2}\right)\left(\frac{2k_BT}{m_i+m_s}\right)^{\frac{3}{2}} \\ &= 2\pi \frac{\sqrt{\pi}}{2}\left(\frac{2k_BT}{m_i+m_s}\right)^{\frac{3}{2}} \qquad (41) \\ &= \left(\frac{2\pi k_BT}{m_i+m_s}\right)^{\frac{3}{2}}. \qquad (42)\end{aligned}$$

Finally, the integral $\mathscr{D}$ can be rewritten as

$$\begin{aligned}\mathscr{D} &= \int_{\mathbb{R}^3} V\mathbf{v} \exp\left(-\frac{\mu_{is}V^2}{2k_BT}\right)\left(\boldsymbol{a}_{is}\cdot\boldsymbol{V}\right) V d\boldsymbol{V} \\ &= \int_{\mathbb{R}^3} V\mathbf{v} \exp\left(-\frac{\mu_{is}V^2}{2k_BT}\right)\left(a_{is}V\cos\theta\right) V d\boldsymbol{V} \\ &= a_{is}\int_{\mathbb{R}^3} V\mathbf{v} \exp\left(-\frac{\mu_{is}V^2}{2k_BT}\right) V^2\cos\theta d\boldsymbol{V}.\end{aligned}$$

Writing the integral $\mathscr{D}$ in spherical coordinates, we obtain

$$\begin{aligned}\mathscr{D} &= a_{is}\int_0^{\infty}\int_0^{\pi}\int_0^{2\pi} V(\hat{\mathbf{x}}\sin\theta\cos\phi + \hat{\mathbf{y}}\sin\theta\sin\phi + \hat{\mathbf{z}}\cos\theta)\,\exp\left(-\frac{\mu_{is}V^2}{2k_BT}\right)\\ &\times V^2\cos\theta V^2\sin\theta d\phi d\theta dV\\ &= a_{is}\underbrace{\int_0^{\infty} V^5\exp\left(-\frac{\mu_{is}V^2}{2k_BT}\right)dV}_{\mathscr{D}_1}\left(\hat{\mathbf{x}}\underbrace{\int_0^{\pi}\sin^2\theta\cos\theta d\theta}_{0}\underbrace{\int_0^{2\pi}\cos\phi d\phi}_{0}\right.\\ &\left.+\hat{\mathbf{y}}\underbrace{\int_0^{\pi}\sin^2\theta\cos\theta d\theta}_{0}\underbrace{\int_0^{2\pi}\sin\phi d\phi}_{0} + \hat{\mathbf{z}}\underbrace{\int_0^{\pi}\sin\theta\cos^2\theta d\theta}_{\frac{2}{3}}\underbrace{\int_0^{2\pi}d\phi}_{2\pi}\right),\end{aligned}$$

where $\hat{\mathbf{x}}, \hat{\mathbf{y}}, \hat{\mathbf{z}}$ are the Cartesian unit vectors in $\mathbb{R}^3$. Evaluating the integral in V using (37), we obtain

$$\begin{aligned}\int_0^{\infty} V^5\exp\left(-\frac{\mu_{is}V^2}{2k_BT}\right)dV &= \frac{1}{2}\Gamma(3)\left(\frac{2k_BT}{\mu_{is}}\right)^3\\ &= \frac{1}{2}2!\left(\frac{2k_BT}{\mu_{is}}\right)^3\\ &= \left(\frac{2k_BT}{\mu_{is}}\right)^3. \qquad (43)\end{aligned}$$

Substituting (43) into the integral $\mathscr{D}$, we obtain

$$\mathscr{D} = a_{is}\left(\frac{2k_BT}{\mu_{is}}\right)^3\left[\hat{\mathbf{x}}(0\times 0) + \hat{\mathbf{y}}(0\times 0) + \hat{\mathbf{z}}\left(\frac{2}{3}\times 2\pi\right)\right] = \boldsymbol{a}_{is}\frac{4\pi}{3}\left(\frac{2k_BT}{\mu_{is}}\right)^3. \qquad (44)$$

Since the integrals $\mathscr{A}$ and $\mathscr{B}$ both vanish, we have that $\mathscr{O}_i$ reduces to

$$\begin{aligned}\mathscr{O}_i &= -\alpha\sum_{\substack{s=1\\ s\neq i}}^{N}\sigma_{is}^2\frac{4\pi\mu_{is}m_s}{3(m_i+m_s)}\frac{(m_im_s)^{\frac{3}{2}}}{(2\pi k_BT)^3}c_i^{\alpha}c_s^{\alpha}\left(\frac{2\pi k_BT}{m_i+m_s}\right)^{\frac{3}{2}}\boldsymbol{a}_{is}\frac{4\pi}{3}\left(\frac{2k_BT}{\mu_{is}}\right)^3 + O(\alpha^2)\\ &= -\alpha\sum_{\substack{s=1\\ s\neq i}}^{N}\sigma_{is}^2\frac{16\mu_{is}^2}{9k_BT}\left(\frac{\mu_{is}}{2\pi k_BT}\right)^{\frac{3}{2}}c_i^{\alpha}c_s^{\alpha}\left(\frac{2\pi k_BT}{\mu_{is}}\right)^2\left(\frac{2k_BT}{\mu_{is}}\right)(\boldsymbol{u}_i^{\alpha}-\boldsymbol{u}_s^{\alpha}) + O(\alpha^2)\\ &= -\alpha\sum_{\substack{s=1\\ s\neq i}}^{N}\sigma_{is}^2\frac{32\mu_{is}}{9}c_i^{\alpha}c_s^{\alpha}\left(\frac{2\pi k_BT}{\mu_{is}}\right)^{\frac{1}{2}}(\boldsymbol{u}_i^{\alpha}-\boldsymbol{u}_s^{\alpha}) + O(\alpha^2)\\ &= -\alpha\frac{32}{9}\sum_{\substack{s=1\\ s\neq i}}^{N}\sigma_{is}^2(2\pi\mu_{is}k_BT)^{\frac{1}{2}}c_i^{\alpha}c_s^{\alpha}(\boldsymbol{u}_i^{\alpha}-\boldsymbol{u}_s^{\alpha}) + O(\alpha^2),\end{aligned}$$

where we have used the definition of $\boldsymbol{a}_{is}$ given in (19). The proof is complete. □

4.3 Formal Asymptotics

Here we present the asymptotic analysis of the species continuity equations and the species momentum balance equations towards a diffusion model where the diffusion process is described by the MS equations. For a diffusion asymptotics of the Boltzmann equations for non-reactive mixtures in a kinetic framework, see, [22].

Theorem 4.1 *The Maxwellians defined in* (17) *are solutions of the initial-boundary value problem* (12) *if* $(c_i^\alpha, \boldsymbol{u}_i^\alpha)$ *solves*

$$\begin{aligned} &\frac{\partial c_i^\alpha}{\partial t} + \frac{\partial}{\partial \boldsymbol{x}}(c_i^\alpha \boldsymbol{u}_i^\alpha) = 0, \quad i = 1, 2, \ldots, N, \\ &\alpha^2 m_i \frac{\partial}{\partial t}\left(c_i^\alpha \boldsymbol{u}_i^\alpha\right) + k_B T \frac{\partial c_i^\alpha}{\partial \boldsymbol{x}} + \alpha^2 m_i \frac{\partial}{\partial \boldsymbol{x}}\left(c_i^\alpha \boldsymbol{u}_i^\alpha \otimes \boldsymbol{u}_i^\alpha\right) = \frac{1}{\alpha}\mathscr{O}_i, \end{aligned} \tag{45}$$

where

$$\frac{1}{\alpha}\mathscr{O}_i = -\frac{32}{9}\sum_{\substack{s=1 \\ s\neq i}}^{N} \sigma_{is}^2 (2\pi \mu_{is} k_B T)^{\frac{1}{2}} c_i^\alpha c_s^\alpha \left(\boldsymbol{u}_i^\alpha - \boldsymbol{u}_s^\alpha\right) + O(\alpha).$$

Moreover, in the limit as $\alpha \to 0$ *Eqs.* (45) *reduces to*

$$\begin{aligned} &\frac{\partial c_i}{\partial t} + \frac{\partial \mathbf{J}_i}{\partial \boldsymbol{x}} = 0, \quad i = 1, 2, \ldots, N, \\ &\frac{\partial c_i}{\partial \boldsymbol{x}} = \frac{32}{9}\sum_{\substack{s=1 \\ s\neq i}}^{N} \sigma_{is}^2 \left(\frac{2\pi \mu_{is}}{k_B T}\right)^{\frac{1}{2}} \left(c_i \mathbf{J}_s - c_s \mathbf{J}_i\right). \end{aligned} \tag{46}$$

Proof Putting together Eqs. (27) and (29) gives (45). To obtain (46), we first set $c_i^\alpha \boldsymbol{u}_i^\alpha = \mathbf{J}_i^\alpha + c_i^\alpha \boldsymbol{u}^\alpha$ in (45), where $\boldsymbol{u}^\alpha$ represents the average velocity of the mixture, next we divide both sides of the second equation of (45) by $k_B T$, then take the limit for $\alpha \to 0$, where

$$c_i = \lim_{\alpha\to 0} c_i^\alpha, \qquad \mathbf{J}_i = \lim_{\alpha\to 0} \mathbf{J}_i^\alpha, \qquad \boldsymbol{u} = \lim_{\alpha\to 0} \boldsymbol{u}^\alpha,$$

and neglect the convective term, that is $\dfrac{\partial}{\partial \boldsymbol{x}}(c_i \boldsymbol{u}) = 0$. □

Observe that summing over all species in both equations given in (46), we obtain that $\dfrac{\partial c}{\partial t} = 0$ and $\dfrac{\partial c}{\partial \boldsymbol{x}} = 0$, respectively where $c = \displaystyle\sum_{i=1}^{N} c_i$. Therefore, we must have that c is uniform in space and constant in time. Hence, the second equation of system (46) can be rewritten as

$$\frac{\partial c_i}{\partial \boldsymbol{x}} = \frac{1}{c}\sum_{\substack{s=1\\ s\neq i}}^{N} \frac{c_i \mathbf{J}_s - c_s \mathbf{J}_i}{D_{is}}, \quad i = 1, 2, \ldots, N, \tag{47}$$

where

$$D_{is} = \frac{9}{32}\left(\frac{k_B T}{2\pi \mu_{is}}\right)^{\frac{1}{2}} \frac{1}{c\,\sigma_{is}^2}. \tag{48}$$

The equations given in (47) are the MS equations and the MS diffusion coefficients are given in (48). Replacing the second equation of (46) with (47), we obtain

$$\begin{aligned} &\frac{\partial c_i}{\partial t} + \frac{\partial \mathbf{J}_i}{\partial \boldsymbol{x}} = 0 \quad i = 1, 2, \ldots, N, \\ &\frac{\partial c_i}{\partial \boldsymbol{x}} = \frac{1}{c}\sum_{\substack{s=1\\ s\neq i}}^{N} \frac{c_i \mathbf{J}_s - c_s \mathbf{J}_i}{D_{is}}. \end{aligned} \tag{49}$$

System (49) above is a diffusion model where the diffusion process is described by the MS equations. Furthermore, the boundary conditions to accompany the system of equations (49) are

$$\nu \cdot \mathbf{J}_i = 0, \quad i = 1, 2, \ldots N, \tag{50}$$

where $\nu(\boldsymbol{x})$ is the outward normal vector at $\boldsymbol{x} \in \partial\Omega$. This boundary conditions ensure that the system is closed.

Remark 4.1 System (49) is a diffusion model where the diffusion process is governed by the MS equations. This diffusion model is similar to the ones obtained in [4, 6, 11]. However, the MS diffusion coefficients in [4] were not given explicitly. In [6, 11], the MS diffusion coefficient were obtained explicitly but they differ from the one obtained in this work. More precisely, the MS diffusion coefficients in [6] are given by

$$D_{ij} = \frac{KT}{2\pi \mu_{ij}} \frac{1}{c||b_{ij}||_{L^1}}, \tag{51}$$

while those of [11] are given by

$$\tilde{D}_{ij} = \frac{1}{\tilde{\Delta}_{ij}}, \quad \text{where} \quad \tilde{\Delta}_{ij} = a_0 \frac{2\pi \mu_{ij} |b_{ij}|_{L^1}}{(m_i + m_j)kT} + \ldots, \tag{52}$$

see Eq. (24) of [11] for the complete expression of $\tilde{\Delta}_{ij}$. The difference σ_{is}^2 and $|b_{ij}|_{L^1}$ is due to the fact that the angular collision kernel in [6, 11] is given by $b_{ij}(\cos\theta)$, whereas in the present paper, it is $\cos\theta$. The differences in the coefficient $\frac{9}{32}$ and the exponent $\frac{1}{2}$ between Eqs. (48) and (51) are consequences of the difference in the considered cross-sections and the definitions of the pre-collision velocities in [6, 11] and the post-collision velocities in the present work. Furthermore, the MS diffusion

coefficients obtained in this work are the same as those obtained in [1] because the cross-sections considered in both cases are of hard-sphere type, and also because of the chemical regime considered in [1], which results in the fact that diffusion effects are not seen on the chemical reactive terms.

5 Conclusion

In this work, we have studied a kinetic model for non-reactive mixtures with hard-sphere cross-sections under isothermal condition and obtained a diffusion model where the diffusion process is described by the Maxwell–Stefan equations. More precisely, the diffusion model of MS type was obtained as a hydrodynamic limit of the scaled kinetic equations. In particular, from the species continuity equations and the species momentum balance equations in the limit as the scaling parameter tends to zero.

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References

1. B. Anwasia, P. Gonçalves, A.J. Soares, From the simple reacting sphere kinetic model to the reaction-diffusion system of Maxwell-Stefan type. Commun. Math. Sci. **17**, 507–538 (2019)
2. B. Anwasia, M. Bisi, F. Salvarani, A.J. Soares, On the Maxwell-Stefan diffusion limit for a reactive mixture of polyatomic gases in non-isothermal setting. Kinet. Relat. Mod. **13**, 63–95 (2020)
3. D. Bothe, On the Maxwell-Stefan approach to multicomponent diffusion. Prog. Nonliniear Differ. Equ. Appl. **80**, 81–93 (2011)
4. L. Boudin, B. Grec, V. Pavan, The Maxwell-Stefan diffusion limit for a kinetic model of mixtures with general cross sections. Nonlinear Anal. **159**, 40–61 (2017)
5. L. Boudin, B. Grec, F. Salvarani, A mathematical and numerical analysis of the Maxwell-Stefan diffusion equations. Discrete Contin. Dyn. Syst. Ser. B **17**, 1427–1440 (2012)
6. L. Boudin, B. Grec, F. Salvarani, The Maxwell-Stefan diffusion limit for a kinetic model of mixtures. Acta Appl. Math. **136**, 79–90 (2015)
7. C. Cercignani, *The Boltzmann Equation and Its Applications* (Springer, New York, 1988)
8. J.B. Duncan, H.L. Toor, An experimental study of three component gas diffusion. AIChE J. **8**, 38–41 (1962)
9. A. Fick, On liquid diffusion. Phil. Mag. **10**, 30–39 (1855)
10. A. Fick, Über Diffusion. Poggendorff's Annel Physik **94**, 59–86 (1855)
11. H. Hutridurga, F. Salvarani, On the Maxwell-Stefan diffusion limit for a mixture of monatomic gases. Math. Meth. Appl. Sci. **40**, 803–813 (2017)
12. H. Hutridurga, F. Salvarani, Maxwell-Stefan diffusion asymptotics for gas mixtures in non-isothermal setting. Nonlinear Anal. **159**, 285–297 (2017)
13. A. Jüngel, I.V Stelzer, Existence analysis of Maxwell-Stefan systems for multicomponent mixtures. J. Math. Anal. **45**, 2421–2440 (2013)
14. R. Krishna, J. Wesselingh, The Maxwell-Stefan approach to mass transfer. Chem. Engin. Sci. **52**, 861–911 (1997)

15. J.C. Maxwell, On the dynamical theory of gases. Phil. Trans. R. Soc. **157**, 49–88 (1866)
16. M. McLeod, Y. Bourgault, Mixed finite element methods for addressing multi-species diffusion using the Maxwell Stefan equations. Comput. Methods Appl. Mech. Engrg. **279**, 515535 (2014)
17. J. Polewczak, A.J. Soares, On modified simple reacting spheres kinetic model for chemically reactive gases. Kinet. Relat. Models **10**, 513–539 (2017)
18. J. Stefan, Über das Gleichgewicht und die Bewegung insbesondere die Diffusion von Gasgemengen. Akad. Wiss. Wien **63**, 63–124 (1871)
19. C. Bardos, F. Golse, C.D. Levermore, Fluid dynamic limits of kinetic equations. I. Formal derivations. J. Stat. Phys. **63**, 323–344 (1991)
20. D. Bothe, W. Dreyer, Continuum thermodynamics of chemically reacting fluid mixtures. Acta Mech. **226**, 1757–1805 (2015)
21. S. Simić, M. Pavić-Čolić, D. Madjarević, Non-equilibrium mixtures of gases: Modelling and computation. Rivista di Matematica della Universita di Parma **6**(1), 135214 (2015)
22. L. Boudin, B. Gréc, M. Pavić, F. Salvarani, Diffusion asymptotics of a kinetic model for gaseous mixtures. Kinet. Relat. Model **6**(1), 137157 (2013)

An Asymptotic Preserving Scheme for a Stochastic Linear Kinetic Equation in the Diffusion Regime

Nathalie Ayi

Abstract In this paper, we present an Asymptotic Preserving scheme for a stochastic linear kinetic equation. Its construction is based on a micro-macro decomposition. We start by explaining how we build it and then perform the formal numerical limit. After stating some stability results proved in [1], some numerical tests confirming the good performances of our scheme are finally presented.

Keywords Stochastic partial differential equations · Transport equations · Diffusion limit · Asymptotic preserving schemes · Stiff terms

1 Introduction

In some physical contexts such as radiative transfer or rarefied gas dynamics for instance, there exist several levels of description: the microscopic scale where we are interested in the evolution of each particle and the macroscopic one where we deal with macroscopic quantities. There exists also an intermediate scale, called mesoscopic, where we are interested in the evolution of the density of particles f, a function depending on time, position and velocity such that $f(t, x, v)dxdv$ represents the number of particles in the infinitesimal volume $dxdv$. At this level, we study the kinetic equation satisfied by the density of particles. The passage from one scale to another is done by passing to the limit on one parameter of the system. Typically, to go from the microscopic scale to the mesoscopic one, we pass to the limit on the number of particles N, N going to infinity.

In this proceeding, we will focus on the passage from the mesoscopic scale to the macroscopic one, by passing to the limit on the mean free path, denoted by ε. Our goal will be to study this passage from a numerical point of view. Indeed, we want to design a scheme which adapts to this particular scaling limit. Actually, this type of problem can be very challenging numerically. The idea is to construct a

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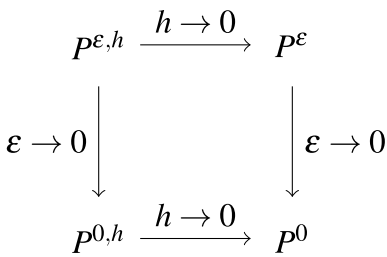

Fig. 1 Property of AP Schemes: $P^{\varepsilon,h}$ is the numerical approximation of the solution of the kinetic equation P^{ε} and converges to the numerical approximation $P^{0,h}$ of the solution of the macroscopic equation P^0

scheme which mimics the asymptotic behavior of the kinetic equation, i.e. reduces to numerical approximations of the macroscopic equation when the scaling parameter goes to 0. This is exactly the purpose of the Asymptotic Preserving (AP) schemes as illustrated in Fig. 1. They have been first studied in neutron transport by Larsen et al. [19], Larsen and Morel [18] and Jin and Levermore [13, 14] for steady problems. For time dependent problems, we can mention the works of Klar [17], Jin et al. [15] who proposed two classes of semi-implicit time discretizations.

One of the difficulties is that, when adopting standard schemes to reach our goal, the time step satisfies a stability condition of the type $h = \mathcal{O}(\varepsilon)$ and this becomes computationally too expensive in "fluid" zone (i.e. for ε small). Therefore, we need to be cautious when constructing our scheme to obtain an h independent of ε.

This type of questions has been widely studied in the literature. The novelty in our problem is that we are interested in that question in a stochastic setting. The kinetic equation we study presents a stochastic perturbation by a Wiener process. Indeed, lately, the study of stochastic perturbation of well known deterministic partial differential equations has been a subject of growing interest, (see [2, 7–9, 11, 12, 16] …). The introduction of such term can be justified to model numerical and empirical uncertainties.

The paper is organized as follows: in Sect. 2, we introduce the model under study, which is a stochastic kinetic linear equation with multiplicative noise. In Sect. 3, we present the diffusion limit and we introduce a new formulation of the problem which will be the key to construct our scheme. In Sect. 4, we construct the scheme and give some results about its behavior. In Sect. 5, we present some numerical tests. Finally, in Sect. 6, we present our perspectives.

2 General Setting

We are interested into the following stochastic linear kinetic equation (see [6])

$$df + \frac{1}{\varepsilon} v \partial_x f dt = \frac{\sigma}{\varepsilon^2} \mathscr{L} f dt + f \circ Q dW_t \tag{1}$$

where f is the distribution function of particles that depends on time $t > 0$, on position $x \in \mathbf{T} = \mathbf{R}/2\pi\mathbf{Z}$ and on velocity $v \in [-1, 1]$, dW_t a cylindrical Wiener process on the Hilbert space $L^2(\mathbf{T})$, $\circ$ referring to the Stratonovich integral. We can define it by setting

$$dW_t = \sum_{k\geq 0} e_k d\beta_k(t)$$

where the $(\beta_k)_{k\geq 0}$ are independent Brownian motions on the real line and $(e_k)_{k\geq 0}$ a complete orthonormal system in the Hilbert space $L^2(\mathbf{T})$. Q is a linear self-adjoint operator on $L^2(\mathbf{T})$ such that

$$\sum_{k\geq 0} \| Qe_k \|^2_{L^\infty_x} < +\infty. \tag{2}$$

This assumption, borrowed to [6], is used for the existence of a solution to the macroscopic equation that we will introduce later. Moreover, we assume that σ satisfies $0 < \sigma_m \leq \sigma(x) \leq \sigma_M$ for every x and belongs to $\mathscr{C}^3(\mathbf{T})$.

In this Eq. 1, the left-hand side represents the free transport of the particles while the right-hand side models the interaction of particles with the medium.

We define the operator Π such that

$$\Pi\phi = \frac{1}{2}\int_{-1}^{1} \phi(v)dv \tag{3}$$

which is the average of every velocity dependent function ϕ. The linear operator $\mathscr{L}$ that we will consider is given by

$$\mathscr{L} f(v) = \int_{-1}^{1} s(v, v')(f(v') - f(v))dv', \tag{4}$$

where the kernel s is such that $0 < s_m \leq s(v, v') \leq s_M$ for every $v, v' \in [-1, 1]$. We assume that s satisfies $\int_{-1}^{1} s(v, v')dv' = 1$ and that it is symmetric: $s(v, v') = s(v', v)$.

We then have the following properties:

Lemma 1 • *$\mathscr{L}$ acts only on the velocity dependence of f (it is local with respect to t and x).*
- *$\Pi(\mathscr{L}\phi) = 0$ for every $\phi \in L^2([-1, 1])$.*
- *The null space of $\mathscr{L}$ is $\mathscr{N}(\mathscr{L}) = \{\phi = \Pi\phi\}$ (constant functions).*
- *The range of $\mathscr{L}$ is $\mathscr{R}(\mathscr{L}) = \mathscr{N}^\perp(\mathscr{L}) = \{\phi \text{ s.t. } \Pi\phi = 0\}$.*
- *$\mathscr{L}$ is non-positive self-adjoint in $L^2([-1, 1])$ and we have*

$$\Pi(\phi\mathscr{L}\phi) \leq -2s_m\Pi(\phi^2) \tag{5}$$

for every $\phi \in \mathcal{N}^{\perp}(\mathscr{L})$.
- $\mathscr{L}$ *admits a pseudo inverse from* $\mathcal{N}^{\perp}(\mathscr{L})$ *onto* $\mathcal{N}^{\perp}(\mathscr{L})$ *denoted by* $\mathscr{L}^{-1}$.
- *The orthogonal projection from* $L^2([-1,1])$ *onto* $\mathcal{N}(\mathscr{L})$ *is* Π.

All those properties are actually easy to obtain once we have noticed that the assumptions on s imply that $\mathscr{L} + I$ is a self-adjoint Hilbert–Schmidt, and therefore compact operator.

For instance, the one-group transport equation corresponds to

$$\mathscr{L} f = \int_{-1}^{1} \frac{1}{2}(f(v') - f(v))dv' = \Pi f - f,$$

and it is classical in this case to prove that $\mathscr{L}$ satisfies all the previous properties. Equation 1 becomes

$$df + \frac{1}{\varepsilon} v \partial_x f dt = \frac{\sigma}{\varepsilon^2}(\Pi f - f)dt + f \circ Q dW_t. \tag{6}$$

If the velocity set is $\{-1, 1\}$, dv is the discrete measure and the corresponding one-group transport equation is called the telegraph equation. We denote $f(t, x, 1) := p(t, x)$ and $f(t, x, -1) := q(t, x)$. For $\sigma = 1$, the Eq. 1 becomes

$$\begin{cases} dp + \frac{1}{\varepsilon}\partial_x p dt = \frac{1}{\varepsilon^2}\left(\frac{p+q}{2} - p\right)dt + p \circ dW_t \\ dq - \frac{1}{\varepsilon}\partial_x q dt = \frac{1}{\varepsilon^2}\left(\frac{p+q}{2} - q\right)dt + q \circ dW_t. \end{cases} \tag{7}$$

3 The Diffusion Limit

3.1 The Macroscopic Equation

The diffusive limit of (1) when ε goes to 0 is

$$d\rho + \partial_x(\kappa \partial_x \rho)dt = \rho \circ Q dW_t \tag{8}$$

with $\kappa(x) = \dfrac{\Pi(v\mathscr{L}^{-1}v)}{\sigma(x)}$, see [6].
A good approach to see it is to perform Hilbert's expansion:

$$f(t, x, v) = f_0(t, x, v) + \varepsilon f_1(t, x, v) + \varepsilon^2 f_2(t, x, v) + \ldots \tag{9}$$

and to identify the power of ε. Using the properties of $\mathscr{L}$ leads to

$$\begin{aligned} \sigma \mathscr{L} f_0 = 0 \Rightarrow f_0 = \Pi f_0 = \rho_0, \\ v\partial_x f_0 = \sigma \mathscr{L} f_1 \Rightarrow f_1 = \mathscr{L}^{-1}\left(\frac{1}{\sigma} v\partial_x \rho_0\right) \end{aligned} \tag{10}$$

$$df_0 = \sigma \mathscr{L} f_2 dt + f_0 \circ Q dW_t - v\partial_x f_1 dt. \tag{11}$$

Applying Π on (11) and identifying f_1, we obtain

$$d\rho_0 = \rho_0 \circ Q dW_t - \partial_x \left(\Pi\left[v\mathscr{L}^{-1}\left(\frac{v}{\sigma}\right)\right]\partial_x \rho_0\right) dt \tag{12}$$

and so when ε goes to 0, f_ε goes to f_0 which is equal to ρ_0, solution of (8).

3.2 The Micro-Macro Decomposition

The starting point of this article is a scheme proposed by Lemou and Mieussens in [20] based on the micro-macro decomposition of the distribution function into microscopic and macroscopic components. The decomposition only uses basic properties of the collision operator that are common to most of kinetic equations (namely conservation and equilibrium properties) and leads to a coupled system of equations for these two components without any linearity assumption. One of the interest of this approach is that it appears to be very general, as it can be applied to kinetic equations for both diffusion limit (see [20, 21] for linear transport equations and [4] for the nonlinear Kac equation) and hydrodynamic regimes (see [3] for the Boltzmann equation for instance).

We introduce g such that

$$g := \frac{f - \rho}{\varepsilon} \tag{13}$$

with $\rho = \Pi(f)$ so that $f = \rho + \varepsilon g$, adopting the framework of an expansion of Chapman–Enskog type. We notice that g satisfies $\Pi(g) = 0$. The equation becomes

$$d(\rho + \varepsilon g) + \frac{1}{\varepsilon} v\partial_x(\rho + \varepsilon g)dt = \frac{\sigma}{\varepsilon^2}\mathscr{L}(\rho + \varepsilon g)dt + (\rho + \varepsilon g) \circ Q dW_t. \tag{14}$$

We apply Π and since $\pi(\mathscr{L}\phi) = 0$ for every ϕ, we obtain

$$d\rho + \partial_x \Pi(vg)dt = \rho \circ Q dW_t. \tag{15}$$

We do (14), (15) and obtain

$$dg + \frac{1}{\varepsilon}(I - \Pi)(v\partial_x g)dt = \frac{\sigma}{\varepsilon^2}\mathscr{L} g dt + g \circ Q dW_t - \frac{1}{\varepsilon^2} v\partial_x \rho dt. \tag{16}$$

Thus, we obtain an equivalent system to (14):

$$\begin{cases} d\rho + \partial_x \Pi(vg)dt = \rho \circ Q dW_t \\ dg + \dfrac{1}{\varepsilon}(I - \Pi)(v\partial_x g)dt = \dfrac{\sigma}{\varepsilon^2}\mathscr{L} g dt + g \circ Q dW_t - \dfrac{1}{\varepsilon^2} v\partial_x \rho dt. \end{cases} \tag{17}$$

Example 1 For the one group transport equation, the micro-macro decomposition writes

$$\begin{cases} d\rho + \partial_x \Pi(vg)dt = \rho \circ Q dW_t \\ dg + \dfrac{1}{\varepsilon}(I - \Pi)(v\partial_x g)dt = -\dfrac{\sigma}{\varepsilon^2} g dt + g \circ Q dW_t - \dfrac{1}{\varepsilon^2} v\partial_x \rho dt. \end{cases} \tag{18}$$

For the telegraph equation, denoting $g = (\alpha, \gamma)$, it is

$$\begin{cases} d\rho + \partial_x \dfrac{\alpha - \gamma}{2} dt = \rho \circ Q dW_t \\ d\alpha + \dfrac{1}{\varepsilon}\partial_x \dfrac{\alpha + \gamma}{2} dt = -\dfrac{1}{\varepsilon^2}\alpha dt + \alpha \circ Q dW_t - \dfrac{1}{\varepsilon^2}\partial_x \rho dt \\ d\gamma - \dfrac{1}{\varepsilon}\partial_x \dfrac{\gamma + \alpha}{2} dt = -\dfrac{1}{\varepsilon^2}\gamma dt + \gamma \circ Q dW_t + \dfrac{1}{\varepsilon^2}\partial_x \rho dt. \end{cases} \tag{19}$$

3.3 Formal Analytical Limit

Under this form, we can perform the formal analytical limit again. The interest is that it is now straightforward. Moreover, we will study the limit of our numerical scheme with this same approach.

From $dg + \dfrac{1}{\varepsilon}(I - \Pi)(v\partial_x g)dt = \dfrac{\sigma}{\varepsilon^2}\mathscr{L} g dt + g \circ Q dW_t - \dfrac{1}{\varepsilon^2} v\partial_x \rho dt$, we deduce

$$g = \mathscr{L}^{-1}\left(\frac{1}{\sigma} v\partial_x \rho\right) + \mathscr{O}(\varepsilon).$$

Thus, $d\rho + \partial_x \Pi(vg)dt = \rho \circ Q dW_t$ leads to

$$d\rho + \partial_x(\kappa \partial_x \rho)dt = \rho \circ Q dW_t + \mathscr{O}(\varepsilon)$$

where $\kappa(x) = \dfrac{\Pi(v\mathscr{L}^{-1}v)}{\sigma(x)}$ is the diffusion coefficient which satisfies $\kappa(x) < 0\ \forall x$.

4 The Numerical Scheme

4.1 Construction of the Scheme

We start by an illustration of the type of problems that can occur. Let us deal with the stiff term for the one-group transport equation with $\sigma = 1$. We are interested in

$$\partial_t g = -\frac{1}{\varepsilon^2} g. \tag{20}$$

With the explicit Euler method, we obtain

$$\frac{g^{n+1} - g^n}{\Delta t} = -\frac{1}{\varepsilon^2} g^n. \tag{21}$$

Thus, we have $g^{n+1} = \left(1 - \frac{\Delta t}{\varepsilon^2}\right) g^n = \left(1 - \frac{\Delta t}{\varepsilon^2}\right)^{n+1} g^0$. Therefore, we see that stability considerations imply that $\Delta t \leq \varepsilon^2$. In particular for instance, in order to preserve the positivity, we have to satisfy this condition. Thus, it is an issue for small ε. On the other hand, if we adopt the implicit Euler method, we obtain

$$\frac{g^{n+1} - g^n}{\Delta t} = -\frac{1}{\varepsilon^2} g^{n+1} \tag{22}$$

Thus, we have $g^{n+1} = \left(\frac{\varepsilon^2}{\varepsilon^2 + \Delta t}\right) g^n$ and we see that stability issues are independent of the size ε.

Thus, in our scheme, the collision term will be implicit to ensure stability as ε goes to 0. Furthermore, we will adopt the upwind discretization of $(I - \Pi)(v\partial_x g)$ to ensure stability in the kinetic regime while the centered approximations of $\partial_x \Pi(vg)$ and $v\partial_x \rho$ will allow to capture the diffusion limit. Using the formula which links the Itô integral and the Stratonovich one, we can rewrite (17) as follows

$$\begin{cases} d\rho + \partial_x \Pi(vg)dt = \rho Q dW_t + \frac{1}{2}\rho \sum_{k\geq 0} (Qe_k)^2 dt \\ dg + \frac{1}{\varepsilon}(I - \Pi)(v\partial_x g)dt = \frac{\sigma}{\varepsilon^2} \mathscr{L} g dt + g Q dW_t + \frac{1}{2} g \sum_{k\geq 0} (Qe_k)^2 dt - \frac{1}{\varepsilon^2} v\partial_x \rho dt. \end{cases} \tag{23}$$

We study the following numerical scheme for this system with a time step Δt and times $t_n = n\Delta t$ and two staggered grids of step Δx and nodes $x_i = i\Delta x$ and $x_{i+\frac{1}{2}} = (i + \frac{1}{2})\Delta x$ extended by periodicity. We are interested in a semi-discretization in x, and we use the notation $\rho_i^n \approx \rho(t_n, x_i)$ and $g_{i+\frac{1}{2}}^n(v) \approx g(t_n, x_{i+\frac{1}{2}}, v)$.

$$\begin{aligned}
\rho_i^{n+1} &= \rho_i^n - \Delta t\, \Pi\left(v\frac{g_{i+\frac{1}{2}}^{n+1} - g_{i-\frac{1}{2}}^{n+1}}{\Delta x}\right) + \rho_i^n\left(\frac{1}{2}\Delta t\sum_{k\geq 0}(b_{ik})^2 + \sqrt{\Delta t}\sum_{k\geq 0} b_{ik}\xi_k^{n+1}\right)\\
g_{i+\frac{1}{2}}^{n+1} &= g_{i+\frac{1}{2}}^n - \frac{\Delta t}{\varepsilon\Delta x}(I-\Pi)\left(v^+\left(g_{i+\frac{1}{2}}^n - g_{i-\frac{1}{2}}^n\right) + v^-\left(g_{i+\frac{3}{2}}^n - g_{i+\frac{1}{2}}^n\right)\right)\\
&\quad + \frac{\sigma_{i+\frac{1}{2}}}{\varepsilon^2}\mathscr{L}g_{i+\frac{1}{2}}^{n+1}\Delta t + g_{i+\frac{1}{2}}^n\left(\frac{1}{2}\Delta t\sum_{k\geq 0}(b_{i+\frac{1}{2},k})^2 + \sqrt{\Delta t}\sum_{k\geq 0} b_{i+\frac{1}{2},k}\xi_k^{n+1}\right)\\
&\quad - \frac{1}{\varepsilon^2}v\frac{\rho_{i+1}^n - \rho_i^n}{\Delta x}\Delta t,
\end{aligned} \tag{24}$$

where $v^+ = \max(v, 0)$ and $v^- = \min(v, 0)$, $(\xi_k^n)_{n\geq 1, k\geq 0}$ are i.i.d. variables with a normal distribution and we use the notation $b_{ik} := Qe_k(x_i)$ and $b_{i+\frac{1}{2},k} := Qe_k(x_{i+\frac{1}{2}})$.

4.2 Formal Numerical Limit

Similarly as for the kinetic equation, we can obtain the formal limit directly. From the second equation of (24), we obtain $g_{i+\frac{1}{2}}^{n+1} = \dfrac{1}{\sigma_{i+\frac{1}{2}}}\mathscr{L}^{-1}\left(v\dfrac{\rho_{i+1}^n - \rho_i^n}{\Delta x}\right) + \mathscr{O}(\varepsilon)$. Thus, putting this in the first equation of (24), we have

$$\rho_i^{n+1} = \rho_i^n - \frac{\Delta t}{\Delta x}\left(\kappa_{i+\frac{1}{2}}\frac{\rho_{i+1}^n - \rho_i^n}{\Delta x} - \kappa_{i-\frac{1}{2}}\frac{\rho_i^n - \rho_{i-1}^n}{\Delta x}\right) + \rho_i^n\left(\frac{1}{2}\Delta t\sum_{k\geq 0}(b_{ik})^2 + \sqrt{\Delta t}\sum_{k\geq 0} b_{ik}\xi_k^{n+1}\right) + \mathscr{O}(\varepsilon)$$

with $\kappa_{i+\frac{1}{2}} = \dfrac{\Pi(v\mathscr{L}^{-1}v)}{\sigma_{i+\frac{1}{2}}}$. We recognize the usual 3-points stencil explicit scheme for the diffusion equation.

4.3 Stability Results

In this subsection, we will just state the stability results that we have established in [1] and we invite the reader to consult this reference to see the proofs.

4.3.1 The Telegraph Case

We start with the telegraph case with a one dimensional Brownian motion. In that case, as seen previously the micro-macro system writes

$$\begin{cases} d\rho + \partial_x \dfrac{\alpha-\gamma}{2} dt = \rho \circ d\beta(t) \\ d\alpha + \dfrac{1}{\varepsilon}\partial_x \dfrac{\alpha+\gamma}{2} dt = -\dfrac{1}{\varepsilon^2}\alpha dt + \alpha \circ d\beta(t) - \dfrac{1}{\varepsilon^2}\partial_x \rho dt \\ d\gamma - \dfrac{1}{\varepsilon}\partial_x \dfrac{\gamma+\alpha}{2} dt = -\dfrac{1}{\varepsilon^2}\gamma dt + \gamma \circ d\beta(t) + \dfrac{1}{\varepsilon^2}\partial_x \rho dt. \end{cases} \tag{25}$$

For this system, the scheme (24) takes the form

$$\begin{aligned} \rho_i^{n+1} &= \rho_i^n - \tfrac{\Delta t}{2\Delta x}\left[\left(\alpha_{i+\frac12}^{n+1} - \gamma_{i+\frac12}^{n+1}\right) - \left(\alpha_{i-\frac12}^{n+1} - \gamma_{i-\frac12}^{n+1}\right)\right] + \rho_i^n\left(\tfrac{\Delta t}{2} + \sqrt{\Delta t}\,\xi^{n+1}\right) \\ \alpha_{i+\frac12}^{n+1} &= \alpha_{i+\frac12}^n - \frac{\Delta t}{\varepsilon \Delta x}\left[\left(\alpha_{i+\frac12}^n - \alpha_{i-\frac12}^n\right) - \frac12\left(\alpha_{i+\frac12}^n - \alpha_{i-\frac12}^n - \gamma_{i+\frac32}^n + \gamma_{i+\frac12}^n\right)\right] \\ &\quad - \frac{\Delta t}{\varepsilon^2}\alpha_{i+\frac12}^{n+1} + \alpha_{i+\frac12}^n\left(\frac{\Delta t}{2} + \sqrt{\Delta t}\,\xi^{n+1}\right) - \frac{1}{\varepsilon^2}\Delta t\left(\frac{\rho_{i+1}^n - \rho_i^n}{\Delta x}\right) \\ \gamma_{i+\frac12}^{n+1} &= \gamma_{i+\frac12}^n \frac{\Delta t}{\varepsilon \Delta x}\left[-\left(\gamma_{i+\frac32}^n - \gamma_{i+\frac12}^n\right) - \frac12\left(\alpha_{i+\frac12}^n - \alpha_{i-\frac12}^n - \gamma_{i+\frac32}^n + \gamma_{i+\frac12}^n\right)\right] \\ &\quad - \frac{\Delta t}{\varepsilon^2}\gamma_{i+\frac12}^{n+1} + \gamma_{i+\frac12}^n\left(\frac{\Delta t}{2} + \sqrt{\Delta t}\,\xi^{n+1}\right) + \frac{1}{\varepsilon^2}\Delta t\left(\frac{\rho_{i+1}^n - \rho_i^n}{\Delta x}\right) \end{aligned} \tag{26}$$

where $(\xi^n)_{n\geq 1}$ are i.i.d. variables with a normal distribution. We denote $j := \frac{1}{2\varepsilon}(p-q) = \frac12(\alpha-\gamma)$ and the above scheme can be written under the much simpler form

$$\begin{aligned} \rho_i^{n+1} &= \rho_i^n - \tfrac{\Delta t}{\Delta x}\left(j_{i+\frac12}^{n+1} - j_{i-\frac12}^{n+1}\right) + \rho_i^n\left(\tfrac{\Delta t}{2} + \sqrt{\Delta t}\,\xi^{n+1}\right) \\ j_{i+\frac12}^{n+1} &= j_{i+\frac12}^n + \frac{\Delta t}{2\varepsilon \Delta x}\left[j_{i+\frac32}^n - 2j_{i+\frac12}^n + j_{i-\frac12}^n\right] \\ &\quad - \frac{\Delta t}{\varepsilon^2} j_{i+\frac12}^{n+1} + j_{i+\frac12}^n\left(\frac{\Delta t}{2} + \sqrt{\Delta t}\,\xi^{n+1}\right) - \frac{1}{\varepsilon^2}\Delta t\left(\frac{\rho_{i+1}^n - \rho_i^n}{\Delta x}\right) \end{aligned} \tag{27}$$

In [1], we have established the following result for the stability of this scheme.

Theorem 1 *There exist constants L, Δt_0, Δx_0 and ε_0 such that for all $\Delta t \leq \Delta t_0$, $\Delta x \leq \Delta x_0$ and $\varepsilon \leq \varepsilon_0$ satisfying the CFL condition*

$$\Delta t \leq \frac12\left(\frac{\Delta x^2}{2} + \varepsilon \Delta x\right) \tag{28}$$

then we have

$$\mathrm{e}\left[\sum_i (\rho_i^n)^2 + (\varepsilon j_{i+\frac12}^n)^2\right] \leq e^{Ln\Delta t}\,\mathrm{e}\left[\sum_i (\rho_i^0)^2 + (\varepsilon j_{i+\frac12}^0)^2\right] \tag{29}$$

for every n.

The proof is based on a standard Von Neumann analysis. We observe that the diffusive CFL condition $\Delta t \leq \frac{1}{4}\Delta x^2$ is sufficient for stability for small ε, while half of the convection CFL is sufficient for $\varepsilon = O(1)$.

4.3.2 The General Case

We also have established the uniform stability of the general scheme in [1].

Theorem 2 *If Δt satisfies the following CFL condition*

$$\Delta t \leq \frac{2 s_m \sigma_m \Delta x^2}{2(2+\varepsilon)} + \frac{\varepsilon \Delta x}{2+\varepsilon}, \tag{30}$$

then the sequence ρ^n and g^n defined by the scheme (24) satisfy the energy estimate

$$\mathrm{e}\left[\sum_i (\rho_i^n)^2\right] + \varepsilon^2 \mathrm{e}\left[\sum_i \Pi\left((g^n_{i+\frac{1}{2}})^2\right)\right] \leq C(T)\left(\mathrm{e}\left[\sum_i (\rho_i^0)^2\right] + \varepsilon^2 \mathrm{e}\left[\sum_i \Pi\left((g^0_{i+\frac{1}{2}})^2\right)\right]\right) \tag{31}$$

for every n with $C(T)$ a constant which only depends on T. Hence, the scheme (24) is stable.

5 Numerical Tests

We now test the performance of our algorithm on the one-group model (6) with velocity set $[-1, 1]$ and $\sigma = 1$. We denote this equation by

$$df + \frac{v}{\varepsilon}\partial_x f dt = \frac{1}{\varepsilon}(\Pi f - f)dt + f \circ Q dW_t. \tag{32}$$

For the space variable $x \in [0, 1]$, we assume periodic boundary conditions. The noise QW_t is given by

$$(QW)_t(x) = \sum_{k \in \mathbf{Z}} \frac{1}{|k|+1}\left(\cos(2k\pi x) + \sin(2k\pi x)\right) d\beta_k(t)$$

where $(\beta_k)_{k\in\mathbf{Z}}$ are independent brownian motions. Note that, indeed, it fulfills the condition (2). The initial data $f(0, x, v) = f_0(x, v)$ is given by

$$f_0(x, v) = (1 + \cos(2\pi x + \pi)).$$

We denote our scheme SMM N, where N is the number of grid points both in space and velocity variables: $x_j = j\Delta x$ for $\Delta x = N^{-1}$ and $v_j = -1 + j\Delta v$ with

$\Delta v = 2\Delta x = 2N^{-1}$ for $j = 1, \ldots, N-1$. A function $f(x, v)$ will be approximated by numbers f_{jk}, $(j, k) \in \{0, \ldots, N-1\}$ representing $f(x_j, v_k)$ evaluated at the grid point. For a given time step Δt, $f(t_n, x_j, v_k)$ is thus represented by f_{jk}^n for $t_n = n\Delta t$. The operator Π is discretized by the discrete average operator $(\Pi_N f)_j = \frac{1}{2N} \sum_{k=0}^{N-1} f_{jk}$.

To test the performance of our scheme and in particular its asymptotic preserving properties, we calculate some reference solutions to which we will compare our numerical results. We compare our solution with the kinetic equation for $\varepsilon = 1$. More precisely, we compute reference solutions with the explicit schemes

$$f_i^{n+1} = f_i^n - \frac{\Delta t}{\varepsilon \Delta x}(v^+(f_i^n - f_{i-1}^n) + v^-\left(f_{i+1}^n - f_i^n\right)) + \frac{1}{\varepsilon^2}(\Pi f_i^n - f_i^n) + f_i^n\left(\frac{1}{2}\Delta t \sum_{k\geq 0}(b_{ik})^2 + \sqrt{\Delta t}\sum_{k\geq 0} b_{ik}\xi_k^{n+1}\right) \tag{33}$$

referred to as the kinetic (KIN) schemes. Then, we compare our numerical solution with respect to the solution of the diffusion Eq. 8 for smaller ε with $\kappa = \Pi(v\mathscr{L}^{-1}v) = -1/3$, and which is independent of ε. To compute an approximation μ_i^n of the solution of this equation at time t_n and grid points x_i, we use the Crank–Nicholson (CN) scheme

$$\mu_i^{n+1} = \mu_i^n - \frac{\kappa}{2}\frac{\Delta t}{\Delta x^2}\left(\mu_{i+1}^{n+1} - 2\mu_i^{n+1} + \mu_{i-1}^{n+1}\right) - \frac{\kappa}{2}\frac{\Delta t}{\Delta x^2}\left(\mu_{i+1}^n - 2\mu_i^n + \mu_{i-1}^n\right) + \mu_i^n\left(\frac{1}{2}\Delta t\sum_{\ell\geq 0}(b_{i\ell})^2 + \sqrt{\Delta t}\sum_{\ell\geq 0} b_{i\ell}\xi_\ell^{n+1}\right). \tag{34}$$

As we will see, our scheme behaves well in the kinetic regime, and is asymptotic preserving at the limit $\varepsilon \to 0$.

We are interested in the evolution of $\rho(t, x) = (\Pi f)(t, x)$ and we denote by ρ_i^n the approximated value of this function at the point x_j at time $t_n = n\Delta t$.

In all the cases we perform $M = 100$ realizations of the processes and we denote by $(\rho_j^n)_{(m)}$ the realizations obtained, for $m = 1, \ldots, M$. We are interested in the mean $\overline{\rho}^n = (\overline{\rho}_j^n)_{j=0}^{N-1}$ and the standard deviation $\mathbf{S}^n = (\mathbf{S}_j^n)_{j=0}^{N-1}$ defined by

$$\overline{\rho_i^n} = \frac{1}{M}\sum_{m=1}^{M}\left(\rho_i^n\right)_{(m)}, \qquad \mathbf{S}_i^n = \sqrt{\frac{1}{M-1}\sum_{m=1}^{M}\left(\left(\rho_i^n\right)_{(m)} - \overline{\rho_i^n}\right)^2}.$$

In Fig. 2, we consider the case $\varepsilon = 1$, and we plot the means $\overline{\rho}$ of the KIN scheme and our SMM scheme in two cases: 25 grid points and 200 grid points and for various different values of the time t = 0.01, 0.25, 0.4 and 1. In Fig. 3 we consider the diffusion regime $\varepsilon = 10^{-8}$ and compare the numerical solutions $\bar{\rho}$ given by SMM schemes for various values of the number of grid points N, with the numerical solution of the reference CN scheme (CN 200). In Fig. 4, we plot the differences of the mean $\bar{\rho}$ and

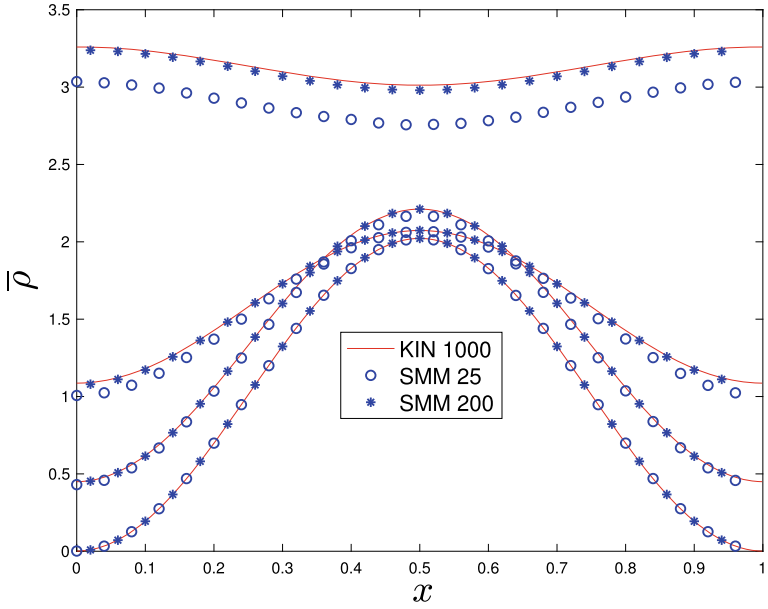

Fig. 2 One-group transport equation $\varepsilon = 1$: comparisons of the mean between KIN and SMM schemes. Results at times t = 0.01, 0.25, 0.4 and 1 (from down to up on the left vertical axis)

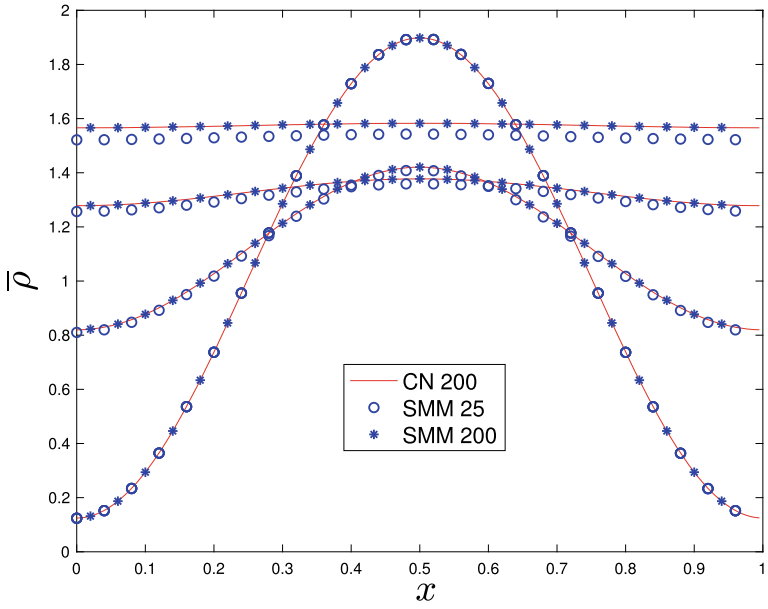

Fig. 3 One-group transport equation $\varepsilon = 10^{-8}$: comparison of the mean between CN and SMM schemes. Results at times t = 0.01, 0.1, 0.25 and 0.4 (from down to up)

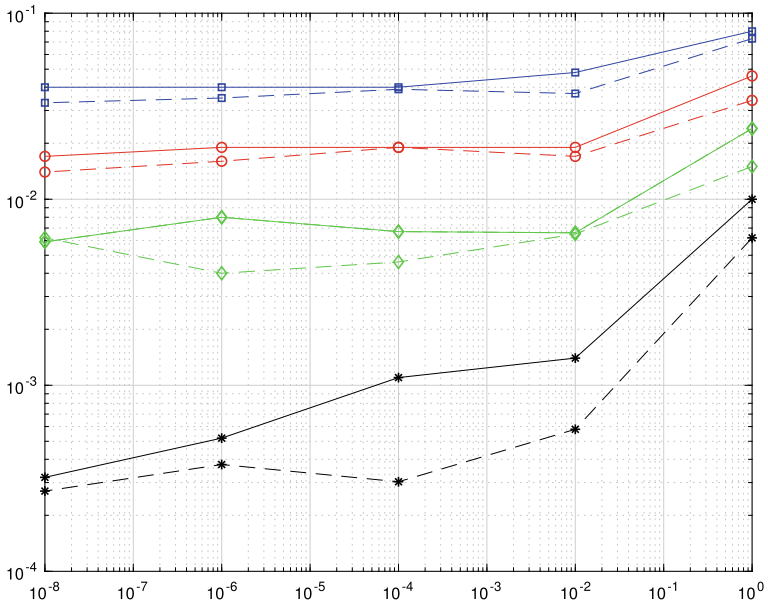

Fig. 4 Error for the mean (solid lines) and the standard deviation (dashed lines) at $t = 0.4$, with respect to ε, with 25 (squares), 50 (circles), 100 (diamonds) and 200 grid points (stars)

standard deviation **S** between the reference scheme (KIN or CNN) and our SMM schemes (with $N = 25, 50, 100$ and 200 points) and for $\varepsilon \in \{10^{-2m}\}, m = 0, \ldots, 4$.

6 Conclusion and Perspectives

The scheme presented in this paper is Asymptotic Preserving and its construction is based on the micro-macro decomposition. We have obtained some numerical results confirming the good performances of the scheme, in particular in the diffusion regime as it can be seen in the figures. In [1], we have established some conditions of CFL type ensuring the stability of our scheme uniformly with respect to ε. The natural perspectives are to use similar techniques to study stochastic perturbations of the nonlinear case which has been studied theoritically in [6], or again of the Boltzmann equation for which one the micro-macro decomposition method works in the deterministic case (see [10]). It is quite relevant to develop a scheme for that stochastic setting regarding the recent advances for the stochastic study of the Boltzmann equation, see [22] for instance. We could also take an interest in some AP schemes for hydrodynamical limits of the previous problems mentioned and for a stochastic version of the Vlasov equation, the deterministic case being treated in [5].

References

1. N. Ayi, E. Faou, Analysis of an asymptotic preserving scheme for stochastic linear kinetic equations in the diffusion limit. SIAM/ASA J. Uncertain. Quantif. **7**, 760–785 (2019)
2. C. Bauzet, G. Vallet, P. Wittbold, The Cauchy problem for conservations laws with a multplicative Stochastic perturbation. J. Hyperbolic Differ. Equ. **09**(04), 661–709 (2012)
3. M. Bennoune, M. Lemou, L. Mieussens, Uniformly stable numerical schemes for the Boltzmann equation preserving the compressible Navier–Stokes asymptotics. J. Comput. Phys. **227**(8), 3781–3803 (2008)
4. M. Bennoune, M. Lemou, L. Mieussens, An asymptotic preserving scheme for the Kac model of the Boltzmann equation in the diffusion limit. Contin. Mech. Thermodyn. **21**(5), 401 (2009)
5. N. Crouseilles, M. Lemou, An asymptotic preserving scheme based on a micro-macro decomposition for collisional Vlasov equations: diffusion and high-field scaling limits. Kinet. Relat. Model. **4**, 06 (2011)
6. A. Debussche, S. De Moor, J. Vovelle, Diffusion limit for the radiative transfer equation perturbed by a Wiener process. Kinet. Relat. Model. **8**(3), 467–492 (2015)
7. A. Debussche, J. Vovelle, Scalar conservation laws with stochastic forcing. J. Funct. Anal. **259**(4), 1014–1042 (2010)
8. E. Weinan, K. Khanin, A. Mazel, Ya. Sinai, Invariant measures for burgers equation with Stochastic forcing. Ann. Math. **151**(3), 877–960 (2000)
9. J. Feng, D. Nualart, Stochastic scalar conservation laws. J. Funct. Anal. **255**(2), 313–373 (2008)
10. I.M. Gamba, S. Jin, L. Liu, Micro-macro decomposition based asymptotic-preserving numerical schemes and numerical moments conservation for collisional nonlinear kinetic equations. J. Comput. Phys. **382**, 264–290 (2019)
11. M. Hofmanova, A Bhatnagar–Gross–Krook approximation to stochastic scalar conservation laws. Annales de l'Institut Henri Poincaré Probabilités et Statistiques **51**(4), 1500–1528 (2015)
12. H. Holden, N.H. Risebro, Conservation laws with a random source. Appl. Math. Optim. **36**(2), 229–241 (1997)
13. S. Jin, D. Levermore, The discrete-ordinate method in diffusive regimes. Transp. Theory Stat. Phys. **20**(5–6), 413–439 (1991)
14. S. Jin, D. Levermore, Fully-discrete numerical transfer in diffusive regimes. Transp. Theory Stat. Phys. **22**(6), 739–791 (1993)
15. S. Jin, L. Pareschi, G. Toscani, Uniformly accurate diffusive relaxation schemes for multiscale transport equations. SIAM J. Numer. Anal. **38**(3), 913–936 (2000)
16. J.U. Kim, On a stochastic scalar conservation law. Indiana Univ. Math. J. (2003)
17. A. Klar, An asymptotic-induced scheme for nonstationary transport equations in the diffusive limit. SIAM J. Numer. Anal. **35**(3), 1073–1094 (1998)
18. E.W. Larsen, J.E. Morel, Asymptotic solutions of numerical transport problems in optically thick, diffusive regimes II. J. Comput. Phys. **83**(1), 212–236 (1989)
19. E.W. Larsen, J.E. Morel, W.F. Miller, Asymptotic solutions of numerical transport problems in optically thick, diffusive regimes. J. Comput. Phys. **69**(2), 283–324 (1987)
20. M. Lemou, L. Mieussens, A new asymptotic preserving scheme based on micro-macro formulation for linear kinetic equations in the diffusion limit. SIAM J. Sci. Comput. **31**(1), 334–368 (2008)
21. J. Liu, L. Mieussens, Analysis of an asymptotic preserving scheme for linear kinetic equations in the diffusion limit. SIAM J. Numer. Anal. **48**(4), 1474–1491 (2010)
22. S. Punshon-Smith, S. Smith, On the Boltzmann equation with stochastic kinetic transport: global existence of renormalized martingale solutions. Arch. Rat. Mech. Anal. **229**(2), 627–708 (2018)

Zero-Range Process in Random Environment

C. Bahadoran, T. S. Mountford, K. Ravishankar, and E. Saada

Abstract We survey our recent articles dealing with one-dimensional attractive zero range processes moving under site disorder. We suppose that the underlying random walks are biased to the right and so hyperbolic scaling is expected. Under the conditions of our model the process admits a maximal invariant measure. The initial focus of the project was to find conditions on the initial law to entail convergence in distribution to this maximal distribution, when it has a finite density. Somewhat surprisingly, necessary and sufficient conditions were found. In this part hydrodynamic results were employed chiefly as a tool to show distributional convergence but subsequently we developed a theory for hydrodynamic limits treating profiles possessing densities that did not admit corresponding equilibria. Finally we derived strong local equilibrium results.

Keywords Asymmetric attractive zero-range process · Site disorder · Phase transition · Condensation · Hydrodynamic limit · Strong local equilibrium · Large-time convergence

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1 Introduction

The asymmetric zero-range processs (AZRP) with site disorder was introduced in [20] to study condensation phenomena. It is a conservative interacting particle system whose dynamics is determined by a jump rate function $g : \mathbb{N} \to \mathbb{N}$, a function $\alpha : \mathbb{Z}^d \to \mathbb{R}_+$ (called the *environment* or *disorder*), and a jump distribution $p(.)$ on $\mathbb{Z}^d$, for $d \geq 1$. A particle leaves site x at rate $\alpha(x)g[\eta(x)]$, where $\eta(x)$ denotes the current number of particles at x, and moves to $x + z$, where site z is chosen at random with distribution $p(.)$. As explained later on, this model has a whole family of product invariant measures carrying different mean densities; it exhibits a *critical density* ρ_c, i.e. no product invariant measure exists above ρ_c [19, 21], if the function g is bounded, α has averaging properties plus a proper tail assumption. This can be interpreted as a *phase transition*.

In this review paper, we consider the one-dimensional attractive nearest neighbour process, that is $d = 1$, $p(1) + p(-1) = 1$ and g nondecreasing. We summarize the papers [13–16], by giving their results and the main ideas of their proofs. In these papers, we developed robust approaches to study various aspects of the phase transition mentioned above.

One aspect is the *mass escape* phenomenon. Suppose the process is started from a given configuration where the global empirical density of particles is greater than ρ_c. One usually expects convergence to the extremal invariant measure carrying the same density as the initial state. However, in this case such a measure does not exist. When $g(n) = \min(n, 1)$ and $p(1) = 1$ it was shown in [6] that the system converges to the maximal invariant measure (thereby implying a loss of mass). This was established in [13, 14] for the general nearest neighbour model under a weak convexity assumption, and we showed that this could fail for non nearest neighbour jump kernels.

Phase transition also arises in the hydrodynamic limit. We show in [15] that the hydrodynamic behaviour of our process is given under hyperbolic time scaling by entropy solutions of a scalar conservation law

$$\partial_t \rho(t, x) + \partial_x [f(\rho(t, x))] = 0 \tag{1}$$

where $\rho(t, x)$ is the local particle density field, with a macroscopic flux function $\rho \mapsto f(\rho)$ that is increasing up to ρ_c and constant thereafter.

The natural question following hydrodynamic limit is that of *local equilibrium*. In general, for a conservative particle system endowed with a family $(\nu_\rho)_\rho$ of extremal invariant measures, the local equilibrium property states that the distribution of the microscopic particle configurations at a macroscopic time $t \geq 0$ around a site with macroscopic location $x \in \mathbb{R}$ is close to $\nu_{\rho(t,x)}$, where $\rho(t, x)$ is the hydrodynamic density, here given by (1). This property has a weak (space-averaged) and a strong (pointwise) formulation, see e.g. [24]. But the local equilibrium property is expected to be *wrong* at *supercritical* hydrodynamic densities, that is, such that $\rho(t, x) > \rho_c$, since a corresponding equilibrum measure does not exist. This already poses a problem at the level of the hydrodynamic limit [15], since in the usual heuristic for

(1), the macroscopic flux function f is the expectation of microscopic flux function under local equilibrium.

In [16], we introduce a new approach for the derivation of *quenched strong* local equilibrium. In the case of subcritical hydrodynamic density, that is, $\rho(t,x) < \rho_c$, we establish not only conservation but also *spontaneous creation* of local equilibrium: we only require starting from a sequence of (possibly deterministic) initial configurations with a given macroscopic profile, but with a distribution possibly far away from initial local equilibrium. In the case of supercritical hydrodynamic density $\rho(t,x) > \rho_c$, we prove that the local equilibrium property fails, and that, locally around "typical points" of the environment, the distribution of the microscopic state is close to the *critical measure* denoted by μ_c^α: this can be viewed as a *dynamic version* of the loss of mass property studied in [6, 13, 14]. In the case of a critical hydrodynamic density, that is, $\rho(t,x) = \rho_c$, we prove that locally around typical points, the distribution of the system approaches the critical measure. This can still be viewed as a local equilibrium creation result, but only in a partial sense. Indeed, outside the situation of an ergodic disorder (to which we are not limited), the critical measure may not have critical density, nor even any well-defined density.

The paper is organized as follows. In Sect. 2, we introduce our results through an illustrating analysis of traffic jams. In Sect. 3, we introduce the model and its basic properties. Section 4 refers to [13, 14], that is, to the convergence to the critical measure μ_c^α from a supercritical or a critical initial configuration. Section 5 refers to [15], that is, to the hydrodynamic limits results (including the supercritical regime). Section 6 refers to [16], that is, to strong local equilibrium in the subcritical and critical regimes (creation or conservation), and to loss of local equilibrium in the supercritical regime.

2 A Preliminary Illustration: Traffic Jams

In this section we describe some heuristics for a particular AZRP, where $g(n) = \min(n,1)$ and $p(1) = 1$. This is a well-known model, namely, a series of $M/M/1$ queues in tandem where each site $x \in \mathbb{Z}$ corresponds to a server with service rate $\alpha(x)$. Then (see e.g. [32]) provided $\lambda < \alpha(x)$ for all x, an invariant measure for this process can be described as follows: if $\eta(x)$ denotes the number of customers waiting for server x, the random variables $\{\eta(x) : x \in \mathbb{Z}\}$ are independent, and the law of $\eta(x)+1$ is the geometric distribution with parameter $1-\lambda/\alpha(x)$; thus $\eta(x)$ has mean value $\lambda/(\alpha(x)-\lambda)$. The parameter λ is the intensity of the Poisson process of departures from each queue, hence it can be interpreted as the mean current (or *flux*) of customers along the system. We assume that

$$\forall x \in \mathbb{Z}, \quad 0 < c := \inf_{y\in\mathbb{Z}} \alpha(y) < \alpha(x) \tag{2}$$

so that the above invariant measure is defined for $\lambda \leq c$. The value $\lambda = c$ corresponds to what we called "critical" in the introduction.

This particular AZRP is isomorphic to a totally asymmetric simple exclusion process (TASEP), that models traffic on a one lane highway where overtaking is forbidden. In this TASEP, cars (particles) are labeled from left to right by integers $n \in \mathbb{Z}$, and each of them moves one step further left as long as it is not blocked by another car in front of it (according to the exclusion rule). Particle n jumps with its own rate $\alpha(n)$, hereafter called its *speed*. This *intrinsic* speed is the one it would reach on an otherwise empty road in the absence of any exclusion rule. Whereas the original AZRP was endowed with *site* disorder, the associated TASEP is endowed with *particle* disorder. Here, (2) means that we can find cars moving at speeds arbitrarily close to but not equal to c.

The isomorphism between AZRP and TASEP is as follows. An AZRP server at site $n \in \mathbb{Z}$ becomes a TASEP car with label n, and customers waiting for this server become vacant TASEP sites between this car and the next one to the left. Thus if we denote by x_n the position of the nth TASEP particle, $\eta(n) = x_n - x_{n-1} - 1$ represents the number of AZRP particles at site n.

Any time the nth TASEP particle jumps to the left (that is x_n decreases by 1), an AZRP customer (i.e. a TASEP hole) is transferred from server n to server $n+1$ at rate $\alpha(n)$ (that is $\eta(n)$ decreases by 1 and $\eta(n+1)$ increases by 1). The displacement of car n corresponds to the flux of customers leaving server n. By the isomorphism between AZRP and TASEP, invariant measures can be obtained for the above TASEP: under these, inter-particle distances $x_{n+1} - x_n$ are independent geometric random variables with parameter $1 - \lambda/\alpha(n+1)$, where $0 \leq \lambda \leq c$.

We illustrate these different cases for TASEP with cars with different speeds (represented by different colors) on a highway. In the corresponding figures, cars are now going from left to right (see Fig. 1), and not from right to left as in the previous explanations. When the traffic is dense, cars tend to be slowed down by the exclusion rule, compared to which the differences of speeds between them play a lesser role (see Fig. 2). There is a phase transition between dense and fluid traffic: when the traffic is fluid (see Fig. 3), the difference of speeds plays a dominant role compared to the exclusion rule. There are traffic jams arising behind the slowest cars, and big gaps ahead of them and behind the jams generated by the next slower car (see Fig. 4). Then big gaps get reduced from back to front: the successive jams merge together (see Fig. 5).

Indeed, to see this, we go back to our explanations (where TASEP particles go left); we can define a subsequence $\{\alpha(n_k)\}$ (of $\{\alpha(n) : n \leq 0\}$) of rates for successive slower cars which strictly decreases to c such that if $n_{k+1} < j < n_k$ then $\alpha(n_k) \leq \alpha(j)$. This is done by defining $n_{k+1} = \sup\{j < n_k : \alpha(j) < \alpha(n_k)\}$ and $n_0 = 0$. Let us see how

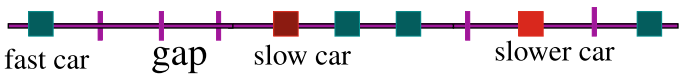

Fig. 1 cars on a highway: fast cars are blue, slow cars are purple, and slower cars are red

Fig. 2 dense traffic: all cars are separated by small gaps

Fig. 3 fluid traffic: all cars are separated by large gaps, but in front of slow cars, the gaps are much larger

Fig. 4 evolution from fluid traffic

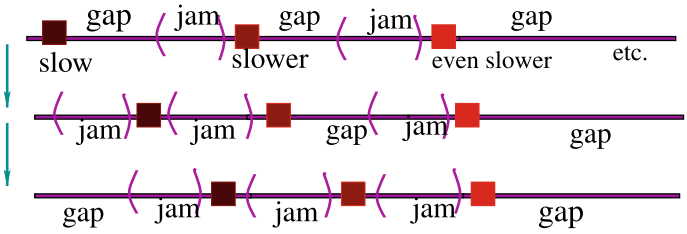

Fig. 5 condensation due to cars regulation: slow cars are dark purple, slower cars are light purple and even slower cars are red

cars with labels in the interval $\mathbb{Z} \cap [n_{k+1}, n_k]$ evolve when we start with large enough gaps. Neglecting the exclusion rule, each car moves at its intrinsic speed as long as it is not slowed down by the motion of the next car ahead. This generates the following scenario:

1. Since car $n_k - 1$ has greater speed than car n_k, its displacement will be bigger, hence the gap between them first grows linearly with time, until:
2. in the long run car n_k becomes slowed down by the *slightly* (if k is large) smaller speed of car n_{k+1} and joins the jam already formed behind it by cars with labels in between (which are indeed faster than n_{k+1}). At this time the existing jam behind car n_k merges with the one between n_{k+1};
3. on a longer time scale, this new bigger jam will in turn catch up with a slightly slower jam behind car n_{k+2}, and so on.

These steps translate as follows into the AZRP picture, starting with large enough occupation numbers (that is, "supercritical density"):

1. The flux from site $n_k - 1$ will be greater than the flux leaving site n_k, and the occupation number of site n_k will first grow linearly with time, which can be interpreted as dynamic condensation;

2. in the long run the region between sites n_{k+1} and n_k will tend towards an equilibrium with incoming flux close to $\alpha(n_{k+1})$ on the left end and an outgoing flux $\alpha(n_k)$ close to matching it, meaning an equilibrium at flux $\alpha(n_{k+1})$;
3. when the effect from the next block to the left (i.e. from n_{k+2} to n_k) reaches n_k, the approximate equilibrium in the site interval $\mathbb{Z} \cap [n_{k+2}, n_k]$ will be one for flux $\alpha(n_{k+2})$ on the left.

Since $\alpha(n_k) \to c$ as $k \to +\infty$, this suggests that as time goes to infinity the measure on the AZRP will converge to a measure parametrized by flux c. A heuristic derivation of the time scale at which merging (or *condensation*) occurs, when the service rates $\alpha(x)$ are i.i.d. random variables, can be found in [26].

If we zoom out and look at servers from far away (corresponding to a scaling limit), one obtains a conservation law with a flux function that grows nonlinearly in the "subcritical" density range (that is, for densities with flux less than c), and is truncated at c in the supercritical range.

While we have described the heuristics for the simple model of totally asymmetric case with a jump rate one if the site is occupied (for AZRP) we obtain the same result for a more complicated case of AZRP (like our general model) where the jumps are asymmetric (but not totally asymmetric), the jump rate is determined by a function depending on the occupation number and the randomness of the disorder is much weaker than independent.

3 Description of the Model, Basic Properties

In the sequel, $\mathbb{R}$ denotes the set of real numbers, $\mathbb{Z}$ the set of signed integers, $\mathbb{N} = \{0, 1, \ldots\}$ the set of nonnegative integers and $\overline{\mathbb{N}} := \mathbb{N} \cup \{+\infty\}$. For $x \in \mathbb{R}$, $\lfloor x \rfloor$ denotes the integer part of x, that is largest integer $n \in \mathbb{Z}$ such that $n \le x$. The notation $X \sim \mu$ means that a random variable X has probability distribution μ.

Let $\overline{\mathbf{X}} := \overline{\mathbb{N}}^{\mathbb{Z}}$ denote the set of particle configurations, and $\mathbf{X} := \mathbb{N}^{\mathbb{Z}}$ the subset of particle configurations with finitely many particles at each site. A configuration in $\overline{\mathbf{X}}$ is of the form $\eta = (\eta(x) : x \in \mathbb{Z})$ where $\eta(x) \in \overline{\mathbb{N}}$ for each $x \in \mathbb{Z}$. The set $\overline{\mathbf{X}}$ is equipped with the coordinatewise order: for $\eta, \xi \in \overline{\mathbf{X}}$, we write $\eta \le \xi$ if and only if $\eta(x) \le \xi(x)$ for every $x \in \mathbb{Z}$; in the latter inequality, $\le$ stands for extension to $\overline{\mathbb{N}}$ of the natural order on $\mathbb{N}$, defined by $n \le +\infty$ for every $n \in \mathbb{N}$, and $+\infty \le +\infty$. This order is extended to probability measures on $\overline{\mathbf{X}}$: For two probability measures μ, ν, we write $\mu \le \nu$ if and only if $\int f d\mu \le \int f d\nu$ for any nondecreasing function f on $\overline{\mathbf{X}}$. We denote by $(\tau_x)_{x \in \mathbb{Z}}$ the group of spatial shifts. For $x \in \mathbb{Z}$, the action of τ_x on particle configurations is defined by $(\tau_x \eta)(y) = \eta(x + y)$ for every $\eta \in \overline{\mathbf{X}}$, $y \in \mathbb{Z}$. Its action on a function f from $\mathbf{X}$ or $\overline{\mathbf{X}}$ to $\mathbb{R}$ is defined by $\tau_x f := f \circ \tau_x$.

3.1 The Process and Its Invariant Measures

Let $p(.)$ be a probability measure on $\mathbb{Z}$ supported on $\{-1, 1\}$. We set $p := p(1), q := p(-1) = 1 - p$, and assume $p \in (1/2, 1]$, so that the mean drift of the associated random walk is $p - q > 0$. Let $g : \mathbb{N} \to [0, +\infty)$ be a nondecreasing function such that

$$g(0) = 0 < g(1) \leq \lim_{n \to +\infty} g(n) =: g_\infty < +\infty .$$

We extend g to $\overline{\mathbb{N}}$ by setting $g(+\infty) = g_\infty$. Without loss of generality, we henceforth assume $g(+\infty) = g_\infty = 1$.

Let $\alpha = (\alpha(x),\ x \in \mathbb{Z})$ (called the environment or disorder) be a $[0, 1]$-valued sequence. The set of environments is denoted by $\mathbf{A} := [0, 1]^{\mathbb{Z}}$.

We consider the Markov process $(\eta_t^\alpha)_{t \geq 0}$ on $\overline{\mathbf{X}}$ with generator given for any cylinder function (also called local function, that is depending on finitely many sites) $f : \overline{\mathbf{X}} \to \mathbb{R}$ by

$$L^\alpha f(\eta) = \sum_{x,y \in \mathbb{Z}} \alpha(x) p(y - x) g(\eta(x)) \left[f\left(\eta^{x,y}\right) - f(\eta) \right] \tag{3}$$

where, if $\eta(x) > 0$, $\eta^{x,y} := \eta - \delta_x + \delta_y$ denotes the new configuration obtained from η after a particle has jumped from x to y (configuration δ_x has one particle at x and no particle elsewhere; addition of configurations is meant coordinatewise). In cases of infinite particle number, the following interpretations hold: $\eta^{x,y} = \eta - \delta_x$ if $\eta(x) < \eta(y) = +\infty$ (a particle is removed from x), $\eta^{x,y} = \eta + \delta_y$ if $\eta(x) = +\infty > \eta(y)$ (a particle is created at y), $\eta^{x,y} = \eta$ if $\eta(x) = \eta(y) = +\infty$.

For the existence and uniqueness of $(\eta_t^\alpha)_{t \geq 0}$ see [14, Appendix B]. Recall from [1] that, since g is nondecreasing, $(\eta_t^\alpha)_{t \geq 0}$ is attractive, i.e. its semigroup, denoted by $S(t)$ for $t \geq 0$, maps nondecreasing functions (with respect to the partial order on $\overline{\mathbf{X}}$) onto nondecreasing functions. A graphical construction via a Harris system [23] will be a crucial tool (see e.g. [14]): attractiveness enables to construct a completely monotone coupling of a finite number of copies of the process.

The process $(\eta_t^\alpha)_{t \geq 0}$ has the property that if $\eta_0 \in \mathbf{X}$, then almost surely, one has $\eta_t \in \mathbf{X}$ for every $t > 0$. In this case, it may be considered as a Markov process on $\mathbf{X}$ with generator (3) restricted to functions $f : \mathbf{X} \to \mathbb{R}$.

When the environment $\alpha(.)$ is identically equal to 1, we recover the *homogeneous* zero-range process (see [1] for its detailed analysis).

For $\beta < 1$, we define the probability measure θ_β on $\mathbb{N}$ by

$$\theta_\beta(n) := Z(\beta)^{-1} \frac{\beta^n}{g(n)!}, \quad n \in \mathbb{N}, \qquad \text{where} \quad Z(\beta) := \sum_{\ell=0}^{+\infty} \frac{\beta^\ell}{g(\ell)!} ,$$

$$g(n)! := \prod_{k=1}^{n} g(k) \quad \text{for} \quad n \in \mathbb{N} \setminus \{0\}, \quad \text{and} \quad g(0)! := 1 .$$

We denote by μ_β^α the invariant measure of L^α defined (see e.g. [19]) as the product measure with marginal $\theta_{\beta/\alpha(x)}$ at site x:

$$\mu_\beta^\alpha(d\eta) := \bigotimes_{x\in\mathbb{Z}} \theta_{\beta/\alpha(x)}[d\eta(x)]\,. \tag{4}$$

Let

$$c := \inf_{x\in\mathbb{Z}} \alpha(x)\,. \tag{5}$$

The measure (4) can be defined on $\overline{\mathbf{X}}$ for $\beta \in [0, c]$, by using the conventions

$$\theta_1 := \delta_{+\infty}\,, \tag{6}$$

$$\frac{\beta}{a} = 0 \text{ if } \beta = 0 \text{ and } a \geq 0\,. \tag{7}$$

Definition 1 With the above conventions, for $\beta = c$,

$$\mu_c^\alpha := \bigotimes_{x\in\mathbb{Z}} \theta_{c/\alpha(x)}[d\eta(x)] \tag{8}$$

is by definition the *critical measure*.

The measure (4) is always supported on $\mathbf{X}$ if $\beta \in (0, c) \cup \{0\}$. When $\beta = c > 0$, conventions (6)–(7) yield a measure supported on configurations with infinitely many particles at all sites $x \in \mathbb{Z}$ that achieve the infimum in (5), and finitely many particles at other sites. In particular, this measure is supported on $\mathbf{X}$ when the infimum in (5) is not achieved. When $c = 0$, the measure (4) is supported on the empty configuration.

Since $(\theta_\beta)_{\beta\in[0,1)}$ is an exponential family, we have a stochastic order relation, that is, for $\beta \in [0, \inf_{x\in\mathbb{Z}} \alpha(x)]$, μ_β^α is weakly continuous and stochastically increasing with respect to β.

3.2 Assumptions on the Environment, and Consequences

To state our results, we introduce two sets of assumptions on α. The first one says that the environment α has "averaging properties", while the second one sets a restriction on the sparsity of "slow sites" (where by "slow sites" we mean sites where the disorder variable becomes arbitrarily close or equal to the infimum value c, which was defined by (5)).

Assumption 1 *If $c > 0$, there exists a probability measure $Q_0 = Q_0(\alpha)$ on $[0, 1]$ such that*

$$Q_0(\alpha) = \lim_{n\to+\infty} \frac{1}{n+1} \sum_{x=-n}^{0} \delta_{\alpha(x)} = \lim_{n\to+\infty} \frac{1}{n+1} \sum_{x=0}^{n} \delta_{\alpha(x)}\,. \tag{9}$$

Assumption 2 *The environment α has* macroscopically dense defects*, that is, there exists a sequence of sites $(x_n)_{n\in\mathbb{Z}}$ such that*

$$\forall n \in \mathbb{Z},\ x_n < x_{n+1}; \quad \lim_{n\to\pm\infty} \alpha(x_n) = c\,, \tag{10}$$

and

$$\lim_{n\to\pm\infty} \frac{x_{n+1}}{x_n} = 1\,.$$

Remark that (10) implies in particular

$$\liminf_{x\to\pm\infty} \alpha(x) = c\,. \tag{11}$$

By (5) and (9), we have

$$c = \inf_{x\in\mathbb{Z}} \alpha(x) \le \inf \operatorname{supp} Q_0\,, \tag{12}$$

and if, for $\beta < 1$, we define the mean value of θ_β by

$$R(\beta) := \sum_{n=0}^{+\infty} n\theta_\beta(n)\,, \tag{13}$$

an *average mean density* exists for all $\beta \in [0, c)$:

$$\overline{R}(\beta) := \lim_{n\to+\infty} \frac{1}{n+1} \sum_{x=-n}^{0} R\left(\frac{\beta}{\alpha(x)}\right) = \lim_{n\to+\infty} \frac{1}{n+1} \sum_{x=0}^{n} R\left(\frac{\beta}{\alpha(x)}\right)\,. \tag{14}$$

Remark 1 When $c > 0$, Assumption 1 is actually *equivalent* to the fact that the two limits in (14) exist and coincide for every $\beta \in [0, c)$.

For reasons of concreteness, we denote by **(EE)** the stronger hypothesis of *environmental ergodicity*.

(EE) *The environment has a distribution Q, for Q a spatially ergodic probability measure on* $\mathbf{A}$ *with marginal Q_0, such that $c = \inf \operatorname{supp} Q_0$.*

For instance, the i.i.d. case $Q = Q_0^{\otimes\mathbb{Z}}$ satisfies **(EE)**.

Assumptions 1 and 2 are satisfied under assumption **(EE)**; in particular, Q-a.e. realization of the environment α satisfies Assumption 2.

By (14), $\overline{R}$ is an increasing C^∞ function on $[0, c)$ if $c > 0$ (see [15, Lemma 3.1]). We define the *critical density* by

$$\rho_c := \overline{R}(c-) := \lim_{\beta\uparrow c} \overline{R}(\beta) \in [0, +\infty]\,, \tag{15}$$

and we define $\overline{R}(c) := \overline{R}(c-) = \rho_c$, making $\overline{R}(.)$ left continuous at c. If $c = 0$, $\overline{R}$ is defined on $\{0\}$ and equal to 0 by convention (7). In this case, we set $\rho_c = 0$.

Moreover, we may define the inverse of $\overline{R}$ on its image $[0, \rho_c)$, and, for $\beta \in [0, c)$, we reindex the invariant measure μ_β^α by setting

$$\mu^{\alpha,\rho} := \mu^\alpha_{(\overline{R})^{-1}(\rho)} \tag{16}$$

The parameter ρ represents the mean particle density in the sense that, for $\mu^{\alpha,\rho}$-almost every configuration $\eta \in \mathbf{X}$,

$$\lim_{n\to+\infty} \frac{1}{n+1} \sum_{x=0}^{n} \eta(x) = \lim_{n\to+\infty} \frac{1}{n+1} \sum_{x=-n}^{0} \eta(x) = \rho\,. \tag{17}$$

Note that under **(EE)**, (11) is satisfied, $\overline{R}(\beta)$ is well-defined by the ergodic theorem for all $\beta \in [0, c]$, and we have

$$\overline{R}(\beta) = \int_{(c,1]} R\left[\frac{\beta}{a}\right] dQ_0[a], \qquad \rho_c = \overline{R}(c)\,, \tag{18}$$

Remark 2 *(i)* Unlike under **(EE)**, under (9), $\lim_{\beta\uparrow c} \overline{R}(\beta)$ could be distinct from $\overline{R}(c)$ as defined by (14) for $\beta = c$. In fact, the limits in (14) may not exist for $\beta = c$, or exist and be different from one another and/or from ρ_c.

(ii) In view of (15), it may be tempting to extend the parametrization (16) to $\rho = \rho_c$ by setting $\mu^{\alpha,\rho_c} = \mu_c^\alpha$. However, this does not make real sense, as under (9), because of *(i)* above, the measure thus defined may not satisfy (17) for $\rho = \rho_c$.

We regard densities below ρ_c as *subcritical*, density ρ_c as *critical* and densities above ρ_c as *supercritical*. In the first case there exists an equilibrium probability measure with this density, while we will see that none exists for supercritical densities.

4 Convergence

A natural question for an interacting particle system with multiple equilibria is, given a particular equilibrium μ, to determine the set of initial configurations for which the particle system converges to μ. Among classical conservative systems this is fully answered for symmetric exclusion processes on $\mathbb{Z}^d$ (see e.g. [29]) but in general seems very hard. It is often softened to finding large classes of initial distributions for which there is convergence. For asymmetric nearest neighbour exclusion processes, the first result of importance was [2], see also [12, 31] which gave conditions for convergence to product measure. The last is important since it does not require an initial translation invariant distribution but only needs a fixed initial distribution satisfying the appropriate law of averages.

Theorems 1 and 2 below, proved respectively in [13, 14], establish a necessary and sufficient condition for our zero range process to converge to μ_c^α. To our knowledge there are no other comparable results for nontrivial assymmetric conservative systems. Certainly the fact (to be justified below), that we consider the maximal equilibrium helps but it is to be noted that, [12] notwithstanding, for the exclusion process it is not clear what a necessary and sufficient condition for convergence in distribution to $\delta_{\underline{0}}$ (and so $\delta_{\underline{1}}$) would be (where $\underline{0}$ and $\underline{1}$ denote the empty and full configurations, defined respectively by $\underline{0}(x) = 1 - \underline{1}(x) = 0$ for every $x \in \mathbb{Z}$).

4.1 Previous Results for Convergence

The main paper we refer to is [6], which considers a TAZRP ($p(1) = 1$), on $\mathbb{Z}$, for $g(n) = \mathbf{1}_{\{n \geq 1\}}$, with $\alpha(x) \in [c, 1]$. Their results are the following:

(a) [6, Theorem 2.1] For α fixed, the geometric product measures μ_β^α, for $\beta < \alpha(x)$ for all $x \in \mathbb{Z}$, are the extremal invariant measures. The range of the parameter β may be either $[0, c)$ (when $\alpha(x) = c$ for some x) or $[0, c]$ (when $\alpha(x) > c$ for all x).

(b) [6, Proposition 2.2] There does not exist any invariant measure with a density above ρ_c.

(c) [6, Theorem 2.3] If $\rho_c < +\infty$, and $\eta_0 \in \mathbb{N}^{\mathbb{Z}}$ satisfies the supercriticality assumption

$$\liminf_{n \to \infty} n^{-1} \sum_{x=-n}^{0} \eta_0(x) > \rho_c \,, \tag{19}$$

then η_t^α converges in distribution to μ_c^α.

Note that under our assumptions, we obtain $\beta \in [0, c]$ in *(a)*.

An immediate consequence of *(c)* is that there is a "loss of mass": for "most" of the sites the local density will be ρ_c but our system is conservative and the hypothesis (19) has a "global" density (at least on the left halfline) strictly higher.

This is an example of *condensation* (as exhibited for instance in [20, 21, 26]). The "lost" mass accumulates at sites with α value close to the minimum c (where "close" decreases with time). If we return to $M/M/1$ queues with service rate $\alpha(x)$ at queue x, or cars, then, informally speaking, many clients remain trapped in far away slow servers, or lots of space in the road is in front of a small number of slow cars.

4.2 Our Results for Convergence

For our convergence results (from [13, 14]), we also need the following assumption on disorder. Recall that c is defined by (5):

Assumption 3 *We have that* $c > 0$, $\rho_c < +\infty$, *and* $\overline{R}$ *satisfies the weak convexity assumption*

(H) $\forall \beta \in [0, c), \quad \overline{R}(\beta) - \overline{R}(c) - (\beta - c)\overline{R}'^{+}(c) > 0$

where $\overline{R}'^{+}(c)$ *is the left-hand derivative at c of the convex envelope of* $\overline{R}$, *that is*

$$\overline{R}'^{+}(c) := \limsup_{\beta \to c} \frac{\overline{R}(c) - \overline{R}(\beta)}{c - \beta}\,.$$

For instance, if R is strictly convex, then for any environment satisfying assumption (14), $\overline{R}$ is strictly convex and **(H)** satisfied. A sufficient condition for R to be strictly convex [17] is that $n \mapsto g(n+1) - g(n)$ is a nonincreasing function.

Theorem 1 ([14, Theorem 2.2]) *Assume (14), Assumptions 2 and 3. Then, for all* $\eta_0 \in \mathbb{N}^{\mathbb{Z}}$ *satisfying the supercriticality assumption*

$$\liminf_{n\to\infty} n^{-1} \sum_{x=-n}^{0} \eta_0(x) \geq \rho_c\,, \tag{20}$$

the process $(\eta_t^\alpha)_{t\geq 0}$ *of initial state the configuration* η_0 *converges in distribution when* $t \to \infty$ *to the critical measure* μ_c^α *defined by (8).*

Theorem 2 ([13, Theorem 2.2]) *Assume (14), Assumptions 2 and 3. Assume further that* η_0 *satisfies*

$$\rho = \liminf_{n\to\infty} n^{-1} \sum_{x=-n}^{0} \eta_0(x) < \rho_c\,.$$

Then η_t^α *does not converge in distribution to* μ_c^α *as* $t \to +\infty$.

Together, as claimed, these two results give a necessary and sufficient condition for convergence to μ_c^α.

Now note that Theorem 1 generalises [6, Theorem 2.3] in the following ways:

1. the underlying random walk kernel is asymmetric nearest neighbour but not necessarily totally asymmetric,
2. the strict inequality in (19) is replaced by the greater than or equal condition of Theorem 1,
3. the special case function $g(n) = \mathbf{1}_{\{n\geq 1\}}$ is removed in favour of any $g(.)$ increasing to a finite limit and compatible with Assumption 3.

In viewing these improvements, one might think that 1. could be improved to at least the condition that kernel $p(.)$ is positive mean and of finite range. In fact,

surprisingly, this is not possible. The nearest neighbour requirement is not to facilitate the argument. The reason is that, loosely speaking, the result holds because the incoming flux to the left of the origin is the maximal value: $c(p-q)$. This balances the outgoing flux to the right of the origin under equilibrium. How the "lim inf" behaviour for the initial particle configuration is achieved is immaterial under nearest neighbour motion and for instance a configuration that is mostly vacant but which has a sparse set of very high peaks at isolated sites poses no problems. This is no longer true if the kernel is not nearest neighbour: an isolated peak with a great number of particles initially surrounded by vacant sites may be unable to furnish the needed maximal flux. The following result is established in [13].

Theorem 3 ([13, Theorem 2.3]) *Assume* (11) *and* (14). *Assume further that the jump kernel* $p(.)$ *is totally asymmetric (but not nearest neighbour) and* $p(1) < 1$. *Then there exists* $\eta_0 \in \mathbb{N}^{\mathbb{Z}}$ *satisfying* (20), *such that* η_t^α *does not converge in distribution to* μ_c^α *as* $t \to +\infty$.

The proof of Theorem 1 comes down to showing that any limit point of the distributions $S(t)\delta_{\eta_0}$ must be "above" and "below" the target distribution. The upper bound almost follows from [22] which gives a strong condition for zero-range processes corresponding to our conditions but with general finite range random walk kernels in $\mathbb{Z}^d$ for all $d \geq 1$ so that $\limsup S(t)\delta_{\eta_0} \leq \mu_c^\alpha$. Unfortunately the following growth condition on η_0 is imposed in [22]:

$$\sum_{n\in\mathbb{N}} e^{-\beta n} \sum_{x:\,|x|=n} \eta_0(x) < +\infty, \quad \forall \beta > 0\,.$$

The approach of [14] is to use (for each $\varepsilon > 0$) a comparison with finite Jackson networks on intervals $(A_\varepsilon, a_\varepsilon)$, where

$$A_\varepsilon := A_\varepsilon(\alpha) = \max\{x \leq 0 : \alpha(x) \leq c + \varepsilon\}\,,$$
$$a_\varepsilon := a_\varepsilon(\alpha) = \min\{x \geq 0 : \alpha(x) \leq c + \varepsilon\}\,.$$

These networks evolve according to the AZRP rules as if the points A_ε and a_ε were permanently occupied by infinitely many particles. As $\varepsilon \to 0$ the left and right endpoints tend respectively to $-\infty$ and $+\infty$. The nontrivial part was to show that this could be done so that:

(a) the resulting "finite AZRP" on $(A_\varepsilon, a_\varepsilon)$ would be positive recurrent for each ε;
(b) the resulting equilibria converged as $\varepsilon \to 0$ to μ_c^α.

The lower bound is harder to show. At root it exploits the following interface property for one-dimensional nearest neighbour processes (which will be substantially deepened in Sect. 5). If two configurations η_0 and ξ_0 satisfy the interface condition

$$\exists\, x_0 : \quad \forall\, y \leq x_0,\ \eta_0(y) \leq \xi_0(y);\ \forall\, y > x_0,\ \eta_0(y) \geq \xi_0(y) \tag{21}$$

and if the AZRP's $(\eta_t)_{t\geq 0}$ and $(\xi_t)_{t\geq 0}$ are generated by the same Harris system, then the interface property is maintained:

$$\forall\, t > 0,\ \exists\, x_t : \quad \forall\, y \leq x_t,\ \eta_t(y) \ \leq\ \xi_t(y);\ \forall\, y > x_t,\ \eta_t(y) \ \geq\ \xi_t(y)\,. \tag{22}$$

This simple property permits a recasting of the property of stochastic domination.

To show that our process η_t^α stochastically dominates μ_c^α in the limit as t becomes large, it is enough to show that for each $\beta < c$, η_t^α in the limit dominates μ_β^α; or equivalently (recalling (16)) that for each $\rho < \rho_c$, η_t^α in the limit dominates $\mu^{\alpha,\rho}$. This will be done if (for ρ fixed) $\eta_t^\alpha(x) \geq \xi_t^{\alpha,\rho}(x)$ for x fixed for $(\xi_s^{\alpha,\rho})_{s\geq 0}$ an AZRP generated with the same Harris system as $(\eta_s^\alpha)_{s\geq 0}$ but initially in $\mu^{\alpha,\rho}$ equilibrium. We cannot use the interface property to compare $\eta_t^\alpha(x)$ and $\xi_t^{\alpha,\rho}(x)$ directly so we introduce an intermediary process $(\eta_s^{\alpha,t})_{s\geq 0}$ that can be compared with both (and indeed everything). This process is itself generated by the same Harris system as the other two and is therefore fully defined by specifying

$$\eta_0^{\alpha,t}(x) = (+\infty)\mathbf{1}_{\{x\leq x_t\}} \tag{23}$$

where x_t is a site that is negative, of order t, with environment value $\alpha(x_t)$ so that as t becomes large, $\alpha(x_t)$ tends to c. The choice of x_t is not straightforward, it requires assumption **(H)**. The initial configuration (23) corresponds to placing source/sinks to the left up to site x_t (but since jumps are nearest neighbour, as seen from the right of x_t, this is equivalent to placing a source/sink only at x_t).

Due to (23), there must be interfaces I_s^1 between $\eta_s^{\alpha,t}$ and η_s^α and I_s^2 between $\eta_s^{\alpha,t}$ and $\xi_s^{\alpha,\rho}$. Our domination result will follow once we have shown that with probability tending to one as t becomes large

- I_t^1 is highly negative and
- I_t^2 is highly positive

as this will imply that around the origin (with high probability)

$$\eta_t^\alpha(x) \geq \eta_t^{\alpha,t}(x) \ \geq\ \xi_t^{\alpha,\rho}(x)\,. \tag{24}$$

for all x near the origin.

To show that e.g. $I_t^1 \leq M_t$ (for some well chosen M_t) it suffices to show that on some interval $[N_t, M_t]$, $\sum_{x=N_t}^{M_t}(\eta_t^\alpha(x) - \eta_t^{\alpha,t}(x)) > 0$ (and similarly for $I_t^2 \geq M_t$). We choose N_t and M_t to both be of order t so that we can use hydrodynamic results to show that at order t both $\sum_{x=N_t}^{M_t}\eta_t^\alpha(x)$ and $\sum_{x=N_t}^{M_t}\eta_t^{\alpha,t}(x)$ are essentially nonrandom and appropriately ordered. In fact in this calculation, it was only necessary to understand the hydrodynamic behaviour and local equilibrium starting from a source initial configuration (23).

The key point regarding this behaviour is the following. The hydrodynamic profile created by the source on its right is nonincreasing and there is a critical speed $v_c \geq 0$ such that a front of uniform density ρ_c propagates from the source at speed v_c. Assumption **(H)** ensures that the profile is continuous at the end of this front. This

enables us to choose x_t of order $-t(v_c + \varepsilon)$ and ensure that (24) holds on $[x_t, 0]$ with any ρ smaller than the hydrodynamic density created by the source around the origin, which can be made arbitrarily close to ρ_c.

A fuller picture of hydrodynamic behaviour and local equilibrium is discussed in the next sections.

5 Hydrodynamics

We begin with the following standard definitions in hydrodynamic limit theory. We denote by $\mathscr{M}(\mathbb{R})$ the set of Radon measures on $\mathbb{R}$. To a particle configuration $\eta \in \mathbf{X}$, we associate a sequence of *empirical measures* $(\pi^N(\eta) : N \in \mathbb{N} \setminus \{0\})$ defined by

$$\pi^N(\eta) := \frac{1}{N} \sum_{y \in \mathbb{Z}} \eta(y) \delta_{y/N} \in \mathscr{M}(\mathbb{R}) .$$

Let $\rho_0(.) \in L^\infty(\mathbb{R})$, and let $(\eta_0^N)_{N \in \mathbb{N} \setminus \{0\}}$ denote a sequence of $\mathbf{X}$-valued random variables. We say this sequence has *limiting density profile* $\rho_0(.)$, if the sequence of empirical measures $\pi^N(\eta_0^N)$ converges in probability to the deterministic measure $\rho_0(.)dx$ with respect to the topology of vague convergence.

Let $f : [0, +\infty) \to \mathbb{R}$ be a Lipschitz function, and consider the conservation law

$$\partial_t \rho(t, x) + \partial_x f[\rho(t, x)] = 0 . \tag{25}$$

Equation (25) means that around a point where the macroscopic particle density is ρ, the instantaneous algebraic flux (or current) is $f(\rho)$. This equation, with given initial condition $\rho_0(.)$ generally does not have strong solutions even if $\rho_0(.)$ is regular, and has infinitely many weak solutions. However, it has a unique so called *entropy* solution, that is considered as the *physical* solution [35]. The sequence $(\eta_t^N, t \geq 0)_{N \in \mathbb{N} \setminus \{0\}}$ is said to have *hydrodynamic limit* $\rho(., .)$ if: for all $t \geq 0$, $(\eta_{Nt}^N)_{N \in \mathbb{N} \setminus \{0\}}$ has limiting density profile $\rho(t, .)$, which is the *entropy solution* to the conservation law (25) with initial datum $\rho_0(.)$.

5.1 Previous Results for Hydrodynamic Limit

The hydrodynamic limit of an attractive *homogeneous* asymmetric zero-range process was derived in [4, 5] for step initial conditions under the assumption of a concave flux function, and in [33] for general initial conditions without the concavity assumption (the latter result applies to more general attractive models with product invariant measures in any space dimension). In [28], the hydrodynamic behavior was studied for an AZRP with a *single* spatial inhomogeneity exhibiting condensation.

The paper [19] derived quenched hydrodynamics in the subcritical regime for an attractive AZRP (i.e. nondecreasing $g(.)$), on $\mathbb{Z}^d$, for $p(.)$ finite range, with a disorder such that $\alpha(x)$ has a finite number of values (thus $\rho_c = +\infty$).

In the paper [34], hydrodynamics were derived through the variational coupling method, which is effective for a totally asymmetric ZRP ($p(1) = 1$), with $g(n) = \mathbf{1}_{\{n\geq 1\}}$, in all regimes (subcritical, critical and supercritical).

Note that condensation also arises for zero-range processes which are not attractive, that is, with non-increasing jump rates. There, condensation is due to fluctuations accumulating mass at some sites, instead of site disorder in our case. The formation of the condensate over a fixed, finite number of sites is described in [18]. Hydrodynamics for this model are proved in [30, 36].

The difficulties to prove hydrodynamic limits in our set-up are the following. At supercritical densities, there are no invariant measures; moreover we have condensation. It is thus impossible to use the traditional approach [24], through block averaging and block estimates, since mesoscopic block densities can blow up around condensation sites.

5.2 Our Results on Hydrodynamic Limits

The main result of [15] is the following.

Theorem 4 ([15, Theorem 2.1]) *Assume the environment α satisfies Assumption 1, and the sequence $(\eta_0^N)_{N\in\mathbb{N}\setminus\{0\}}$ has limiting density profile $\rho_0(.) \in L^\infty(\mathbb{R})$. For each $N \in \mathbb{N}\setminus\{0\}$, let $(\eta_t^{\alpha,N})_{t\geq 0}$ denote the process with initial configuration η_0^N and generator (3). Assume either that the initial data is subcritical, that is $\rho_0(.) < \rho_c^\alpha$; or, that Assumption 2 holds. Let $\rho(.,.)$ denote the entropy solution to (25) with initial datum $\rho_0(.)$, where f is the flux function defined by (26)–(27) below. Then for any $t > 0$, the sequence $(\eta_{Nt}^{\alpha,N})_{N\in\mathbb{N}\setminus\{0\}}$ has limiting density profile $\rho(t,.)$.*

To complete the above theorem, we explain how the flux function in (25) is obtained. Let $x_. : t \mapsto x_t$ be a $\mathbb{Z}$-valued path representing the position of a moving "observer" on the lattice.

Definition 2 We let $\Gamma_{x_.}(t,\eta)$ denote the algebraic current across $x_.$, that is the algebraic number of particles crossing the "observer" to the right, between times 0 and t, when starting from the initial configuration η.

In the special case where $x_.$ is identically 0, we obtain in Definition 2 the current through the origin between times 0 and t, simply denoted by $\Gamma_0^\alpha(t,\eta)$: that is, the number of jumps from 0 to 1 minus the number of jumps from 1 to 0. Then the flux function $\rho \mapsto f(\rho)$ is defined by

$$f(\rho) := \lim_{t\to+\infty} t^{-1}\Gamma_0^\alpha(t,\eta^\rho)\,.$$

We can show that this limit exists and depends only on ρ (and not on the choice of η^ρ nor on α), where η^ρ denotes a configuration with density ρ, that is a configuration satisfying (17). For $\beta \in [0, c)$, we can compute the stationary current under μ^α_β, as follows.

$$\int_{\mathbf{X}} [p\alpha(x)g(\eta(x)) - q\alpha(x+1)g(\eta(x+1))]d\mu^\alpha_\beta(\eta) = (p-q)\beta\,.$$

Recall the function $\overline{R}$ defined by (14). As a function of the mean density $\rho = \overline{R}(\beta)$, we define the flux for our system as

$$f(\rho) := (p-q)\overline{R}^{-1}(\rho)\,. \tag{26}$$

And we extend f to $[\rho_c, +\infty)$ by

$$f(\rho) = (p-q)c, \quad \forall \rho \geq \rho_c\,. \tag{27}$$

Remark 3 Under Assumption **(EE)** of an ergodic environment, the flux function depends only on the marginal Q_0 of the environment. Under the more general Assumptions 1–2, the flux function depends on the pair (Q_0, c) defined in (12)–(14). In the latter case, the inequality in (12) can be strict, so c should be regarded as an additional parameter not contained in Q_0, whereas in the ergodic case, equality always holds in (12). A simple non-ergodic example is given in Sect. 5.3 below.

To prove Theorem 4, we use a reduction principle established in [7–11] for one-dimensional conservative attractive processes. This method reduces the proof of hydrodynamics for a Cauchy initial condition to that for a Riemann initial condition, that is, of the form

$$\rho_0(x) = R_{\lambda,\rho}(x) := \lambda \mathbf{1}_{\{x<0\}} + \rho \mathbf{1}_{\{x\geq 0\}} \tag{28}$$

for $\lambda, \rho \in \mathbb{R}$. The passage from one to the other is similar in spirit to Riemann-based numerical schemes for scalar conservation laws; the difficulty is to control the propagation of the error committed at successive time steps when replacing the actual entropy solution with a piecewise constant approximation. Crucial tools in this reduction are:

(i) The *finite propagation* property, that is, the fact that discrepancies between two AZRP's, and similarly between two entropy solutions of (25), propagate with bounded speed.

(ii) The *macroscopic stability* property, which states that if two AZRP configurations are initially close macroscopically, they remain so at later times. In our case this is a consequence of the fact that jumps are nearest neighbour and $g(.)$ is nondecreasing.

To prove hydrodynamics for the Riemann initial condition (28), we use a variational characterization (see e.g. [11]) of the entropy solution $R_{\lambda,\rho}(t,.)$ of the *Riemann problem* (that is, (25) with initial datum (28)). Namely, define

$$\mathscr{G}_{\lambda,\rho}(v) = \begin{cases} \min_{r\in[\lambda,\rho]}[f(r) - vr] \text{ if } \lambda \le \rho\,, \\ \max_{r\in[\rho,\lambda]}[f(r) - vr] \text{ if } \lambda \ge \rho\,. \end{cases} \tag{29}$$

For such values, we define

$$R_{\lambda,\rho}(t, vt) := \begin{cases} \operatorname{argmin}_{r\in[\lambda,\rho]}[f(r) - vr] \text{ if } \lambda \le \rho \\ \operatorname{argmax}_{r\in[\rho,\lambda]}[f(r) - vr] \text{ if } \lambda \ge \rho \end{cases} \tag{30}$$

that is, the minimizer (resp. maximizer) in (29) if $\lambda \le \rho$ (resp. $\lambda \ge \rho$). This optimizer is unique for all but countably many values of v (see [15, Proposition 3.2]).

In order to prove (29) at the microscopic level, the main issue is to show that

$$\lim_{t\to+\infty} t^{-1} \Gamma_{x_\cdot}(t, \xi^{\alpha,\lambda,\rho}) = \mathscr{G}_{\lambda,\rho}(v) \tag{31}$$

in probability, where $x_\cdot$ is a path with asymptotic speed v, and $\xi^{\alpha,\lambda,\rho}$ is a random configuration with profile $R_{\lambda,\rho}(.)$ given in (28); this is the content of [15, Proposition 4.2]. Assume for instance $\lambda < \rho$. To define a suitable configuration $\xi^{\alpha,\lambda,\rho}$ in (31), we use a family of AZRP's $\xi_\cdot^{\alpha,r,r}$, where $r \ge 0$, and $\xi_\cdot^{\alpha,r,r}$ has homogeneous macroscopic density r at time 0. For $r < \rho_c$, we can choose $\xi_\cdot^{\alpha,r,r}$ to be an equilibrium process with density r (that is, with distribution $\mu^{\alpha,r}$, cf. (16)). For $r > \rho_c$, such equilibria do not exist. Instead, we use what we call "pseudo-equilibria", that is, configurations $\xi^{\alpha,r,r}$ with a supercritical homogeneous macroscopic density profile. We choose $\xi^{\alpha,\lambda,\rho}$ in (31) as the configuration whose restriction to $x \le 0$ is $\xi^{\alpha,\lambda,\lambda}$ and whose restriction to $x > 0$ is $\xi^{\alpha,\rho,\rho}$. The following main ideas are then involved to derive (31):

(a) We prove convergence (31) for equilibria and pseudo-equilibria, that is $\lambda = \rho = r$. This follows from ergodicity in the case $r < \rho_c$ of equilibria, but novel arguments are necessary in the case $r > \rho_c$ of pseudo-equilibria.

(b) The upper bound in (31) (proving that the l.h.s. is dominated with high probability by the r.h.s.) is the simpler part. It follows from a coupling argument showing that the current in $\xi_\cdot^{\alpha,\lambda,\rho}$ cannot exceed the one in $\xi_\cdot^{\alpha,r,r}$. This property can be regarded as "intuitive" because, since $r \in [\lambda, \rho]$, the latter system has initially more particles to the left and more space to the right. However, mathematically, this is related to the macroscopic stability property.

(c) For the lower bound in (31), we introduce a novel "interface process", which gives a more adapted (in our setting) version of the local particle density than the usual block average. This is a random spatially nondecreasing lattice field $\rho_t(x)$ taking values in $[\lambda, \rho]$ with the following property: in a space region where ρ_t does not fluctuate much, the system is approximately at local equilibrium or pseudo-equilibrium, in the sense that $\xi_t^{\alpha,\lambda,\rho}$ is close to $\xi_t^{\alpha,r,r}$ for a random $r = \rho_t(x)$. As a nondecreasing function cannot jump too often, for "most" values

of v, using *(a)*, the macroscopic current across a path with velocity v is close to $f[\rho_t(vt)] - v\rho_t(vt)$, which dominates the minimum in (29). Whence the desired lower bound.

The interface process is obtained by looking at simultaneous interfaces of $\xi_\cdot^{\alpha,\lambda,\rho}$ in the sense of (21)–(22) with all equilibria and pseudo-equilibria $\xi_\cdot^{\alpha,r,r}$ for $r \in [\lambda, \rho]$. Precisely, we can define a simultaneous evolution of interfaces $x_\cdot^r$ between $\eta_\cdot^\alpha$ and $\xi_\cdot^{\alpha,r,r}$ so that x_t^r is nondecreasing with respect to r, and define $x \mapsto \rho_t(x)$ as a generalized inverse of $r \mapsto x_t^r$.

5.3 Examples

In this subsection, we illustrate the behaviour of the flux function and of solutions to (25) with some examples.

Dilute limit (see [15, Sect. 3.4]). It is natural to compare the "disordered" flux function (26)–(27) to the "homogeneous" flux function f_{hom} obtained from the same AZRP in a homogeneous environment $\alpha_{\text{hom}}(x) \equiv 1$. In general, there is no simple relation between these two fluxes. However, the relation becomes simple and natural in the so-called *dilute limit* where $\alpha(x) = 1$ at "most" sites. More precisely, let Q_0 be the probability measure in Assumption 1, **(EE)** and (18). We consider an i.i.d. random environment in which, for each $x \in \mathbb{Z}$, $\alpha(x)$ is chosen according to Q_0 with probability $\varepsilon \geq 0$, and equal to 1 with probability $(1 - \varepsilon)$. Thus $\alpha(x)$ has distribution

$$Q_0^\varepsilon := (1 - \varepsilon)\delta_1 + \varepsilon Q_0 \,. \tag{32}$$

The value $\varepsilon = 0$ corresponds to the homogeneous environment α_{hom}, while $\varepsilon = 1$ corresponds to the i.i.d. environment with marginal Q_0. The dilute limit is the limit $\varepsilon \to 0+$. Let f^ε denote the flux function (26)–(27) produced by the environment with marginal (32). For $\varepsilon = 0$, $f^0 = f_{\text{hom}}$ is the flux function for the homogenous AZRP. It follows from (26)–(27) that

$$f_{\text{hom}}(\rho) = (p - q)R^{-1}(\rho) \,. \tag{33}$$

For $\varepsilon \in (0, 1]$, there is no simple relation between f^ε and f_{hom}. However, using (26)–(27) and (18), we can show that

$$\lim_{\varepsilon \to 0} f^\varepsilon(\rho) = f_d(\rho)$$

where f_d is the dilute limit of the flux function, defined by

$$f_d(\rho) := \left\{ \begin{array}{ll} f_{\text{hom}}(\rho) & \text{if } \rho < \rho_c \\ (p - q)c & \text{if } \rho \geq \rho_c \end{array} \right\} = f_{\text{hom}}(\rho) \wedge (p - q)c \,. \tag{34}$$

This limit can be understood intuitively as follows. As $\varepsilon \to 0$, slow sites are very rare, hence the system exhibits long homogeneous stretches where it behaves as a homogeneous process. Thus the memory of slow sites is only retained by the flux truncation, but not by the shape of the flux function prior to truncation. Note in particular that only the infimum of the support of Q_0 in (32) (but not details of the distribution) is involved in the dilute limit.

We defined above the dilute limit from the limit of a sequence of random environments. Another point of view is to construct a *single deterministic* environment equal to 1 except on a 0 density subset of $\mathbb{Z}$, where it asymptotically approaches its infimum value c. Precisely, let $\alpha(.)$ be an environment satisfying the conditions of Assumption 2, with values in $[c, 1]$, and such that

$$\alpha(x) = 1 \text{ if } x \notin \{x_n : n \in \mathbb{Z}\}.$$

Assume moreover $\lim_{n\to\pm\infty}(n/x_n) = 0$. For such an environment, the flux function defined by (26)–(27) is exactly f_d given by (34). As announced in Remark 3, this example shows that, outside the case of an ergodic random environment, the flux function is not entirely determined by the empirical distribution Q_0 in (10). Indeed, in this case we have $Q_0 = \delta_1$, which does not give any information on c.

Supercritical entropy solutions. We now describe the consequences of the flat line (27) on the behaviour of entropy solutions through the analysis of the so-called *Riemann* problem with initial data of the form (28). The following result can be obtained using (29) and (30).

Proposition 1 ([15, Proposition 3.1]) *Assume* $+\infty > \lambda \geq \rho_c > \rho$. *Let*

$$v_c(\rho) := \inf_{r\in[\rho,\rho_c)} \frac{f(\rho_c) - f(r)}{\rho_c - r} = \inf_{r\in[\rho,\rho_c)} \frac{\widehat{f}(\rho_c) - \widehat{f}(r)}{\rho_c - r} = \widehat{f}'(\rho_c-) \tag{35}$$

where $\widehat{f}$ *denotes the concave envelope of* f *on* $[\rho, \rho_c]$. *In particular, if* f *is concave,*

$$v_c(\rho) = f'(\rho_c-) = \left\{\int_{[c,1]} \frac{1}{a} R'\left[\frac{c}{a}\right] dQ_0(a)\right\}^{-1}.$$

Then, for every $t > 0$, *we have*

$$R_{\lambda,\rho}(x,t) = \lambda, \quad \forall x < 0 \tag{36}$$

$$R_{\lambda,\rho}(x,t) = R_{\rho_c,\rho}(x,t), \quad \forall x > 0 \tag{37}$$

$$\lim_{t\to+\infty} R_{\lambda,\rho}(x,t) = \rho_c, \quad \forall x \geq 0 \tag{38}$$

$$R_{\lambda,\rho}(0+,t) = \rho_c \tag{39}$$

$$R_{\lambda,\rho}(x,t) = \rho_c, \quad \forall x \in (0, tv_c(\rho)) \tag{40}$$

$$R_{\lambda,\rho}(x,t) < \rho_c, \quad \forall x > tv_c(\rho) \tag{41}$$

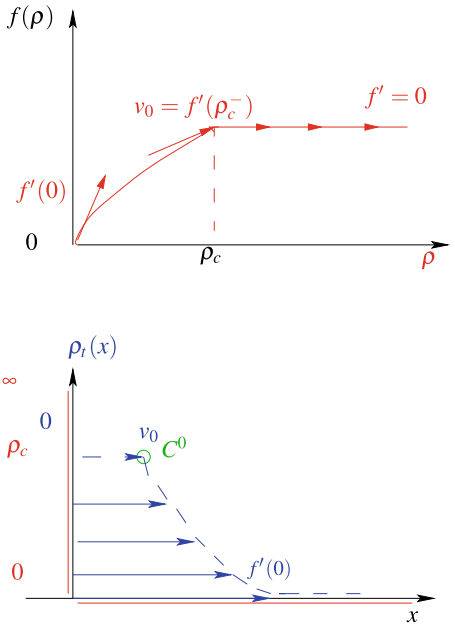

Fig. 6 Illustration of the critical front in (40), (41), with here $\lambda = \rho_c$ and $\rho = 0$. On the lower picture, each arrow represents the characteristic speed of the corresponding density level, that is the derivative of the flux function on the upper picture; we denote $v_0 = v_c(0)$. The critical density has a whole fan of speeds ranging from 0 to v_0 due to the cusp on the flux function. This accounts for the flat part of the front. We chose a concave flux on this example; if it is not, it should be replaced by its concave envelope on $[0, \rho_c]$

Property (36) states that the initial constant density is not modified to the left of the origin. This is related to the fact that f is nondecreasing, hence characteristic velocities are always nonnegative.

Property (37) states that the solution to the right of the origin does not depend on the supercritical initial density λ on the left. Formally, we may thus consider that this is also the solution for "$\lambda = +\infty$", which corresponds to placing sources to the left of the origin. In particular, for $\rho = 0$, we recover the source solution used in Sect. 4.2, that is the hydrodynamic limit starting from the particular source configuration (23).

Properties (38), (39), (40) are signatures of the phase transition. They express the fact that, regardless of the supercritical value on the left side, supercritical densities are blocked, and the right side is dominated by the critical density. In particular, (40)–(41) state that a front of critical density propagates to the right from the origin at speed v_c if $v_c(\rho) > 0$. This is illustrated in Fig. 6.

An explicit case: $M/M/1$ queues in series. Consider the $M/M/1$ queues in series, that is $g(n) = \min(n, 1)$, with total asymmetry ($p = 1, q = 0$), cf. Sect. 2. With this choice of g, (13) and (33) write

$$R(\beta) = \frac{\beta}{1-\beta}, \quad f_{\text{hom}}(\rho) = \frac{\rho}{1+\rho}. \tag{42}$$

In view of (42), the dilute limit f_d defined in (34) writes here

$$f_d(\rho) = \left[\frac{\rho}{1+\rho}\right] \wedge c = \begin{cases} \dfrac{\rho}{1+\rho} & \text{if } \rho < \rho_c := \dfrac{c}{1-c}\,, \\ c & \text{if } \rho \geq \rho_c\,. \end{cases} \tag{43}$$

Since f_d defined by (43) is concave, (35) yields

$$v_c(\rho) = f'_{\text{hom}}(\rho_c^-) = (1-c)^2\,.$$

6 Local Equilibrium

We now come to results from [16] on strong local equilibrium with respect to the hydrodynamic limit (25).

A natural extension of the convergence theorems is to establish results for the following question. Let us fix a realization of the environment $\alpha(.)$ and suppose given a sequence of initial configurations $\{\eta_0^N\}_{N\geq 0}$ which correspond to a "profile" ρ_0 in the sense that, for every $a, b \in \mathbb{R}$,

$$\frac{1}{N} \sum_{aN<k<bN} \eta_0^N(k) \;-\; \int_a^b \rho_0(x)dx \;\to\; 0\,. \tag{44}$$

Let $x_N \in \mathbb{Z}$ satisfy $N^{-1}x_N \to u \in (-\infty, \infty)$. What can be said about the behaviour of $\eta_{Nt}^{\alpha,N}$ around x_N?

We suppose that the entropy solution $\rho(.,.)$ to the associated hydrodynamic equation (25) is continuous at (t, u). It is reasonable to believe that $\tau_{[x_N]}\eta_{Nt}^{\alpha,N}$ "looks" like the equilibrium corresponding to $\rho(t, u)$ (with environment α suitably shifted). This question is anticipated by several works on conservative systems without disorder. In translation invariant cases where there is a family of equilibria $\{\mu^r\}_{r\geq 0}$ and the initial configurations are random there is *conservation of local equilibrium* if, when

$$\lim_{N\to\infty} \tau_{[uN]}\eta_0^N = \mu^{\rho_0(u)}$$

in distribution for each continuity point u of $\rho_0(.)$, then for each (t, u) as above,

$$\lim_{N\to\infty} \tau_{[uN]}\eta_{Nt}^N = \mu^{\rho(t,u)} \tag{45}$$

in distribution. In [27], conservation of local equilibrium was proved for a homogeneous zero-range process with a strictly convex flux, under an initial product local equilibrium measure. Following [2, 12] showed for finite range nonzero mean exclusion processes, that (45) held with no further assumptions on η_0^N beyond the profile hypothesis (44). We call this a "spontaneous creation of local equilibrium."

In our family of models it is natural to hope for similar results. We discuss three differences: We denote by $\mathbf{E}$ the expectation w.r.t. the process $(\eta_t^\alpha)_{t\geq 0}$.

1. Our system is not translation invariant and in fact we cannot expect a limit as in (45) because the environment varies as $N \to +\infty$: given appropriate (t, u) it is possible to find sequences x_N and y_N that converge macroscopically to x so that $\mathbf{E}(f(\tau_{x_N}\eta^{\alpha,N}_{Nt})) - \mathbf{E}(f(\tau_{y_N}\eta^{\alpha,N}_{Nt}))$ does not converge to zero as N becomes large.
2. Around a fixed point, say 0, the environment is fixed and will satisfy $\alpha(x) < c$ for x close to the point, however when considering x_N which (in scale N) converges to, say the origin, it is perfectly possible that $\alpha(x_N)$ converges to c.
3. The value $\rho(t, u)$ may be supercritical, that is strictly greater than ρ_c the maximum density for an equilibrium.

The first point is dealt with by a simple reformulation of the result but the second and third questions require a more substantive response. The second requires us to consider AZRP for which the occupation number $+\infty$ is permitted. For the third, as with other papers analyzing condensation phenomena, we expect that the limiting density will be ρ_c and not $\rho(t, u)$.

Our first results concern cases where the entropy solution $\rho(.,.)$ is continuous at (t, u) and has a value strictly below ρ_c.

Theorem 5 ([16, Theorem 2]) *Under assumptions of Theorem 4, the following holds for every $(t, u) \in (0, +\infty) \times \mathbb{R}$: let $\psi : \mathbf{X} \to \mathbb{R}$ be a bounded local function, and $(x_N)_{N\in\mathbb{N}}$ a sequence of sites such that $u = \lim_{N\to+\infty} N^{-1}x_N$. Then if $\rho(.,.)$ is continuous at (t, u) and $\rho(t, u) < \rho_c$,*

$$\lim_{N\to+\infty}\left[\mathbf{E}\psi\left(\tau_{x_N}\eta^{\alpha,N}_{Nt}\right) - \int_{\mathbf{X}} \psi(\eta)d\mu^{\tau_{x_N}\alpha,\rho(t,u)}(\eta)\right] = 0\,. \tag{46}$$

This result relied upon coupling. It is sufficient to show the desired convergence for increasing cylinder functions ψ. So it is sufficient to show that for $r < \rho(t, u)$ we have

$$\liminf_{N\to\infty} \mathbf{E}\psi\left(\tau_{x_N}\eta^{\alpha,N}_{Nt}\right) - \int_{\mathbf{X}} \psi(\eta)d\mu^{\tau_{x_N}\alpha,r}(\eta) \geq 0$$

for N large; and similarly for $r > \rho(t, u)$. So it will be sufficient to show that for N large in a N order interval centered around x_N, the process $\eta^{\alpha,N}_{tN}$ dominates $\xi^{\alpha,r}_{Nt}$ where as before $\xi^{\alpha,r}_{.t}$ is a AZRP run with the given Harris system in $\mu^{\alpha,r}$ equilibrium.

Our approach shadows that of [12] but is a bit more complicated than this argument which dealt with the exclusion process. In particular the key tool of [25], which relies on global strict concavity or convexity of the flux function, is no longer available here.

Under the general assumptions on function $g(.)$, the flux function f need not be globally convex or globally concave. Nonetheless away from the critical value the function f is analytic and therefore in any interval of densities, there will exist subintervals on which the flux is either globally convex or globally concave. Thus given $r < \rho(t, u)$ we can find $r < r_1 < r_2 < \rho(t, u)$ so that f is either convex or concave on (r_1, r_2). For concreteness suppose it is concave, then we may "impose" a system of *priorities* (or *classes*, cf. [3]) on $\eta^{\alpha,N}_s$ particles that are not coalesced with $\xi^{\alpha,r}_s$ particles. This means that higher priority particles will be faster than lower priority

ones. So a given small, but order N, interval I can be placed between two similar intervals J_l and J_r. In a short time (unless they become coalesced) fast particles in J_l will overtake slow particles in J_r. This entails coalescence of many uncoalesced $\xi_s^{\alpha,r}$ particles originally in I. This argument is repeated until in an interval around x_N, the "density" of uncoalesced $\xi_s^{\alpha,r}$ particles will be very small. We can then argue as in [12] to show the required domination.

Next, we consider points at which the hydrodynamic density is supercritical or critical. As discussed above, there does not (in the supercritical case) or may not (in the critical case) exist a corresponding equilibrium measure, so one cannot expect the same type of convergence as above. We expect and to some extent show one has local convergence to the *critical* quenched invariant measure. We now introduce an additional assumption that is needed.

Definition 3 ([16, Definition 1]) Let $(x_N)_{N\in\mathbb{N}}$ be a sequence of sites such that $N^{-1}x_N$ converges to $u \in \mathbb{R}$ as $N \to +\infty$. The sequence $(x_N)_{N\in\mathbb{N}}$ is *typical* if and only if any subsequential limit $\overline{\alpha}$ of $(\tau_{x_N}\alpha)_{N\in\mathbb{N}}$ has the following properties:

(i) For every $z \in \mathbb{Z}$, $\overline{\alpha} \in \mathbf{B} := (c, 1]^{\mathbb{Z}}$.
(ii) $\liminf_{z\to-\infty} \overline{\alpha}(z) = c$.

The interpretation of the word "typical" is the following. When α does not achieve its infimum value c (that is $\alpha \in \mathbf{B}$), *(i)–(ii)* says that the environment as seen from x_N shares key properties of the environment seen from a fixed site (say the origin).

The typicality assumption will in fact be needed only to show that the microscopic distribution is locally dominated by the critical measure (8). We observe however that even in the critical case, if the invariant measure does not (in the supercritical case) or may not (in the critical case), we are not able to prove the statement without the typicality assumption.

Theorem 6 ([16, Theorem 3]) *Under assumptions of Theorem 4, the following holds for every $(t, u) \in (0, +\infty) \times \mathbb{R}$. Let $\psi : \mathbf{X} \to \mathbb{R}$ be a bounded local function, and $(x_N)_{N\in\mathbb{N}}$ a typical sequence of sites such that $u = \lim_{N\to+\infty} N^{-1}x_N$. Then:*

(i) *If ψ is nondecreasing,*

$$\lim_{N\to+\infty} \left[\mathbf{E}\psi\left(\tau_{x_N}\eta_{Nt}^{\alpha,N}\right) - \int_{\mathbf{X}} \psi(\eta) d\mu_c^{\tau_{x_N}\alpha}(\eta) \right]^+ = 0\,. \tag{47}$$

(ii) *If $\rho_*(t, u) \geq \rho_c$ (where $\rho_*(t, u) := \liminf_{(t',u')\to(t,u)} \rho(t', u')$), then*

$$\lim_{N\to+\infty} \left[\mathbf{E}\psi\left(\tau_{x_N}\eta_{Nt}^{\alpha,N}\right) - \int_{\mathbf{X}} \psi(\eta) d\mu_c^{\tau_{x_N}\alpha}(\eta) \right] = 0\,. \tag{48}$$

The argument we give for the upper bound is now close to that for the convergence upper bound: we show that we can find $y_N < x_N < z_N$ so that the "finite" AZRP on (y_N, z_N) with infinitely many particles at y_N and z_N has an equilibrium very close to μ_c^α. The lower bound is essentially supplied by the arguments for Theorem 5.

Without the above typicality assumption, we are not able to prove such a statement at given times, but we can obtain a weaker time-integrated result.

Theorem 7 ([16, Theorem 4]) *Under assumptions and notations of Theorem 4, the following holds. Let $t > 0$, and $(x_N)_{N\in\mathbb{N}}$ be an* arbitrary *sequence of sites such that $\lim_{N\to+\infty} N^{-1}x_N = u$, where $u \in \mathbb{R}$ is such that $\rho_*(t,u) \geq \rho_c$. Let $\psi : \overline{\mathbf{X}} \to \mathbb{R}$ be a continuous local function. Then*

$$\lim_{\delta\to 0} \limsup_{N\to+\infty} \left| \frac{1}{\delta} \int_{t-\delta}^{t} \mathbf{E}\psi\left(\tau_{x_N}\eta_{Ns}^{\alpha,N}\right) ds - \int_{\overline{\mathbf{X}}} \psi(\eta) d\mu_c^{\tau_{x_N}\alpha}(\eta) \right| = 0\,. \tag{49}$$

Remark 4 Whereas in Theorems 5 and 6, the test function ψ is defined on $\mathbf{X}$, in Theorem 7, it is defined on $\overline{\mathbf{X}}$. Indeed in Theorem 5, the fact that $\rho(t,u) < \rho_c$ implies that the subcritical measure $\mu^{\tau_{x_N}\alpha,\rho(t,u)}$ in (46) is supported on $\mathbf{X}$. In Theorem 6, statement *(i)* in Definition 3 of the typicality assumption ensures that the critical measure $\mu_c^{\tau_{x_N}\alpha}$ in (47)–(48) is still supported on $\mathbf{X}$. However in Theorem 7, owing to the absence of the typicality assumption, the critical measure $\mu_c^{\tau_{x_N}\alpha}$ in (49) may have infinitely many particles at sites $x \in \mathbb{Z}$ such that $\alpha(x) = c$.

Our approach is to first note that, again, the lower bound is achieved via Theorem 5. The upper bound is more intricate. We argue that in the supercritical regime the current through any point must ("on average") equal c. We then argue that any invariant measure that dominates μ_c^α and has current c must equal μ_c^α. The (unfortunately necessary) Cesàro means are to give an invariant measure for any limit measure and to ensure that the limit measure must have flux c.

Example An illuminating particular case of the above theorems is when the initial datum is uniform. Assume

$$\rho_0(x) \equiv \rho \tag{50}$$

for some $\rho \geq 0$. Then $\rho(t,x) \equiv \rho$ for all $t > 0$. Specializing Theorems 5 and 6 to $u = 0$, we obtain that $\eta_{Nt}^{\alpha,N}$ converges in distribution to $\mu^{\alpha,\rho}$ if $\rho < \rho_c$, or to μ_c^α if $\rho \geq \rho_c$. Therefore a mass condensation phenomenon is somehow present, even at hyperbolic scaling. We may in particular achieve (50) as follows by a sequence of initial configurations $\eta_0^N = \eta_0$ independent of N.

(i) Stationary initial state. Let $\eta_0^N = \eta_0 \sim \mu^{\alpha,\rho}$, with $\rho < \rho_c$. Since $\mu^{\alpha,\rho}$ is an invariant measure for the process with generator (3), for every $t > 0$, we have $\eta_{Nt}^{\alpha,N} \sim \mu^{\alpha,\rho}$. As a result, the expression between brackets in (46) vanishes for every $N \in \mathbb{N}\setminus\{0\}$ and $t \geq 0$. Hence there is *conservation* of local equilibrium (since (46) already holds for $t = 0$), but there is in fact nothing to prove, since this conservation follows form stationarity.

(ii) Deterministic initial state. Let $\eta_0^N = \eta_0$, where $\eta_0 \in \mathbf{X}$ has density ρ, cf. (17). This implies that the sequence $(\eta_0^N)_{N\in\mathbb{N}\setminus\{0\}}$ has density profile $\rho_0(x) \equiv \rho$. Here Theorems 5 and 6 are no longer void statements as in *(i)*. When specialized to $u = 0$, they yield a large-time convergence result for our process. Namely, Theorem 5 implies that $\eta_t^\alpha \to \mu^{\alpha,\rho}$ in distribution if $\rho < \rho_c$, and Theorem 6 implies $\eta_t^\alpha \to \mu_c^\alpha$ if $\rho \geq \rho_c$.

Pushing the analysis of *(ii)* further, we can show that the first limit in (17) is irrelevant, and derive from Theorems 5 and 6 the following convergence result.

Theorem 8 ([16, Theorem 5]) *Let $\eta_0 \in \mathbf{X}$ be such that, for some $\rho > 0$,*

$$\lim_{n\to+\infty} \frac{1}{n} \sum_{x=-n}^{0} \eta_0(x) = \rho\,.$$

Then η_t^α converges in distribution as $t \to +\infty$ to $\mu^{\alpha,\rho\wedge\rho_c}$.

Remark 5 *(i)* In the case $\rho < \rho_c$, Theorem 8 solves the convergence problem posed in [19, pp 195–196].

(ii) In the case $\rho \geq \rho_c$, Theorem 8 is a partial improvement over Theorem 1. It improves the latter in the sense that we do not need a weak convexity assumption on g, but is it less general with respect to initial conditions.

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References

1. E.D. Andjel, Invariant measures for the zero-range process. Ann. Prob. **10**, 525–547 (1982)
2. E.D. Andjel, The asymmetric simple exclusion process on $\mathbb{Z}^d$. Z. Wahrscheinlichkeitstheor. Verw. Geb. **58**, 423–432 (1981)
3. E.D. Andjel, C. Kipnis, Derivation of the hydrodynamical equation for the zero-range interaction process. Ann. Prob. **12**(2), 325–334 (1984)
4. E.D. Andjel, M.E. Vares, Hydrodynamic equations for attractive particle systems on $\mathbb{Z}$. J. Stat. Phys. **47**(1–2), 265–288 (1987)
5. E.D. Andjel, M.E. Vares, Correction to: Hydrodynamic equations for attractive particle systems on $\mathbb{Z}$. J. Stat. Phys. **113**(1–2), 379–380 (2003)
6. E. Andjel, P.A. Ferrari, H. Guiol, C. Landim, Convergence to the maximal invariant measure for a zero-range process with random rates. Stoch. Process. Appl. **90**, 67–81 (2000)
7. C. Bahadoran, H. Guiol, K. Ravishankar, E. Saada, A constructive approach to Euler hydrodynamics for attractive particle systems. Application to k-step exclusion. Stoch. Process. Appl. **99**(1), 1–30 (2002)
8. C. Bahadoran, H. Guiol, K. Ravishankar, E. Saada, Euler hydrodynamics of one-dimensional attractive particle systems. Ann. Prob. **34**(4), 1339–1369 (2006)
9. C. Bahadoran, H. Guiol, K. Ravishankar, E. Saada, Strong hydrodynamic limit for attractive particle systems on $\mathbb{Z}$. Elect. J. Prob. **15**(1), 1–43 (2010)
10. C. Bahadoran, H. Guiol, K. Ravishankar, E. Saada, Euler hydrodynamics for attractive particle systems in random environment. Ann. Inst. H. Poincaré Prob. Stat. **50**(2), 403–424 (2014)
11. C. Bahadoran, H. Guiol, K. Ravishankar, E. Saada, Constructive Euler hydrodynamics for one-dimensional attractive particle systems, in *Sojourns in Probability Theory and Statistical*

Physics—III—Interacting Particle Systems and Random Walks, A Festschrift for Charles M. Newman, ed. by V. Sidoravicius; Springer PROMS, vol. 300 (Springer, Singapore 2019), pp. 43–89
12. C. Bahadoran, T.S. Mountford, Convergence and local equilibrium for the one-dimensional nonzero mean exclusion process. Prob. Theory Relat. Fields **136**(3), 341–362 (2006)
13. C. Bahadoran, T.S. Mountford, K. Ravishankar, E. Saada, Supercriticality conditions for the asymmetric zero-range process with sitewise disorder. Braz. J. Prob. Stat. **29**(2), 313–335 (2015)
14. C. Bahadoran, T.S. Mountford, K. Ravishankar, E. Saada, Supercritical behavior of zero-range process with sitewise disorder. Ann. Inst. H. Poincaré Prob. Stat. **53**(2), 766–801 (2017)
15. C. Bahadoran, T.S. Mountford, K. Ravishankar, E. Saada, Hydrodynamics in a condensation regime: the disordered asymmetric zero-range process. Ann. Prob. **48**(1), 404–444 (2020)
16. C. Bahadoran, T.S. Mountford, K. Ravishankar, E. Saada, Quenched convergence and strong local equilibrium for asymmetric zero-range process with sitewise disorder. Prob. Theory Relat. Fields **176**(1–2), 149–202 (2020)
17. M. Balázs, T. Seppäläinen, A convexity property of expectations under exponential weights (2007), Arxiv: PR07074273
18. J. Beltrán, M. Jara, C. Landim, A martingale problem for an absorbed diffusion: the nucleation phase of condensing zero range processes. Prob. Theory Relat. Fields **169**, 1169–1220 (2017)
19. I. Benjamini, P.A. Ferrari, C. Landim, Asymmetric conservative processes with random rates. Stoch. Process. Appl. **61**(2), 181–204 (1996)
20. M.R. Evans, Bose–Einstein condensation in disordered exclusion models and relation to traffic flow. Europhys. Lett. **36**(1), 13 (1996)
21. P. Ferrari, J. Krug, Phase transitions in driven diffusive systems with random rates. J. Phys. A. **29**, L465–L471 (1996)
22. P.A. Ferrari, V.V. Sisko, Escape of mass in zero-range processes with random rates, in *Asymptotics: Particles, Processes and Inverse Problems*. IMS Lecture Notes Monograph Series, Institute of Mathematical Statistics, vol. 55, Beachwood, OH (2007), pp. 108–120
23. T.E. Harris, Nearest-neighbour Markov interaction processes on multidimensional lattices. Adv. Math. **9**, 66–89 (1972)
24. C. Kipnis, C. Landim, *Scaling Limits for Interacting Particle Systems* (Springer, Berlin 1999)
25. E. Kosygina, The behaviour of specific entropy in the hydrodynamic scaling limit. Ann. Prob. **29**(3), 1086–1110 (2001)
26. J. Krug, Phase separation in disordered exclusion models. Braz. J. Phys. **30**, 97–104 (2000)
27. C. Landim, Conservation of local equilibrium for attractive particle systems on $\mathbb{Z}$. Ann. Prob. **21**(4), 1782–1808 (1993)
28. C. Landim, Hydrodynamical limit for space inhomogeneous one-dimensional totally asymmetric zero-range processes. Ann. Prob. **24**, 599–638 (1996)
29. T.M. Liggett, *Interacting Particle Systems*. Reprint of the 1985 original. Classics in Mathematics (Springer, Berlin, 2005)
30. M. Loulakis, M.G. Stamatakis, Generalized Young measures and the hydrodynamic limit of condensing zero range processes (2019), ArXiv:1910.00493
31. T. Mountford, An extension of a result of Andjel. Ann. Appl. Prob. **11**, 321–337 (2001)
32. E. Pardoux, *Processus de Markov et applications* (Dunod, Paris, 2007)
33. F. Rezakhanlou, Hydrodynamic limit for attractive particle systems on $\mathbb{Z}$. Commun. Math. Phys. **140**(3), 417–448 (1991)
34. T. Seppäläinen, J. Krug, Hydrodynamics and platoon formation for a totally asymmetric exclusion process with particlewise disorder. J. Stat. Phys. **95**, 525–567 (1999)
35. D. Serre, Systems of conservation laws. 1. Hyperbolicity, entropies, shock waves. Translated from the 1996 French original by I.N. Sneddon (Cambridge University Press, Cambridge, 1999)
36. M.G. Stamatakis, Hydrodynamic limit of mean zero condensing zero range processes with sub-critical initial profiles. J. Stat. Phys. **158**(1), 87–104 (2015)

On Non-equilibrium Fluctuations for the Stirring Process with Births and Deaths

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Abstract We study the density fluctuation field for the stirring process with births and deaths at two sites at the boundary which tend to impose a current into the system. Assuming correlation estimates (to be proved in a companion paper [2]) we derive an equation for the limiting kernel of the variance of the fluctuation field. The key difficulty lies in closing the martingales, with respect to the density fluctuation field, due to the boundary effects and we present a strategy on how to deal with more general boundary conditions.

Keywords Stirring process · Births and deaths · Current reservoir · Boundary conditions · Non-equilibrium fluctuations · Closure of martingale

1 Introduction

Interacting particle systems coupled with reservoirs can demonstrate a rich macroscopic behaviour sensitive to the effective boundary conditions. From the technical point of view a key issue is the closure of the corresponding equations as boundary effects propagate and create non vanishing correlations. One can design different types of reservoirs corresponding to different physical mechanisms, such as density (i.e., fixing the density as in the Fourier law) or current (fixing the current which tends to propagate in the medium). This is done by tuning the strength of the boundary action, namely, when it is strong the density is fixed and when it is weak the density

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is no longer fixed but instead the current is. Macroscopically, the reservoirs' action, if restricted to a finite number of sites, gives rise to a boundary condition, while if the reservoirs' action is in the bulk, then it gives rise to a reaction term. The hydrodynamic limit for the current reservoir with a medium consisting of the symmetric simple exclusion process (SSEP) has been considered in [4–6]. Instead, the density reservoir case has been explored in [1] in the presence of only one reservoir and in [7] for the case of two reservoirs. The hydrodynamic equation is the heat equation (thanks to the SSEP dynamics), with either Robin-type boundary conditions (see (18)), in the case of current reservoirs, or Dirichlet boundary conditions in the case of density reservoirs.

The main difficulty one faces when dealing with a reservoir that acts in more than one site and which injects/removes particles from the system at a particular site x depending at the configuration of all the neighbouring sites, is that one has to know a lot of information about the boundary behaviour in order to control the correlations of the boundary variables. Actually, the proof of hydrodynamics of the SSEP with a strong boundary action from a reservoir consisting of more than one sites is an open problem due to the fact that correlation estimates are difficult to establish (as a result of the competition between the bulk exchange dynamics and the boundary Glauber dynamics).

In these notes we focus on the properties of the density fluctuation field around the hydrodynamic limit and we present a systematic way of closing the corresponding martingale problem associated to this field. Our result is compatible with previous work for the special case when the reservoirs act at one boundary point (see [8]) and provides some more insight on how to treat more complex scenarios. Other cases of the SSEP superposed with a Glauber dynamics acting at only one site in the boundary have been studied in [12] where the intensity of the density reservoir is strong and in [9] for the case of a weaker intensity for both density and current reservoirs.

The key idea in dealing with the fluctuations for boundary mechanisms is to view the problem as a linearization of the limiting equations both at the bulk and at the boundary. As it will be shown, this allows to "guess" the space in which one should describe the fluctuation field. In all the aforementioned problems, the space where the density field is defined is independent of the hydrodynamic profile since the boundary dynamics only acts at one site and the hydrodynamic equation is the heat equation with linear Robin boundary conditions (see (18) for $K = 1$). In the case where the boundary acts in more than one site and the current is fixed, the boundary conditions become non-linear Robin and the choice of the space of test functions will depend on the hydrodynamical profile which requires, from a technical point of view, further decay properties of higher order correlation functions. We leave this issue for a more technical subsequent paper [2].

These notes are organized as follows: we start (Sect. 2) with the presentation of the model and some relevant results for the hydrodynamic limit. Then, in Sect. 2.3 we define the fluctuation field and describe the problem, presenting the corresponding martingale decomposition. The strategy of closure of the martingale is described in Sect. 3 where a linearization argument is given for the appropriate choice of the test function space in which to define the limiting fluctuation field. Finally, in Sect. 4 we

give a comparison between a direct microscopic derivation of the variance of the fluctuation field and another based on the martingale decomposition using Holley-Stroock's theory. The comparison of the two provides another way of dictating the right choice for the test functions. We conclude with the derivation of an equation for the kernel of the macroscopic fluctuation field.

2 Preliminaries

2.1 The Model

Let $N \in \mathbb{N}$ denote the scaling parameter which will be taken to infinity and fix an integer $K \leq N$ which does not scale with N. We consider the stirring process evolving on the discrete subset $\Lambda_N := [-N, N]$ of $\mathbb{Z}$. The configurations of particles are elements η in $\{0, 1\}^{\Lambda_N}$, so that $\eta(x) = 1$ if there is a particle at site x and $\eta(x) = 0$ otherwise. The stirring process with births and deaths is a Markov process defined by its infinitesimal generator given by

$$L_\varepsilon := \varepsilon^{-2}\big(L_0 + \varepsilon L_{b,-} + \varepsilon L_{b,+}\big), \quad \varepsilon \equiv \frac{1}{N}, \tag{1}$$

where L_0 is the generator of the stirring process in Λ_N, namely

$$L_0 f(\eta) := \frac{1}{2} \sum_{x=-N}^{N-1} [f(\eta^{x,x+1}) - f(\eta)] \tag{2}$$

and

$$L_{b,\pm} f(\eta) := \frac{j}{2} \sum_{x \in I_\pm} D_\pm \eta(x) [f(\eta^x) - f(\eta)\Big], \tag{3}$$

with $j > 0$, $I_+ = [N - K + 1, N]$, $I_- = [-N, -N + K - 1]$, and for any function $u : \Lambda_N \to \mathbb{R}$, $D_\pm$ are defined as follows:

$$D_+ u(x) = [1 - u(x)]u(x + 1)u(x + 2) \cdots u(N), \ x \in I_+,$$
$$D_- u(x) = u(x)[1 - u(x - 1)][1 - u(x - 2)] \cdots [1 - u(-N)], \ x \in I_- .$$

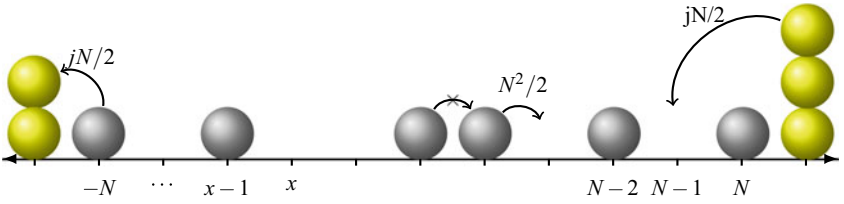
Observe that K fixes the size of the window where the reservoirs act. In the sequel we will be switching between the use of ε and N (depending on the context) in order to describe the small parameter for the passage from micro to macro. We hope this does not create confusion to the reader. Above, $\eta^{x,x+1}$, $-N \leq x \leq N - 1$, is the configuration obtained from η by exchanging the occupation variables $\eta(x)$ and $\eta(x + 1)$:

$$(\eta^{x,x+1})(y) = \begin{cases} \eta(x+1), & y = x\ , \\ \eta(x), & y = x+1\ , \\ \eta(y), & y \neq x, x+1\ , \end{cases}$$

while for $x \in I_{\pm}$, η^x is the configuration obtained by flipping the occupation variable $\eta(x)$:

$$(\eta^x)(y) = \begin{cases} \eta(x), & y \neq x\ , \\ 1-\eta(y), & y = x\ . \end{cases}$$

The generator $N^2 L_0$ describes a process where nearest neighbour sites are exchanged at rate $N^2/2$ and $NL_{b,+}$ describes a birth process: at rate $jN/2$ a particle is created in the first (starting from N and going down up to $N-K+1$) empty site in I_+, if no site is empty the birth is aborted. Symmetrically $NL_{b,-}$ describes deaths: at rate $jN/2$ the first particle (starting from $-N$) in I_- is removed, if I_- is empty there is no death.



2.2 Hydrodynamic Limit

For $x \in \Lambda_N$ and $t \geq 0$, let us denote

$$\rho_t^{\varepsilon}(x) := \mathbb{E}_{\varepsilon}[\eta_t(x)], \tag{4}$$

where by $\mathbb{E}_{\varepsilon}$ we denote the expectation of the process with generator L_{ε} and starting from the product measure μ^{ε}. It readily follows from the structure of the generators that $\rho_t^{\varepsilon}(x)$ satisfies the relations:

$$\partial_t \rho_t^{\varepsilon}(x) = \frac{1}{2}\Delta_{\varepsilon,1}\rho_t^{\varepsilon}(x) + \varepsilon^{-1}\frac{j}{2}\left(\mathbf{1}_{x\in I_+}\mathbb{E}_{\varepsilon}[D_+\eta_t(x)] - \mathbf{1}_{x\in I_-}\mathbb{E}_{\varepsilon}[D_-\eta_t(x)]\right) \tag{5}$$

for any $x \in \Lambda_N$ and $t > 0$, where

$$\begin{aligned} &\Delta_{\varepsilon,1}u(x) = \varepsilon^{-2}\Big(u(x+1)+u(x-1)-2u(x)\Big), \qquad x \in \Lambda_N \setminus \{-N, N\}, \\ &\Delta_{\varepsilon,1}u(\pm N) = \varepsilon^{-2}\Big(u(\pm(N-1)) - u(\pm N)\Big) \end{aligned} \tag{6}$$

for any function $u : \Lambda_N \to \mathbb{R}$. On the other hand, for $x \in \Lambda_N$ let us denote by $\rho_\varepsilon(x,t)$ (note the slight difference in notation with (4)) the solution of

$$\begin{cases} \partial_t \rho_\varepsilon(x,t) = \frac{1}{2}\Delta_{\varepsilon,1}\rho_\varepsilon(x,t) + \varepsilon^{-1}\frac{j}{2}\Big(\mathbf{1}_{x\in I_+} D_+\rho_\varepsilon(x,t) - \mathbf{1}_{x\in I_-} D_-\rho_\varepsilon(x,t)\Big) \\ \rho_\varepsilon(x,0) = \rho_0^\varepsilon(x), \end{cases} \tag{7}$$

for any $x \in \Lambda_N$. Observe that the previous equation is the closed version of (5), that is, the previous equation would be obtained from (5), if we had assumed that, for any $x \in I_\pm$ and any time t, it holds $\mathbb{E}[D_\pm \eta_t(x)] = D_\pm \mathbb{E}[\eta_t(x)]$, which translates into uncorrelatedness of occupation variables at the boundary for any time t. Below we recall Eq. (3.9) from [5], which allows the control of discrete gradients of $\rho_\varepsilon(x,t)$.

Lemma 1 *For any $\zeta > 0$ and $\tau > 0$, there is c so that*

$$\sup_{x,y\in\Lambda_N : |x-y|\le 1} |\rho_\varepsilon(x,t) - \rho_\varepsilon(y,t)| \le \frac{c}{(\varepsilon^{-2}t)^{1/2-\zeta} + 1} \tag{8}$$

for any $t \le \tau \log \varepsilon^{-1}$.

Observe that the difference between the solutions of the two Eqs. (5) and (7), can be quantified by estimates on the following quantities, called v-functions:

$$v_n^\varepsilon(\underline{x},t) := \mathbb{E}_\varepsilon\left[\prod_{i=1}^n (\eta_t(x_i) - \rho_\varepsilon(x_i,t))\right], \quad \underline{x} \in \Lambda_N^{n,\neq}, n \ge 1, \tag{9}$$

where $\Lambda_N^{n,\neq}$ is the set of all sequences $(x_1,\dots,x_n) \in \Lambda_N^n$ with $x_i \neq x_j$. Such estimates have been derived in [4, Theorem 2.1]: for any $\beta^* > 0$ and for any positive integer n, there is a constant $c_n < \infty$ so that for every $\varepsilon > 0$, any initial product measure μ^ε,

$$\sup_{\underline{x}\in\Lambda_N^{n,\neq}} |v_n^\varepsilon(\underline{x},t)| \le \begin{cases} c_n(\varepsilon^{-2}t)^{-c^*n}, & \text{for } t \le \varepsilon^{\beta^*} \\ c_n\varepsilon^{(2-\beta^*)c^*n}, & \text{for } \varepsilon^{\beta^*} \le t \le \tau\log\varepsilon^{-1}, \end{cases} \tag{10}$$

for some $\tau > 0$ and $c^* > 0$.

As a result of (10), empirical averages of the microscopic process are close to the functions ρ_ε satisfying (7); hence the following theorem (which is proved in [4]) identifies the hydrodynamics of the microscopic system:

Theorem 1 ([4, Theorem 1]) *Suppose that the initial datum $\rho_\varepsilon(\cdot,0)$ defined on Λ_N, with values in $[0,1]$ converges weakly as $\varepsilon \to 0$ to $u_0(\cdot) \in L^\infty([-1,1],[0,1])$ in the sense*

$$\lim_{\varepsilon\to 0} \varepsilon \sum_{x\in\Lambda_N} \rho_\varepsilon(\cdot,0)\phi(\varepsilon x) = \int_{[-1,1]} u_0(r)\phi(r)dr, \quad \text{for every } \phi \in L^\infty([-1,1],\mathbb{R}). \tag{11}$$

Then, there is $\rho(r,t)$, $r \in [-1,1]$, $t > 0$ *so that for any* $t_1 > t_0 > 0$

$$\lim_{\varepsilon \to 0} \sup_{x \in \Lambda_N} \sup_{t_0 \le t \le t_1} |\rho_\varepsilon(x,t) - \rho(\varepsilon x, t)| = 0, \tag{12}$$

where the function $\rho(r,t)$ *is the unique solution of the integral equation*

$$\begin{aligned} \rho(r,t) = &\int_{[-1,1]} P_t(r,r')u_0(r')dr' + \frac{j}{2}\int_0^t P_s(r,1)(1-\rho(1,t-s)^K) \\ &-P_s(r,-1)(1-(1-\rho(-1,t-s))^K)ds \end{aligned} \tag{13}$$

where $P_t(r,r')$ *is the density kernel of the semigroup (also denoted as* P_t*) with generator* $\Delta/2$, Δ *the Laplacian in* $[-1,1]$ *with reflecting, Neumann, boundary conditions.*

Remark 1 The density kernel $P_t(r,r')$ can be expressed in terms of the Gaussian kernel

$$G_t(r,r') = \frac{e^{-(r-r')^2/2t}}{\sqrt{2\pi t}} \tag{14}$$

as follows: if $\psi : \mathbb{R} \to [-1,1]$ denotes the usual reflection map, i.e. $\psi(x) = x$ for $x \in [-1,1]$, $\psi(x) = 2 - x$ for $x \in [1,3]$, with ψ extended to the whole line as periodic of period 4, then

$$P_t(r,r') = \sum_{\psi(r'')=r'} G_t(r,r''), \quad \text{for } r, r' \neq \pm 1 \tag{15}$$

$$P_t(r,\pm 1) = \sum_{\psi(r'')=\pm 1} 2G_t(r,r''). \tag{16}$$

Furthermore, by a simple computation one can check that $\rho(r,t)$ for $t > 0$ and $r \in (-1,1)$ satisfies the heat equation

$$\partial_t \rho(r,t) = \frac{1}{2}\partial_{rr}^2 \rho(r,t) \tag{17}$$

with boundary conditions:

$$\partial_r \rho(r,t)\Big|_{r=1} = j(1-\rho(1,t)^K), \quad \partial_r \rho(r,t)\Big|_{r=-1} = j(1-(1-\rho(-1,t))^K). \tag{18}$$

See also [6] for an alternative derivation using the entropy method of [10].

2.3 Fluctuations

The main goal of this note is to suggest a systematic way of choosing the proper test functions for the definition of the limiting fluctuation field. So let H be a test function in a space $\mathbb{S}$ which will be determined later on. Let $\mathscr{D}([0,T],\mathbb{S}')$ be the space of trajectories which are right continuous, with left limits and taking values in $\mathbb{S}'$, the dual of $\mathbb{S}$.

Definition 1 (*Density fluctuation field*) We define the density fluctuation field $Y^\varepsilon_\cdot$ as the time-trajectory of linear functionals acting on functions $H : [-1,1]\times[0,T]\to\mathbb{R}$ as

$$Y^\varepsilon_t(H) \;=\; \sqrt{\varepsilon}\sum_{x\in\Lambda_N} H(\varepsilon x,t)\bar{\eta}_t(x), \tag{19}$$

where $\bar{\eta}_t(x) := \eta_t(x) - \rho^\varepsilon_t(x)$ and $\rho^\varepsilon_t(x)$ was defined in (4).

For each $\varepsilon>0$, let $\mathbb{Q}^\varepsilon_{\mu^\varepsilon}$ be the probability measure on $\mathscr{D}([0,T],\mathbb{S}')$ induced by the density fluctuation field $Y^\varepsilon_\cdot$ and the measure μ^ε. For every n positive integer and $x_1,\dots,x_n\in\Lambda_N^{n,\neq}$, we define:

$$C^{n,\varepsilon}_t(x_1,\dots,x_n) := \mathbb{E}_\varepsilon[\bar{\eta}_t(x_1)\dots\bar{\eta}_t(x_n)]. \tag{20}$$

Note the difference between the v-function defined in (9) and the correlation function $C^{n,\varepsilon}_t$, that is ρ^ε_t is the solution to the discrete equation (5) whose closed version is exactly (7). In order to find the limiting equation for the density fluctuation field defined in (19), one needs an improved version of (10) due to the softer scaling of the quantity of interest ($\varepsilon^{1/2}$ instead of ε). Hence, for the purpose of this note, we will assume an improved version of this estimate see (44) and (45), to be proven in a forthcoming article [2].

In order to find the distribution of the fluctuation field, for any $F\in C^\infty(\mathbb{R})$ and for any $H:[-1,1]\times[0,T]\to\mathbb{R}$ a test function, we define

$$\mathscr{M}^{F,\varepsilon}_t(H) := F(Y^\varepsilon_t(H)) - F(Y^\varepsilon_0(H)) - \int_0^t (\partial_s + L_\varepsilon)F(Y^\varepsilon_s(H))ds. \tag{21}$$

For special choices of F we can write:

$$M^\varepsilon_t(H) := Y^\varepsilon_t(H) - Y^\varepsilon_0(H) - \int_0^t (\partial_s + L_\varepsilon)Y^\varepsilon_s(H)ds, \tag{22}$$

$$N^\varepsilon_t(H) := (M^\varepsilon_t(H))^2 - \int_0^t \Big(L_\varepsilon(Y^\varepsilon_s(H))^2 - 2Y^\varepsilon_s(H)L_\varepsilon Y^\varepsilon_s(H)\Big)ds. \tag{23}$$

It is easy to check that these are martingales with respect to the natural filtration $\mathscr{F}_t := \sigma(\{\eta_s : s\le t\})$. Furthermore, using the general form (21), there is a function $R^\varepsilon(t,H)$ uniformly bounded in ε such that:

$$(\partial_t + L_\varepsilon)F(Y_t^\varepsilon(H)) = F'(Y_t^\varepsilon(H))\gamma_1^\varepsilon(t,H) + \frac{1}{2}F''(Y_t^\varepsilon(H))\gamma_2^\varepsilon(t,H) + R^\varepsilon(t,H), \tag{24}$$

where

$$\gamma_1^\varepsilon(t,H) = (\partial_t + L_\varepsilon)Y_t^\varepsilon(H) \tag{25}$$

and

$$\gamma_2^\varepsilon(t,H) = L_\varepsilon(Y_t^\varepsilon(H))^2 - 2Y_t^\varepsilon(H)L_\varepsilon Y_t^\varepsilon(H). \tag{26}$$

Above, by noticing that $\partial_t Y_t^\varepsilon(H) = Y_t^\varepsilon(\partial_t H) - \sqrt{\varepsilon}\sum_{x\in\Lambda_N} H(\varepsilon x)\partial_t\rho_t^\varepsilon(x)$ and that, from Kolmogorov's equation $\partial_t\rho_t^\varepsilon(x) = \mathbb{E}_\varepsilon[L_\varepsilon\eta_t(x)]$, we get

$$\gamma_1^\varepsilon(t,H) = L_\varepsilon Y_t^\varepsilon(H) + Y_t^\varepsilon(\partial_t H) - \mathbb{E}_\varepsilon(L_\varepsilon Y_t^\varepsilon(H)). \tag{27}$$

Before proceeding we give a small remark which will be useful in the sequel.

Remark 2 For the particular case $F(r) = r^2$, noting that

$$L_\varepsilon(Y_t^\varepsilon(H))^2 = 2Y_t^\varepsilon(H)L_\varepsilon Y_t^\varepsilon(H) + L_\varepsilon(Y_t^\varepsilon(H))^2 - 2Y_t^\varepsilon(H)L_\varepsilon Y_t^\varepsilon(H) \tag{28}$$

and comparing with (24) as well as $\gamma_1^\varepsilon(t,H)$ and $\gamma_2^\varepsilon(t,H)$ defined in (27) and (26), respectively, we obtain that $R^\varepsilon(t,H) = 0$.

3 Closure of the Martingale

The main purpose of this note is to propose a strategy on how to close the martingales (22) and (23) with respect to the macroscopic quantity Y_t^ε. This is equivalent to determining the distribution of the limiting field using (24) and in particular its variance from expression (26).

To give an intuition why we will have to consider test functions with a certain type of boundary conditions, we first present an heuristic argument derived from the macroscopic PDE (17) with the boundary conditions given in (18). Therefore, we consider an order ε variation of the value of the density $\rho(1,t)$ at the boundary. Then Eq. (18) becomes:

$$\partial_r(\rho(r,t) + \varepsilon\xi(r,t))|_{r=1} = j(1 - ((\rho+\varepsilon\xi)(1,t))^K), \tag{29}$$

similarly at $r = -1$. The first order correction ξ should satisfy:

$$\partial_r\xi(r,t)|_{r=1} = -jK\rho(1,t)^{K-1}\xi(1,t). \tag{30}$$

On the other hand, in the bulk we have $\partial_t \xi(r,t) = \frac{1}{2}\partial^2_{rr}\xi(r,t)$ and by performing integration by parts against the test function H (depending on both space and time), we obtain:

$$\begin{aligned} -\xi\,\partial_t H = H\partial_t \xi &= H\tfrac{1}{2}\partial^2_{rr}\xi \\ &= \partial^2_{rr} H\tfrac{1}{2}\xi + \tfrac{1}{2}(H\partial_r\xi)|^1_{-1} - \tfrac{1}{2}(\partial_r H\xi)|^1_{-1} \\ &= \partial^2_{rr} H\tfrac{1}{2}\xi + \tfrac{1}{2}[-jK\rho(1,t)^{K-1}H(1,t) - \partial_r H(1,t)]\xi(1,t) + \cdots \end{aligned}$$

and similarly at the left boundary. Since the latter should be true for all ξ one should choose H such that

$$\partial_t H(r,t) = \tfrac{1}{2}\partial^2_{rr}H(r,t), \quad \partial_r H(1,t) = -jK\rho(1,t)^{K-1}H(1,t) \qquad \text{and}$$
$$\partial_r H(-1,t) = jK(1-\rho(-1,t))^{K-1}H(-1,t). \tag{31}$$

Motivated by the previous argument we are now in position to define what we believe that will be the proper space of test functions $\mathbb{S}$.

Definition 2 Fix a solution of the hydrodynamic equation $\rho(t,r)$ and let $\mathbb{S}$ denote the subspace of functions in $C^{1,2}([-1,1]\times[0,T])$ that satisfy

$$\begin{aligned} &\partial_r H(-1,t) = jK(1-\rho(-1,t))^{K-1}H(-1,t), \\ &\partial_r H(1,t) = jK\rho(1,t)^{K-1}H(1,t) \end{aligned} \tag{32}$$

for all $t \in [0,T]$.

Now, we are back to the microscopic level and our goal is to check whether the choice of the space of test functions defined above is the correct one or not. The first task now is to compute the compensator of the martingale defined in (21), which corresponds to γ_1 defined in (27). Since in the next calculations we want to pass from differences in η to differences in H we need to perform a (discrete) summation by parts which is summarized in the next two formulas:

$$\begin{aligned} \sum_{x=a+1}^{b-1} H(x)(u(x+1)-u(x)) &= H(b-1)u(b) - H(a+1)u(a+1) \\ &\quad - \sum_{x=a+2}^{b-1}(H(x)-H(x-1))u(x) \end{aligned} \tag{33}$$

$$\begin{aligned} \sum_{x=a+1}^{b-1} H(x)(u(x)-u(x-1)) &= H(b-1)u(b-1) - H(a+1)u(a) \\ &\quad - \sum_{x=a+2}^{b-1}(H(x)-H(x-1))u(x-1) \end{aligned} \tag{34}$$

in a discrete domain $\{a, a+1, \dots, b\}$. Above, just for ease of notation, we did not index the test function H in time. Thus, for the first term on the right hand side of (27), by the summation by parts formulas, we obtain:

$$\begin{aligned}\varepsilon^{-2} L_0 Y_t^\varepsilon(H) =& \sqrt{\varepsilon} \sum_{x=-N+1}^{N-1} H(\varepsilon x, t) \Delta_{\varepsilon,1} \eta_t(x) \\ &+ \frac{1}{2\sqrt{\varepsilon}} \nabla_\varepsilon^+ H(-1,t)\eta_t(-N) - \frac{1}{2\sqrt{\varepsilon}} \nabla_\varepsilon^- H(1,t)\eta_t(N), \end{aligned} \tag{35}$$

where

$$\begin{aligned}\varepsilon \nabla_\varepsilon^- H(1,t) &:= H(\varepsilon(N-1),t) - H(1,t), \\ \varepsilon \nabla_\varepsilon^+ H(-1,t) &:= H(\varepsilon(-N+1),t) - H(-1,t), \end{aligned} \tag{36}$$

i.e., for a smooth function H the quantities $\nabla_\varepsilon^\pm H$ are of order one in ε. We observe that the last term of (35) is "closed" with respect to Y_t^ε, but we also obtain the gradients of H evaluated at ± 1 with a diverging factor $\varepsilon^{-\frac{1}{2}}$. The purpose of this section is to suggest a strategy how to treat the latter. For simplicity and transparency of the key steps we perform the boundary calculations for the case $K = 2$, but the same strategy can be followed for the general K case.

In addition, for the generators acting at the boundary we have:

$$L_{b,+} Y_t^\varepsilon(H) = \frac{j}{2\sqrt{\varepsilon}} H(\varepsilon(N-1),t)(1-\eta_t(N-1))\eta_t(N) + \frac{j}{2\sqrt{\varepsilon}} H(1,t)(1-\eta_t(N)) \tag{37}$$

and

$$L_{b,-} Y_t^\varepsilon(H) = \frac{j}{2\sqrt{\varepsilon}} H(-\varepsilon(N-1),t)\eta_t(-N+1)(1-\eta_t(-N)) + \frac{j}{2\sqrt{\varepsilon}} H(-1,t)\eta_t(-N). \tag{38}$$

Putting together (35) and the two previous displays, we obtain that $L_\varepsilon Y_t^\varepsilon(H)$ equals to

$$\begin{aligned}&\frac{1}{2\sqrt{\varepsilon}} \nabla_\varepsilon^+ H(-1,t)\eta_t(-N) - \frac{1}{2\sqrt{\varepsilon}} \nabla_\varepsilon^- H(1,t)\eta_t(N) + \sqrt{\varepsilon} \sum_{x \in \Lambda_N} H(\varepsilon x, t) \Delta_{\varepsilon,1} \eta_t(x) \\ &+\sqrt{\varepsilon}\Big(\frac{j}{2} H(\varepsilon(N-1),t)(1-\eta_t(N-1))\eta_t(N) + \frac{j}{2} H(1,t)(1-\eta_t(N))\Big) \\ &+\sqrt{\varepsilon}\Big(\frac{j}{2} H(-\varepsilon(N-1),t)\eta_t(-N+1)(1-\eta_t(-N)) + \frac{j}{2} H(-1,t)\eta_t(-N)\Big). \end{aligned} \tag{39}$$

Also recall (5) and observe its contribution to (27). Next, we show how the combination of the above formulas together with an appropriate intuitive choice for the test functions H gives a martingale which is closed in terms of Y_t^ε. For the first,

since macroscopically the points $\varepsilon(N-1)$ and εN in the second line of (39) are the same, we can consider the test function evaluated at the same point $H(1,t)$ with a vanishing error of order ε (by performing a Taylor expansion on H). Then we observe the cancellation of the $\eta_t(N)$ term in the second line of (39). Note that a similar cancellation takes place in the derivation of the hydrodynamic limit for the general K case, where by adding the boundary contributions—denoted here by ρ—(i.e., considering them at the same site) we obtain:

$$\sum_{x=N-K+1}^{N}(1-\rho)\rho^{N-x} = (1-\rho)\rho^{K-1} + \cdots + (1-\rho)\rho + (1-\rho) = 1-\rho^K.$$

Note that the 1 cancels with the corresponding contribution from the third term of (27). Thus, we are left with the term $-\eta_t(N-1)\eta_t(N)$ on the second line of (39) (corresponding to $-\rho^2$ in the example just above for $K=2$) and the second term from (35). Both are at the boundary and we want to combine them in some way in order to get a martingale closed with respect to Y_t^ε. Note that the reasoning at the left boundary is completely analogous and we will not repeat it here. Thus, we need to get some information from the boundary conditions and the equation that these satisfy in the hydrodynamic equation. Furthermore, since we are looking at the fluctuations (rather than the hydrodynamic limit) maybe we should be looking at the linearized version of these conditions and mimic them at the microscopic level.

The heuristic argument presented in the beginning of this section suggests that we may match the second (diverging) term of (35) with some terms from (37) by "mimicking" the linearization (30). Following this reasoning, the first step is to use the same test function $H(\pm 1,t)$ in front of both terms, Then, in the same way of finding the order ε term of $(\rho+\varepsilon\xi)^2$ in (29) we write:

$$\begin{aligned}
\eta_t(N-1)\eta_t(N) &= \left\{\bar{\eta}_t(N-1)+\rho_t^\varepsilon(N-1)\right\}\left\{\bar{\eta}_t(N)+\rho_t^\varepsilon(N)\right\}\\
&= \bar{\eta}_t(N-1)\rho_t^\varepsilon(N)+\bar{\eta}_t(N)\rho_t^\varepsilon(N-1)\\
&\quad +\bar{\eta}_t(N-1)\bar{\eta}_t(N)+\rho_t^\varepsilon(N-1)\rho_t^\varepsilon(N)\\
&= 2\bar{\eta}_t(N)\rho_t^\varepsilon(N)\\
&\quad +[\bar{\eta}_t(N-1)-\bar{\eta}_t(N)]\rho_t^\varepsilon(N)+\bar{\eta}_t(N)(\rho_t^\varepsilon(N-1)-\rho_t^\varepsilon(N))\\
&\quad +\bar{\eta}_t(N-1)\bar{\eta}_t(N)+\rho_t^\varepsilon(N-1)\rho_t^\varepsilon(N)
\end{aligned} \tag{40}$$

It is also easy to check that

$$\mathbb{E}_\varepsilon[\bar{\eta}_t(N-1)\bar{\eta}_t(N)] = \mathbb{E}_\varepsilon[\eta_t(N-1)\eta_t(N)] - \rho_t^\varepsilon(N-1)\rho_t^\varepsilon(N). \tag{41}$$

Thus, considering the bulk with only the right boundary (the left is completely analogous), we obtain:

$$\gamma_1^\varepsilon(t,H) = -\frac{1}{2\sqrt{\varepsilon}}\nabla_\varepsilon^- H(1,t)\bar{\eta}_t(N) + Y_t^\varepsilon\Big(\frac{1}{2}\Delta_\varepsilon H\Big) + Y_t^\varepsilon(\partial_t H)$$
$$-\frac{j}{2\sqrt{\varepsilon}}H(1,t)\left\{\eta_t(N-1)\eta_t(N) - \mathbb{E}_\varepsilon[\eta_t(N-1)\eta_t(N)]\right\} + \cdots$$

where the second term in last line comes from the second term on the right hand side of (5). Above the dots represent the extra terms coming from the left boundary and

$$\Delta_\varepsilon H(\varepsilon x,t) = \varepsilon^{-2}\Big(H(\varepsilon(x+1),t) + H(\varepsilon(x-1),t) - 2H(\varepsilon x,t)\Big). \quad (42)$$

Therefore we have

$$\begin{aligned}\gamma_1^\varepsilon(t,H) &= Y_t^\varepsilon\Big(\frac{1}{2}\Delta_\varepsilon H\Big) + Y_t^\varepsilon(\partial_t H)\\ &\quad -\frac{1}{2\sqrt{\varepsilon}}\nabla_\varepsilon^- H(1,t)\bar{\eta}_t(N) - \frac{j}{2\sqrt{\varepsilon}}H(1,t)\Big\{2\bar{\eta}_t(N)\rho_t^\varepsilon(N)\\ &\quad +[\bar{\eta}_t(N-1) - \bar{\eta}_t(N)]\rho_t^\varepsilon(N) + \bar{\eta}_t(N)[\rho_t^\varepsilon(N-1) - \rho_t^\varepsilon(N)]\\ &\quad +\bar{\eta}_t(N-1)\bar{\eta}_t(N) + \rho_t^\varepsilon(N-1)\rho_t^\varepsilon(N) - \mathbb{E}_\varepsilon[\eta_t(N-1)\eta_t(N)]\Big\} + \cdots\\ &= Y_t^\varepsilon\Big(\frac{1}{2}\Delta_\varepsilon H\Big) + Y_t^\varepsilon(\partial_t H) \quad (43)\\ &\quad -\frac{1}{2\sqrt{\varepsilon}}\nabla_\varepsilon^- H(1,t)\bar{\eta}_t(N) - \frac{1}{2\sqrt{\varepsilon}}H(1,t)\Big\{2\bar{\eta}_t(N)\rho_t^\varepsilon(N)\\ &\quad +[\bar{\eta}_t(N-1) - \bar{\eta}_t(N)]\rho_t^\varepsilon(N) + \bar{\eta}_t(N)(\rho_t^\varepsilon(N-1) - \rho_t^\varepsilon(N))\\ &\quad +\bar{\eta}_t(N-1)\bar{\eta}_t(N) - \mathbb{E}_\varepsilon[\bar{\eta}_t(N-1)\bar{\eta}_t(N)]\Big\} + \cdots\end{aligned}$$

where $\mathbb{E}_\varepsilon[\bar{\eta}_t(N)] = 0$. In the last equality we used (41). The second line in last equality vanishes by the choice of test functions (31) and by approximating $\rho_t^\varepsilon(N)$ by $\rho(1,t)$ using (12) and the v-estimate for the one point correlation given in (10).

For the first term on the third line of the last equality of (43), we use the following estimate which holds for $x \in \Lambda_N \setminus \{N-1\}$ and $t \le \tau \log \varepsilon^{-1}$:

$$\mathbb{E}_{\mu_\varepsilon}\Big[\Big(\int_0^t (\bar{\eta}_s(x) - \bar{\eta}_s(x+1))\,ds\Big)^2\Big] \le C\varepsilon^{1+a}, \quad (44)$$

for some $a > 0$ and $C > 0$. This estimate will be proved in the subsequent work [2]. For the second term on the third line in the last equality of (43), we recall Lemma 1, so that

$$\mathbb{E}\Big[\Big(\int_0^t \frac{j}{2\sqrt{\varepsilon}}H(1,s)\bar{\eta}_s(N)(\rho_s^\varepsilon(N-1) - \rho_s^\varepsilon(N))ds\Big)^2\Big]$$
$$= \frac{j^2}{2\varepsilon}\mathbb{E}\Big[\int_0^t\int_0^s H(1,s)H(1,r)\bar{\eta}_s(N)\bar{\eta}_r(N)(\rho_s^\varepsilon(N-1) - \rho_s^\varepsilon(N))(\rho_r^\varepsilon(N-1) - \rho_r^\varepsilon(N))dr\,ds\Big]$$

$$\leq C\varepsilon^{-1}\int_0^t\int_0^s(\rho_s^\varepsilon(N-1)-\rho_s^\varepsilon(N))(\rho_r^\varepsilon(N-1)-\rho_r^\varepsilon(N))dr\,ds$$
$$\leq C\varepsilon^{-1}\int_0^t\int_0^s\frac{1}{(\varepsilon^{-2}s)^{1/2-\zeta}}\frac{1}{(\varepsilon^{-2}r)^{1/2-\zeta}}\,dr\,ds\leq C\varepsilon^{1-4\zeta}(\tau\log\varepsilon^{-1})^{1+2\zeta}$$

where we use that $\mathbb{E}\Big[\bar{\eta}_s(N)\bar{\eta}_r(N)\Big]$ is bounded by 1. Last display vanishes as $\varepsilon\to 0$ for any choice of $0<\zeta<\frac{1}{4}$. For the fourth line we use the following inequality which holds for any subset $X\subset\Lambda_N$:

$$\mathbb{E}_{\mu_\varepsilon}\left[\left(\int_0^t\prod_{x\in X}\bar{\eta}_s(x)\,ds\right)^2\right]\leq C\varepsilon^{1+a},\tag{45}$$

for some $a>0$ and $C>0$, which will be proved in a subsequent work [2]. These arguments show that (22) can be rewritten as

$$M_t^\varepsilon(H):=Y_t^\varepsilon(H)-Y_0^\varepsilon(H)-\int_0^t(Y_s^\varepsilon(\tfrac{1}{2}\Delta_\varepsilon H)+Y_s^\varepsilon(\partial_s H))ds,$$

plus terms that vanish in L^2, as $\varepsilon\to 0$.

Analogously and by repeating similar computations to the ones above, we see that for (26) we obtain

$$\gamma_2^\varepsilon(t,H)=\varepsilon\sum_{x=-N}^{N}(\nabla_\varepsilon^+H(\varepsilon x,t))^2(\eta_t(x)-\eta_t(x+1))^2+$$
$$+\frac{j}{2}\sum_{x=N-K+1}^{N}H(\varepsilon x,t)^2D_+\eta_t(x)+\frac{j}{2}\sum_{x=-N}^{-N+K-1}H(\varepsilon x,t)^2D_-\eta_t(x),$$

where

$$\varepsilon\nabla_\varepsilon^+H(\varepsilon x,t):=H(\varepsilon(x+1),t)-H(\varepsilon x,t).$$

We observe that all terms in $\gamma_2^\varepsilon(t,H)$ survive in the limit $\varepsilon\to 0$. Recalling Remark 2, the second moment becomes:

$$L_\varepsilon(Y_t^\varepsilon(H))^2=2Y_t^\varepsilon(H)\gamma_1^\varepsilon(t,H)+\gamma_2^\varepsilon(t,H)+R^\varepsilon(t,H)\tag{46}$$
$$=2Y_t^\varepsilon(H)Y_t^\varepsilon(\frac{1}{2}\Delta_\varepsilon H)+\gamma_2^\varepsilon(t,H)+o_\varepsilon(1).\tag{47}$$

We note that the contribution of the boundary terms has been registered in the choice of the test functions H as well as in $\gamma_2^\varepsilon(t,H)$ in a "closed" form. Thus, in the next section we will be looking for the limiting field as $\varepsilon\to 0$ of Y_t^ε for an appropriate choice of test function space satisfying (31).

4 Macroscopic Limit of the Fluctuation Field

The purpose of this section is to find an equation for the continuous kernel of the variance of the limiting fluctuation field. This will also motivate another way of "guessing" the appropriate test function space alternative to the one of the previous section, but of the same flavour. The strategy is as follows. Let us assume for a moment that the limiting fluctuation field exists. Its variance should coincide with the limit as $\varepsilon \to 0$ of $\mathbb{E}_\varepsilon[Y_t^\varepsilon(H)^2]$. We can compute the latter in two ways: either directly or using the martingale decomposition (24) by computing γ_1 and γ_2 separately. Note that the difference between the two approaches lies on the fact that in the former some cancellations take place making disappear the "dangerous" diverging terms in γ_1. Instead, for the latter, in order to control the dangerous terms, one has to choose a proper test function space and then apply the Holley-Stroock theory [11] obtaining a martingale for the limiting field from which an equation for the kernel follows. Summarizing, we notice that in the second approach the catch lies in the fact that using the martingale decomposition we have to obtain closed forms and for that an assumption for the test functions is in order.

In the previous section this choice was motivated by the linearization argument and it will be used here for the derivation of the macroscopic equation for the kernel. Then, we will further validate it by a comparison to the direct calculation of $\mathbb{E}_\varepsilon[Y_t^\varepsilon(H)^2]$ since a term-by-term correspondence can be established. Moreover, the latter could also serve as an alternative (to the linearization) way of determining the test functions.

4.1 Direct Calculation of the Variance

We have:

$$\begin{aligned}\partial_t \mathbb{E}_\varepsilon[Y_t^\varepsilon(H)^2] = \varepsilon \sum_{x\neq y} H(\varepsilon x)H(\varepsilon y)\partial_t \mathbb{E}_\varepsilon[\bar{\eta}_t(x)\bar{\eta}_t(y)] \\ +2\varepsilon \sum_{x\neq y} \partial_t H(\varepsilon x)H(\varepsilon y)\mathbb{E}_\varepsilon[\bar{\eta}_t(x)\bar{\eta}_t(y)] \\ +\varepsilon \sum_{x} H(\varepsilon x)^2(1-2\rho_t^\varepsilon(x))\partial_t \rho_t^\varepsilon(x) \\ +2\varepsilon \sum_{x} H(\varepsilon x)\partial_t H(\varepsilon x)(1-(\rho_t^\varepsilon(x))^2). \qquad (48)\end{aligned}$$

Recalling (20), the factor $\partial_t \mathbb{E}_\varepsilon[\bar{\eta}_t(x)\bar{\eta}_t(y)]$ for $x \neq y$ and $K = 2$ yields:

$$\begin{aligned}\partial_t C_t^{2,\varepsilon}(x,y) &= \mathbf{1}_{-N\le x,y\le N}\frac{1}{2}\Delta_{\varepsilon,2}C_t^{2,\varepsilon}(x,y) - \varepsilon^{-2}\mathbf{1}_{|x-y|=1}\frac{1}{2}(\rho_t^\varepsilon(x)-\rho_t^\varepsilon(y))^2\\ &+\varepsilon^{-1}\frac{j}{2}\mathbf{1}_{x=N-1,y=N}\left[-C_t^{2,\varepsilon}(N-1,N)(2-\rho_t^\varepsilon(N))\right.\\ &\left.+(1-\rho_t^\varepsilon(N-1))\rho_t^\varepsilon(N)(1-\rho_t^\varepsilon(N))\right]\\ &+\varepsilon^{-1}\frac{j}{2}\mathbf{1}_{y=N-1}\left[(1-\rho_t^\varepsilon(N-1))C_t^{2,\varepsilon}(x,N)-\rho_t^\varepsilon(N)C_t^{2,\varepsilon}(x,N-1)\right.\\ &\left.-C_t^{3,\varepsilon}(x,N-1,N)\right]\\ &+\varepsilon^{-1}\frac{j}{2}\mathbf{1}_{y=N}\left[-C_t^{2,\varepsilon}(x,N)\right]\\ &+\cdots \end{aligned} \tag{49}$$

where the ... stand for the corresponding terms at the left boundary. Moreover, by $\Delta_{\varepsilon,2}$ we denote the discrete Laplacian acting on both entries of $C_t^{2,\varepsilon}$, namely for $-N+1\le x,y\le N-1$ we have:

$$\begin{aligned}\Delta_{\varepsilon,2}C^{2,\varepsilon}(x,y) =&\varepsilon^{-2}\Big(C^{2,\varepsilon}(x+1,y)+C^{2,\varepsilon}(x-1,y)+C^{2,\varepsilon}(x,y+1)\\ &+C^{2,\varepsilon}(x,y+1)-4C^{2,\varepsilon}(x,y)\Big),\end{aligned} \tag{50}$$

while for $x=-N,N$, we have

$$\Delta_{\varepsilon,2}C^{2,\varepsilon}(N,y) = \varepsilon^{-2}\Big(C^{2,\varepsilon}(N-1,y)-C^{2,\varepsilon}(N,y)\Big) \tag{51}$$

$$\Delta_{\varepsilon,2}C^{2,\varepsilon}(-N,y) = \varepsilon^{-2}\Big(C^{2,\varepsilon}(-N+1,y)-C^{2,\varepsilon}(-N,y)\Big). \tag{52}$$

Note that $\Delta_{\varepsilon,2}C^{2,\varepsilon}(x,N)$ and $\Delta_{\varepsilon,2}C^{2,\varepsilon}(x,-N)$ are defined analogously. Similarly, for the second term of (48) we have:

$$\begin{aligned}\partial_t\rho_t^\varepsilon(x) = \mathbb{E}_\varepsilon[L_\varepsilon\eta_t(x)] = \mathbf{1}_{-N+1\le x\le N-1}&\frac{1}{2}\Delta_{\varepsilon,1}\rho_t^\varepsilon(x)-\frac{1}{2}\Delta_{\varepsilon,1}\rho_t^\varepsilon(N)\\ &+\frac{j}{2}\mathbf{1}_{x=N-1}\left[\rho_t^\varepsilon(N)(1-\rho_t^\varepsilon(N-1))(1-2\rho_t^\varepsilon(N))\right.\\ &\left.-(1-2\rho_t^\varepsilon(N-1))C_t^{2,\varepsilon}(N-1,N)\right]\\ &+\frac{j}{2}\mathbf{1}_{x=N}\left[(1-2\rho_t^\varepsilon(N))(1-\rho_t^\varepsilon(N))\right]\\ &+\cdots\end{aligned} \tag{53}$$

and similarly at the left boundary. We remark that the previous display is exactly (5) but now it is written with respect to the correlation function. Based on the correlation function estimates (still to be established in [2]), we expect that the higher order correlation $C_t^{3,\varepsilon}(x,N-1,N)$ is of lower order in ε with respect to the one and the two point correlations. As mentioned before, at this point one option would be to

pass to the limit $\varepsilon \to 0$ and obtain an equation for the kernel of the variance of the limiting field (without need of introducing the martingales). But since our purpose is to see how to work with the martingales, we keep Eq. (49) at finite ε and we will use it later for comparison. Hence, in the next subsection we pass to the limit $\varepsilon \to 0$ in the context of the Holley-Stroock theory [11] using the martingale decomposition and the choice of the test functions motivated by the linearization argument given in the beginning of Sect. 3. Alternatively, we observe that the same choice of test functions is dictated by the comparison with Eq. (49) given in this subsection.

4.2 Continuous Kernel Variance Using Martingales

To pass to the limit for the fluctuation field, we follow the strategy presented in [3]. One needs the following ingredients:

1. The process at time 0, $\{Y_0^\varepsilon\}_{\varepsilon>0}$ converges as $\varepsilon \to 0$ to a mean-zero Gaussian field Y with some covariance kernel.
2. The sequence $Y^\varepsilon \equiv \{Y_t^\varepsilon(H),\ t \geq 0,\ H \in \mathbb{S}\}$ is tight in $\mathscr{D}([0,T], \mathbb{S}')$.
3. Any limiting point Y of Y^ε satisfies the martingale problem: for any $F \in C^\infty([-1,1])$ and for any $H \in \mathbb{S}$:

$$F(Y_t(H)) - \int_0^t F'(Y_s(H))(Y_s(AH) + Y_s(\partial_s H)) - ds \int_0^t \frac{1}{2}\|B_s H\|^2_{L^2(\rho_s)} F''(Y_s(H))\, ds \tag{54}$$

is a martingale for a choice of the operators A and B_s and the norm $L^2(\rho_s)$ is defined below. Based on the decomposition (24) as well as $\gamma_1^\varepsilon(t, H)$ and $\gamma_2^\varepsilon(t, H)$ defined in (27) and (26), respectively, the operators A and B_s in the above formulation will be given by:

$$A := \frac{1}{2}\Delta \quad \text{and} \quad B_s := \sqrt{\chi(\rho_s)}\nabla, \tag{55}$$

where $\Delta H(r) = \partial^2_{rr} H(r)$ and $\nabla H(r) = \partial_r H(r)$. For $s > 0$ and $H \in \mathbb{S}$

$$\|B_s H\|^2_{L^2(\rho_s)} = \frac{j}{2}(H(-1,s))^2(1-(1-\rho(-1,s))^K) + \frac{j}{2}(H(1,s))^2(1-\rho(1,s)^K) + \int_{-1}^1 (\nabla H(r,s))^2 \chi(\rho(r,s))\, dr \tag{56}$$

where $\chi(\rho(r,s)) = \rho(r,s)(1-\rho(r,s))$ with $\rho(r,t)$ being the solution of the hydrodynamic equation given in Sect. 2.2.

Suppose for a moment that we have tightness, which will be proved using correlation estimates in [2]. From the arguments derived in the previous sections and if we assume that $\{Y_0^\varepsilon\}_\varepsilon$ converges, as $\varepsilon \to 0$, to a mean-zero Gaussian field Y_0,

then, the limit field, obtained by taking $\varepsilon \to 0$ in a proper topology, is a generalized Ornstein–Uhlenbeck (O.U.) process, which is the formal solution of the equation:

$$\partial_t Y_t = AY_t dt + \sqrt{\chi(\rho_t)}\nabla W_t\,, \tag{57}$$

where W_t is a space-time white noise of unit variance.

Following the previous section one sees that the time integral of $\gamma_2^\varepsilon(s, H)$ converges in mean to $\int_0^t \frac{1}{2}\|B_s H\|^2_{L^2(\rho_s)}\, ds$ and the time integral of $\gamma_1^\varepsilon(s, H)$ converges in L^2 to $\int_0^t Y_s(AH)+Y_s(\partial_s H)\, ds$ under some assumption on the space of test functions. The latter was based on a linearization argument but here, the choice of test functions can be derived by comparing to the direct calculation of the previous subsection as we show next.

Definition 3 We define the variance kernel $C_t^*(r, r')$ by the relation

$$\mathbb{E}[Y_t(H)Y_t(G)] = \int_{-1}^1 \int_{-1}^1 H(r)G(r')C_t^*(r, r')dr dr' \tag{58}$$

for any H, G test functions and where $\mathbb{E}$ is the expectation with respect to the law of the limiting process Y_t.

Since $Y = \{Y_t(H) : t \geq 0,\ H \in \mathbb{S}\}$ satisfies the martingale problem given in (54), choosing $F(r) = r^2$ and taking the expected value we obtain:

$$\mathbb{E}[Y_t(H)Y_t(H)] = \int_0^t ds\, 2\mathbb{E}[Y_s(H)Y_s(AH)+Y_s(H)Y_s(\partial_s H)] + \int_0^t ds \|B_s H\|^2_{L^2(\rho_s)}. \tag{59}$$

By substituting the expression from Definition 3, we obtain the following equation for the kernel variance $C_t^*(r, r')$:

$$\begin{aligned}\int_{-1}^1 \int_{-1}^1 H(r,t)H(r',t)C_t^*(r,r')\,dr\,dr' &= \int_0^t \int_{-1}^1 \int_{-1}^1 \partial^2_{rr} H(r,s)H(r',s)C_s^*(r,r')\,dr\,dr'\,ds \\ &+2\int_0^t \int_{-1}^1 \int_{-1}^1 H(r,s)\partial_s H(r',s)C_s^*(r,r')\,dr\,dr'\,ds \\ &+\int_0^t \int_{-1}^1 (\partial_r H(r,s))^2 \chi(\rho(r,s))dr\,ds + \frac{j}{2}\int_0^t H(1,s)^2(1-\rho(1,s)^K)\,ds \\ &+\frac{j}{2}\int_0^t H(-1,s)^2(1-(1-\rho(-1,s))^K)\,ds.\end{aligned} \tag{60}$$

Note that for the above expression we have used so far only the bulk part of operator A as well as the operator B_s which is closed, so no closure issues arised. But now, the boundary conditions come into play as we need to perform integration by parts in order to obtain an equation for the kernel. It will be also useful to split the kernel variance in the following way: for any $t \geq 0$ and $r, r' \in (-1, 1)$

$$C_t^*(r,r') = C_t(r,r') + \delta(r,r')\chi(\rho(r,t)), \tag{61}$$

where we introduced the new kernel $C_t(r,r')$. The calculation leading to the equation for $C_t(r,r')$ is summarized in the next lemma.

Lemma 2 *Let $H \in \mathbb{S}$. The kernel $C_t(r,r')$ defined in (61) satisfies the following equation:*

$$\begin{aligned}
&\int_{-1}^{1}\int_{-1}^{1} H(r,t)H(r',t)\partial_t C_t(r,r')\,dr\,dr' = \int_{-1}^{1}\int_{-1}^{1} H(r,t)H(r',t)\partial_{rr}^2 C_t(r,r')\,dr\,dr' \\
&-\int_{-1}^{1}(H(r,t))^2(\partial_r\rho(r,t))^2\,dr \\
&-Kj\rho(1,t)^{K-1}H(1,t)\int_{-1}^{1}H(r,t)C_t(1,r)\,dr \\
&-Kj(1-\rho(-1,t))^{K-1}H(-1,t)\int_{-1}^{1}H(r,t)C_t(-1,r)\,dr \\
&-\int_{-1}^{1}H(r,t)H(1,t)\partial_r C_t(1,r)dr + \int_{-1}^{1}H(r,t)H(-1,t)\partial_r C_t(-1,r)\,dr \\
&+j(H(1,t))^2\left[\rho(1,t)(1-\rho(1,t)^K) - K\rho(1,t)^K(1-\rho(1,t))\right] \\
&+j(H(-1,t))^2\left[(1-(1-\rho(-1,t))^K)(1-\rho(-1,t)) - K(1-\rho(-1,t))^K\rho(-1,t)\right].
\end{aligned}$$

Proof We first substitute (61) into (60) and perform integration by parts. For the first term we have

$$\begin{aligned}
&\int_{-1}^{1}\int_{-1}^{1}\partial_{rr}^2 H(r,t)H(r',t)C_t(r,r')\,dr\,dr' = \int_{-1}^{1}\int_{-1}^{1}H(r,t)H(r',t)\partial_{rr}^2 C_t(r,r')\,dr\,dr' \\
&-\int_{-1}^{1}H(1,t)H(r',t)\partial_r C_t(1,r')\,dr' + \int_{-1}^{1}H(-1,t)H(r',t)\partial_r C_t(-1,r')\,dr' \\
&+\int_{-1}^{1}\partial_r H(1,t)H(r',t)C_t(1,r')\,dr' - \int_{-1}^{1}\partial_r H(-1,t)H(r',t)C_t(-1,r')\,dr',
\end{aligned}$$

where $\partial_r C_t(1,r')$ is the derivative with respect to the first entry and then evaluated at $r=1$. For the third term,

$$\begin{aligned}
\int_{-1}^{1}(\partial_r H(r,t))^2\chi(\rho(r,t))dr &= \frac{1}{2}\int_{-1}^{1}(H(r,t))^2\partial_{rr}^2(\chi(\rho(r,t)))dr \\
&-\int_{-1}^{1}H(r,t)\partial_{rr}^2 H(r,t)\chi(\rho(r,t))dr - \frac{1}{2}(H(1,t))^2(1-2\rho(1,t))\partial_r\rho(1,t) \\
&+\frac{1}{2}(H(-1,t))^2(1-2\rho(-1,t))\partial_r\rho(-1,t) \\
&+H(1,t)\partial_r H(1,t)\chi(\rho(1,t)) - H(-1,t)\partial_r H(-1,t)\chi(\rho(-1,t)).
\end{aligned}$$

In the above formula the second term of the right hand side cancels when we go from C_t^* to C_t. Furthermore, the first term can be written as

$$\frac{1}{2}\int_{-1}^{1}(H(r,t))^2\partial_{rr}^2(\chi(\rho(r,t)))dr = -\int_{-1}^{1}(H(r,t))^2(\partial_r\rho(r,t))^2dr + \frac{1}{2}\int_{-1}^{1}(H(r,t))^2(1-2\rho(r,t))\partial_{rr}^2\rho(r,t)dr.$$

Substituting to (60) we obtain:

$$\begin{aligned}
&\int_{-1}^{1}\int_{-1}^{1}H(r,t)H(r',t)\partial_t C_t^*(r,r')\,dr\,dr' + 2\int_{-1}^{1}\int_{-1}^{1}H(r,t)\partial_t H(r',t)C_t^*(r,r')dr\,dr' \\
&= \int_{-1}^{1}\int_{-1}^{1}H(r,t)H(r',t)\partial_{rr}^2 C_t(r,r')drdr' \\
&\quad -\int_{-1}^{1}H(1,t)H(u,t)\partial_r C_t(1,u)du + \int_{-1}^{1}H(-1,t)H(u,t)\partial_r C_t(-1,u)du \\
&\quad +\int_{-1}^{1}\partial_r H(1,t)H(u,t)C_t(1,u)du - \int_{-1}^{1}\partial_r H(-1,t)H(u,t)C_t(-1,u)du \\
&\quad -\int_{-1}^{1}(H(r,t))^2(\partial_r\rho(r,t))^2dr + \frac{1}{2}\int_{-1}^{1}(H(r,t))^2(1-2\rho(r,t))\partial_{rr}^2\rho(r,t)dr \\
&\quad -\frac{1}{2}(H(1,t))^2(1-2\rho_t(1))\partial_r\rho(1,t) + \frac{1}{2}(H(-1,t))^2(1-2\rho(-1,t))\partial_r\rho(-1,t) \\
&\quad +H(1,t)\partial_r H(1,t)\chi(\rho(1,t)) - H(-1,t)\partial_r H(-1,t)\chi(\rho(-1,t)) \\
&\quad +\frac{j}{2}(H(1,t))^2(1-\rho(1,t)^K) + \frac{j}{2}(1-(1-\rho(-1,t))^K)(H(-1))^2 \\
&\quad +2\int_{-1}^{1}\int_{-1}^{1}H(r,t)\partial_t H(r',t)C_t(r,r')dr\,dr' + 2\int_{-1}^{1}H(r,t)\partial_t H(r)\chi(\rho(r,t)). \qquad (62)
\end{aligned}$$

Note that the second term of the left hand side cancels with the last line of the right hand side. Moreover, the first term of the left hand side combined with the second term of the fifth line gives

$$\int_{-1}^{1}\int_{-1}^{1}H(r,t)H(r',t)\partial_t C_t(r,r')drdr'.$$

Then we can conclude by using the choice of test functions H given in (31).

Alternatively, we observe that it is easy to establish the connection between the last expression and formulas (49) and (53) of the direct calculation of the variance and as a result obtain the same choice of test functions as in (31). For example, the first term of the fourth line of (62) corresponds to the terms of the fourth and sixth line of (49) and similar arguments hold for the other terms. As a result, one obtains a condition for $\partial_r H(1,t)$ which agrees with (31). □

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References

1. R. Baldasso, O. Menezes, A. Neumann, R. Souza, Exclusion process with slow boundary. J. Stat. Phys. **167**, 1112–1142 (2017)
2. P. Birmpa, P. Gonçalves, D. Tsagkarogiannis, In preparation
3. A. De Masi, P. Presutti, E. Scacciatelli, The weakly asymmetric simple exclusion process. Ann. de l'I.H.P. B. **25**(1), 1–38 (1989)
4. A. De Masi, E. Presutti, D. Tsagkarogiannis, M.E. Vares, Current reservoirs in the simple exclusion process. J. Stat. Phys. **144**, 1151–1170 (2011)
5. A. De Masi, E. Presutti, D. Tsagkarogiannis, M.E. Vares, Truncated correlations in the stirring process with births and deaths. Electron. J. Probab. **17**(6), 1–35 (2012)
6. C. Erignoux, P. Gonçalves, G. Nahum, Hydrodynamics for SSEP with non-reversible slow boundary dynamics: Part I, the critical regime and beyond. J. Stat. Phys. **181**(4), 1433–1469 (2020)
7. C. Erignoux, P. Gonçalves, G. Nahum, Hydrodynamics for SSEP with non-reversible slow boundary dynamics: Part II, the critical regime and beyond ALEA. Lat. Am. J. Probab. Math. Stat. 17, 791–823 (2020). http://alea.impa.br/articles/v17/17-31.pdf
8. T. Franco, P. Gonçalves, A. Neumann, Non-equilibrium and stationary fluctuations for a slowed boundary symmetric exclusion process. Stoch. Proc. Appl. **129**(4), 1413–1442 (2019)
9. P. Gonçalves, M. Jara, A. Neumann, O. Menezes, Non-equilibrium and stationary fluctuations for a slowed boundary symmetric exclusion. Stoch. Proc. Appl. **130**(7), 4326–4357 (2020)
10. M.Z. Guo, G.C. Papanicolaou, S.R.S. Varadhan, Nonlinear diffusion limit for a system with nearest neighbor interactions. Commun. Math. Phys. **118**, 31–59 (1988)
11. R. Holley, D. Stroock, Generalized Ornstein-Uhlenbeck processes and infinite particle branching Brownian motions. Publ. Res. Inst. Math. Sci. **14**(3), 741–788 (1978)
12. C. Landim, A. Milanes, S. Olla, Stationary and nonequilibrium fluctuations in boundary driven exclusion processes. Markov Proc. Rel. Fields **14**(2), 165–184 (2008)

On Existence, Uniqueness and Banach Space Regularity for Solutions of Boltzmann Equations Systems for Monatomic Gas Mixtures

Erica de la Canal, Irene M. Gamba, and Milana Pavić-Čolić

Abstract This review manuscript reports on two recent results for a time dynamics model for a non-linear system of Boltzmann equations in a space homogeneous setting that describes multi-component monatomic gas mixtures for binary interactions. This model describes the evolution of an arbitrary finite set of probability density functions, depending on time and molecular velocity in $\mathbb{R}^N$, corresponding to each gas component described by its mass parameter. The existence and uniqueness of the initial value problem of the vector-valued solution associated to the mixture in the case of hard potentials with integrable angular scattering kernels corresponding to each pair of interacting species is addressed. This result is obtained by means of an abstract ODE theory in Banach spaces localized in the molecular velocity state. It relies on a lower bound of the collision frequency as much as on an energy identity for gas mixtures that enables a new angular averaging (Povzner) lemma associated to the vector of collisional integrals. Moreover, for collisional transition probability rate given by hard potentials with integrable angular part, the unique vector-valued solution $L^1(\mathbb{R}^N)$ polynomially and exponentially weighted norm is generated and propagated. Further, by means of a Carleman representation for the collision operator associated to the binary mixing of two components, $L^p(\mathbb{R}^N)$ weighted norms are propagated with polynomial and/or exponential weights, $p \in (1, \infty]$. These results are obtained by gain of integrability $L^p(\mathbb{R}^N)$ estimates for the multi-species collision operator.

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1 Introduction

This manuscript reviews the recent progress in the theory for monatomic gas mixtures modeled by time dynamical system of Boltzmann equations for binary molecular interactions associated to identical spherical molecules with a finite number of different masses in the space homogeneous setting. This presentation will simply merge the work on existence and uniqueness theory from [14] of global in time vector-valued probability density function solution, showing the propagation and generation of polynomial and exponential weighted norm bounds in $L^1(\mathbb{R}^3)$ Banach spaces in molecular velocity; and recently extended to $L^1(\mathbb{R}^N)$, $N \geq 3$, as well as the complete global in time theory of propagation of $L^p(\mathbb{R}^N)$, $N \geq 3$ norms, both in [12], for a system of Boltzmann equations in a unified frame. Hence, this manuscript will state and connect results of these two manuscripts in a review presentation, without including rigorous proofs presented in [12, 14]. For a self-contained narrative, we start with a full introduction presenting the system model.

Kinetic theory for monatomic gas mixtures in a space homogeneous setting describes each mixture component $\mathscr{A}_i$, $i = 1, \ldots, I$, with its own distribution function $f_i := f_i(t, v)$, that depends on time $t \geq 0$ and velocity of molecules $v \in \mathbb{R}^N$. Each particle density function f_i changes due to binary collisions with other particles. In the mixture framework, these particles interactions can belong to the same species $\mathscr{A}_i$ or a pair of different one $\mathscr{A}_j$, $j \neq i$ when a particle from species $\mathscr{A}_i$ collide with another particle from $\mathscr{A}_j$, for some $j \neq i$. Thus, the collision operator needs to take into account the influence of all species $\mathscr{A}_j$ for all $j = 1, \ldots, I$, to the fixed one, $\mathscr{A}_i$. In other words, the measure of change of distribution function f_i is a sum $\sum_{j=1}^{I} Q_{ij}(f_i, f_j)$, where the pair-wise collision operator $Q_{ij}(f_i, f_j)$ describes influence of $\mathscr{A}_j$ on $\mathscr{A}_i$.

Considering all species simultaneously, a vector-valued problem is described by a set of both distribution functions and collision operators,

$$\mathbb{F} := [f_i]_{1 \leq i \leq I}, \quad \mathbb{Q}(\mathbb{F}, \mathbb{F}) = \left[\sum_{j=1}^{I} Q_{ij}(f_i, f_j) \right]_{1 \leq i \leq I}. \tag{1}$$

Then in a space homogeneous setting, the system of Boltzmann equations describing a monatomic gas mixture reads

$$\partial_t \mathbb{F}(t, v) = \mathbb{Q}(\mathbb{F}, \mathbb{F})(t, v). \tag{2}$$

Reference [14] shows global in time existence and uniqueness of solutions $\mathscr{C}([0,\infty),\Omega)\cap\mathscr{C}^1\left((0,\infty),L^1_2\right)$, where the set Ω, to be defined in (42), is a subset of a vector-valued Banach space with a norm depending on the species mass fractions, for the initial value problem associated to system (2) . These results may be obtained by following a general ODE theory in Banach spaces and relies on a stability condition, depending on the first few moments of the initial data as well as the transition probability rate parameters, that secures the existence of a unique global in time solution, without imposing initial entropy boundedness. These techniques were inspired by the work in [6] for the scalar classical N-dimensional Boltzmann equation for elastic binary interactions in integrable angular transition, and hard potentials or Maxwell type of interactions. This approach to existence may be view as a revision from the notes in [11], where the ODE on Banach spaces approach is proposed as a main tool to tackle the Cauchy problem for hard spheres in three dimensions with constant angular transition rate and for which the work by [6], as much as related ones by [1, 7], provide complete proof that the sub-tangency condition is fulfilled by the Boltzmann flow.

The path to obtain these results, i.e. the existence and uniqueness of the vector-valued solution $\mathbb{F}$ to the initial valued problem for the Boltzmann system (2), have recently been extended to vector valued in Banach spaces in $L^1(\mathbb{R}^N)$. Their analysis involve the development of global in time propagation and generation of $L^1(\mathbb{R}^N)$ polynomial as much as exponential weighted norms. It is based, on one hand, on a lower bound of the sum collision frequencies that depends on the Lebesgue bracket associated to a fixed species with order $\bar{\gamma}$ defined by the minimum of all potential rates of the binary system mixture. On the other hand, it relies on an energy identity for gas mixtures that enables a new angular averaging (Povzner) lemma associated to the system of collisional integrals, showing the emergence of a constant, smaller than unity, depending on the Lebesgue bracket order decaying to zero for any higher order. These results were presented first in [14] for $\mathbb{R}^3$, and extended to $\mathbb{R}^N$ in [12], where relevant estimates taking into the account the extension to the N-dimensional account are developed. These two estimates yield sufficient control for the evolution of polynomially weighted $L^1(\mathbb{R}^N)$ estimates of the collisional integral system, referred to as moments estimates. They show positive contributions from collectively the moments of the mixture gain collision term expressed in binary sums forms that are dominated in moment order by the negative contribution from the loss collision term. Moreover, the unique vector-valued solution propagates and generates $L^1(\mathbb{R}^N)$ polynomially weighted (Lebesgue bracket) norms of order $k > k_*$, whose bounds depend on specific conditions on the collision transition probabilities to be specified in this manuscript.

In addition, the authors rigorously studied propagation of polynomially and exponentially weighted L^p norms, for the extended range of $p \in (1,\infty]$ in [12]. These results rely on a new explicit Carleman integral representation for the positive contribution associated to each binary collisional operator, referred by the gain operator $Q^+_{ij}(f_i, f_j)$, $1 \le i, j \le I$. By means of this new representation, a gain of integrability estimate for each $Q^+_{ij}(f_i, f_j)$ can be obtained first, by the control of the weighted

L^p norm of $Q_{ij}^+(f_i, f_j)$ by a sublinear weighted L^p norm of the input function, say f_i . Then, such estimate is invoked in the propagation of L^p norms, with both polynomial and exponential weights, provided that a control of the negative part of the collisional form, denoted by $Q_{ij}^-(f_i, f_j)$, by a linear form of weighted L^p norm for the same input function f_i holds, depending on the integrability properties of the angular transition function and the intramolecular potential rates as will be described in these pages. More precisely, in this review we look at the at the weighted integrability properties which strongly depends on the transition probability rates (also called collision kernels in the classical elastic setting for single monoatomic elastic gasses) associated to binary molecular interactions. For a complete and comprehensive list of references, readers can look at manuscripts [12, 14].

2 Kinetic Model

The kinetic model is first described along with the notation used throughout this manuscript.

2.1 Collision Process

A binary collision law is obtained by fixing a pair of interacting particles, each in $\mathbb{R}^N$, one of species $\mathscr{A}_i$ having mass m_i and pre-collisional velocity v' and the other one belonging to the species $\mathscr{A}_j$, with mass m_j and velocity v'_*; producing a pair of post-collisional velocities v and v_* respectively. When interactions are assumed elastic, then the momentum and kinetic energy of the two interacting molecular velocities pairs are conserved, that is

$$m_i v' + m_j v'_* = m_i v + m_j v_* \tag{3}$$

$$m_i |v'|^2 + m_j |v'_*|^2 = m_i |v|^2 + m_j |v_*|^2. \tag{4}$$

If the center-of-mass velocity V_{ij} and the relative velocity u both in $\mathbb{R}^N$ are introduced by

$$V_{ij} = \frac{m_i}{m_i + m_j} v + \frac{m_i}{m_i + m_j} v_*, \quad u = v - v_*,$$

then conservation laws (3) during collision process are equivalent to

$$V'_{ij} = V_{ij}, \quad |u'| = |u| . \tag{5}$$

As done in the case of a single gas, these equations can be parameterized with the vector-parameter $\sigma \in \mathbb{S}^{N-1}$, so that

$$u' = |u|\,\sigma.$$

Now pre-collisional velocities can be written in terms of post-collisional ones as

$$v' = V_{ij} + \frac{m_j}{m_i + m_j}\,|u|\,\sigma, \quad v'_* = V_{ij} - \frac{m_i}{m_i + m_j}\,|u|\,\sigma. \tag{6}$$

Thus, introducing the parameter $r_{ij} \in (0, 1)$ as the mass contribution of the molecule of species $\mathscr{A}_i$ to the sum of masses of the two colliding molecules of species $\mathscr{A}_i$ and $\mathscr{A}_j$, that is,

$$r_{ij} := \frac{m_i}{m_i + m_j} \quad \Rightarrow \quad r_{ji} := 1 - r_{ij} = \frac{m_j}{m_i + m_j}, \tag{7}$$

then the coordinate pair v', v'_* (6) becomes

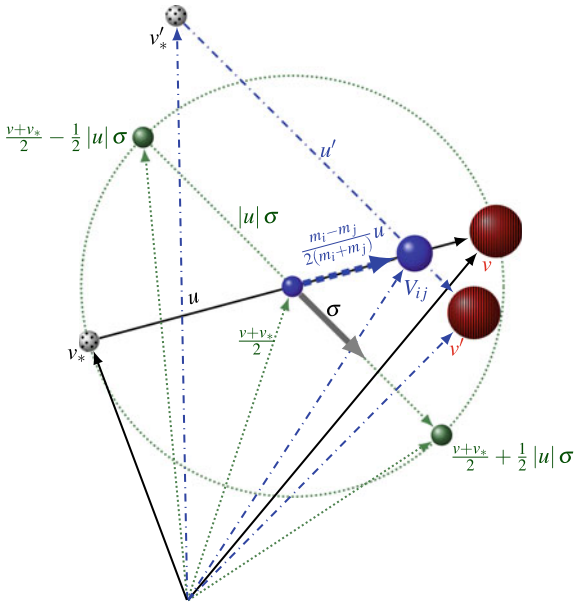

Fig. 1 Illustration of the collision transformation for $N = 3$. Solid lines denote vectors after collision, or given data. Dash-dotted vectors represent primed (pre-collisional) quantities that can be calculated from the given data, and compared to the case $m_i = m_j$, represented by dotted vectors. The dashed vector direction is the displacement along the direction of the relative velocity u proportional to the half difference of relative masses, (which clearly vanishes for $m_i = m_j$, reducing the model to a classical collision). Note that the scattering direction σ is preserved as the pre-collisional relative velocity u' keeps the same magnitude as the post-collisional u, u' is parallel to the reference elastic pre-collisional relative velocity $|u|\sigma$

$$v' = v + (1 - r_{ij})(|u|\,\sigma - u), \quad v'_* = v_* - r_{ij}(|u|\,\sigma - u), \tag{8}$$

which will be used in the sequel as well. It is noticeable that in the case of the single species the mass fraction is $r_{ij} = 1/2$ for all $i, j = 1, \cdots, I$. The difference between this representation for a single species and the collision transformation given in (8) for a binary mixture of monatomic gases can be clear when looking at the Fig. 1, presented for $N = 3$.

2.2 The System of Boltzmann Equations

When fixing i, the distribution function f_i changes due to binary interactions of the particle of species $\mathscr{A}_i$ with particles of the same or different species; therefore, it solves a Boltzmann type equation where the collision operator takes into account the influence of all particles of species $\mathscr{A}_j$ over our fixed particle. The Boltzmann type equation in this case is

$$\partial_t f_i(t, v) = \sum_{j=1}^{I} Q_{ij}(f_i, f_j)(t, v), \qquad i = 1, \ldots, I. \tag{9}$$

The form of Q_{ij}, for any $i, j = 1, \ldots I$, is given by the non-local bilinear form

$$\begin{aligned} Q_{ij}(f_i, f_j)(v) &= \int_{\mathbb{R}^N} \int_{\mathbb{S}^{N-1}} \left(f_i(v') f_j(v'_*) - f_i(v) f_j(v_*) \right) \mathscr{B}_{ij}(|u|, \hat{u} \cdot \sigma)\, \mathrm{d}\sigma\, \mathrm{d}v_* \\ &=: Q^+_{ij}(f_i, f_j)(v) \; - \; Q^-_{ij}(f_i, f_j)(v) \end{aligned} \tag{10}$$

where the pre-collisional velocity pair v', v'_*, and post-collisional corresponding ones v, v_*, are related as stated on (8) and $\hat{u} := u/|u|$. The transition probability rates $\mathscr{B}_{ij}$ are positive a.e. measures that satisfy the micro-reversibility assumptions given by an invariance when switching the post- and pre-collisional velocities or the particles themselves. This means that

$$\mathscr{B}_{ij}(|u|\,, \hat{u} \cdot \sigma) = \mathscr{B}_{ij}(\left|u'\right|\,, \hat{u}' \cdot \sigma') = \mathscr{B}_{ji}(|u|\,, \hat{u} \cdot \sigma), \tag{11}$$

where σ and u' are defined as in the previous subsection (note that then $\sigma' = u'/\,|u|$). Some additional assumptions are also listed in Sect. 4 below.

Note that (10) has introduced the gain and loss operator forms, namely

$$\begin{aligned} Q^+_{ij}(f_i, f_j)(v) \; &:= \; \int_{\mathbb{R}^N} \int_{\mathbb{S}^{N-1}} f_i(v') f_j(v') \mathscr{B}_{ij}(|u|, \hat{u} \cdot \sigma)\, \mathrm{d}\sigma\, \mathrm{d}v_*\,, \\ Q^-_{ij}(f_i, f_j)(v) \; &:= \int_{\mathbb{R}^N} \int_{\mathbb{S}^{N-1}} f_i(v) f_j(v_*) \mathscr{B}_{ij}(|u|, \hat{u} \cdot \sigma)\, \mathrm{d}\sigma\, \mathrm{d}v_* \; = \; f_i(v) \nu_{ij}(v)\,. \end{aligned} \tag{12}$$

where $\nu_{ij}(v)$ is the local collision frequency for each collision pair (i, j), $1 \leq i, j \leq I$.

When the mixture is considered as a whole, a vector-valued notation is introduced for both the probability distribution functions as well as for the collision operators as given in (1). Then the Boltzmann collisional system in (9) takes the vector form (2).

2.3 Representations of the Collision Operator

The proposed approach strongly relies on different estimates of the positive contribution of the collision operator, namely the gain term $Q_{ij}^{+}(f_i, f_j)(v)$ given in (12). Different formulations of this operator are used throughout the paper, where properties of the transition probability rates (or collision kernels) may vary.

2.3.1 The Kernel Form for the Gain Term

Inspired by the work [5] of gain of integrability estimate for the scalar single species model, the authors [12] found a new representation of strong form for the gain term $Q_{ij}^{+}(f_i, f_j)(v)$ by means of an associated Carleman integral representation associated to the vector-valued collisional forms.

This new Carleman representation for the strong collisional form associated to the gain operator for a binary interaction is formulated in the next statement, where all the parameters are determined by functions of the corresponding mass ratio. This is a key step in the proof of propagation of L^p norms.

Theorem 1 (Carleman representation of the gain term) *Let*

$$P_{r_{ij}}(v, v') = \frac{\big(v - (2r_{ij} - 1)v'\big)}{2(1 - r_{ij})}, \quad r_{ij} \in (0, 1).$$

Denote with $E_{vv'}$ the hyperplane orthogonal to the vector $v - v'$, that is

$$E_{vv'} = \big\{ y \in \mathbb{R}^N : (v - v') \cdot y = 0 \big\} \subset \mathbb{R}^{N-1}. \tag{13}$$

Let f and g be nonnegative functions. Then the gain term can be represented as follows

$$Q_{ij}^{+}(f, g)(v) = (1 - r_{ij})^{-N+1} \int_{x \in \mathbb{R}^N} \frac{f(x)}{|x - v|} \int_{z \in E_{vx}} g(z + P_{r_{ij}}(v, x)) \tag{14}$$

$$\times \left| \frac{(v - x)}{2(1 - r_{ij})} + z \right|^{2-N} \mathscr{B}_{ij} \left(\left| \frac{(v - x)}{2(1 - r_{ij})} + z \right|, 1 - \frac{|x - v|^2}{2(1 - r_{ij})^2 \left| \frac{(v-x)}{2(1-r_{ij})} + z \right|^2} \right) \mathrm{d}z \, \mathrm{d}x.$$

By means of the Carleman representation, the operator $\mathbb{Q}^+(\mathbb{F}, \mathbb{G})$ can be written in a kernel form as follows.

Lemma 1 (Kernel form of the gain operator) *Let* $\mathbb{F} = [f_i]_{1\le i\le I}$ *and* $\mathbb{G} = [g_i]_{1\le i\le I}$, *where* $f_i(v) \ge 0$ *and* $g_i(v) \ge 0$ *for all* $v \in \mathbb{R}^N$ *and all* $1 \le i \le I$. *Then the gain operator* $\mathbb{Q}^+(\mathbb{F}, \mathbb{G})$ *can be written in the following kernel form*

$$\left[\mathbb{Q}^+(\mathbb{F}, \mathbb{G})\right]_i (v) = \int_{\mathbb{R}^N} f_i(x)\, K_i[\mathbb{G}](v, x)\, \mathrm{d}x, \tag{15}$$

where the kernel is

$$K_i[\mathbb{G}](v, x) = \sum_{j=1}^{I} \tau_x\, Q_{ij}^+(\delta_0, \tau_{-x} g_j)(v),$$

with δ_0 *the Dirac mass at the origin and the translation operator* τ_w *defined by*

$$\tau_w g(v) = g(v - w), \quad \textit{for any} \quad v, w \in \mathbb{R}^N.$$

2.3.2 Weak Formulation of Collisional Integrals for Gas Mixtures

The weak form associated to the system is obtained by integrating each equation after multiplying by a test function $\psi_i(v)$ and performing the classical interchange of coordinates $(v, v_*, \sigma) \leftrightarrow (v', v'_*, \sigma')$ and $(v, v_*, \sigma) \leftrightarrow (v_*, v, -\sigma)$. That yields

$$2\sum_{i=1}^{I} \int_{\mathbb{R}^N} [\mathbb{Q}(\mathbb{F}, \mathbb{F})]_i\, \psi_i(v)\mathrm{d}v = \sum_{i=1}^{I}\sum_{j=1}^{I} \iiint_{\mathbb{R}^N\times\mathbb{R}^N\times\mathbb{S}^{N-1}} f_i(v) f_j(v_*) \times \left(\psi_i(v') + \psi_j(v'_*) - \psi_i(v) - \psi_j(v_*)\right) \mathscr{B}_{ij}(v, v_*, \sigma)\mathrm{d}\sigma\,\mathrm{d}v_*\mathrm{d}v, \tag{16}$$

where now the primed velocity pair v', v'_* refers to post collisional velocities, and the unprimed associated pair v, v_* to pre collisional ones, and are defined as in (8).

This formulation enables the classical functions that annihilate the weak form associated to the system, called collision invariants, given by

$$\psi_\ell(x) = 1, \quad \psi_\ell(x) = m_\ell x \quad \text{and} \quad \psi_\ell(x) = m_\ell\, |x|^2, \quad \ell = 1, \ldots, I, \quad x \in \mathbb{R}^N, \tag{17}$$

to satisfy the total conservation laws during collision process (3).

2.3.3 A Different Weak Formulation

Following the representation introduced in [4], we define the collision weight angular integral operator acting on the test functions φ and χ, bounded and continuous,

$$\mathscr{P}_{ij}(\varphi,\chi)(u) := \int_{\mathbb{S}^{N-1}} \varphi(u_{ij}^-)\,\chi(u_{ij}^+)\,b_{ij}(\hat{u}\cdot\sigma)\,\mathrm{d}\sigma, \tag{18}$$

where u^+ and u^- are defined by

$$u_{ij}^- := (1-r_{ij})(u-|u|\sigma) \;\text{ and }\; u_{ij}^+ := u - u_{ij}^- = r_{ij}u + (1-r_{ij})|u|\sigma.$$

Moreover, let τ and $\mathscr{R}$ denote the translation and reflection operators,

$$\tau_v\psi(x) := \psi(x-v) \;\text{ and }\; \mathscr{R}\psi(x) := \psi(-x),\; v, x \in \mathbb{R}^N.$$

Therefore, from the weak formulation (16) of the gain part of the collision operator when $\mathscr{B}_{ij}(|u|,\hat{u}\cdot\sigma) = |u|^{\gamma_{ij}}\; b_{ij}(\hat{u}\cdot\sigma)$, yields

$$\begin{aligned}\int_{\mathbb{R}^N} Q_{ij}^+(f,g)(v)\psi(v)\mathrm{d}v &= \int_{\mathbb{R}^N}\int_{\mathbb{R}^N} f(v)g(v-u)|u|^{\gamma_{ij}}\,\mathscr{P}_{ij}(\tau_{-v}(\mathscr{R}\psi),1)(u)\mathrm{d}u\,\mathrm{d}v\\ &= \int_{\mathbb{R}^N}\int_{\mathbb{R}^N} f(v-u)g(v)|u|^{\gamma_{ij}}\,\mathscr{P}_{ij}(1,\tau_{-v}(\mathscr{R}\psi))(u)\mathrm{d}u\,\mathrm{d}v.\end{aligned}$$

3 Moments and Functional Space

Set first the following Lebesgue brackets that yield weighted polynomial moment in the Banach space topology with a suitable norm to handle the mixture system,

$$\langle v\rangle_i := \left(1+\frac{m_i}{\sum_{j=1}^I m_j}|v|^2\right)^{1/2},\quad v\in\mathbb{R}^N, i=1,\dots,I. \tag{19}$$

Thus, scalar Lebesgue bracket polynomial moments of order $q \geq 0$, for both vector-valued $\mathbb{F}(t,v)$ and $\mathbb{Q}(\mathbb{F},\mathbb{F})$ taking values on the vector space $\mathbb{R}^I$, are independent of mass density units. They are given by

$$\mathfrak{m}_q[\mathbb{F}](t) = \sum_{i=1}^I \int_{\mathbb{R}^N} f_i(t,v)\,\langle v\rangle_i^q\,\mathrm{d}v \quad\text{and}\quad \mathfrak{m}_q[\mathbb{Q}(\mathbb{F},\mathbb{F})](t) = \sum_{i=1}^I \int_{\mathbb{R}^N} [\mathbb{Q}(\mathbb{F},\mathbb{F})]_i\,\langle v\rangle_i^q\,\mathrm{d}v. \tag{20}$$

The associated Banach space is defined by the kth-polynomial weighted Lebesgue space associated to the ith-component, namely,

$$L_{k,i}^p(\mathbb{R}^N) := \left\{ g : \|g\|_{L_{k,i}^p}^p := \int_{\mathbb{R}^N} \left(|g(v)|\,\langle v\rangle_i^k\right)^p \mathrm{d}v < \infty, k\geq 0, 1\leq p<\infty \right\}.$$

The corresponding $L_{k,i}^\infty(\mathbb{R}^N)$ space is defined in the usual way, as

$$L^{\infty}_{k,i} := \left\{ g : \|g\|_{L^{\infty}_{k,i}} = \operatorname*{ess\,sup}_{v\in\mathbb{R}^N} \left(|g(v)| \langle v \rangle_i^k \right) < \infty,\ k \geq 0 \right\}.$$

When summed over all species, the corresponding Lebesgue space for the whole mixture takes the form, for any $1 \leq p < \infty$,

$$L^p_k(\mathbb{R}^N) := \left\{ \mathbb{F} = [f_i]_{1\leq i\leq I} : \|\mathbb{F}\|^p_{L^p_k} := \sum_{i=1}^{I} \int_{\mathbb{R}^N} \left(|f_i(v)| \langle v \rangle_i^k \right)^p \mathrm{d}v < \infty, \quad k \geq 0, \right\}, \tag{21}$$

with $L^{\infty}_k(\mathbb{R}^N)$ defined as

$$L^{\infty}_k := \left\{ \mathbb{F} = [f_i]_{1\leq i\leq I} : \sum_{i=1}^{I} \operatorname{ess\,sup}_{v\in\mathbb{R}^N} \left(|f_i(v)| \langle v \rangle_i^k \right) < \infty,\ k \geq 0 \right\}.$$

It is clear that $\mathbb{F}$ in L^p_k is related to the norm of its components f_i in the space $L^p_{k,i}$ via

$$\|\mathbb{F}\|^p_{L^p_k} = \sum_{i=1}^{I} \|f_i\|^p_{L^p_{k,i}}, \quad \|\mathbb{F}\|_{L^{\infty}_k} = \sum_{i=1}^{I} \|f_i\|_{L^{\infty}_{k,i}}.$$

Remark 1 Lebesgue bracket weighted polynomial norms $\|\mathbb{F}\|_{L^1_k}$, as defined in (21) coincide with the corresponding polynomial moment $\mathfrak{m}_k[\mathbb{F}]$ if each component $f_i(t, v)$ of $\mathbb{F}$ is non-negative. However, it is important to stress that, on one hand, by (16) and (17), both $\mathfrak{m}_0[\mathbb{Q}(\mathbb{F}, \mathbb{F})] = \mathfrak{m}_1[\mathbb{Q}(\mathbb{F}, \mathbb{F})] = 0$, giving rise to conservation of both total number density $\mathfrak{m}_0[\mathbb{F}](t) = \|\mathbb{F}\|_{L^1_0}(t) = \|\mathbb{F}_0\|_{L^1_0}$ and total kinetic energy $\mathfrak{m}_2[\mathbb{F}](t) = \|\mathbb{F}\|_{L^1_2}(t) = \|\mathbb{F}_0\|_{L^1_2}$ of the mixture,

$$\partial_t \|\mathbb{F}\|_{L^1_{0,i}} = 0, \quad \partial_t \|\mathbb{F}\|_{L^1_0} = 0, \quad \partial_t \|\mathbb{F}\|_{L^1_2} = 0.$$

On the other hand, the k-moment of the collision operator $\mathfrak{m}_k[\mathbb{Q}(\mathbb{F}, \mathbb{F})]$ is expected to take negative values for $k > k_*$, sufficiently large. This property is essential for the global in time solutions for the Cauchy problem associated to system (1) as it will be addressed in sections to come.

4 Statement of the Problem

The Cauchy problem for the Boltzmann system (2) for a binary gas mixture of an arbitrary number I of species is given by

$$\begin{cases} \partial_t \mathbb{F}(t, v) = \mathbb{Q}(\mathbb{F}, \mathbb{F})(t, v), \quad t > 0,\ v \in \mathbb{R}^N, \\ \mathbb{F}(0, v) = \mathbb{F}_0(v). \end{cases} \tag{22}$$

This problem is uniquely solved globally in time by the authors in [14] with initial data $\mathbb{F}_0(v) \in \Omega \subset L^1_k(\mathbb{R}^N)$, for $k \geq k_*$ (with Ω and k_* defined as below), showing that the Lebesgue moments are propagated, and also generated, obtaining that the solution is globally in L^1_k for all $k \geq k_*$.

If, in addition, the initial data is in $L^p_\ell(\mathbb{R}^N)$, with $p \in [1, \infty]$ for $\ell \geq 0$ then the property of propagation also holds, as shown in [12].

The proofs consist in showing that Lebesgue polynomial moments of vector-valued solutions $\mathbb{F}$ propagate the Banach space regularity of the initial data by means of constructing an Ordinary Differential Inequality for the $L^p_\ell(\mathbb{R}^N)$-norms, for $\ell \geq 0$, as well as the full range of $p \in [1, \infty]$. The base case $p = 1$ actually generates all $L^1_k(\mathbb{R}^N)$-norms, with just initial data $\mathbb{F}_0(v) \in \Omega \subset L^1_{k_*}(\mathbb{R}^N)$ and propagates them with the additional requirement on the initial data $\mathbb{F}_0(v) \in L^1_k(\mathbb{R}^N)$, $k \geq k_*$. It is important to stress that the $L^p_\ell(\mathbb{R}^N)$-norm propagation, $\ell \geq 0$, $p \in [1, \infty]$, as much as exponentially weighted norms propagation (and generation for $p = 1$) hold under restricted conditions on the transition probabilities forms depending on the intramolecular rates and integrability properties of the angular transition function, which are being described next. These properties are consequence of the conservation laws associated to the mixture.

The assumption on the form of the transition probability rates $\mathscr{B}_{ij}, i, j = 1, \ldots, I$ which corresponds to hard potentials with a potential γ_{ij}, are

$$\mathscr{B}_{ij}(|u|, \hat{u} \cdot \sigma) = |u|^{\gamma_{ij}} \; b_{ij}(\hat{u} \cdot \sigma), \text{ with } \gamma_{ij} \in (0, 1], \tag{23}$$

and angular transition rates $b_{ij}(\hat{u} \cdot \sigma)$ satisfying the integrability conditions

$$b_{ij}(\hat{u} \cdot \sigma) \in L^1(\mathbb{S}^{N-1}) \tag{24}$$

for L^1_k theory in Sect. 6 and existence and uniqueness theory in Sect. 7; and

$$b_{ij}(\hat{u} \cdot \sigma) \in L^\infty(\mathbb{S}^{N-1}) \tag{25}$$

for L^p_ℓ theory, $p \in (1, \infty]$ in Sects. 8–9. However, our studies of moment propagation and generation of summability of moments giving rise to exponentially weighted norms in L^p, for the complete range of $p \in [1, \infty]$ requires that potentials γ_{ij} are the same for all $i, j = 1, \ldots, I$.

Whenever needed, the following notation will be employed

$$\bar{\gamma} = \min_{1 \leq i, j \leq I} \gamma_{ij}, \quad \bar{\bar{\gamma}} = \max_{1 \leq i \leq I} \gamma_{ij}. \tag{26}$$

In addition, the following control by below is fundamental to estimate the collision frequency factor in the loss term under the assumption (23) for the transition probability rate.

Lemma 2 *Let $\gamma_{ij} \in [0, 2]$, for any $i, j \in \{1, \ldots, I\}$, and assume $0 \leq \left\{\mathbb{F}(t) = [f_1(t) \ldots f_I(t)]^T\right\}_{t \geq 0} \subset L^1_2$ satisfies*

$$c \le \sum_{i=1}^{I} \int_{\mathbb{R}^N} m_i \, f_i(t,v) \mathrm{d}v \le C, \qquad c \le \sum_{i=1}^{I} \int_{\mathbb{R}^N} f_i(t,v) m_i \, |v|^2 \, \mathrm{d}v \le C,$$

$$\sum_{i=1}^{I} \int_{\mathbb{R}^N} f_i(t,v) m_i v \mathrm{d}v = 0,$$

for some positive constants c and C. Assume also boundedness of the moment

$$\sum_{i=1}^{I} \int_{\mathbb{R}^N} f_i(t,v) m_i \, |v|^{2+\varepsilon} \, \mathrm{d}v \le B, \quad \varepsilon > 0.$$

Then, there exists a constant c_{lb} depending on m_i, c, C and B such that

$$\sum_{i=1}^{I} \int_{\mathbb{R}^N} m_i f_i(t,w) \, |v-w|^{\gamma_{ij}} \, \mathrm{d}w \ge c_{lb} \langle v \rangle_j^{\bar{\gamma}}, \tag{27}$$

for any $j \in \{1, \ldots, I\}$, with $\bar{\gamma} = \min_{1 \le i,j \le I} \gamma_{ij}$.

The proof of this Lemma, originally written in [14, Appendix], extends concepts from a single monatomic gas case given in [6, 9]. A revised version reflecting the notation of the current statement of this lemma can be found in [14, ArXiv:1806.09331v3, Appendix].

5 Angular Averaging Estimate for the Mixture System Gain Operators

This key estimate may be viewed as the extension of the angular averaging lemma used in [5, 10, 13], referred as a sharper form of the original Povzner lemma for the classical theory of single species of monoatomic elastic gases with binary interactions. It is a crucial step for the theory since it ensures the dominance of polynomially weighted norms of an order k in L^1 space associated to the negative contribution from the loss part of the collision operator with respect to those same norms of the positive contribution, i.e. gain part, for sufficiently large k. In the mixture setting, k grows with disparateness of masses measured with deviations of r_{ij} from $1/2$.

Lemma 3 (Angular averaging for the mixing model) *Suppose that b_{ij} satisfies (24). Let v' and v'_* be functions of v, v_*, σ as in (6), with $m_i, m_j > 0$. Then, the following estimate holds for any fixed i, j,*

$$\int_{\mathbb{S}^{N-1}} \left(\langle v' \rangle_i^k + \langle v'_* \rangle_j^k \right) b_{ij}(\sigma \cdot \hat{u}) \, \mathrm{d}\sigma \le \mathscr{C}_{\frac{k}{2}}^{ij} \left(\langle v \rangle_i^2 + \langle v_* \rangle_j^2 \right)^{\frac{k}{2}}, \tag{28}$$

where constant $\mathscr{C}^{ij}_{\frac{k}{2}}$ *tends to zero as* k *grows and moreover*

$$\mathscr{C}^{ij}_{\frac{k}{2}} - \left\|b_{ij}\right\|_{L^1(\mathrm{d}\sigma)} < 0, \qquad \text{for any } k \geq k^{ij}_*, \quad 1 \leq i, j \leq I, \tag{29}$$

where each k^{ij}_* *depends on* b_{ij} *and* r_{ij}.

The proof strongly relies on an *energy identity*, which encodes double-convex combination form of velocities v' and v'_* written in brackets (19). More precisely, define first the total energy E_{ij} of two colliding particles in $\langle\cdot\rangle$ bracket forms, which is conserved during collision process by (3),

$$E_{ij} := \langle v\rangle_i^2 + \langle v_*\rangle_j^2 = \left\langle v'\right\rangle_i^2 + \left\langle v'_*\right\rangle_j^2.$$

Then, there exists a couple of functions $p_{ij} = p_{ij}(v, v_*, m_i, m_j)$ and $q_{ij} = q_{ij}(v, v_*, m_i, m_j)$ such that, $p_{ij} + q_{ij} = E_{ij}$ and a function $\lambda_{ij} = \lambda_{ij}(v, v_*, m_i, m_j)$ so that the following representation holds

$$\langle v'_{ij}\rangle_i^2 = p_{ij} + \lambda_{ij}\,\sigma\cdot\hat{V}_{ij}, \qquad \langle v'_{*ij}\rangle_j^2 = q_{ij} - \lambda_{ij}\,\sigma\cdot\hat{V}_{ij}. \tag{30}$$

These Eq. (30) allow to write left-hand side of (28) in terms of a Taylor expansion up to second order with a reminder in the integral form. Thus, denoting

$$\bar{\bar{r}}_{ij} = \max\{r_{ij}, 1 - r_{ij}\}, \quad \bar{r}_{ij} = \min\{r_{ij}, 1 - r_{ij}\},$$

the following estimate holds

$$\int_{\mathbb{S}^{N-1}} \left(\left\langle v'\right\rangle_i^k + \left\langle v'_*\right\rangle_j^k\right) b_{ij}(\sigma\cdot\hat{u})\,\mathrm{d}\sigma \leq E_{ij}^{k/2} \begin{cases} \left((k+2)\tilde{C}^{ij}_{k/2} + \bar{C}^{ij}_{k/2} + \hat{C}^{ij}_{k/2}\right)\left\|b_{ij}\right\|_{L^1(\mathrm{d}\sigma)} + \check{C}^{ij}_{k/2}, & k > 4 \\ 2\tilde{C}^{ij}_{k/2}\left\|b_{ij}\right\|_{L^1(\mathrm{d}\sigma)}, & 2 < k \leq 4 \end{cases},$$

with explicit expressions for constants

$$\tilde{C}^{ij}_n = \left(\bar{\bar{r}}_{ij}\right)^n, \qquad \bar{C}^{ij}_n = -2\left(\frac{\bar{\bar{r}}_{ij}}{\bar{r}_{ij}}\right)^2 (1 - \bar{r}_{ij})^n, \qquad \hat{C}^{ij}_n = 2\left(\frac{\bar{\bar{r}}_{ij}}{\bar{r}_{ij}}\right)^2 n\,(1 - \bar{r}_{ij})^{n-1},$$

and

$$\check{C}^{ij}_n = 2\left(\frac{\bar{\bar{r}}_{ij}}{\bar{r}_{ij}}\right)^2 \int_{\mathbb{S}^{N-1}} \left(1 + \bar{r}_{ij}(|\sigma\cdot\hat{u}| - 1)\right)^n b_{ij}(\sigma\cdot\hat{u})\,\mathrm{d}\sigma.$$

Under a more restrictive assumption on b_{ij} which is $b_{ij}(\sigma\cdot\hat{u}) \in L^\infty(\mathbb{S}^{N-1}; \mathrm{d}\sigma)$, it is possible to calculate the constant $\check{C}^{ij}_n$ as well. Namely,

$$\check{C}_n^{ij} = 2\left|\mathbb{S}^{N-1}\right| \frac{\bar{\bar{r}}^2}{\bar{r}^3} \left\|b_{ij}\right\|_{L^\infty(\mathrm{d}\sigma)} \left(\frac{1}{n+1} - \frac{(1-\bar{r})^{n+1}}{n+1}\right),$$

where $\left|\mathbb{S}^{N-1}\right|$ is the volume of a unit N-dimensional ball.

Since these constants are explicitly calculated, it is clear that the Povzner constant $\mathscr{C}_n^{ij}$ decays to zero as $n \to \infty$ (for $\check{C}_n^{ij}$ when $b_{ij} \in L^1(\mathbb{S}^{N-1}; \mathrm{d}\sigma)$ it follows from the Monotone Convergence Theorem). This ensures existence of a n_*^{ij} such that

$$\mathscr{C}_n^{ij} < \left\|b_{ij}\right\|_{L^1(\mathrm{d}\sigma)}, \quad n > n_*^{ij}. \tag{31}$$

It is worthwhile to mention the rate of convergence of the Povzner constant $\mathscr{C}_n^{ij}$ and the difference in the mixture setting with respect to the single component case. For the single component gas, when $r_{ij} = 1/2$ the convergence rate of $\mathscr{C}_n^{ij}$ is $1/n$ when $n \to \infty$, which implies that (31) will hold for any $n > 1$ or we can take $n_* = 1$. In the mixture case, the $\mathscr{C}_n^{ij}$ decay power strongly depends on r_{ij}, and as r_{ij} deviates from $1/2$ it decays slower, and thus n_*^{ij} which guarantees (31) will be greater. This fact is illustrated in the following Fig. 2 for the case $b_{ij}(\sigma \cdot \hat{u}) \in L^\infty(\mathbb{S}^{N-1}; \mathrm{d}\sigma)$ after introducing $\mathscr{C}_n^\infty(r_{ij})$ via

$$\mathscr{C}_n^{ij} = \left|\mathbb{S}^{N-1}\right| \left\|b_{ij}\right\|_{L^\infty(\mathrm{d}\sigma)} \mathscr{C}_n^\infty(r_{ij}), \tag{32}$$

and compared $\mathscr{C}_n^\infty(r_{ij})$ with respect to 1.

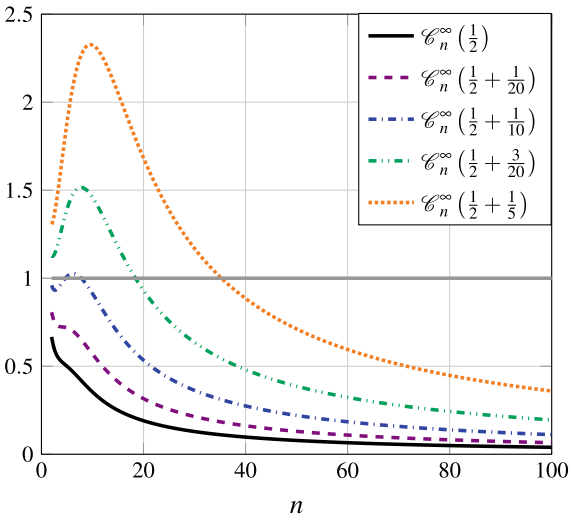

Fig. 2 Constant $\mathscr{C}_n^\infty(r_{ij})$ defined in (32) and related to the constant from Povzner Lemma 3 for some fixed value of $r_{ij} =: r_*$, and $N = 3$. This figure illustrates the non-monotonic behavior in n variable, and the growth of n needed to ensure that $\mathscr{C}_n^\infty(r_*) < 1$ caused by a deviation of r_{ij} with respect to $\frac{1}{2}$

6 Polynomially and Exponentially Weighted L^1 Theory

Next, the focus is on a priori estimates in k-polynomially and exponentially weighted L^1-norms in order to solve the Cauchy problem (22) in a suitable Banach space. The techniques in this section have been inspired by the ones developed for single species scalar binary elastic interactions case in [2, 3, 10, 13, 16], and extended to hard potentials with the angular part of the transition probability being integrable. All these results were extended to the case of Maxwell type of interactions, (i.e. $\gamma = 0$), where the polynomially and exponentially weighted L^1 theory [17] can only propagate, due to the nature of the Maxwell type of interaction model.

6.1 Polynomially Weighted L^1 Norms

The kth moment associated to the system of Eq. (22) is given by

$$\frac{\mathrm{d}}{\mathrm{d}t}\,\|\mathbb{F}\|_{L^1_k}(t) = \frac{\mathrm{d}}{\mathrm{d}t}\mathfrak{m}_k[\mathbb{F}](t) = \mathfrak{m}_k[\mathbb{Q}(\mathbb{F},\mathbb{F}](t) = \sum_{i=1}^{I}\int_{\mathbb{R}^N}[\mathbb{Q}(\mathbb{F},\mathbb{F})]_i\,(t)\,\langle v\rangle_i^k\,\mathrm{d}v. \quad (33)$$

In order to find an upper control to the right-hand side of (33), it is important to notice that such term has a negative and positive contributions that can be associated to moments of the vector-valued solutions, whose all its components $f_i(t, v)$ are a priori assumed to be non-negative. These estimates are due to, on one hand, the Povzner Lemma 3 which allows to control kth polynomial moments of the collision operator gain terms, and, on the other hand, the lower bound from Lemma 2 which provides a lower estimate for the loss term. More precisely, it was shown in [14], that the right hand side of (33) is bounded by a superlinear function of the k-moments of $\|\mathbb{F}\|_{L^1_k}(t)$ that recover the classical Bernoulli form associated to the generation and propagation of moments of solutions. All these results are summarized in the following two lemmas.

Lemma 4 (Ordinary differential inequality for polynomial moments in L^1_k) *If* $\mathbb{F} = [f_i]_{i=1,\dots,I} \in L^1_2$ *is a solution of the Boltzmann system* (22) *with the transition rate* (23)–(24)*, then the following Ordinary Differential Inequality (ODI) for norms in* L^1_k *space holds*

$$\frac{\mathrm{d}}{\mathrm{d}t}\,\|\mathbb{F}\|_{L^1_k}(t) \le -A_{k_*}\,\|\mathbb{F}\|_{L^1_k}(t)^{1+\frac{\tilde{\gamma}}{k}} + B_k\,\|\mathbb{F}\|_{L^1_k}(t), \quad (34)$$

for positive constants A_{k_*} *and* B_k*, large enough* $k \ge k_*$*, with* k_* *defined by*

$$k_* = \max\{2 + 2\bar{\bar{\gamma}},\ \bar{k}\}, \quad with \quad \bar{k} = \max_{1\le i,j\le I}\{k_*^{ij}\}, \tag{35}$$

for $\bar{\bar{\gamma}}$ *and* $\bar{\gamma}$ *defined in* (26) *and* k_*^{ij} *as in* (29).

The constant A_{k_*} which depends on c_{lb} from (27), $\mathscr{C}^{ij}_{k_*/2}$ from (29) and the mass and energy of the initial data, as well as the moment of order k_* and $\bar{\gamma}$, may be viewed as a coercive constant for the Boltzmann flow system that induces a global in time bound for its vector value solutions. Both constants, A_{k_*} and B_k depend only on the data associated to the Boltzmann system (22), as described in [14].

This ODI for the Lebesgue bracket weighted norms in L^1_k paves the way to the following result on generation and propagation of such norms.

Theorem 2 (Generation and propagation of polynomially weighted L^1 norms) *Under the same conditions of Lemma 4, the following estimates hold.*

1. *(Generation) Let* $\mathfrak{C}^{\mathfrak{m}} = \left(A_{k_*}/B_k\right)^{-k/\bar{\gamma}}$ *be the constants from* (34), $\bar{\gamma}$ *from* (26), *and* $\mathfrak{B}^{\mathfrak{m}} = \mathfrak{C}^{\mathfrak{m}} \max\left\{(\bar{\gamma}/(B_k k))^{-k/\bar{\gamma}}\, e^{\frac{B_k}{2}}, \left(1 - e^{-\bar{\gamma}/(B_k k)}\right)^{-k/\bar{\gamma}}\right\}$ *and* k_* *defined in* (35). *Then,*

$$\|\mathbb{F}\|_{L^1_k}(t) \le \mathfrak{B}^{\mathfrak{m}}\ \max\{1, t^{-k/\bar{\gamma}}\}, \quad for\ any\ k > k_*, \quad \forall t > 0. \tag{36}$$

2. *(Propagation) Moreover, if* $\|\mathbb{F}\|_{L^1_k}(0) < \infty$, *then*

$$\|\mathbb{F}\|_{L^1_k}(t) \le \max\{\mathfrak{C}^{\mathfrak{m}}, \|\mathbb{F}\|_{L^1_k}(0)\}, \quad for\ any\ k > k_*, \quad \forall t > 0. \tag{37}$$

The idea of the proof is to find upper solutions to an associate super-linear ODE of Bernoulli type to (34), namely $y'(t) = -a\, y(t)^{1+c} + b\, y(t)$, whose explicit solution, given by

$$y(t) = \left(\frac{a}{b}\left(1 - e^{-c\,b\,t}\right) + y(0)^{-c} e^{-c\,b\,t}\right)^{-\frac{1}{c}}, \tag{38}$$

$y(t) \le (\frac{a}{b}(1 - e^{-c\,b\,t}))^{-\frac{1}{c}}$, for $t > 0$, which yields the generation estimate (36) after setting $y(t) := \|\mathbb{F}\|_{L^1_k}$, $a := A_k$, $b := B_k$ and $c := \bar{\gamma}/k$. Moreover, when the initial data is finite, then $y(t) \le \max\{y(0), (a/b)^{-1/c}\}$, for $t > 0$, which concludes the propagation result (37).

6.2 Exponentially Weighted L^1 Norms

The results that hold for polynomially weighted L^1-norms, can be extended to L^1-norms with exponential weight for the solution of the Boltzmann system for the case when $\bar{\bar{\gamma}} = \bar{\gamma}$, i.e., all γ_{ij} coincide, $i, j \in \{1, \ldots, I\}$.

Theorem 3 (Generation and propagation of exponentially weighted L^1 norms) *Let $\bar{\gamma} = \bar{\bar{\gamma}} = \gamma_{ij}$, $i, j \in \{1, \ldots, I\}$. Then, under the same conditions of Lemma 4 and Theorem 2 the summability of $k-$moments imply the following properties of L^1 exponentially weighted norms for the solution $\mathbb{F}$ of the mixture Cauchy problem (22).*

(a) (Generation) There exist constants $\alpha > 0$ and $\mathfrak{B}^{\mathscr{E}} > 0$ such that

$$\left\| \mathbb{F} e^{\alpha \min\{t,1\}\langle\cdot\rangle^{\bar{\gamma}}} \right\|_{L^1_0} \leq \mathfrak{B}^{\mathscr{E}}, \quad \forall t \geq 0.$$

(b) (Propagation) Let $0 < s \leq 2$. Suppose that there exists a constant $\alpha_0 > 0$, such that

$$\left\| \mathbb{F}_0 e^{\alpha_0 \langle\cdot\rangle^s} \right\|_{L^1_0} \leq M_0 < \infty. \tag{39}$$

Then there exist constants $0 < \alpha \leq \alpha_0$ and $\mathfrak{C}^{\mathscr{E}} > 0$ such that

$$\left\| \mathbb{F} e^{\alpha \langle\cdot\rangle^s} \right\|_{L^1_0} \leq \mathfrak{C}^{\mathscr{E}}, \qquad \forall t \geq 0. \tag{40}$$

The idea of the proof is to write exponential function in terms of its Taylor series and then to apply results obtained in Theorem 2.

7 Existence and Uniqueness Theory

As mentioned in the introduction, abstract ODE theory in Banach spaces was employed to solve the Cauchy Problem in order to prove existence and uniqueness of the vector-valued solution $\mathbb{F}$ to (22). This technique was adapted to the system setting from the work in [1] for the scalar, single species elastic Boltzmann equation for Maxwell type and hard potentials and integrable angular transition functions. Thus, a natural Banach space to solve the system of Boltzmann equations is L^1_2 defined in (21). The crucial point is to find an invariant region $\Omega \subset L^1_2$ in which the collision operator $\mathbb{Q} : \Omega \to L^1_2$ will satisfy (i) Hölder continuity, (ii) Sub-tangent and (iii) one-sided Lipschitz conditions. To that end, we have studied the map $\mathscr{L}_{\bar{\gamma},k} : [0, \infty) \to \mathbb{R}$, with $\bar{\gamma}$ from (26), motivated by the upper control of the k-moment of the collision operator generating the ODI discussed in (34). More precisely, such estimate results motivates the study of the map

$$\mathscr{L}_{\bar{\bar{\gamma}},k}(x) = -Ax^{1+\frac{\bar{\gamma}}{k_*}} + Bx, \quad x \geq 0,$$

where A and B are positive constants, and $\bar{\gamma}$, k_* are defined by (35). This map has only one non-zero root, denoted with $x^*_{\bar{\gamma},k_*}$, at which $\mathscr{L}_{\bar{\gamma},k_*}$ changes from positive to negative. Thus, for any $x \geq 0$, define

$$\mathscr{L}_{\bar{\gamma},k_*}(x) \leq \max_{0\leq x\leq x^*_{\bar{\gamma},k_*}} \mathscr{L}_{\bar{\gamma},k_*}(x) =: \mathscr{L}^*_{\bar{\gamma},k_*}.$$

and denote

$$C_{k_*} := x^*_{\bar{\gamma},k_*} + \mathscr{L}^*_{\bar{\gamma},k_*}. \tag{41}$$

Now, one can formulate an invariant region $\Omega \subset L^1_2$,

$$\begin{aligned}\Omega = \Big\{ \mathbb{F}(t,\cdot) \in L^1_2(\mathbb{R}^N) : \mathbb{F} \geq 0 \text{ in } v, \sum_{i=1}^{I} \int_{\mathbb{R}^N} m_i v\, f_i(t,v)\mathrm{d}v = 0,\\ \exists\, c_0, C_0, c_2, C_2, C_{2+\varepsilon} > 0, \text{ and } C_0 < c_2, \text{ such that } \forall t \geq 0,\\ c_0 \leq \|\mathbb{F}\|_{L^1_0}(t) \leq C_0,\ c_2 \leq \|\mathbb{F}\|_{L^1_2}(t) \leq C_2,\\ \|\mathbb{F}\|_{L^1_{2+\epsilon}}(t) \leq C_{2+\varepsilon},\ \text{for } \varepsilon > 0,\\ \|\mathbb{F}\|_{L^1_{k_*}}(t) \leq C_{k_*},\ \text{with } k_* \text{ as in (35), and } C_{k_*} \text{ is constructed in (41)} \Big\},\end{aligned} \tag{42}$$

and solve the Cauchy problem (22), as stated in the following theorem.

Theorem 4 (Existence and Uniqueness) *Assume that* $\mathbb{F}(0,v) = \mathbb{F}_0(v) \in \Omega$. *Then the Boltzmann system* (22) *for a transition function satisfying* (23) *and* (24) *has a unique solution in* $C\left([0,\infty), \Omega\right) \cap C^1\left((0,\infty), L^1_2(\mathbb{R}^N)\right)$.

We stress that no conditions on initial entropy are necessary. However, if the initial data has finite entropy, then the entropy inequality implies that the total entropy will remain globally bounded for all times.

8 Polynomial and Exponential Weighted L^p Theory, $1 < p < \infty$

The proof for the propagation of L^p norms follows, after the generalization to the multi-species problem, the strategy devised in [5], which consists in first showing the control of a weighted L^2 norm of the positive part of the pairwise collision operator by a lower order weighted L^2 norm of the input vector-valued function in a suitable Banach space. After the L^2 control, one can obtain a Young's type inequality for the gain term of the vector-valued collision operator for mixture of gases by means of a weak form of the positive term of the collisional operator as an extension of the original strategy developed in [4] and a subsequent interpolation argument obtained now for the whole system describing a gas mixture.

Estimates in L^2 space. The first result we need is a gain of integrability estimate, whose proof will follow from the kernel form of the gain term.

Lemma 5 *Let $N \geq 3$ and let $\mathbb{F}$ and $\mathbb{G}$ be distribution functions, such that $\mathbb{F} \in L^1_\ell(\mathbb{R}^N)$ and $\mathbb{G} \in L^1_{\frac{N-3}{1-\theta}+\ell}(\mathbb{R}^N) \cap L^2_\ell(\mathbb{R}^N)$, $\ell \geq 0$. For the transition probability terms choose (23) and (25). Then, for any $\varepsilon > 0$, the following estimate holds*

$$\left\|\mathbb{Q}^+(\mathbb{F},\mathbb{G})\right\|_{L^2_\ell} \leq \left(\sqrt{2Ik_0}\,\epsilon^{\bar{\bar{\gamma}}}\,\|\mathbb{G}\|_{L^2_\ell} + \sqrt{2Ik_N}\,\varepsilon^{2(2-N+\bar{\gamma})}\,\|\mathbb{G}\|^{1-\theta}_{L^1_{\frac{N-3}{1-\theta}+\ell}}\,\|\mathbb{G}\|^{\theta}_{L^2_\ell}\right)\|\mathbb{F}\|_{L^1_\ell},$$

where $\bar{\bar{\gamma}}$ and $\bar{\gamma}$ as defined in (26) and the constants k_N and k_0 depending on r_{ij}, m_j, and $\|b_{ij}\|_{L^\infty}(\mathbb{S}^{N-1})$, and $\theta = \frac{1}{N}$.

Young's-type estimate. Using the operator (18) and the different weak formulation of the gain term of the collision operator we can prove the following estimate. Note that this theorem is stated for a more general version of the cross section.

Theorem 5 *Let $\mathbb{F} \in L^p_\lambda(\mathbb{R}^N)$ and $\mathbb{G} \in L^q_\lambda(\mathbb{R}^N)$, for $p, q, r \in [1, \infty]$ with $\frac{1}{p} + \frac{1}{q} = 1 + \frac{1}{r}$. Assume that $\mathscr{B}_{ij}$ takes the form*

$$\mathscr{B}_{ij}(x, y) = x^{\lambda_{ij}}\, b_{ij}(y), \quad \lambda_{ij} \geq 0, \quad \text{and} \quad b_{ij} \in L^1([-1, 1]; \mathrm{d}\xi_N^{b_{ij}}(s)),$$

for any $i, j = 1, \ldots, I$, with the measure as $\mathrm{d}\xi_N^{b_{ij}}(s) = b_{ij}(s)(1 - s^2)^{\frac{N-3}{2}}$. Then,

$$\left\|\mathbb{Q}^+(\mathbb{F},\mathbb{G})\right\|_{L^r_0} \leq C^{\mathbb{Q}^+}_{p,q,r}\,\|\mathbb{F}\|_{L^p_\lambda}\,\|\mathbb{G}\|_{L^q_\lambda}, \qquad \text{with} \quad \lambda = \max_{1\leq i,j\leq I}\lambda_{ij}, \tag{43}$$

and the constant $C^{\mathbb{Q}^+}_{p,q,r}$ depends on m_i, m_j and $\|b_{ij}\|_{L^1(\mathbb{S}^{N-1})}$.

By Riesz–Thorin Interpolation, and the use of Lemma 5 and Theorem 5, yields the following Theorem. It is noteworthy that by gain of integrability, we mean that the L^p_k norm of the positive part of the collision operator is controlled sublinearly by the L^p_k norms of the input functions.

Theorem 6 (Gain of integrability) *Under the same conditions of Theorem 5, for any $\epsilon > 0$, $p \in (1, \infty)$ and $\ell \geq 0$ the collision operator can be estimated by*

$$\left\|\mathbb{Q}^+(\mathbb{F},\mathbb{G})\right\|_{L^p_\ell} \leq I^{1-\frac{1}{p}}\,2^{\frac{p-1}{p}}\,\|\mathbb{F}\|_{L^1_\ell}\left(\epsilon^{\bar{\bar{\gamma}}}C^{\mathbb{Q}^+}_{p,1,p}\|\mathbb{G}\|_{L^p_\ell} + \hat{C}_N\epsilon^{2+\bar{\gamma}-N}\|\mathbb{G}\|^{1-\theta}_{L^1_{\frac{N-2}{1-\theta}+\ell}}\,\|\mathbb{G}\|^{\theta}_{L^p_\ell}\right) \tag{44}$$

with $C^{\mathbb{Q}^+}_{p,1,p}$ from Theorem 5, $\hat{C}_N$ depending on N, M_{ij}, b_{ij} and θ defined as

$$\theta = \theta_{p,N} := \begin{cases} \frac{1}{N}, & \text{if } p \in (1, 2] \\ \frac{N(p-2)+1}{N(p-1)}, & \text{if } p \in [2, \infty), \end{cases} \tag{45}$$

These estimates, together with the lower bound estimate (27), the following lemmas are proven, whose complete proofs can be found on Sects. 5, 6 and 7 of [12].

Lemma 6 (ODI for L^p_ℓ-moments) *Let* $\mathbb{F}_0 \in \Omega \cap L^1_{\frac{N-2}{1-\theta}+\ell}(\mathbb{R}^N) \cap L^p_\ell(\mathbb{R}^N)$, *with* $0 < \theta < 1$ *from* (45), $\ell \geq 0$, $1 < p < \infty$ *and the solvability set* Ω *from* (42). *If* $\mathbb{F}$ *is the solution of the Boltzmann system* (22) *with the transition probability rates* (23) *and* (25), *then*

$$\frac{1}{p}\partial_t \|\mathbb{F}\|^p_{L^p_\ell} \leq B_{\ell p}\|\mathbb{F}\|^{p-1+\theta}_{L^p_\ell} - A_{\ell p}\,\|\mathbb{F}\|^p_{L^p_\ell}\,, \tag{46}$$

with $B_{\ell p}$ *and* $A_{\ell p}$ *positive constants, both depending on the constants* A_{k_*} *and* B_k *introduced in* (34), *for* $k \geq k_*$ *from* (35), *expressed on the bounds to solutions constructed in Theorem 2.*

These L^p_ℓ-moments ODI is different from the one in the previous section, since (46) is associated to a *sub-linear* ODE of Bernoulli type

$$y'(t) = by(t)^{1-c} - ay(t), \tag{47}$$

with $a, b, c > 0$, whose solution will be an upper bound for $\|\mathbb{F}\|^p_{L^p_\ell}$. Note that the right hand side of (47) is linear with respect to $y(t)$, which implies the lack of generation estimates, contrary to the L^1_k-theory and equation super-linear Bernoulli ODE.

Indeed, explicitly solving (47) we get the solution

$$y(t) = \left(\frac{b}{a}\left(1 - e^{-act}\right) + y(0)^c e^{-act}\right)^{\frac{1}{c}}.$$

The difference of this solution with respect to (38) is now clear, and since we cannot have an analogue of Jensen's inequality for L^p, $p > 1$, we can not obtain generation of L^p norms. However, choosing $y(t) = \|\mathbb{F}\|^p_{L^p_\ell}$, $b = pB_{\ell p}$, $a = pA_{\ell p}$, and $c = \frac{1-\theta}{p}$ we obtain the propagation as stated in the following Theorem.

Theorem 7 (Propagation of polynomially weighted L^p norms) *If* $\mathbb{F}$ *is the solution of the Boltzmann system* (22) *with* $\mathbb{F}_0 \in \Omega \cap L^1_{\frac{N-2}{1-\theta}+\ell}(\mathbb{R}^N) \cap L^p_\ell(\mathbb{R}^N)$, *with* θ *given in* (45), $\ell \geq 0$, $1 < p < \infty$, *the set* Ω *from* (42), *and the transition probability rates satisfying* (23) *and* (25), *then*

$$\|\mathbb{F}\|^p_{L^p_\ell} \leq \max\{D_{\ell p}, \|\mathbb{F}_0\|^p_{L^p_\ell}\}, \tag{48}$$

where $D_{\ell p} = (B_{\ell p}/A_{\ell p})^{(1-\theta)/p}$, *with* $A_{\ell p}$ *and* $B_{\ell p}$ *from* (46).

Invoking this previous estimate, the following theorem extends to propagation of L^p norms with exponential weights, for $p \in (1, \infty)$, when $\bar{\bar{\gamma}} = \bar{\gamma}$ as follows.

Theorem 8 (Propagation of exponentially weighted L^p norms) *Let $\mathbb{F}$ be the solution of the Boltzmann system with the transition probability rates satisfying (23) and (25) and additionally $\bar{\gamma} = \bar{\bar{\gamma}} = \gamma_{ij}$, $i, j \in \{1, \ldots, I\}$. If*

$$\left\| \mathbb{F}_0 e^{\alpha_0 \langle \cdot \rangle^s} \right\|_{L^1_0 \cap L^p_0} = C^e_0 < \infty,$$

for some $s \in (0, 1]$, $p \in (1, \infty)$ and positive constants α_0 and C^e_0, then, there exist positive constants α and $\hat{D}_0$ such that

$$\left\| \mathbb{F} e^{\alpha \langle \cdot \rangle^s} \right\|_{L^p_0} \leq \max \left\{ \hat{D}_0, \| \mathbb{F}_0 e^{\alpha \langle \cdot \rangle^s} \|_{L^p_0} \right\}, \quad t \geq 0. \tag{49}$$

9 Polynomial and Exponential L^∞ Theory

Theorem 5 and the Lower Bound Lemma 2 are enough to complete the proof of the propagation of L^∞ norm as stated in the following Theorem. The complete version can be found in [12], Sect. 9, which extends the arguments of [8, 15] for a single monatomic gas.

Theorem 9 (Propagation of polynomially weighted L^∞ norms) *Let $\mathbb{F}$ be the solution of the Boltzmann system (22) from Theorem 4 with the assumption (25). Let $\mathbb{F}_0 \in \Omega \cap L^1_{2N-4+\ell+\bar{\bar{\gamma}}}(\mathbb{R}^N) \cap L^2_{\ell+\bar{\bar{\gamma}}}(\mathbb{R}^N)$, with the set Ω from (42), and assume there exists some positive constant $\mathscr{C}_0$ such that*

$$\| \mathbb{F}_0 \|_{L^\infty_\ell} = \mathscr{C}_0,$$

for $\ell \geq 0$. Then there exists a constant $\mathscr{C}(\mathbb{F}_0)$ depending on $\bar{\bar{\gamma}}$ from (26), m_i, b_{ij}, ℓ such that

$$\| \mathbb{F}(t, \cdot) \|_{L^\infty_\ell} \leq \mathscr{C}(\mathbb{F}_0), \quad t \geq 0. \tag{50}$$

Clearly, whenever $\bar{\bar{\gamma}} = \bar{\gamma}$, Theorem 9 extends to the propagation property of L^∞ exponentially weighted norms, as follows.

Theorem 10 (Propagation of exponentially weighted L^∞ norms) *Let $\mathbb{F}$ be the solution of the Boltzmann system (22) with the transition probability rates satisfying (23) and (25) and additionally $\bar{\gamma} = \bar{\bar{\gamma}} = \gamma_{ij}$, $i, j \in \{1, \ldots, I\}$. Assume that the initial data $\mathbb{F}_0 := \mathbb{F}(0, \cdot) \in \Omega$ and that*

$$\| \mathbb{F}_0 e^{\alpha_0 \langle \cdot \rangle^s} \|_{(L^1_0 \cap L^2_0 \cap L^\infty_0)} = C^e_0 < \infty,$$

for some $s \in (0, 1]$, and positive constants α_0 and C^e_0, then, there exist positive constants α and $\hat{D}_\infty$ such that

$$\| \mathbb{F} e^{\alpha \langle \cdot \rangle^s} \|_{L^\infty_0} \leq \hat{D}_\infty(\mathbb{F}_0), \quad t \geq 0. \tag{51}$$

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References

1. R. Alonso, V. Bagland, Y. Cheng, B. Lods, One-dimensional dissipative Boltzmann equation: measure solutions, cooling rate, and self-similar profile. SIAM J. Math. Anal. **50**(1), 1278–1321 (2018)
2. R. Alonso, J.A. Cañizo, I.M. Gamba, C. Mouhot, A new approach to the creation and propagation of exponential moments in the Boltzmann equation. Comm. Part. Differ. Equ. **38**(1), 155–169 (2013)
3. R. Alonso, E. Carneiro, Estimates for the Boltzmann collision operator via radial symmetry and Fourier transform. Adv. Math. **223**(2), 511–528 (2010)
4. R. Alonso, E. Carneiro, I.M. Gamba, Convolution inequalities for the Boltzmann collisionn operator. Comm. Math. Phys. **298**(2), 293–322 (2010)
5. R. Alonso, I.M. Gamba, Gain of integrability for the Boltzmann collisional operator. Kinet. Relat. Models **4**(1), 41–51 (2011)
6. R.J. Alonso, I.M. Gamba, Revisiting the Cauchy problem for the Boltzmann equation for hard potentials with integrable cross section: from generation of moments to propagation of L^∞ bounds. Preprint (2020)
7. R.J. Alonso, I.M. Gamba, M.B. Tran, The Cauchy problem and BEC stability for the quantum Boltzmann-Condensation system for bosons at very low temperature. arXiv:1609.07467.v2
8. R. Alonso, I.M. Gamba, M. Taskovic, Exponentially-tailed regularity and decay rate to equilibrium for the Boltzmann equation. arXiv:1711.06596v2 (2019)
9. R.J. Alonso, I.M. Gamba, S. Tharkabhushanam, Convergence and error estimates for the Lagrangian-based conservative spectral method for Boltzmann equations. SIAM J. Numer. Anal. **56** (2016)
10. A.V. Bobylev, Moment inequalities for the Boltzmann equation and applications to spatially homogeneous problems. J. Statist. Phys. **88**, 1183–1214 (1997)
11. A. Bressan, *Notes on the Boltzmann Equation*. Lecture notes for a summer course, S.I.S.S.A (2005), http://www.math.psu.edu/bressan/
12. E. de la Canal, I.M. Gamba, M. Pavić-Čolić, Propagation of solutions to Boltzmann systems modeling monatomic gas mixtures in weighted Banach spaces (2020). arXiv:2001.09204
13. I.M. Gamba, V. Panferov, C. Villani, Upper Maxwellian bounds for the spatially homogeneous Boltzmann equation. Arch. Ration. Mech. Anal. **194**, 253–282 (2009)
14. I.M. Gamba, M. Pavić-Čolić, On existence and uniqueness to homogeneous Boltzmann flows of monatomic gas mixtures. Arch. Ration. Mech. Anal. **235**(1), 723–781 (2020). arXiv:1806.09331v3
15. I.M. Gamba, N. Pavlović, M. Tasković, Propagation of pointwise exponentially weighted estimates for the Boltzmann equation. SIAM J. Math. Anal. **51**(5), 39211755 (2019)
16. C. Mouhot, Rate of convergence to equilibrium for the spatially homogeneous Boltzmann equation with hard potentials. Comm. Math. Phys. **261**, 629–672 (2006)

17. M. Pavić-Čolić, M. Tasković, Propagation of stretched exponential moments for the Kac equation and Boltzmann equation with Maxwell molecules. Kinet. Relat. Models **11**(3), 597–613 (2018)

Hydrodynamics of Weakly Asymmetric Exclusion with Slow Boundary

Pedro Capitão and Patrícia Gonçalves

Abstract In this article we discuss the hydrodynamic limit of the weakly asymmetric simple exclusion process, whose asymmetry is regulated by a factor N^γ with $\gamma \geq 1$, and in contact with stochastic reservoirs, which are regulated by two factors N^θ and N^δ for, respectively, the symmetric and asymmetric parts of the jump rate at the boundary. Depending on the strength of the asymmetry, that is on the parameter γ, we derive the heat equation (when $\gamma > 1$) as in the purely symmetric case studied in [1], or the viscous Burgers equation (when $\gamma = 1$). In both cases, the PDEs have several boundary conditions which depend on the range of the parameters δ and θ.

Keywords Exclusion process · Weakly asymmetric rates · Slow boundary · Hydrodynamic limits

1 Introduction

Interacting particle systems are a class of Markov processes, which were introduced around 1970 (see [15]) and since then they have been widely studied, see [13, 14]. These systems are used as toy models in contexts such as statistical physics, neural networks, spread of infections and evolution of biological populations. Other than the exclusion process, which is our process of interest, examples of interacting particle systems include the stochastic Ising model, the voter model, the contact process and the zero-range process (see, for example [13]).

The main defining features of interacting particle systems are the following: they usually have state spaces of the form $\Omega = \{0, 1\}^\Lambda$ or $\Omega = \mathbb{N}^\Lambda$, where Λ is a countable set, and they can be seen as a superposition of processes, each describing the movement of a single particle. These individual particle processes, with values in

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Λ, would behave like independent random walks, if it were not for the interaction mechanics. In this interpretation, a state of the process $\eta \in \Omega$ is seen as a configuration of particles and $\eta(x)$ represents the number of particles at site $x \in \Lambda$. Each model is characterized by its state space and the set of laws that dictate how particles interact. These laws determine the evolution of the system as a whole, which is always assumed to be Markovian.

The process we are going to study is a simple exclusion process on the discrete space $\Lambda_N = \{1, \ldots, N-1\}$, for some $N \in \mathbb{N}$. This means that at most one particle can occupy each site (hence the state space is $\Omega_N = \{0, 1\}^{\Lambda_N}$), each transition affects two sites and corresponds to the jump of a particle from one to the other, and particles can only jump to their nearest neighbours. This process can be thought of as a superposition of random walks, with the law for interaction being that jumps to sites that are already occupied are suppressed. For each possible jump, the time until that jump occurs is exponentially distributed. Furthermore, all these times are independent of each other and depend only on the current configuration. This ensures that the system is a Markov process. Note that these exponentially distributed random variables do not necessarily have all the same rate.

The particular model we want to study is the weakly asymmetric simple exclusion process (abbreviated WASEP) in contact with reservoirs. The particles move on $\Lambda_N = \{1, \ldots, N-1\}$, which is called the bulk, and the state space of the process is $\Omega_N = \{0, 1\}^{\Lambda_N}$. The sites 0 and N act as reservoirs: they have an infinite number of particles and can add or remove particles from the sites in the bulk immediately next to them. The process is weakly asymmetric in the sense that the rate at which particles jump to the left or right is not the same (jumps to the right are slightly preferred and happen at rate $1 + \frac{E}{N^\gamma}$, while to the left they happen at rate 1), but this difference between the two rates becomes smaller as N increases. We restrict the parameter γ to be greater or equal to 1. A representation of these dynamics is given in Fig. 1.

Our goal is to study the density of particles in the limit as the scaling parameter N tends to infinity. More precisely, we want to show that the empirical measure, which is a random measure on $[0, 1]$ weighted by the number of particles, converges to an absolutely continuous deterministic measure whose density is the solution of some partial differential equation, called the *hydrodynamic equation*. This is the equation that governs the macroscopic evolution of the density of the system. According to

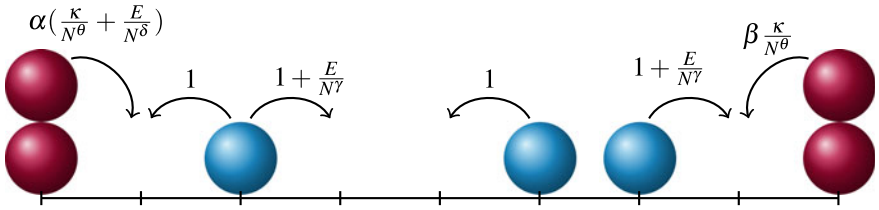

Fig. 1 Possible transitions in the WASEP with reservoirs

the parameters of the model, we will identify the equations that should be obtained for each one of their values. Depending on the value of γ the nature of the PDE changes, more precisely, for $\gamma > 1$ we derive the heat equation while for $\gamma = 1$ we derive the viscous Burgers equation. Depending on the values of the parameters that regulate the intensity of the reservoirs we obtain these equations with several boundary conditions. We give the description of the hydrodynamics for the cases $\theta \geq 0$ and $\delta \geq 1$ and the case $\delta = \theta \in [0, 1)$. The remaining cases are left for a future work.

We employ the entropy method developed in [11] and the main reason for the method not to work in the case we left open is the fact that we do not have enough information on the stationary measure of the model to derive good bounds to compare the Dirichlet form operator and the carré du champ operator, which is crucial when proving replacement lemmas. We remark that the case of symmetric jumps was analyzed in [1] where the heat equation was derived with several boundary conditions and corresponds to our case when $E = 0$ (no asymmetry). The case when jumps are arbitrarily large and given by a symmetric transition probability $p(\cdot)$ with finite variance was studied in [2] and the case of infinite variance was studied both in [3, 4].

The motivation for the study of the model we consider in this article is to have intuition for the case where long jumps are present, as in the aforementioned articles, but considering a transition probability which is weakly asymmetric. The goal will be to derive the fractional viscous Burgers equation with several (fractional) boundary conditions. This is left for a future work.

Once the hydrodynamic limit is established, there are several possibilities to attack as, for example, the Fick's Law, the large deviation principle, the fluctuations, among others. Let us just briefly discuss one of the paths we want to pursue: the fluctuations. We observe that for our model in the case $\kappa = 1, \gamma = 1, \theta = 0, \delta = 1$ the equilibrium fluctuations were established in [6], while the non-equilibrium fluctuations were analysed in [9]. When the asymmetry increases, the equilibrium fluctuations in the case $\kappa = 1$, $\gamma \in [\frac{1}{2}, +\infty)$, $\theta = 0$, $\delta = \gamma$ and $\alpha = \beta$, were derived in [10], and for $\gamma > \frac{1}{2}$ the limit is an Ornstein–Uhlenbeck process; while for $\gamma = 1/2$ the limit is an energy solution of the stochastic Burgers equation, both with Dirichlet boundary conditions. As a continuation of our study we intend to analyse the remaining cases in a future work, specially for the case of a strong asymmetric regime.

This article is organized as follows. In Sect. 2 we present the models that we study, the hydrodynamic equations that we derive and the respective notions of weak solutions, and we state our main result, the hydrodynamic limit. We assume that the PDEs we obtain have a unique weak solution, according to Definitions 2 and 3, since the equations are quite classical in the PDE's literature. In Sect. 3 we give a heuristic argument on how to derive the notions of weak solutions for each one of the regimes that we study. This is done through auxiliary martingales that can be associated to Markov Processes by Dynkin's formula, which gives a discretization of the notion of weak solution. Then one just has to justify that the limit in N converges to the integral solution given either in (3) or (5). In Sect. 4 we prove tightness of

the sequence of empirical measures. In Sect. 5 we prove all the replacement lemmas that we need along the arguments, in order to recognize the limit of the martingales as the solution of the respective PDE.

2 Statement of Results

2.1 The Models

Fix the following parameters: $E, \kappa > 0$, $\alpha, \beta \in (0, 1)$, $\gamma \geq 1$, and $\theta, \delta \geq 0$. Let N be a natural number. Denote by $\{\eta_t : t \geq 0\}$, the one-dimensional, boundary driven, weakly asymmetric simple exclusion process with state space $\Omega_N = \{0, 1\}^{\Lambda_N}$, where $\Lambda_N = \{1, \dots, N-1\}$. The configurations of the state space are denoted by the symbol η, so that $\eta(x) = 1$ if site $x \in \Lambda_N$ is occupied for the configuration η and $\eta(x) = 0$ if site x is empty. The infinitesimal generator of the Markov process $\{\eta_t : t \geq 0\}$ is denoted by $\mathscr{L}_N$ and acts on functions $f : \Omega_N \to \mathbb{R}$ as $\mathscr{L}_N = \mathscr{L}_N^B + \mathscr{L}_N^L + \mathscr{L}_N^R$, where the terms on the right are the generators corresponding to the dynamics of the bulk, the left boundary, and the right boundary, respectively:

$$\begin{aligned} (\mathscr{L}_N^B f)(\eta) &= \sum_{x=1}^{N-2} c_{x,x+1}(\eta)\,\{f(\eta^{x,x+1}) - f(\eta)\}\,, \\ (\mathscr{L}_N^L f)(\eta) &= c_{0,1}(\eta)\,\{f(\eta^1) - f(\eta)\}\,, \\ (\mathscr{L}_N^R f)(\eta) &= c_{N-1,N}(\eta)\,\{f(\eta^{N-1}) - f(\eta)\}\,. \end{aligned} \tag{1}$$

where, for $1 \leq x \leq N-2$,

$$\begin{aligned} c_{x,x+1}(\eta) &= \Big(1 + \frac{E}{N^\gamma}\Big)\eta(x)\,[1 - \eta(x+1)] \;+\; \eta(x+1)\,[1 - \eta(x)]\,, \\ c_{0,1}(\eta) &= \Big(\frac{\kappa}{N^\theta} + \frac{E}{N^\delta}\Big)\,\eta(0)\,[1 - \eta(1)] + \frac{\kappa}{N^\theta}\eta(1)\,[1 - \eta(0)]\,, \\ c_{N-1,N}(\eta) &= \Big(\frac{\kappa}{N^\theta} + \frac{E}{N^\delta}\Big)\eta(N-1)\,[1 - \eta(N)] \;+\; \frac{\kappa}{N^\theta}\eta(N)\,[1 - \eta(N-1)], \end{aligned}$$

with the convention that $\eta(0) = \alpha$ and $\eta(N) = \beta$. In these formulas, for $1 \leq x \leq N-2$, $\eta^{x,x+1}$ is the configuration obtained from η by exchanging the occupation variables $\eta(x)$ and $\eta(x+1)$:

$$(\eta^{x,x+1})(y) = \begin{cases} \eta(x+1), & y = x\,, \\ \eta(x), & y = x+1\,, \\ \eta(y), & y \neq x, x+1\,, \end{cases}$$

while for $x \in \{1, N-1\}$, η^x is the configuration obtained by flipping the occupation variable $\eta(x)$, that is $(\eta^x)(y) = \eta(y)\mathbf{1}_{y\neq x} + (1-\eta(y))\mathbf{1}_{y=x}$.

From now on we fix a finite time horizon $[0, T]$. The trajectories of our process $\{\eta_t : t \geq 0\}$ are elements of the Skorohod space $\mathscr{D}([0, T], \Omega_N)$, which is defined as the set of all functions $\eta_\cdot : [0, T] \to \Omega_N$ that are right continuous with left limits.

We observe that, since our process is a finite state Markov process, there exists a unique stationary measure. For $\alpha = \beta = \rho$ and $E = 0$ or $\gamma = \delta$ the invariant measure is the Bernoulli product measure ν_ρ^N with marginals

$$\nu_\rho^N\{\eta : \eta(x) = 1\} = \rho,$$

for $x \in \Lambda_N$. In fact, one can show that, when $\alpha = \beta = \rho$ and $E = 0$ this measure is also reversible. Nevertheless, for other values of the parameters, we do not have information about the stationary measure, except some partial description that can be given by the matrix ansatz method, but which, in fact, we do not use in this article.

2.2 Hydrodynamic Equations

We denote by $\langle \cdot, \cdot \rangle_\mu$ the inner product in $L^2([0, 1])$ with respect to a measure μ defined in $[0, 1]$ and $\| \cdot \|_{L^2(\mu)}$ is the corresponding norm. When μ is the Lebesgue measure we write $\langle \cdot, \cdot \rangle$ and $\| \cdot \|_{L^2}$ for the corresponding norm.

We denote by $C^{m,n}([0, T] \times [0, 1])$ the set of functions defined on $[0, T] \times [0, 1]$ that are m times continuously differentiable on the first variable and n times continuously differentiable on the second variable. For a function $G := G_t(q) \in C^{m,n}([0, T] \times [0, 1])$ we denote by $\partial_t G$ its derivative with respect to the time variable t and by ∇G and ΔG its first and second derivatives, respectively, with respect to the space variable q. The supremum norm is denoted by $\| \cdot \|_\infty$. Finally, $C_0^{m,n}([0, T] \times [0, 1])$ is the set of functions $G \in C^{m,n}([0, T] \times [0, 1])$ such that for any time t the function G_t vanishes at the boundary, that is, $G_t(0) = G_t(1) = 0$.

Now we want to define the space on which the solutions of the hydrodynamic equations will live, namely the Sobolev space $\mathscr{H}_1$ on $[0, 1]$. For that purpose, we define the semi inner-product $\langle \cdot, \cdot \rangle_1$ on the set $C^\infty([0, 1])$ by

$$\langle G, H \rangle_1 = \int_0^1 (\nabla G)(q)\,(\nabla H)(q)\,dq,$$

for $G, H \in C^\infty([0, 1])$ and the corresponding semi-norm is denoted by $\| \cdot \|_1$.

Definition 1 The Sobolev space $\mathscr{H}_1$ on $[0, 1]$ is the Hilbert space defined as the completion of $C^\infty([0, 1])$ for the norm $\| \cdot \|_{\mathscr{H}_1}^2 := \| \cdot \|_{L^2}^2 + \| \cdot \|_1^2$. Its elements coincide a.e. with continuous functions. The space $L^2([0, T], \mathscr{H}_1)$ is the set of measurable functions $f : [0, T] \to \mathscr{H}_1$ such that $\int_0^T \| f_s \|_{\mathscr{H}_1}^2 ds < \infty$.

We can now give the definition of the weak solutions of the hydrodynamic equations that will be derived. In what follows, $\rho_0 : [0, 1] \to [0, 1]$ is a measurable function and it is the initial condition of all the partial differential equations that we define below.

Definition 2 We say that $\rho : [0, T] \times [0, 1] \to [0, 1]$ is a weak solution of the viscous Burgers equation with Dirichlet boundary conditions

$$\begin{cases} \partial_t \rho(t, q) = \Delta\rho(t, q) - \mathfrak{e}\, \nabla\sigma(\rho(t, q)) \,, \quad t \in [0, T] \,, \quad q \in [0, 1] \,, \\ \rho(t, 0) = a \,, \quad \rho(t, 1) = b \,, \quad t \in [0, T], \\ \rho(0, q) = \rho_0(q) \,, \quad q \in [0, 1] \,, \end{cases} \tag{2}$$

if the following two conditions hold:

- $\rho \in L^2([0, T], \mathscr{H}_1)$;
- ρ satisfies the weak formulation

$$\begin{aligned} &\int_0^1 \rho_t(q) G_t(q)\, dq - \int_0^1 \rho_0(q) G_0(q)\, dq - \int_0^t \int_0^1 \rho_s(q) \Big(\Delta + \partial_s\Big) G_s(q)\, dq\, ds \\ &- \int_0^t \int_0^1 \mathfrak{e}\sigma(\rho_s(q)) \nabla G_s(q) dq ds + \int_0^t \big(b \nabla G_s(1) - a \nabla G_s(0)\big)\, ds = 0, \end{aligned} \tag{3}$$

for all $t \in [0, T]$ and any function $G \in C_0^{1,2}([0, T] \times [0, 1])$.

Above $\sigma(\rho)$ represents the mobility and it is given by $\sigma(\rho) = \rho(1 - \rho)$.

Observe that when $\mathfrak{e} = 0$ the equation above reduces to the heat equation.

Definition 3 We say that $\rho : [0, T] \times [0, 1] \to [0, 1]$ is a weak solution of the viscous Burgers equation with Robin boundary conditions

$$\begin{cases} \partial_t \rho(t, q) = \Delta\rho(t, q) - \mathfrak{e}\, \nabla\sigma(\rho(t, q)) \,, \quad t \in [0, T] \,, \quad q \in [0, 1] \,, \\ \nabla\rho(t, 0) = a\rho(t, 0) + b + \mathfrak{e}\sigma(\rho(t, 0)) \,, \quad t \in [0, T], \\ \nabla\rho(t, 1) = c\rho(t, 1) + d + \mathfrak{e}\sigma(\rho(t, 1)) \,, \quad t \in [0, T], \\ \rho(0, q) = \rho_0(q) \,, \quad q \in [0, 1] \,, \end{cases} \tag{4}$$

if the following two conditions hold:

- $\rho \in L^2([0, T], \mathscr{H}_1)$;
- ρ satisfies the weak formulation

$$\begin{aligned} &\int_0^1 \rho_t(q) G_t(q)\, dq - \int_0^1 \rho_0(q) G_0(q)\, dq - \int_0^t \int_0^1 \rho_s(q) \Big(\Delta + \partial_s\Big) G_s(q)\, dq\, ds \\ &- \int_0^t \int_0^1 \mathfrak{e}\sigma(\rho_s(q)) \nabla G_s(q)\, dq\, ds + \int_0^t \rho_s(1) \nabla G_s(1)\, ds - \int_0^t \rho_s(0) \nabla G_s(0)\, ds \\ &- \int_0^t \big(c\rho_s(1) + d\big) G_s(1)\, ds + \int_0^t \big(a\rho_s(0) + b\big) G_s(0)\, ds = 0, \end{aligned} \tag{5}$$

for all $t \in [0, T]$ and any function $G \in C^{1,2}([0, T] \times [0, 1])$.

The proof of the uniqueness of weak solutions in the case $\mathfrak{e} = 0$, which corresponds to the heat equation with Dirichlet, linear Robin or Neumann boundary conditions can be seen in Sect. 7 of [1]. For completeness we included in the Appendix the proof of uniqueness of weak solutions in the case $\mathfrak{e} \neq 0$ for Dirichlet or Neumann boundary conditions. Nevertheless, we assume the uniqueness of weak solutions for Robin boundary conditions in the case $\mathfrak{e} \neq 0$, but we believe that the proof could be adapted from the one in Sect. 7 of [5]. We leave this for a future work.

2.3 Hydrodynamic Limit

In this section we want to state the hydrodynamic limit of the process $\{\eta_{tN^2} : t \geq 0\}$ with state space Ω_N and infinitesimal generator $N^2\mathscr{L}_N$, where $\mathscr{L}_N$ is as defined in (1). Note that we are accelerating time by a factor of N^2. Let $\mathscr{M}^+$ be the space of positive measures on $[0, 1]$ with total mass bounded by 1 equipped with the weak topology. For any configuration $\eta \in \Omega_N$ we define the empirical measure $\pi^N(\eta, dq)$ on $[0, 1]$ by

$$\pi^N(\eta, dq) = \frac{1}{N-1} \sum_{x \in \Lambda_N} \eta(x) \delta_{\frac{x}{N}}(dq),$$

where δ_a is a Dirac mass on $a \in [0, 1]$, and

$$\pi_t^N(\eta_\cdot, dq) := \pi^N(\eta_{tN^2}, dq).$$

This measure gives weight $\frac{1}{N-1}$ to each occupied site of the configuration η.

We denote by $\mathbb{P}_{\mu_N}$ the probability measure on the Skorohod space $\mathscr{D}([0, T], \Omega_N)$ induced by the Markov process $\{\eta_{tN^2} : t \geq 0\}$ and initial distribution μ_N on Ω_N, and we denote by $\mathbb{E}_{\mu_N}$ the expectation with respect to $\mathbb{P}_{\mu_N}$. Now let $\{\mathbb{Q}_N\}_{N \geq 1}$ be the sequence of probability measures on $\mathscr{D}([0, T], \mathscr{M}^+)$ induced by the Markov process $\{\pi_t^N : t \geq 0\}$ and by $\mathbb{P}_{\mu_N}$.

At this point we need to fix an initial profile $\rho_0 : [0, 1] \to [0, 1]$ which is measurable and an initial distribution $\mu_N \in \Omega_N$. We are going to consider the following set of initial measures:

Definition 4 A sequence of probability measures $\{\mu_N\}_{N \geq 1}$ in Ω_N is associated with the profile $\rho_0(\cdot)$ if for any continuous function $G : [0, 1] \to \mathbb{R}$ and any $\varepsilon > 0$

$$\lim_{N \to \infty} \mu_N \Big(\eta \in \Omega_N : \Big| \frac{1}{N-1} \sum_{x \in \Lambda_N} G\left(\tfrac{x}{N}\right) \eta(x) - \int_0^1 G(q) \rho_0(q) dq \Big| > \varepsilon \Big) = 0.$$

Our main result is summarized in the following theorem.

Theorem 1 *Let $\rho_0 : [0, 1] \to [0, 1]$ be a measurable function and let $\{\mu_N\}_{N \geq 1}$ be a sequence of probability measures in Ω_N associated with $\rho_0(\cdot)$. Then, for any $t \in$*

$[0, T]$ and any $\varepsilon > 0$,

$$\lim_{N\to\infty} \mathbb{P}_{\mu_N}\left(\eta. : \left|\frac{1}{N-1}\sum_{x=1}^{N-1} G\left(\tfrac{x}{N}\right)\eta_{tN^2}(x) - \int_0^1 G(q)\rho_t(q)dq\right| > \varepsilon\right) = 0,$$

where $\rho_t(\cdot)$ is:

- *for $\gamma = 1$ the unique weak solution of*
  1. *for $\theta > 1$ and $\delta > 1$, the PDE (4) with $\mathfrak{e} = E$ and $a = b = c = d = 0$.*
  2. *for $\theta = 1$ and $\delta > 1$, the PDE (4) with $\mathfrak{e} = E$, $a = \kappa$, $b = -\kappa\alpha$, $c = -\kappa$ and $d = \kappa\beta$.*
  3. *for $\delta = 1$ and $\theta > 1$, the PDE (4) with $\mathfrak{e} = E$, $a = E\alpha$, $b = -E\alpha$, $c = -E(1-\beta)$ and $d = 0$.*
  4. *for $\theta = \delta = 1$, the PDE (4) with $\mathfrak{e} = E$, $a = \kappa + E\alpha$, $b = -(\kappa + E)\alpha$, $c = -(\kappa + E(1-\beta))$ and $d = \kappa\beta$.*
  5. *for $\theta = \delta \in [0, 1)$, the PDE (2) with $\mathfrak{e} = E$, $a = \frac{\alpha(\kappa+E)}{\kappa+\alpha E}$ and $b = \frac{\kappa\beta}{\kappa+E(1-\beta)}$.*
  6. *for $\theta \in [0, 1)$ and $\delta \geq 1$, the PDE (2) with $\mathfrak{e} = E$, $a = \alpha$ and $b = \beta$.*
- *for $\gamma > 1$ the unique weak solution of heat equation with the same boundary conditions as in the case $\gamma = 1$.*

The partial differential equations corresponding to the values of the parameters θ and δ are summarized in Fig. 2.

We note that above we obtained in the first four cases, for $\gamma = 1$ (resp. $\gamma > 1$) the viscous Burgers equation (resp. heat equation) with non-linear Robin boundary

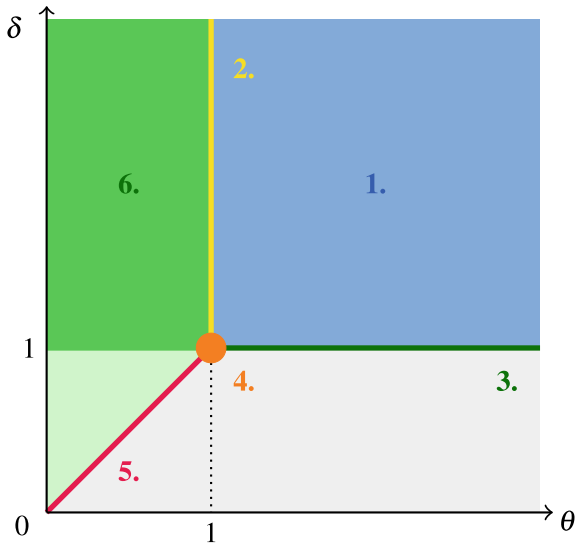

Fig. 2 Boundary conditions for the viscous Burgers equation (when $\gamma = 1$) and for the heat equation (when $\gamma > 1$) as functions of the model parameters θ and δ. The numbering refers to the equations above. The study of the regions in light green and grey is left for future work

conditions (resp. linear Robin or Neumann boundary conditions); and in the last two cases, the boundary conditions are of Dirichlet type.

Remark 1 We observe that, by changing the value of E to $\tilde{E}$ only on the rates $c_{0,1}(\eta)$ and changing E to E' only on the rates $c_{N-1,N(\eta)}$ we would obtain the same PDEs as above, except that on the boundary conditions, we would replace in both a and b the value E by $\tilde{E}$ and in both c and d we would replace the value E by E'.

The analysis of the region $\delta \in [0, 1)$ and $\theta \geq 0$ (apart the red line in Fig. 2) is left for a future work. Nevertheless, we conjecture that the green zone should continue up to the red line (the region in light green) and the remaining region (the region in grey) should correspond to the PDE (2) with $a = 1$ and $b = 0$ and with $\mathfrak{e} = 0$ when $\gamma > 1$ and $\mathfrak{e} = E$ when $\gamma = 1$.

The proof of last theorem follows the usual approach of convergence in distribution of stochastic processes: we have to prove tightness of the sequence $\{\mathbb{Q}_N\}_{N\geq 1}$ (which is done in Sect. 4) from where we conclude that the sequence $\{\mathbb{Q}_N\}_{N\geq 1}$ has a subsequence that converges weakly to some measure that we denote by $\mathbb{Q}$. Then we characterize this measure by showing that it is supported on trajectories of measures that satisfy $\pi_t(dq) = \rho_t(q)dq$ where $\rho_t(q)$ is the unique weak solution of the hydrodynamic equation. These two results combined give the convergence of $\{\mathbb{Q}_N\}_{N\geq 1}$ to $\mathbb{Q}$, as $N \to \infty$. Showing that the limit point $\mathbb{Q}$ is concentrated on trajectories of measures that are absolutely continuous with respect to the Lebesgue measure is a consequence of the fact that our process is an exclusion process (we refer the reader to [12] for a proof), and the proof that the density $\rho_t(\cdot)$ is a weak solution of the hydrodynamic equation goes through the help of auxiliary martingales associated to the empirical measure, this is done in Sect. 3. We only present the heuristic argument of this derivation, but since we prove all the replacement lemmas (see Sect. 5) that are necessary, the rigorous proof is simple and is left to the reader. From the uniqueness of the weak solutions of the equations, we conclude that $\{\mathbb{Q}_N\}_{N\geq 1}$ has a unique limit point $\mathbb{Q}$.

3 Heuristics for Hydrodynamic Equations

In this section we give the main ideas which are behind the identification of limit points as weak solutions of the partial differential equations given in Sect. 2.2. Now we argue that the density $\rho_t(\cdot)$ is a weak solution of the corresponding hydrodynamic equation for each regime of the parameters γ, θ, δ. In order to prove that $\rho_t(\cdot)$ satisfies the weak formulation we use auxiliary martingales associated to the Markov process $\{\eta_{tN^2} : t \geq 0\}$. For that purpose, fix a function $G \in C^{1,2}([0, T] \times [0, 1])$. By Dynkin's formula, see for example Lemma 5.1 of [12],

$$M_t^N(G) = \langle \pi_t^N, G\rangle - \langle \pi_0^N, G\rangle - \int_0^t (N^2\mathscr{L}_N + \partial_s)\langle \pi_s^N, G\rangle\, ds \tag{6}$$

is a martingale with respect to the natural filtration $\{\mathscr{F}_t\}_{t\geq 0}$, where for each $t \geq 0$, $\mathscr{F}_t := \sigma(\eta_s : s < t)$. By expanding the last term above and using the notation $\nabla_N^+ G_s(\frac{x}{N}) := N(G_s(\frac{x+1}{N}) - G_s(\frac{x}{N}))$, $\nabla_N^- G_s(\frac{x}{N}) := N(G_s(\frac{x}{N}) - G_s(\frac{x-1}{N}))$, $\Delta_N G_s(\frac{x}{N}) := N^2(G_s(\frac{x+1}{N}) - 2G_s(\frac{x}{N}) + G_s(\frac{x-1}{N}))$, we get the following expression:

$$
\begin{aligned}
M_t^N(G) = \langle \pi_t^N, G_t\rangle - \langle \pi_0^N, G_0\rangle - \int_0^t \langle \pi_s^N, \Delta_N G_s\rangle\, ds - \int_0^t \langle \pi_s^N, \partial_s G_s\rangle\, ds \\
- E\int_0^t \frac{N^{1-\gamma}}{N-1}\sum_{x=1}^{N-2} \nabla_N^+ G_s(\tfrac{x}{N})\eta_{sN^2}(x)(1-\eta_{sN^2}(x+1))\, ds \\
- \int_0^t \frac{N}{N-1}\nabla_N^+ G_s(\tfrac{1}{N})\eta_{sN^2}(1)\, ds + \int_0^t \frac{N}{N-1}\nabla_N^- G_s(\tfrac{N-1}{N})\eta_{sN^2}(N-1)\, ds \\
- \frac{N^2}{N-1}\int_0^t G_s(\tfrac{1}{N})\Big\{\frac{\kappa}{N^\theta}(\alpha - \eta_{sN^2}(1)) + \frac{E}{N^\delta}\alpha(1-\eta_{sN^2}(1))\Big\}\, ds \\
- \frac{N^2}{N-1}\int_0^t G_s(\tfrac{N-1}{N})\Big\{\frac{\kappa}{N^\theta}(\beta - \eta_{sN^2}(N-1)) - \frac{E}{N^\delta}(1-\beta)\eta_{sN^2}(N-1)\Big\}\, ds.
\end{aligned}
\tag{7}
$$

From this expression we will deduce the notion of weak solution of the equations presented above for several regimes of the parameters. We do not present the complete proof but we only highlight what are the ingredients one needs to obtain the results. First we observe that from Sect. 4 we see that $\mathbb{E}_{\mu_N}[(M_t^N(G))^2]$ vanishes as $N \to \infty$. Now we analyse the remaining terms. For that purpose we introduce some notation. We define $\Lambda_N^\varepsilon = \{1 + \varepsilon N, \ldots, N - 1 - \varepsilon N\}$ and denote by $\overrightarrow{\eta}_{sN^2}^{\varepsilon N}(x)$ (resp. $\overleftarrow{\eta}_{sN^2}^{\varepsilon N}(x)$) the empirical density in the box of size εN, which is given on $x \in \Lambda_N^\varepsilon$ by

$$
\overrightarrow{\eta}_{sN^2}^{\varepsilon N}(x) = \frac{1}{\varepsilon N}\sum_{y=x+1}^{x+\varepsilon N} \eta_{sN^2}(y) \qquad \Big(\text{resp.} \quad \overleftarrow{\eta}_{sN^2}^{\varepsilon N}(x) = \frac{1}{\varepsilon N}\sum_{y=x-\varepsilon N+1}^{x} \eta_{sN^2}(y)\Big).
\tag{8}
$$

Note that above, εN should be understood as $\lfloor \varepsilon N \rfloor$ and that $\overrightarrow{\eta}_{sN^2}^{\varepsilon N}(x) = \langle \pi_{sN^2}^N, \iota_\varepsilon^x\rangle$, where $\iota_\varepsilon^x(u) = \frac{1}{\varepsilon}\mathbf{1}_{(\frac{x}{N}, \frac{x}{N}+\varepsilon)}(u)$ and analogously for the definition of the left average. Heuristically, $\langle \pi_{sN^2}^N, \iota_\varepsilon^x\rangle$ converges, when $N \to \infty$, to $\langle \pi_s, \iota_\varepsilon^x\rangle = \int_0^1 \rho_s(u)\iota_\varepsilon^x(u)\, du$, where $\rho_s(\cdot)$ is the density profile that we want to characterize. Then, by taking the limit as $\varepsilon \to 0$ we obtain that $\langle \pi_s, \iota_\varepsilon^x\rangle$ converges to $\rho_s(\frac{x}{N})$. From the observation above we say that $\overrightarrow{\eta}_{sN^2}^{\varepsilon N}(x) \sim \rho_s(\frac{x}{N})$.

Now observe that a simple computation shows that the fifth term on the RHS of (7) vanishes if $\gamma > 1$, while for $\gamma = 1$, a simple application of Lemma 6 twice shows that we can replace that term by

$$
-E\int_0^t \frac{1}{N-1}\sum_{x=1}^{N-2} \nabla_N^+ G_s(\tfrac{x}{N})\,\overleftarrow{\eta}_{sN^2}^{\varepsilon N}(x)(1-\overrightarrow{\eta}_{sN^2}^{\varepsilon N}(x+1))\, ds.
$$

Indeed, to do that observe that the fifth term on the RHS of (7) can be written as

$$-E\int_0^t \frac{1}{N-1}\sum_{x\in\Lambda_N^\varepsilon}\nabla_N^+ G_s(\tfrac{x}{N})\eta_{sN^2}(x)(1-\eta_{sN^2}(x+1))\,ds+O(\varepsilon)$$

and now one applies Lemma 6 once to replace $\eta(x)$ by the average to the left and then again to replace $\eta(x+1)$ by the average to the right.

This term is the one that will change the nature of the PDE, so that for $\gamma>1$ we will derive the heat equation while for $\gamma=1$ we will derive the viscous Burgers equation.

Now we look at the boundary terms. The next terms are those on the third line of (7). From Lemma 5 we see that for $\theta,\delta<1$ (see the restriction on the parameters below) they can be replaced by

$$-\int_0^t \frac{N}{N-1}\nabla_N^+ G_s(0)r_\alpha\,ds+\int_0^t \frac{N}{N-1}\nabla_N^- G_s(1)r_\beta\,ds$$

(where r_α, r_β are defined in Sect. 5) while from Lemma 6 they can be replaced, for $\theta\geq 1$, by

$$-\int_0^t \frac{N}{N-1}\nabla_N^+ G_s(0)\overrightarrow{\eta}^{\varepsilon N}_{sN^2}(1)\,ds+\int_0^t \frac{N}{N-1}\nabla_N^- G_s(\tfrac{N-1}{N})\overleftarrow{\eta}^{\varepsilon N}_{sN^2}(N-1)\,ds.$$

The next terms on the list are those on the fourth line of (7), which, for $\theta=\delta<1$ or $\theta<1,\delta\geq 1$ and by using the fact that in this regime the space of test functions is $G\in C_0^{1,2}([0,T]\times[0,1])$, vanish as $N\to+\infty$. For $\theta>1$ and $\delta>1$ those terms vanish as $N\to+\infty$. Finally for $\theta=\delta=1$, as a consequence of Lemma 6 these terms can be replaced by

$$-\frac{N^2}{N-1}\int_0^t G_s(\tfrac{1}{N})\Big\{\frac{\kappa}{N}(\alpha-\overrightarrow{\eta}^{\varepsilon N}_{sN^2}(1))-\frac{E}{N}\alpha(1-\overleftarrow{\eta}^{\varepsilon N}_{sN^2}(N-1))\Big\}\,ds.$$

For $\theta=1$ and $\delta>1$ those terms can be replaced by

$$-\frac{N^2}{N-1}\int_0^t G_s(\tfrac{1}{N})\Big\{\frac{\kappa}{N}(\alpha-\overrightarrow{\eta}^{\varepsilon N}_{sN^2}(1))\Big\}\,ds$$

and for $\delta=1$ and $\theta>1$ those terms can be replaced by

$$-\frac{N^2}{N-1}\int_0^t G_s(\tfrac{1}{N})\Big\{\frac{E}{N}\alpha(1-\overrightarrow{\eta}^{\varepsilon N}_{sN^2}(1))\Big\}\,ds.$$

The terms related to the right boundary can be analysed as we just did for the left boundary. Then, taking the limit $N\to\infty$ and $\varepsilon\to 0$ in each of the expressions that we have derived, we obtain for $\gamma=1$ (for $\gamma>1$ just ignore the nonlinear term in the equation):

1. $\theta > 1$ and $\delta > 1$:

$$0 = \langle \rho_t^N, G_t \rangle - \langle \rho_0^N, G_0 \rangle - \int_0^t \langle \rho_s, \Delta G_s \rangle \, ds - \int_0^t \langle \rho_s, \partial_s G_s \rangle \, ds$$
$$- E \int_0^t \langle \nabla G_s, \rho_s(1-\rho_s) \rangle \, ds - \int_0^t \nabla G_s(0) \rho_s(0) \, ds + \int_0^t \nabla G_s(1) \rho_s(1) \, ds$$

which corresponds to (4) with $\mathfrak{e} = E$ and $a = b = c = d = 0$.

2. $\theta = 1$ and $\delta > 1$:

$$0 = \langle \rho_t^N, G_t \rangle - \langle \rho_0^N, G_0 \rangle - \int_0^t \langle \rho_s, \Delta G_s \rangle \, ds - \int_0^t \langle \rho_s, \partial_s G_s \rangle \, ds$$
$$- E \int_0^t \langle \nabla G_s, \rho_s(1-\rho_s) \rangle \, ds - \int_0^t \nabla G_s(0) \rho_s(0) \, ds + \int_0^t \nabla G_s(1) \rho_s(1) \, ds$$
$$- \int_0^t G_s(0) \kappa(\alpha - \rho_s(0)) \, ds - \int_0^t G_s(1) \kappa(\beta - \rho_s(1)) \, ds$$

which corresponds to (4) with $\mathfrak{e} = E$ and $a = \kappa$, $b = -\kappa\alpha$, $c = -\kappa$ and $d = \kappa\beta$.

3. $\delta = 1$ and $\theta > 1$:

$$0 = \langle \rho_t^N, G_t \rangle - \langle \rho_0^N, G_0 \rangle - \int_0^t \langle \rho_s, \Delta G_s \rangle \, ds - \int_0^t \langle \rho_s, \partial_s G_s \rangle \, ds$$
$$- E \int_0^t \langle \nabla G_s, \rho_s(1-\rho_s) \rangle \, ds - \int_0^t \nabla G_s(0) \rho_s(0) \, ds + \int_0^t \nabla G_s(1) \rho_s(1) \, ds$$
$$- \int_0^t G_s(0) E\alpha(1 - \rho_s(0)) \, ds + \int_0^t G_s(1) E(1-\beta) \rho_s(1) \, ds$$

which corresponds to (4) with $\mathfrak{e} = E$ and $a = E\alpha$, $b = -E\alpha$, $c = -E(1-\beta)$ and $d = 0$.

4. $\delta = \theta = 1$:

$$0 = \langle \rho_t^N, G_t \rangle - \langle \rho_0^N, G_0 \rangle - \int_0^t \langle \rho_s, \Delta G_s \rangle \, ds - \int_0^t \langle \rho_s, \partial_s G_s \rangle \, ds$$
$$- E \int_0^t \langle \nabla G_s, \rho_s(1-\rho_s) \rangle \, ds - \int_0^t \nabla G_s(0) \rho_s(0) \, ds + \int_0^t \nabla G_s(1) \rho_s(1) \, ds$$
$$- \int_0^t G_s(0)((\kappa + E)\alpha - \rho_s(0)(\kappa + E\alpha)) \, ds$$
$$- \int_0^t G_s(1)(\kappa\beta - (\kappa + E(1-\beta)) \rho_s(1) \, ds$$

which corresponds to (4) with $\mathfrak{e} = E$ and $a = \kappa + E\alpha$, $b = -(\kappa + E)\alpha$, $c = -(\kappa + E(1-\beta))$ and $d = \kappa\beta$.

5. $\delta = \theta < 1$:

$$0 = \langle \rho_t^N, G_t \rangle - \langle \rho_0^N, G_0 \rangle - \int_0^t \langle \rho_s, \Delta G_s \rangle \, ds - \int_0^t \langle \rho_s, \partial_s G_s \rangle \, ds$$
$$- E \int_0^t \langle \nabla G_s, \rho_s(1-\rho_s) \rangle \, ds - \int_0^t \nabla G_s(0) \frac{\alpha(\kappa + E)}{\kappa + \alpha E} \, ds + \int_0^t \nabla G_s(1) \frac{\kappa \beta}{\kappa + E - \beta E}, \, ds$$

which corresponds to (2) with $\mathfrak{e} = E$ and $a = \frac{\alpha(\kappa+E)}{\kappa+\alpha E}$ and $b = \frac{\kappa\beta}{\kappa+E-\beta E}$.

6. $\theta \in [0, 1)$ and $\delta \geq 1$:

$$0 = \langle \rho_t^N, G_t \rangle - \langle \rho_0^N, G_0 \rangle - \int_0^t \langle \rho_s, \Delta G_s \rangle \, ds - \int_0^t \langle \rho_s, \partial_s G_s \rangle \, ds$$
$$- E \int_0^t \langle \nabla G_s, \rho_s(1-\rho_s) \rangle \, ds - \int_0^t \nabla G_s(0) \alpha \, ds + \int_0^t \nabla G_s(1) \beta \, ds$$

which corresponds to (2) with $\mathfrak{e} = E$ and $a = \alpha$ and $b = \beta$.

The remaining cases of θ and δ are left open for a future work.

4 Tightness

In this section we show that the sequence of probability measures $\{\mathbb{Q}_N\}_{N\geq 1}$ is tight in the Skorohod space $\mathscr{D}([0, T], \mathscr{M}^+)$. Tightness of this sequence implies that every subsequence of $\{\mathbb{Q}_N\}_{N\in\mathbb{N}}$ has a further subsequence which is weakly convergent.

Since $C^1([0, 1])$ is dense in $C([0, 1])$ in the uniform topology, by Proposition 1.7 of Chap. 4 in [12] it is enough to show that for every $G \in C^1([0, 1])$ the sequence of measures associated with the real-valued processes $\langle \pi_t^N, G \rangle$ is tight. In order to do that, we invoke Aldous' criterion [12], stated as follows:

Lemma 1 *A sequence $\{P_N\}_{N\geq 1}$ of probability measures on $\mathscr{D}([0, T], \mathscr{M}^+)$ is tight if these two conditions hold:*
a. *For every $t \in [0, T]$ and every $\varepsilon > 0$, there exists a compact set $K_\varepsilon^t \subset \mathscr{M}^+$ such that*

$$\sup_{N\geq 1} P_N\big(\pi_t \notin K_\varepsilon^t\big) < \varepsilon$$

b. *For every $\varepsilon > 0$*

$$\lim_{l\to 0} \limsup_{N\to\infty} \sup_{\tau\in\mathscr{T}_T, t\leq l} P_N\big(d(\pi_\tau, \pi_{\tau+t}) > \varepsilon\big) = 0,$$

where $\mathscr{T}_T$ denotes the set of stopping times with respect to the canonical filtration, bounded by T, and d is any metric in the space $\mathscr{M}^+$ inducing the weak topology.

In our case, condition **a.** reduces to

$$\lim_{A\to\infty} \sup_{N\geq 1} \mathbb{P}_{\mu_N}\big(|\langle \pi_t^N, G \rangle| > A\big) = 0. \tag{9}$$

To prove this, note that for any $A > 0$ and any $N \in \mathbb{N}$, by Markov's inequality,

$$\mathbb{P}_{\mu_N}\big(|\langle \pi_t^N, G\rangle| > A\big) \le \frac{1}{A}\mathbb{E}_{\mu_N}\big[|\langle \pi_t^N, G\rangle|\big] = \frac{1}{A}\mathbb{E}_{\mu_N}\Big[\Big|\frac{1}{N-1}\sum_{x\in\Lambda_N} G(\tfrac{x}{N})\eta_{tN^2}(x)\Big|\Big].$$

Since $|\eta_{tN^2}(x)| \le 1$, the last expression is bounded by $\frac{1}{A}\|G\|_\infty$, and (9) holds.

To establish condition **b.** above, we must show that, for every $\varepsilon > 0$ and $G \in C^1([0,1])$,

$$\lim_{l\to 0}\limsup_{N\to\infty}\sup_{\tau\in\mathscr{T}_T, t\le l}\mathbb{P}_{\mu_N}\Big(\eta_\cdot : \big|\langle \pi_{\tau+t}^N, G\rangle - \langle \pi_\tau^N, G\rangle\big| > \varepsilon\Big) = 0, \tag{10}$$

where all stopping times are bounded by T (thus $\tau + t$ should be understood as $(\tau + t) \wedge T$, where $\wedge$ denotes the minimum).

Let $C_c^m([0,1])$ denote the set of all m times continuously differentiable real-valued functions with compact support contained in $(0,1)$. We begin by showing that (10) holds for functions $G \in C_c^2([0,1])$. Recall (6). Then

$$\begin{aligned}
&\mathbb{P}_{\mu_N}\Big(\eta_\cdot : \Big|\langle \pi_{\tau+t}^N, G\rangle - \langle \pi_\tau^N, G\rangle\Big| > \varepsilon\Big)\\
&= \mathbb{P}_{\mu_N}\Big(\eta_\cdot : \Big|M_{\tau+t}^N(G) - M_\tau^N(G) + \int_\tau^{\tau+t} N^2\mathscr{L}_N\langle \pi_s^N, G\rangle\, ds\Big| > \varepsilon\Big)\\
&\le \mathbb{P}_{\mu_N}\Big(\eta_\cdot : \Big|M_{\tau+t}^N(G) - M_\tau^N(G)\Big| > \frac{\varepsilon}{2}\Big) + \mathbb{P}_{\mu_N}\Big(\eta_\cdot : \Big|\int_\tau^{\tau+t} N^2\mathscr{L}_N\langle \pi_s^N, G\rangle\, ds\Big| > \frac{\varepsilon}{2}\Big).
\end{aligned}$$

Applying, to the first term on the RHS of last inequality, Chebyshev's (resp. Markov's) inequality to the first (resp. second), we can bound the previous expression by

$$\frac{4}{\varepsilon^2}\mathbb{E}_{\mu_N}\Big[\Big(M_{\tau+t}^N(G) - M_\tau^N(G)\Big)^2\Big] + \frac{2}{\varepsilon}\mathbb{E}_{\mu_N}\Big[\Big|\int_\tau^{\tau+t} N^2\mathscr{L}_N\langle \pi_s^N, G\rangle\, ds\Big|\Big].$$

Therefore it is enough to show the next two limits:

$$\lim_{l\to 0}\limsup_{N\to\infty}\sup_{\tau\in\mathscr{T}_T, t\le l}\mathbb{E}_{\mu_N}\Big[\Big|\int_\tau^{\tau+t} N^2\mathscr{L}_N\langle \pi_s^N, G\rangle\, ds\Big|\Big] = 0 \tag{11}$$

$$\lim_{l\to 0}\limsup_{N\to\infty}\sup_{\tau\in\mathscr{T}_T, t\le l}\mathbb{E}_{\mu_N}\Big[\Big(M_{\tau+t}^N(G) - M_\tau^N(G)\Big)^2\Big] = 0. \tag{12}$$

Since we are assuming that $G \in C_c^2([0,1])$, there exists $N_0 \in \mathbb{N}$ such that $G(0) = G(\frac{1}{N}) = G(\frac{N-1}{N}) = G(1) = 0$ for all $N \ge N_0$. Since $|\eta_{sN^2}(x)| \le 1$, we have

$$\left|N^2\mathscr{L}_N\langle\pi_s^N, G\rangle\right| = \left|\langle\pi_s^N, \Delta_N G\rangle + \frac{E}{N-1}\sum_{x=1}^{N-2}\nabla_N^+ G(\tfrac{x}{N})\eta_{sN^2}(x)(1-\eta_{sN^2}(x+1))\right|$$
$$\leq \|G''\|_\infty + E\|G'\|_\infty$$

for $N \geq N_0$. Therefore there exists a constant C such that $|N^2\mathscr{L}_N\langle\pi_s^N, G\rangle| \leq C$ for all $N \in \mathbb{N}$, and (11) follows.

Let us now prove (12). By Dynkin's formula, see for example Lemma 5.1 of [12],

$$M_t^N(G)^2 - \int_0^t N^2[\mathscr{L}_N\langle\pi_s^N, G\rangle^2 - 2\langle\pi_s^N, G\rangle\mathscr{L}_N\langle\pi_s^N, G\rangle]\,ds$$

is a martingale with respect to $\{\mathscr{F}_t\}_{t\geq 0}$. From this, and since τ is a stopping time, it follows that

$$\mathbb{E}_{\mu_N}\Big[\Big(M_{\tau+t}^N(G) - M_\tau^N(G)\Big)^2\Big] = \mathbb{E}_{\mu_N}\Big[\int_\tau^{\tau+t} N^2[\mathscr{L}_N\langle\pi_s^N, G\rangle^2 - 2\langle\pi_s^N, G\rangle\mathscr{L}_N\langle\pi_s^N, G\rangle]ds\Big].$$

A computation shows that, for $N \geq N_0$,

$$N^2[\mathscr{L}_N\langle\pi_s^N, G\rangle^2 - 2\langle\pi_s^N, G\rangle\mathscr{L}_N\langle\pi_s^N, G\rangle]$$
$$= \frac{1}{(N-1)^2}\sum_{x=1}^{N-2} c_{x,x+1}(\eta_{sN^2})(\eta_{sN^2}(x) - \eta_{sN^2}(x+1))^2(\nabla_N^+ G(\tfrac{x}{N}))^2.$$

Since $|c_{x,x+1}(\eta_{sN^2})| \leq 2 + E$, the last expression is bounded by $\frac{2+E}{N}\|G'\|_\infty$, and therefore it goes to zero as $N \to \infty$. This finishes the proof for $G \in C_c^2([0,1])$.

Assume now that $G \in C^1([0,1])$. Since $C_c^2([0,1])$ is dense in $C^1([0,1])$ wrt the $\mathbb{L}^1$ topology, there exists a sequence $\{G_k\}_{k\geq 1}$ of functions in $C_c^2([0,1])$ such that $\|G_k - G\|_1 \to 0$. Since the probability in (10) is less than or equal to

$$\mathbb{P}_{\mu_N}\Big(\eta_\cdot : \Big|\langle\pi_{\tau+t}^N, G_k\rangle - \langle\pi_\tau^N, G_k\rangle\Big| > \frac{\varepsilon}{2}\Big) + \mathbb{P}_{\mu_N}\Big(\eta_\cdot : \Big|\langle\pi_{\tau+t}^N, G - G_k\rangle - \langle\pi_\tau^N, G - G_k\rangle\Big| > \frac{\varepsilon}{2}\Big)$$

and $G_k \in C_c^2([0,1])$, by the computation above it remains only to check that the last probability vanishes as $N \to \infty$ and then $k \to \infty$. For that purpose, note that

$$\big|\langle\pi_{\tau+t}^N, G - G_k\rangle - \langle\pi_\tau^N, G - G_k\rangle\big| \leq \frac{2}{N}\sum_{x=1}^{N-1}\big|(G - G_k)(\tfrac{x}{N})\big|$$
$$\leq 2\sum_{x=1}^{N-1}\int_{\frac{x}{N}}^{\frac{x+1}{N}}\big|(G - G_k)(\tfrac{x}{N}) - (G - G_k)(q)\,dq\big| + 2\int_0^1\big|(G - G_k)(q)\big|\,dq$$
$$\leq \frac{2}{N}\|(G - G_k)'\|_\infty + 2\int_0^1\big|(G - G_k)(q)\big|\,dq.$$

The result follows by taking $N \to \infty$ and then $k \to \infty$.

5 Replacement Lemmas

This section is devoted to the proof of the two lemmas mentioned in Sect. 3, using methods similar to those in [2, 8].

5.1 Estimates on Dirichlet Forms

We consider $\rho : [0,1] \to [0,1]$ to be a Lipschitz continuous function and we take $r_\alpha, r_\beta \in (0,1)$ satisfying $r_\alpha \le \rho(q) \le r_\beta$ for $q \in [0,1]$ such that $\rho(0) = r_\alpha$, $\rho(1) = r_\beta$. Denote by $\nu^N_{\rho(\cdot)}$ the Bernoulli product measure on Ω_N with marginals

$$\nu^N_{\rho(\cdot)}\{\eta : \eta(x) = 1\} = \rho(\tfrac{x}{N}),$$

for $x \in \Lambda_N$. For functions $f, g : \Omega_N \to \mathbb{R}$ and a probability measure μ on Ω_N, the inner product in $L^2(\Omega_N, \mu)$ is denoted by $\langle f, g\rangle_\mu = \int_{\Omega_N} f(\eta) g(\eta) d\mu$.

Lemma 2 *Let $T : \Omega_N \to \Omega_N$ be a transformation, (either the exchange $\eta^{x,y}$ or the flip η^x), $c : \Omega_N \to \mathbb{R}$ a positive function and f a density with respect to a probability measure μ on Ω_N. Then*

$$\begin{aligned}\int c(\eta)\left[\sqrt{f(T(\eta))} - \sqrt{f(\eta)}\right]\sqrt{f(\eta)}\, d\mu \\ = -\frac{1}{2}\int c(\eta)\left[\sqrt{f(T(\eta))} - \sqrt{f(\eta)}\right]^2 d\mu \\ + \frac{1}{2}\int \left[\sqrt{f(T(\eta))}\right]^2 \left[c(\eta) - c(T(\eta))\frac{\mu(T(\eta))}{\mu(\eta)}\right] d\mu.\end{aligned} \tag{13}$$

Proof To prove the result, it is enough to write the term at the LHS of (13) as its half plus its half and to sum and subtract the term needed to complete the square.

We recall Lemmas 5.1 and 5.2 of [2]:

Lemma 3 *Let $T : \Omega_N \to \Omega_N$ be a transformation, $c : \Omega_N \to \mathbb{R}$ a positive function and f a density with respect to a probability measure μ on Ω_N. Then*

$$\begin{aligned}
&\Big\langle c(\eta)\Big(\sqrt{f(T(\eta))}-\sqrt{f(\eta)}\Big),\sqrt{f(\eta)}\Big\rangle_{\mu}\\
&\leq -\frac{1}{4}\int_{\Omega_N} c(\eta)\Big(\sqrt{f(T(\eta))}-\sqrt{f(\eta)}\Big)^2 d\mu\\
&+\frac{1}{16}\int_{\Omega_N}\frac{1}{c(\eta)}\Big[c(\eta)-c(T(\eta))\frac{\mu(T(\eta))}{\mu(\eta)}\Big]^2\Big(\sqrt{f(T(\eta))}+\sqrt{f(\eta)}\Big)^2 d\mu
\end{aligned}$$

Lemma 4 *Let $\rho(\cdot)$ be as described above. There exists a constant C such that, for any $N\in\mathbb{N}$ and any density f with respect to $\nu^N_{\rho(\cdot)}$,*

$$\sup_{1\leq x\leq N-2}\int_{\Omega_N} f(\eta^{x,x+1})d\nu^N_{\rho(\cdot)}(\eta)\leq C,\quad \sup_{x\in\{1,N-1\}}\int_{\Omega_N} f(\eta^{x})d\nu^N_{\rho(\cdot)}(\eta)\leq C.$$

We introduce the following non-negative functions, defined for densities f with respect to $\nu^N_{\rho(\cdot)}$:

$$\begin{aligned}
\mathscr{D}^L_N(\sqrt{f},\nu^N_{\rho(\cdot)}) &= \int_{\Omega_N} c_{0,1}(\eta)\Big(\sqrt{f(\eta^1)}-\sqrt{f(\eta)}\Big)^2 d\nu^N_{\rho(\cdot)},\\
\mathscr{D}^R_N(\sqrt{f},\nu^N_{\rho(\cdot)}) &= \int_{\Omega_N} c_{N-1,N}(\eta)\Big(\sqrt{f(\eta^{N-1})}-\sqrt{f(\eta)}\Big)^2 d\nu^N_{\rho(\cdot)},\\
\mathscr{D}^B_N(\sqrt{f},\nu^N_{\rho(\cdot)}) &= \sum_{x=1}^{N-2}\int_{\Omega_N} c_{x,x+1}(\eta)\Big(\sqrt{f(\eta^{x,x+1})}-\sqrt{f(\eta)}\Big)^2 d\nu^N_{\rho(\cdot)}.
\end{aligned}$$

As a consequence of Lemma 2 we conclude that

Corollary 1 *Let $\rho(\cdot)$ be a profile. There exists a constant $C>0$ such that, for any density f and $N\in\mathbb{N}$,*

$$\langle\mathscr{L}^L_N\sqrt{f},\sqrt{f}\rangle_{\nu^N_{\rho(\cdot)}}\leq -\frac{1}{2}\mathscr{D}^L_N(\sqrt{f},\nu^N_{\rho(\cdot)})+C\Big|\frac{\kappa}{N^\theta}\Big(\rho(\tfrac{1}{N})-\alpha\Big)+\frac{\alpha E}{N^\delta}\Big(\rho(\tfrac{1}{N})-1\Big)\Big|, \tag{14}$$

$$\begin{aligned}
\langle\mathscr{L}^R_N\sqrt{f},\sqrt{f}\rangle_{\nu^N_{\rho(\cdot)}} &\leq -\frac{1}{2}\mathscr{D}^R_N(\sqrt{f},\nu^N_{\rho(\cdot)})\\
&\quad + C\Big|\frac{\kappa}{N^\theta}\Big(\rho(\tfrac{N-1}{N})-\beta\Big)+\frac{(1-\beta)E}{N^\delta}\rho(\tfrac{N-1}{N})\Big|.
\end{aligned} \tag{15}$$

Proof We present the proof for the left boundary since the other case is analogous. By Lemma 2,

$$\langle \mathscr{L}_N^L \sqrt{f}, \sqrt{f} \rangle_{\nu^N_{\rho(\cdot)}} = -\frac{1}{2} \mathscr{D}_N^L(\sqrt{f}, \nu^N_{\rho(\cdot)}) + \frac{1}{2} \int_{\Omega_N} \Big[c_{0,1}(\eta) - c_{0,1}(\eta^1) \frac{\nu^N_{\rho(\cdot)}(\eta^1)}{\nu^N_{\rho(\cdot)}(\eta)} \Big] \Big(\sqrt{f(\eta^1)} \Big)^2 d\nu^N_{\rho(\cdot)}.$$

Let $\bar{\eta} \in \{0,1\}^{\{2,\dots,N-1\}}$ denote the configuration obtained from η by discarding its value at 1, so that $\eta = (1, \bar{\eta})$ if $\eta(1) = 1$ and $\eta = (0, \bar{\eta})$ if $\eta(1) = 0$. The second term on the RHS of last expression inside can be written as

$$\begin{aligned} &\frac{1}{2} \sum_{\bar{\eta}} \left[\frac{(1-\alpha)\kappa}{N^\theta} - \alpha \Big(\frac{\kappa}{N^\theta} + \frac{E}{N^\delta} \Big) \frac{(1 - \rho(\frac{1}{N}))}{\rho(\frac{1}{N}))} \right] f(0, \bar{\eta}) \nu^N_{\rho(\cdot)}(1, \bar{\eta}) \\ &+ \frac{1}{2} \sum_{\bar{\eta}} \left[\alpha \Big(\frac{\kappa}{N^\theta} + \frac{E}{N^\delta} \Big) - \frac{(1-\alpha)\kappa}{N^\theta} \frac{\rho(\frac{1}{N})}{(1 - \rho(\frac{1}{N}))} \right] f(1, \bar{\eta}) \nu^N_{\rho(\cdot)}(0, \bar{\eta}) \\ &\leq C \Big| \frac{\kappa}{N^\theta} \Big(\rho(\tfrac{1}{N}) - \alpha \Big) + \frac{\alpha E}{N^\delta} \Big(\rho(\tfrac{1}{N}) - 1 \Big) \Big|. \end{aligned}$$

Corollary 2 *Let $\rho(\cdot)$ be a Lipschitz continuous function. There exists a constant $C > 0$ such that, for any density f and $N \in \mathbb{N}$,*

$$\langle \mathscr{L}_N^B \sqrt{f}, \sqrt{f} \rangle_{\nu^N_{\rho(\cdot)}} \leq -\frac{1}{4} \mathscr{D}_N^B(\sqrt{f}, \nu^N_{\rho(\cdot)}) + C \Big(\frac{1}{N} + \frac{1}{N^{2\gamma - 1}} \Big).$$

Proof By Lemma 3,

$$\begin{aligned} \langle \mathscr{L}_N^B \sqrt{f}, \sqrt{f} \rangle_{\nu^N_{\rho(\cdot)}} \leq &-\frac{1}{4} \mathscr{D}_N^B(\sqrt{f}, \nu^N_{\rho(\cdot)}) \\ &+ \frac{1}{16} \sum_{x=1}^{N-2} \int_{\Omega_N} \frac{1}{c_{x,x+1}(\eta)} \Big[c_{x,x+1}(\eta) - c_{x,x+1}(\eta^{x,x+1}) \frac{\nu^N_{\rho(\cdot)}(\eta^{x,x+1})}{\nu^N_{\rho(\cdot)}(\eta)} \Big]^2 \times \\ &\times \Big(\sqrt{f(\eta^{x,x+1})} + \sqrt{f(\eta)} \Big)^2 d\nu^N_{\rho(\cdot)}. \end{aligned}$$

For any $1 \leq x \leq N-2$, the expression inside last sum is equal to

$$\begin{aligned} &\sum_{\zeta} \frac{1}{1 + \frac{E}{N^\gamma}} \left[1 + \frac{E}{N^\gamma} - \frac{\rho(\frac{x+1}{N})(1 - \rho(\frac{x}{N}))}{(1 - \rho(\frac{x+1}{N}))\rho(\frac{x}{N})} \right]^2 \Big(\sqrt{f(\zeta)} + \sqrt{f(\zeta^{x,x+1})} \Big)^2 \nu^N_{\rho(\cdot)}(\zeta) \\ &+ \sum_{\zeta} \left[1 - \Big(1 + \frac{E}{N^\gamma} \Big) \frac{\rho(\frac{x}{N})(1 - \rho(\frac{x+1}{N}))}{(1 - \rho(\frac{x}{N}))\rho(\frac{x+1}{N})} \right]^2 \Big(\sqrt{f(\zeta)} + \sqrt{f(\zeta^{x,x+1})} \Big)^2 \nu^N_{\rho(\cdot)}(\zeta) \end{aligned}$$

where the first sum is over all configurations $\zeta \in \Omega_N$ satisfying $\zeta(x) = 1, \zeta(x+1) = 0$, and the second sum over those $\zeta \in \Omega_N$ such that $\zeta(x) = 0$, $\zeta(x+1) = 1$. By Lemma 4, we conclude that

$$\langle \mathscr{L}_N^B \sqrt{f}, \sqrt{f} \rangle_{\nu^N_{\rho(\cdot)}} \leq -\frac{1}{4} \mathscr{D}_N^B(\sqrt{f}, \nu^N_{\rho(\cdot)}) + C \sum_{x=1}^{N-2} \left(\left| \rho\left(\tfrac{x+1}{N}\right) - \rho\left(\tfrac{x}{N}\right) \right| + \frac{E}{N^\gamma} \right)^2$$

for some constant C. Since $\rho(\cdot)$ is Lipschitz continuous, we get

$$\langle \mathscr{L}_N^B \sqrt{f}, \sqrt{f} \rangle_{\nu^N_{\rho(\cdot)}} \leq -\frac{1}{4} \mathscr{D}_N^B(\sqrt{f}, \nu^N_{\rho(\cdot)}) + C\Big(\frac{1}{N} + \frac{1}{N^{2\gamma-1}} \Big).$$

Remark 2 Now, we analyze the bounds obtained above in different regimes of θ and δ. Observe that the bound above simplifies to (without requiring anything on the values of the profile $\rho(\cdot)$ at $q = 0$ nor at $q = 1$)

$$\langle \mathscr{L}_N \sqrt{f}, \sqrt{f} \rangle_{\nu^N_{\rho(\cdot)}} \leq -\frac{1}{4} \mathscr{D}_N(\sqrt{f}, \nu^N_{\rho(\cdot)}) + C\Big(\frac{1}{N^\theta} + \frac{1}{N} + \frac{1}{N^\delta} + \frac{1}{N^{2\gamma-1}} \Big). \quad (16)$$

This will be useful in the cases $\theta \geq 1$ and $\delta \geq 1$ below. When $\theta = \delta < 1$, we ask that $\rho(0) = r_\alpha$ and $\rho(1) = r_\beta$, where r_α and r_β are defined as

$$r_\alpha = \frac{\alpha(\kappa + E)}{\kappa + \alpha E}, \quad r_\beta = \frac{\kappa\beta}{\kappa + E - \beta E}, \quad (17)$$

and, since we assumed $\rho(\cdot)$ to be Lipschitz, we get the bound:

$$\langle \mathscr{L}_N \sqrt{f}, \sqrt{f} \rangle_{\nu^N_{\rho(\cdot)}} \leq -\frac{1}{4} \mathscr{D}_N(\sqrt{f}, \nu^N_{\rho(\cdot)}) + C\Big(\frac{1}{N^{\theta+1}} + \frac{1}{N} + \frac{1}{N^{2\gamma-1}} \Big). \quad (18)$$

In the case $\delta \geq 1$ and $\theta \in [0, 1)$, by asking that $\rho(0) = \alpha$ (and $\rho(1) = \beta$) and $\rho(\cdot)$ to be Lipschitz we get the bound:

$$\langle \mathscr{L}_N \sqrt{f}, \sqrt{f} \rangle_{\nu^N_{\rho(\cdot)}} \leq -\frac{1}{4} \mathscr{D}_N(\sqrt{f}, \nu^N_{\rho(\cdot)}) + C\Big(\frac{1}{N^{\theta+1}} + \frac{1}{N^\delta} + \frac{1}{N} + \frac{1}{N^{2\gamma-1}} \Big). \quad (19)$$

Now that we have all the ingredients we need we state and prove the replacement lemmas we need. The next lemma will be used in the Dirichlet case.

Lemma 5 *Let $F : \mathbb{N} \times [0, T] \to \mathbb{R}$ be a bounded function and suppose that*

(1) $\theta = \delta < 1$
(2) $\theta \in [0, 1)$ *and* $\delta \geq 1$.

Then, for any $t \in [0, T]$,

$$\lim_{N\to\infty} \mathbb{E}_{\mu_N}\left[\left|\int_0^t F(N,s)(\eta_{sN^2}(1)-r_\alpha)\,ds\right|\right]=0,$$

where in

(1) r_α *and* r_β *where defined in* (17).
(2) $r_\alpha=\alpha$ *and* $r_\beta=\beta$.

The same estimate above holds replacing $\eta(1)$ *by* $\eta(N-1)$ *and* r_α *by* r_β.

The next lemma will be used in the Robin cases for $x=1$ and $x=N-1$ to deal with the boundary terms and in all the cases for $x\in\Lambda_n^\varepsilon$ to treat the bulk term coming from the weak asymmetry.

Lemma 6 *Fix* x. *Let* $F:\mathbb{N}\times\Omega_N\times[0,T]\to\mathbb{R}$ *be a bounded function whose support does not intersect the set of points* $\{x+1,\dots,x+\varepsilon N\}$. *Then, for any* $t\in[0,T]$ *and for any* x

$$\lim_{\varepsilon\to 0}\lim_{N\to\infty}\mathbb{E}_{\mu_N}\left[\left|\int_0^t F(N,\eta_{sN^2},s)(\eta_{sN^2}(x)-\overrightarrow{\eta}^{\varepsilon N}_{sN^2}(x))\,ds\right|\right]=0$$

where $\overrightarrow{\eta}^{\varepsilon N}_{sN^2}(x)$ *was defined in* (8). *The same result holds replacing* $\overrightarrow{\eta}^{\varepsilon N}_{sN^2}(x)$ *by* $\overleftarrow{\eta}^{\varepsilon N}_{sN^2}(x)$, *but in this case the support of* F *cannot intersect the set of points* $\{x-\varepsilon N+1,\dots,x\}$. *The values above of* x *are restricted to the cases when the averages make sense.*

In order to prove Lemmas 5 and 6, we need some intermediate results. First observe that if $H(\mu_N|\nu^N_{\rho(\cdot)})$ is the relative entropy of the measure μ_N with respect to $\nu^N_{\rho(\cdot)}$, then there exists a constant $C_{\alpha,\beta}$ such that $H(\mu_N|\nu^N_{\rho(\cdot)})\le C_{\alpha,\beta}N$. To see this it is enough to observe that

$$\nu^N_{\rho(\cdot)}(\eta)=\prod_{x=1}^{N-1}\rho(\tfrac{x}{N})^{\eta(x)}(1-\rho(\tfrac{x}{N}))^{1-\eta(x)}\ge(r_\alpha\wedge(1-r_\beta))^N:=(C_{\alpha,\beta})^N,$$

and by the explicit formula for the entropy, it holds

$$H(\mu_N|\nu^N_{\rho(\cdot)})=\sum_{\eta\in\Omega_N}\mu_N(\eta)\log\left(\frac{\mu_N(\eta)}{\nu^N_{\rho(\cdot)}(\eta)}\right)\le N\log\left(\frac{1}{C_{\alpha,\beta}}\right)\sum_{\eta\in\Omega_N}\mu_N(\eta)=C_{\alpha,\beta}N.$$

Lemma 7 *Let* $G_N:[0,T]\times\Omega_N\to\mathbb{R}$, $N\in\mathbb{N}$, *be a sequence of functions and* $t\in[0,T]$. *Then, for any* $N\in\mathbb{N}$ *and for any* $B>0$,

$$\mathbb{E}_{\mu_N}\left[\left|\int_0^t G_N(s,\eta_{sN^2})\,ds\right|\right]\le\frac{C_{\alpha,\beta}}{B}+\int_0^t\sup_f\left\{\langle G_N(s,\eta),f\rangle_{\nu^N_{\rho(\cdot)}}+\frac{N}{B}\langle\mathscr{L}_N\sqrt{f},\sqrt{f}\rangle_{\nu^N_{\rho(\cdot)}}\right\}ds,$$

where the supremum is taken over all densities f with respect to $\nu^N_{\rho(\cdot)}$, and $C_{\alpha,\beta}$ is a positive constant.

Proof By the entropy inequality and Jensen's inequality, for any $B > 0$ the expectation in the statement of the theorem is bounded by

$$\frac{C_0}{B} + \frac{1}{NB} \log \mathbb{E}_{\nu^N_{\rho(\cdot)}} \left[e^{|\int_0^t BNG_N(s,\eta_{sN^2})\, ds|} \right]. \tag{20}$$

Since $e^{|x|} \leq e^x + e^{-x}$ and

$$\limsup_{N\to\infty} \tfrac{1}{N} \log(a_N + b_N) \leq \max\left\{ \limsup_{N\to\infty} \tfrac{1}{N} \log(a_N), \limsup_{N\to\infty} \tfrac{1}{N} \log(b_N) \right\},$$

we can remove the absolute value from expression (20). By Feynman–Kac's formula (see Lemma 7.3 in [1]), (20) is bounded by

$$\frac{C_{\alpha,\beta}}{B} + \int_0^t \sup_f \left\{ \langle G_N(s,\eta), f \rangle_{\nu^N_{\rho(\cdot)}} + \frac{N}{B} \langle \mathscr{L}_N \sqrt{f}, \sqrt{f} \rangle_{\nu^N_{\rho(\cdot)}} \right\} ds,$$

with the supremum taken over all densities f with respect to $\nu^N_{\rho(\cdot)}$.

In the next lemma we do not assume any condition on the profile $\rho(\cdot)$.

Lemma 8 *There exists a positive constant C such that, for any $A > 0$, any $N \in \mathbb{N}$ and any density f with respect to $\nu^N_{\rho(\cdot)}$,*

$$\left| \langle \eta(1) - r_\alpha, f \rangle_{\nu^N_{\rho(\cdot)}} \right| \leq \frac{C}{A} \mathscr{D}^L_N(\sqrt{f}, \nu^N_{\rho(\cdot)}) + CAN^\theta + C\left|\rho(\tfrac{1}{N}) - r_\alpha\right|,$$

Proof By summing and subtracting the appropriate term,

$$\begin{aligned} \left| \langle \eta(1) - r_\alpha, f \rangle_{\nu^N_{\rho(\cdot)}} \right| \leq{}& \frac{1}{2} \left| \int_{\Omega_N} (\eta(1) - r_\alpha)(f(\eta) - f(\eta^1)) d\nu^N_{\rho(\cdot)} \right| \\ &+ \frac{1}{2} \left| \int_{\Omega_N} (\eta(1) - r_\alpha)(f(\eta) + f(\eta^1)) d\nu^N_{\rho(\cdot)} \right|. \end{aligned} \tag{21}$$

By multiplying and dividing by $\sqrt{c_{0,1}(\eta)}$ and applying Young's inequality we have, for any $A > 0$, that the first term on the RHS of (21) can be bounded by

$$\begin{aligned} &\frac{A}{4} \int_{\Omega_N} \frac{(\eta(1) - r_\alpha)^2}{c_{0,1}(\eta)} \left(\sqrt{f(\eta)} + \sqrt{f(\eta^1)} \right)^2 d\nu^N_{\rho(\cdot)} + \frac{1}{4A} \mathscr{D}^L_N(\sqrt{f}, \nu^N_{\rho(\cdot)}) \\ \leq{}& C' AN^\theta + \frac{1}{A} \mathscr{D}^L_N(\sqrt{f}, \nu^N_{\rho(\cdot)}), \end{aligned}$$

where the last inequality holds, for some constant C', by Lemma 4 and by the fact that $(\eta(1) - r_\alpha)^2 c_{0,1}(\eta)^{-1}$ is bounded by a constant times N^θ.

Now we analyze the second term on the RHS of (21). Let $\bar{\eta} \in \{0,1\}^{\{2,\dots,N-1\}}$ denote the configuration obtained from η by discarding its value at 1, so that $\eta = (1,\bar{\eta})$ if $\eta(1) = 1$ and $\eta = (0,\bar{\eta})$ if $\eta(1) = 0$. Since $\nu^N_{\rho(\cdot)}$ is a product measure with $\nu^N_{\rho(\cdot)}(\eta(1) = 1) = \rho(\frac{1}{N})$, the second term on the RHS of (21) is equal to

$$\begin{aligned}
&\frac{1}{2}\Big|\sum_{\bar{\eta}}\Big[(1-r_\alpha)\rho(\tfrac{1}{N}) - r_\alpha(1-\rho(\tfrac{1}{N}))\Big](f(0,\bar{\eta}) + f(1,\bar{\eta}))\nu^N_{\rho(\cdot)}(\bar{\eta})\Big| \\
&\quad = \frac{1}{2}\Big|\sum_{\bar{\eta}}(\rho(\tfrac{1}{N}) - r_\alpha)(f(1,\bar{\eta}) + f(0,\bar{\eta}))\nu^N_{\rho(\cdot)}(\bar{\eta})\Big| \\
&\quad \le C''\big|\rho(\tfrac{1}{N}) - r_\alpha\big|\sum_{\bar{\eta}}\big[\rho(\tfrac{1}{N})f(1,\bar{\eta})\nu^N_{\rho(\cdot)}(\bar{\eta}) + (1-\rho(\tfrac{1}{N}))f(0,\bar{\eta})\nu^N_{\rho(\cdot)}(\bar{\eta})\big] \\
&\quad = C''\big|\rho(\tfrac{1}{N}) - r_\alpha\big|\sum_{\eta} f(\eta)\nu^N_{\rho(\cdot)}(\eta) = C''\big|\rho(\tfrac{1}{N}) - r_\alpha\big|,
\end{aligned}$$

where $C'' = \max\left\{\frac{1}{2r_\alpha}, \frac{1}{2(1-r_\beta)}\right\} \ge \max\left\{\frac{1}{2\rho(\frac{1}{N})}, \frac{1}{2(1-\rho(\frac{1}{N}))}\right\}$.

Now we have all set to prove the lemma. We start with the proof of Lemma 5.

5.2 *Proof of Lemma 5*

The main difference in the proof between the two cases (1) and (2) is that we change from μ_N to a measure $\nu^N_{\rho(\cdot)}$ where the profile $\rho : [0,1] \to [0,1]$ is Lipschitz, but we assume $\rho(0) = r_\alpha$ and $\rho(1) = r_\beta$ where in (1) (resp. (2)) these values are given in (17) (resp. $r_\alpha = \alpha$ and $r_\beta = \beta$). By Lemma 7, since $|F(N,s)| \le C_1$ for some constant $C_1 > 0$, the expectation in the statement of the lemma is bounded from above by

$$\frac{C_{\alpha,\beta}}{B} + t\sup_f\left\{C_1\big|\langle\eta(1) - r_\alpha, f\rangle_{\nu^N_{\rho(\cdot)}}\big| + \frac{N}{B}\langle\mathscr{L}_N\sqrt{f},\sqrt{f}\rangle_{\nu^N_{\rho(\cdot)}}\right\}. \tag{22}$$

If $\theta = \delta < 1$, we recall (18) and the term inside the supremum in the last expression is bounded from above by

$$C_1\big|\langle\eta(1) - r_\alpha, f\rangle_{\nu^N_{\rho(\cdot)}}\big| - \frac{N}{4B}\mathscr{D}_N(\sqrt{f},\nu^N_{\rho(\cdot)}) + \frac{C}{B}\Big(1 + \frac{1}{N^\theta}\Big).$$

If $\theta \in [0,1)$ and $\delta \ge 1$, we recall (19) and the term inside the supremum in (22) is bounded from above by

$$C_1\big|\langle\eta(1) - r_\alpha, f\rangle_{\nu^N_{\rho(\cdot)}}\big| - \frac{N}{4B}\mathscr{D}_N(\sqrt{f},\nu^N_{\rho(\cdot)}) + \frac{C}{B}\Big(1 + \frac{1}{N^\theta}\Big).$$

Furthermore, from Lemma 8, and choosing $A = cBN^{-1}$ where c is a suitable constant, the last bounds obtained above for both cases give that the term in the supremum in (22) is bounded from above by a constant times

$$\frac{BN^{\theta}}{N} + \left|\rho(\tfrac{1}{N}) - r_{\alpha}\right| + \frac{C}{B}\Big(1 + \frac{1}{N^{\theta}}\Big).$$

Since we assumed $\rho(0) = r_{\alpha}$ (on the case $\theta = \delta$) or $\rho(0) = \alpha$ (on the case $\theta \in [0, 1)$ and $\delta \geq 1$) and that $\rho(\cdot)$ is Lipschitz continuous, all the terms above depending on N vanish as $N \to \infty$. To finish the proof we just need to send $B \to +\infty$.

5.3 *Proof of Lemma 6*

This result is necessary in all the regimes of θ and δ. The main difference in the proof between these cases is the fact that we change from μ_N to a measure $\nu^N_{\rho(\cdot)}$, where the profile $\rho : [0, 1] \to [0, 1]$ is Lipschitz continuous, but in the case $\delta > 1$ and $\theta > 1$ we do not need to impose any extra restriction on the profile. In the other cases we assume the extra conditions as in the proof of last lemma. Using the same arguments as above, the expectation in the statement of the lemma is bounded from above by

$$\frac{C_{\alpha,\beta}}{B} + \int_0^t \sup_f \left\{ \left|\langle F(N,\eta,s)(\eta(x) - \overrightarrow{\eta}^{\varepsilon N}(x)), f\rangle_{\nu^N_{\rho}}\right| + \frac{N}{B}\langle \mathscr{L}_N\sqrt{f}, \sqrt{f}\rangle_{\nu^N_{\rho(\cdot)}} \right\} ds, \tag{23}$$

for any $B > 0$. By writing the term above as a telescopic sum, summing and subtracting terms, we write

$$\begin{aligned}
&\langle F(N,\eta,s)(\eta(x) - \overrightarrow{\eta}^{\varepsilon N}(x)), f\rangle_{\nu^N_{\rho(\cdot)}} \\
&= \frac{1}{2\varepsilon N}\sum_{y=x+1}^{x+\varepsilon N}\sum_{z=x}^{y-1}\int F(N,\eta,s)(\eta(z) - \eta(z+1))\Big(f(\eta) - f(\eta^{z,z+1})\Big)d\nu^N_{\rho(\cdot)} \\
&+ \frac{1}{2\varepsilon N}\sum_{y=x+1}^{x+\varepsilon N}\sum_{z=x}^{y-1}\int F(N,\eta,s)(\eta(z) - \eta(z+1))\Big(f(\eta) + f(\eta^{z,z+1})\Big)d\nu^N_{\rho(\cdot)}.
\end{aligned}$$

By Young's inequality, the first term on the RHS of last expression can be bounded from above by a constant times

$$\begin{aligned}
&\frac{\|F\|^2_{\infty}A}{\varepsilon N}\sum_{y=x+1}^{x+\varepsilon N}\sum_{z=x}^{y-1}\int c_{z,z+1}(\eta)\big(\sqrt{f(\eta^{z,z+1})} - \sqrt{f(\eta)}\big)^2 d\nu^N_{\rho(\cdot)} \\
&+ \frac{\|F\|^2_{\infty}}{A\varepsilon N}\sum_{y=x+1}^{x+\varepsilon N}\sum_{z=x}^{y-1}\int \frac{1}{c_{z,z+1}(\eta)}\big(\sqrt{f(\eta^{z,z+1})} + \sqrt{f(\eta)}\big)^2(\eta(z+1) - \eta(z))^2 d\nu^N_{\rho(\cdot)}
\end{aligned}$$

for any $A > 0$. The first term in last expression can be bounded by $A\|F\|_\infty^2 \mathscr{D}_N^B(\sqrt{f}, \nu^N_{\rho(\cdot)})$ and by Lemma 4, the second term can be bounded by a constant times $A^{-1}\|F\|_\infty^2 \varepsilon N$.

The remaining term in last display can be treated using a similar argument to the one as in the last part of the proof of Lemma 8, invoking the fact that the profile is Lipschitz, and can be bounded from above by ε.

Now we split the proof according to the regimes of δ and θ. For simplicity of the presentation we restrict to the case $\theta \geq 1$ and $\delta \geq 1$. The other cases are left to the reader. From (16) we get

$$\langle \mathscr{L}_N \sqrt{f}, \sqrt{f} \rangle_{\nu^N_\rho} \leq -\frac{1}{4} \mathscr{D}_N(\sqrt{f}, \nu^N_{\rho(\cdot)}) + \frac{C}{N}.$$

Then (23) becomes bounded from above by

$$\frac{C_{\alpha,\beta}}{B} + \int_0^t \sup_f \left\{ A\|F\|_\infty^2 \mathscr{D}_N^B(\sqrt{f}, \nu^N_{\rho(\cdot)}) + \frac{\|F\|_\infty^2 \varepsilon N}{A} + \varepsilon - \frac{N}{4B} \mathscr{D}_N(\sqrt{f}, \nu^N_{\rho(\cdot)}) + \frac{C}{4B} \right\} ds,$$

Therefore, choosing $A = N(C_1 B)^{-1}$, where C_1 is an appropriate constant, the expression in last supremum is bounded by a constant times

$$B\varepsilon + \frac{1}{B} + \varepsilon.$$

The result follows by taking the limit $\varepsilon \to 0$ and then $B \to \infty$.

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Appendix: Uniqueness of Weak Solutions

In this section we prove uniqueness of weak solutions of (2). We use the method taken from Appendix 2 of [12] but an alternative proof can be seen in, for example, Sect. 7 of [7]. Take ρ^1 and ρ^2 two weak solutions of (2) with the same initial condition and call $\bar{\rho}$ their difference $\bar{\rho} = \rho^1 - \rho^2$. Let us recall that the set $\{\psi_k\}_k$ of eigenfunctions of the Laplacian with Dirichlet boundary conditions, given by $\psi_k(u) = \sqrt{2}\sin(k\pi u)$ for $k \geq 1$ and $\psi_0(u) = 1$ is an orthonormal basis of $L^2([0,1])$. Consider

$$V(t) = \sum_{k \geq 0} \frac{1}{2a_k} < \bar{\rho}_t, \psi_k >^2$$

where $a_k = (k\pi)^2 + 1$. We claim that $V'(t) \leq CV(t)$, where C is a positive constant and since $V(0) = 0$, from Gronwall's inequality we conclude that $V(t) \leq 0$, and we are done. Now,

$$V'(t) = \sum_{k\geq 0} \frac{1}{a_k} < \bar{\rho}_t, \psi_k > \frac{d}{dt} < \bar{\rho}_t, \psi_k > . \tag{24}$$

and from (3), $\frac{d}{dt} < \bar{\rho}_t, \psi_k >$ can be replaced by

$$< \bar{\rho}_t, \Delta\psi_k > + \mathfrak{e} < \sigma(\rho_t^1) - \sigma(\rho_t^2), \partial_u \psi_k > = -(k\pi)^2 < \bar{\rho}_t, \psi_k > + \mathfrak{e} < \sigma(\rho_t^1) - \sigma(\rho_t^2), \partial_u \psi_k >$$

and we get

$$V'(t) = -\sum_{k\geq 0} \frac{(k\pi)^2}{a_k} < \bar{\rho}_t, \psi_k >^2 + \sum_{k\geq 0} \frac{\mathfrak{e}}{a_k} < \bar{\rho}_t, \psi_k > < \sigma(\rho_t^1) - \sigma(\rho_t^2), \partial_u \psi_k > .$$

From Young's inequality the rightmost term in last display is bounded from above by

$$\frac{1}{2A} \sum_{k\geq 0} \frac{\mathfrak{e}}{a_k} < \bar{\rho}_t, \psi_k >^2 + \frac{A}{2} \sum_{k\geq 0} \frac{\mathfrak{e}}{a_k} < \sigma(\rho_t^1) - \sigma(\rho_t^2), \partial_u \psi_k >^2,$$

for any $A > 0$. Observe that $\partial_u \psi_k(u) = -k\pi\, \varphi_k(u)$, with $\varphi_k(u) = \sqrt{2}\cos(k\pi u)$, for $k \geq 1$ and $\varphi_0(u) = 1$. Therefore, the rightmost term in last display can be bounded from above by

$$\frac{A}{2} \sum_{k\geq 0} \frac{\mathfrak{e}(k\pi)^2}{a_k} < \sigma(\rho_t^1) - \sigma(\rho_t^2), \varphi_k >^2 \leq \frac{A}{2}\mathfrak{e} \sum_{k\geq 0} < \sigma(\rho_t^1) - \sigma(\rho_t^2), \varphi_k >^2 ,$$

because of the choice of a_k. Observe that, since $\{\varphi_k\}_k$ is an orthonormal basis of $\mathbb{L}^2$, the rightmost term in last display is equal to $\frac{A}{2}\mathfrak{e} \int_0^1 \left(\sigma(\rho_t^1) - \sigma(\rho_t^2)\right)^2 du$. Since $(\sigma(\rho_t^1) - \sigma(\rho_t^2))^2 \leq 5\bar{\rho}_t$, last display is bounded from above by $\frac{5A}{2}\mathfrak{e}\|\bar{\rho}_t\|_2^2$. Putting all this together we conclude that

$$V'(t) \leq \sum_{k\geq 0} \Big(-\frac{(k\pi)^2}{a_k} + \frac{\mathfrak{e}}{2Aa_k} + \frac{5A}{2}\mathfrak{e} \Big) < \bar{\rho}_t, \psi_k >^2 .$$

Taking $A = 2(5\mathfrak{e})^{-1}$ we get $V'(t) \leq 2(\frac{5\mathfrak{e}^2}{4} + 1)V(t)$ and we are done.

In the Neumann case the proof above can be adapted by observing that the set $\{\psi_k\}_k$ of eigenfunctions of Laplacian with Neumann boundary conditions is $\psi_k(u) = \sqrt{2}\cos(k\pi u)$. Observe that the previous proof also includes the case when $\mathfrak{e} = 0$, that is for the heat equation with Dirichlet or Neumann boundary conditions.

References

1. R. Baldasso, O. Menezes, A. Neumann, R. Souza, Exclusion process with slow boundary. J. Stat. Phys. **167**, 1112–1142 (2017)
2. C. Bernardin, P. Gonçalves, B. Jiménez-Oviedo, Slow to Fast infinitely extended reservoirs for the symmetric exclusion process with long jumps. Markov Proc. Relat. Fields **25**, 217–274 (2019)
3. C. Bernardin, P. Gonçalves, B. Jiménez Oviedo. A microscopic model for the regional fractional Laplacian with Dirichlet boundary conditions. Arch. Rat. Mech. Anal. **239**, 1–48 (2021)
4. C. Bernardin, P. Gonçalves, S. Scotta. Hydrodynamic limit for a boundary driven super-diffusive symmetric exclusion. submitted (2020)
5. L. Bonorino, R. De Paula, P. Gonçalves, A. Neumann, Hydrodynamics for the porous medium model with slow reservoirs. J. Stat. Phys. **179**, 748–788 (2020)
6. A. De Masi, E. Presutti, E. Scacciatelli, The weakly asymmetric simple exclusion process. Annales de l'Institut Henri Poincaré **25**, 1–39 (1989)
7. J. Farfan, C. Landim, M. Mourragui, Hydrostatics and dynamical large deviations of boundary driven gradient symmetric exclusion processes. Stoch. Proc. Appl. **121**, 725–758 (2011)
8. P. Gonçalves, Hydrodynamics for symmetric exclusion in contact with reservoirs. Stochastic Dynamics Out of Equilibrium, Institut Henri Poincaré, Paris, France, 2017, Springer Proceedings in Mathematics and Statistics book series (2019), pp. 137–205
9. P. Gonçalves, C. Landim, A. Milanes, Nonequilibrium fluctuations of one-dimensional boundary driven weakly asymmetric exclusion processes. Ann. Appl. Probab. **27**(1), 140–177 (2017)
10. P. Gonçalves, N. Perkowski, M. Simon, Derivation of the Stochastic Burgers equation with Dirichlet boundary conditions from the WASEP. Ann. Henri Lebesgue **3**, 87–167 (2020)
11. M.Z. Guo, G.C. Papanicolaou, S.R.S. Varadhan, Nonlinear diffusion limit for a system with nearest neighbor interactions. Commun. Math. Phys. **118**, 31–59 (1988)
12. C. Kipnis, C. Landim, *Scaling Limits of Interacting Particle Systems* (Springer, New York, 1999)
13. T. Liggett, *Interacting Particles Systems* (Springer, New York, 1985)
14. T. Liggett, *Stochastic Interacting Systems: Contact, Voter and Exclusion Processes* (Springer, New York, 1999)
15. F. Spitzer, Interaction of Markov processes. Adv. Math. **5**(2), 246–290 (1970)

Recent Developments on the Modelling of Cell Interactions in Autoimmune Diseases

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Abstract In this paper, we give an overview of our recent results concerning the mathematical modelling of autoimmune diseases in absence [1] and in presence [2] of immunotherapeutic treatment. Then we complement the model description given in [2], by developing here a kinetic system describing the cellular dynamics corresponding to the macroscopic model presented in [2]. This is the main new contribution in these proceedings and it allows us to investigate the effect of an external drug therapy at the cellular level. The relevant properties on existence, uniqueness, positivity and asymptotic behaviour of the solution to the new kinetic system are stated. Some numerical simulations are also performed for the models in absence and in presence of immunotherapy, to analyse both the effect of optimal treatment strategies and the sensitivity of the solutions to certain parameters of the model with biological significance.

Keywords Mathematical biology · Modelling · Kinetic theory · Autoimmune diseases · Optimal immunotherapy

1 Introduction

The potential of mathematical models in giving valuable predictions concerning the biological development of a disease and its optimal medical treatment is well recognized by specialists both in mathematical and in medical sciences. This recognition

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has become more widespread due to the current epidemiological situation that we are living.

In particular, many interesting problems can be investigated in the context of mathematical modelling of autoimmune diseases. Some of these problems are interesting due to particular mathematical aspects, but other challenging problems can arise due to the scientific interchange between mathematicians and immunologists or biologists.

Our work is motivated by the idea of developing advanced mathematical methods for describing, in a rigorous form, the complex dynamics of the variables involved in autoimmunity, and also to better understand and predict, biologically, the effect of certain populations of cells on the outcome of the disease. We believe that the kinetic approach, being developed at the cellular scale, can give some important insights concerning the effect of certain interactions between cells on the development and control of the disease. At the same time, suitable averaging processes may provide information on the macroscopic observables, so that the advantage of the kinetic approach is that it offers both microscopic and macroscopic descriptions of the biological processes involved in autoimmunity.

In this paper, we give an overview of recent developments concerning the mathematical modelling of autoimmune diseases. We start by presenting the model developed in [1], which is based on a kinetic theory description and where three interacting populations are considered in the development of the disease. In this model, the well-posedness of the kinetic system is proven and the existence of biologically realistic solutions is investigated. Then, a new variable representing the population of IL-2 cytokines, that are believed to be important players in the control of the autoimmune reaction, is introduced in the macroscopic analogue of the kinetic model given in [1]. This extended model is presented in [2] and was developed with the aim of studying optimal policies for the immunotherapeutic treatment of autoimmune diseases.

The main contribution in these proceedings is to present a kinetic system whose macroscopic analogue is the model given in [2]. Accordingly, a fourth population of IL-2 cytokines is considered in the kinetic system and an artificial inlet for the external drug therapy is also introduced in the equations in the same manner as it was done for corresponding macroscopic system.

From the mathematical point of view, our work follows the research line initiated in [3–5], on the study of the tumour-immune system interactions, and then used by other researchers, for instance in [6–10] concerning the immune system response to certain diseases.

2 The Biological Scenario

Autoimmune diseases can affect just about any part of the body, and more than 100 types have been identified so far (some of the most common include type 1 diabetes, rheumatoid arthritis, multiple sclerosis, lupus, psoriasis, thyroid diseases, and inflammatory bowel disease). Most of these diseases are chronic, and so patients

can face a lifetime of debilitating symptoms, loss of organ function, and in extreme cases even death. However, as common and serious they might be, much about autoimmune diseases remains a mystery. The number of patients suffering from these conditions are steadily increasing, particularly in the developed world, yet specialists do not know why, although environmental changes associated with industrialization have been long suspected.

The Role of Self-Reactive T Cells

T cells originate from the common lymphoid progenitor cells in the bone marrow. They migrate as immature precursor T cells via the bloodstream into the thymus, where they undergo several different maturation phases. More than 98 per cent of these cells die during maturation by apoptosis, as they undergo positive selection for those T cells that recognize self major histocompatibility complex molecules and negative selection against those T cells that react to self-antigens. In healthy individuals, T cells that escape thymic negative selection are usually controlled by intrinsic (inhibitory receptors) and extrinsic (regulatory cell populations) mechanisms of tolerance in the periphery. In individuals genetically prone to autoimmunity, one or several of these checkpoints are defective, resulting in expansion of self-reactive T cells due to their exposure to self-antigens by self-antigen presenting cells (SAPCs), that cannot be controlled by regulatory cells. Then, self-reactive T cells migrate to their targeted tissue where cytotoxic mechanisms and uncontrolled inflammation result in tissue damage.

The Role of Regulatory T Cells and Natural Killer Cells

Regulatory T cells (Tregs) are believed to be important mediators within the immune system [11–15]. In fact, Tregs are central to the peripheral tolerance since they are effective in preventing or even reversing disease, whereas autoimmunity commonly results from the genetic absence or loss of Tregs. In autoimmunity, the main functional properties of Tregs involve suppression by modulation of SAPCs maturation or function and suppression by direct or indirect killing of SRTCs and SAPCs. Increasing evidence shows that Natural Killer Cells (NKCs) play a relevant role in organic-specific and systemic autoimmune diseases [16–18]. The decreased NKC frequency and impaired NKC cytotoxicity observed in a variety of autoimmune diseases implies a protective role of NKCs in controlling autoimmunity. In fact, NKCs may limit autoimmune responses by inhibiting the proliferation and activation of SAPCs and SRTCs.

Tregs and NKCs constitute the great majority of immunosuppressive cells (ISCs).

Various immunotherapeutic strategies target different steps in the processes of autoimmunity. The ultimate goal of immunotherapy is to alter the balance of pathogenic versus regulatory T cells to restore tolerance.

Our models focus on the cellular dynamics when an autoimmune episode occurs, particularly on the interplay between SAPCs, SRTCs and ISCs, that can either result in an autoimmune cascade and consequently in illness or in an aborted autoimmune

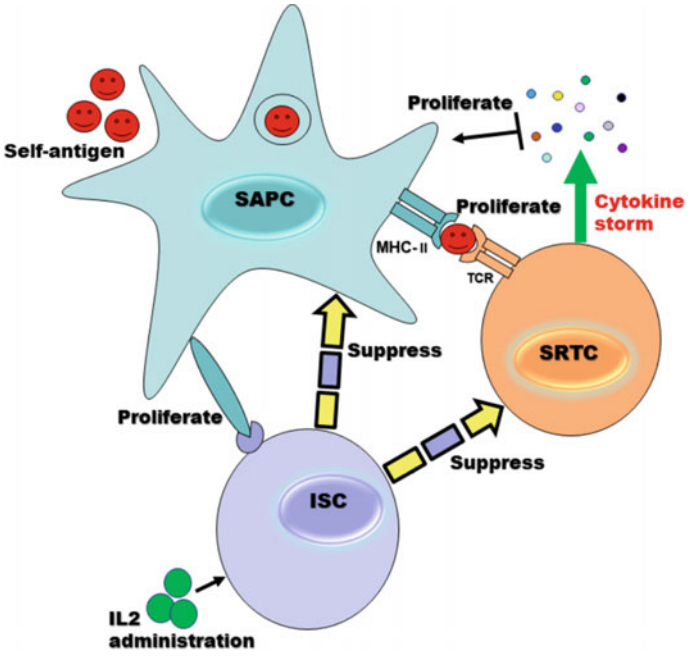


Fig. 1 Flowchart for the models of papers [1, 2]. Cellular dynamics involving SAPCs, SRTCs, ISCs and IL-2 cytokines

response by regulation via ISCs. When the population of IL-2 cytokines is introduced in the model, the control of the autoimmune reaction by external drug therapy takes part of the dynamics.

The cellular interactions among the populations considered in our models are illustrated in the diagram of Fig. 1.

3 The Model for Autoimmune Diseases

The immune system can be regarded, at the cellular level, as a system constituted by a large number of cells belonging to several interacting populations. In our model, we consider three interacting cell populations $p_i, i = 1, 2, 3$, that are involved in the autoimmune competition. More precisely, we consider the population p_1 of SAPCs, the population p_2 of SRTCs, and the population p_3 of ISCs.

In simple terms, the dynamics of these populations can be described as follows. SAPCs transport self-antigens to their encounter with SRTCs. SRTCs are activated when they encounter a SAPC that has digested a self-antigen. ISCs regulate the activity of SRTCs and SAPCs.

The biological system can be modelled using a kinetic theory approach described in terms of the statistical distribution of all states possessed by each cell population.

3.1 The Kinetic Description of the Cellular Interactions

The functional state of the cells of each population is described by a positive real variable $u \in [0, 1]$, called *activation variable* or *activity*, whose biological meaning varies from one population to another and will be specified below.

The Cellular Activity
The activity u of self-antigen presenting cells is defined as the ability to stimulate and activate self-reactive T cells. In particular, $u = 0$ means that the stimulation by SAPCs does not activate SRTCs and, therefore, does not induce an autoimmune response.

In turn, the activity u of self reactive T cells is defined as the ability of promoting the secretion of cytokines. In particular, $u = 0$ means that the SRTCs do not produce cytokines; in other words, SRTCs are not sensitive to the stimulus by SAPCs and no inflammatory process is triggered.

Finally, the activity u of the immunosupressive cells is defined as the ability to inhibit the autoimmune response by either suppressing the activity of SAPCs and SRTCs or eliminating SAPCs or SRTCs. In particular, $u = 0$ means that the ISCs are neither able to inhibit the activity of SAPCs and SRTCs nor to eliminate SAPCs or SRTCs.

The Cellular Dynamics
The interactions among cells of different populations can modify the activity of the cells and can also modify the size of populations. When the interactions only modify the activity of the cells, they are of conservative type, whereas when they increase or reduce the size of the populations, they are of proliferative or destructive type, respectively.

Based on the biological scenario presented above concerning the activity of our populations, we consider interactions of the following type:

Conservative interactions

- ISCs–SAPCs that decrease the activity of SAPCs;
- ISCs–SRTCs that decrease the activity of SRTCs;
- SAPCs–SRTCs that increase the activity of SAPCs and also that of SRTCs;

Proliferative interactions

- SAPCs–SRTCs that increase the number of SRTCs and also that of SAPCs;
- SAPCs–ISCs that increase the number of ISCs;

Destructive interactions

- ISCs–SAPCs that decrease the number SAPCs;
- ISCs–SRTCs that decrease the number SRTCs.

Our Assumptions

In our mathematical model, as a simplification of the biological reality, we consider the following assumptions.

(A) Only binary interactions among cells are significant.
(B) Interactions among cells are instantaneous and homogeneous in space.
(C) The binary interactions between cells of populations p_1 (SAPCs), p_2 (SRTCs) and p_3 (ISCs) can change the activation of SAPCs and SRTCs as well as the size of each population, either by creating more SAPCs, SRTCs and ISCs or by destroying SAPCs and SRTCs. In the first case, the interactions are conservative, whereas in the second case they are either proliferative or destructive interactions.
(D) The population p_3 (ISCs) is homogeneous with respect to its biological activity, since the effect of the cellular interactions on the activity of Tregs and NKCs (ISCs) is not considered in our model. Therefore, the distribution function of the population p_3 is independent of its functional state, that is $f_3 = f_3(t)$.

The Kinetic Equations

The internal state of the biological system is described by the distribution functions associated to the considered populations, namely $f_i : [0, \infty] \times [0, 1] \to \mathbb{R}^+$, $i = 1, 2, 3$, with $f_i(t, u)$ giving the number of cells of population p_i with activity $u \in [0, 1]$ at time $t \geq 0$. The expected number of cells belonging to each population p_i, at time $t \geq 0$, is then given by

$$n_i(t) = \int_0^1 f_i(t, u)\mathrm{d}u, \qquad i = 1, 2, 3. \tag{1}$$

The evolution equations for the distribution functions f_i, $i = 1, 2, 3$, with $t \in \mathbb{R}^+$ and $u \in [0, 1]$, are given by the following coupled system of integro-differential equations, that describe the interactions presented above:

$$\begin{aligned}
\frac{\partial f_1}{\partial t}(t, u) &= 2c_{12}\int_0^u (u - v) f_1(t, v)\mathrm{d}v \int_0^1 f_2(t, w)\mathrm{d}w - c_{12}(u - 1)^2 f_1(t, u)\int_0^1 f_2(t, w)\mathrm{d}w \\
&\quad + 2c_{13} f_3(t)\int_u^1 (v - u) f_1(t, v)\mathrm{d}v - c_{13}u^2 f_1(t, u) f_3(t) \\
&\quad + p_{12}\, f_1(t, u)\int_0^1 f_2(t, w)\mathrm{d}w - d_{13}\, f_1(t, u) f_3(t), \qquad (2) \\
\frac{\partial f_2}{\partial t}(t, u) &= 2c_{21}\int_0^u (u - v) f_2(t, v)dv \int_{w^\star}^1 f_1(t, w)dw - c_{21}(u - 1)^2 \\
&\quad f_2(t, u)\int_{w^*}^1 f_1(t, w)dw + 2c_{23} f_3(t)\int_u^1 (v - u) f_2(t, v)dv - c_{23}u^2 f_2(t, u) f_3(t)
\end{aligned}$$

$$+ p_{21} f_2(t,u) \int_0^1 f_1(t,w)dw - d_{23} f_2(t,u) f_3(t), \tag{3}$$

$$\frac{df_3}{dt}(t) = p_{31} f_3(t) \int_0^1 f_1(t,w)dw. \tag{4}$$

The initial conditions for system (2)–(4) are given by

$$f_1(0,u) = f_1^0(u), \quad f_2(0,u) = f_2^0(u), \quad f_3(0) = f_3^0. \tag{5}$$

The parameters p_{ij}, d_{ij} and c_{ij} in equations (2)–(4) indicate constant rates of proliferative, destructive and conservative interactions, respectively. Furthermore, $w^* \in]0, 1[$ is a parameter of the model, that is related to the tolerance of SRTCs to self-antigens. For more details on the model, please see paper [1].

The description obtained with the kinetic system (2)–(4) is rather detailed and reflects how the cellular interactions affect the activity of the various populations and how they contribute to the evolution of the distribution functions $f_i, i = 1, 2, 3$.

3.2 The Macroscopic Equations

From the kinetic equations (2)–(4), we formally derive the corresponding macroscopic balance equations describing the time evolution of the cellular density of each population, namely $n_i(t), i = 1, 2, 3$. These balance equations are obtained by suitable integration of the kinetic equations (2)–(4) over the biological activity variable $u \in [0, 1]$. As expected, conservative interactions do not give any contribution to the equations for $n_i(t)$, since they do not modify the number of cells of each population and are lost through the integration process. Therefore, the system of ordinary differential equations (ODEs) obtained in this way is

$$\frac{dn_1}{dt}(t) = p_{12} n_1(t) n_2(t) - d_{13} n_1(t) n_3(t), \tag{6}$$

$$\frac{dn_2}{dt}(t) = p_{21} n_2(t) n_1(t) - d_{23} n_2(t) n_3(t), \tag{7}$$

$$\frac{dn_3}{dt}(t) = p_{31} n_3(t) n_1(t). \tag{8}$$

For this system, we consider the following initial data

$$n_1(0) = n_1^0, \quad n_2(0) = n_2^0, \quad n_3(0) = n_3^0, \quad \text{with} \quad n_i^0 > 0 \quad \text{for} \quad i = 1, 2, 3. \tag{9}$$

The description obtained with the balance equations (6)–(8) gives information at a global or macroscopic scale and only reflects information concerning the changes on the number of cells of each population.

3.3 The Wellposedeness of the Model

In this subsection, we state the mathematical properties of the biological model expressed both by the kinetic formulation given by system (2)–(4) and by its macroscopic analogue described by system (6)–(8).

These properties are important, not only from a mathematical point of view, in order to guarantee consistency of the model, but also from the biological point of view, to obtain solutions that are biologically significant. In particular, the positivity and the boundedness of the solution are essential features in the present context.

Local existence of solutions is proven in paper [4] for a rather vast class of kinetic systems with conservative, proliferative and destructive interactions. In general, the solution does not exist globally in time, since a blow-up can occur due to the proliferative interactions. However, a local result is enough when the system is solved numerically and an approximate solution is obtained in the considered biological context.

Theorem 1 (Local existence) *Assume initial data* $f_i^0(u)$ *in* $L^1[0, 1]$. *Then, there exists* $T_0 > 0$ *such that a unique positive solution to the Cauchy problem* (2)–(4) *exists in* $L^1[0, 1]$, *for* $t \in [0, T_0]$.

On the other hand, considering local existence of solution guaranteed by Theorem 1 and assuming that the proliferation and destruction rates are constant, it can be shown that the boundedness of the solution to the macroscopic system (6)–(8) implies the boundedness of the L^1-norm $||f_i(t, \cdot)||_1$. This result is proven in paper [5] and is an immediate consequence of the positivity of the local L^1-solution stated in Theorem 1. In this case, the estimates on the solution to the macroscopic system provide a priori estimates on the solution to the kinetic system, precisely because of the relation kinetic-macro given by Eq. (1) of the population densities $n_i(t)$ in terms of the distribution functions $f_i(t, u)$.

Therefore, we go on to obtain the following results on the existence of a global, positive solution of the Cauchy problem (6)–(8) and (9).

Theorem 2 (Positivity) *Let* $\underline{n}(t) = (n_1(t), n_2(t), n_3(t))$ *be a solution of the Cauchy problem* (6)–(8) *and* (9) *defined on* $[0, T]$, $0 < T < +\infty$. *Then* $n_1(t) > 0$, $n_2(t) > 0$, $n_3(t) > 0$, *for* $t \in [0, T]$.

Theorem 3 (Global solution and asymptotic behaviour) *Assume that* $p_{21} < p_{31}$. *Then the Cauchy problem* (6)–(8) *and* (9) *has a unique solution* $\underline{n}(t) = \big(n_1(t), n_2(t), n_3(t)\big)$ *defined on* $\mathbb{R}_+$, *satisfying the conditions*

$$\lim_{t \to +\infty} n_1(t) = 0, \quad \lim_{t \to +\infty} n_2(t) = 0, \quad \lim_{t \to +\infty} n_3(t) = \sigma < +\infty,$$

whatever are the corresponding initial data.

From the biological point of view, condition $p_{21} < p_{31}$ considered in Theorem 3 corresponds to assuming that the proliferation of SRTCs resulting from the encounters

with SAPCs is dominated by the proliferation of ISCs resulting from the encounters with SAPCs. In this case, the solution of the system does not possess blowups.

Theorems 2 and 3 have been proven by the authors in [1], extending the technique proposed in [5] in the context of tumour dynamics. These results are crucial to assure the consistency of the model and also to perform numerical simulations of the system.

In conclusion, the basic information on the behaviour of the solution to the kinetic system (2)–(4) can be "extracted" from the information concerning the solution to the corresponding macroscopic system (6)–(8).

3.4 Numerical Solutions of the Model

We have solved numerically the kinetic system (2)–(4) by discretizing the equations in the activation variable u and using a trapezoidal quadrature rule. The details of the numerical scheme are given in paper [1].

We have performed several numerical tests in view of analysing different scenarios, investigating some trends or reactions that are typical in autoimmune diseases and studying the influence of certain parameters of the model on the behaviour of the solution.

In our simulations, the choice of the parameter values is based on biological considerations presented in the literature and summed up in Sect. 2.

The initial data are taken to be $f_i^0 = 10^{-2}$, $i = 1, 2, 3$, and the values for the parameters that are not investigated are fixed and are given by

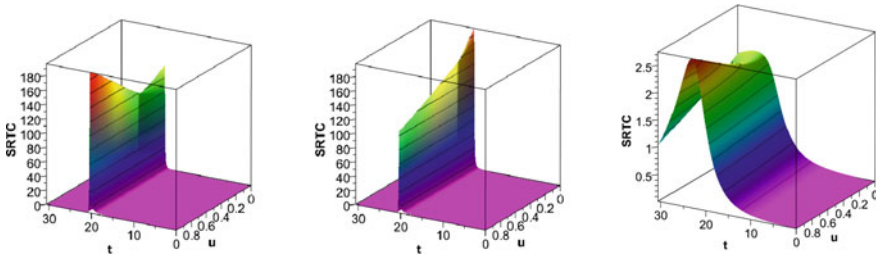
$$\begin{aligned} c_{12} = c_{12} = 2, \quad c_{13} = c_{23} = 0.01, \\ p_{21} = 19, \quad p_{12} = 1, \quad d_{13} = 0.45, \quad d_{23} = 0.01. \end{aligned} \tag{10}$$

In particular, we have studied a scenario describing the trend to illness and two other scenarios in which the autoimmune reaction is controlled to a certain extent.

(a) The scenario where there is *development of an autoimmune disease* corresponds to the situation in which the ISCs are unable to regulate the autoimmune reaction, resulting in a full autoimmune cascade. The corresponding solution is depicted in Fig. 2a. We can observe the mass proliferation of very active SRTCs due to insufficient regulation by ISCs and low tolerance of SRTCs to SAPCs.

(b) The scenario where SRTCs *become more tolerant to* SAPCs corresponds to the situation in which SAPCs are less efficient in increasing the activity of SRTCs. The corresponding solution is illustrated in Fig. 2b and shows this effect. We can observe that, in comparison with Fig. 2a, a moderate decrease in the proliferation of very active SRTCs is observed.

(c) The scenario where there is *immunosuppression of the autoimmune reaction* corresponds to the situation in which the number of ISCs produced by the biological system are enough to abort the autoimmune reaction in an efficient



(a) *Trending to illness* (b) *Immunotolerance* (c) *Immunosupression*

Fig. 2 Evolution of SRTCs determined by the kinetic system (2)–(4), for **(a)** $p_{31} = 20$ and $w^\star = 1/30$, **(b)** $p_{31} = 20$ and $w^\star = 29/30$, **(c)** $p_{31} = 22$ and $w^\star = 1/30$

manner. The corresponding solution is shown in Fig. 2c. We can observe a very low proliferation of active SRTCs due to an efficient regulation by ISCs.

4 The Extended Model with Immunotherapy

We have extended the model presented in Sect. 3 in order to include the effect of immunotherapy on the autoimmune response and investigate optimal therapeutical strategies for the treatment of autoimmune diseases. This study has been recently developed in [2] and we present here a brief description of the relevant aspects, concerning both the model and the obtained results.

In brief, in [2] the macroscopic model with immunotherapy is obtained by extending the balance equations (6)–(8) to include a drug therapy. The mathematical analysis of this new model is developed and some numerical simulations are performed. In particular, we have proven the existence of an optimal control and, under certain conditions on the parameters involved in the model, we have concluded that the optimal control is of bang bang type. This analysis completely characterizes the optimal dosage of drug therapy.

4.1 The Model

Here, we extend the kinetic model given in [1] and written in (2)–(4) such that its the macroscopic analogue is the macroscopic model given in [2]. In other words, we derive a kinetic system by extending equations (2)–(4), when a fourth population of Interleukin-2 cytokines is considered and an artificial inlet for an external drug therapy is also considered, as obtained for the macroscopic model of paper [2].

The fourth population, namely the I-population of Interleukin-2 cytokines, is denoted by p_4, and an artificial inlet for the external drug therapy is denoted by $x(t)$.

The activity of I-cells is the ability of these to promote the ISCs. Moreover, I-cells interact with ISCs resulting in the proliferation of ISCs.

The Kinetic Equations

We introduce the distribution function f_4 of the I-population, and, similarly to what we have assumed for the immunosupressive population, we also assume that f_4 is independent of the biological activity of the I-cells.

Then, we derive a kinetic system by extending equations (2)–(4), when the external drug therapy, $x(t)$, is also considered, as obtained for the macroscopic model in [2].

Therefore, the kinetic equations of the new model have the form

$$\begin{aligned}
\frac{\partial f_1}{\partial t}(t,u) &= 2c_{12}\int_0^u (u-v) f_1(t,v)\mathrm{d}v \int_0^1 f_2(t,w)\mathrm{d}w - c_{12}(u-1)^2 f_1(t,u)\int_0^1 f_2(t,w)\mathrm{d}w \\
&\quad + 2c_{13} f_3(t)\int_u^1 (v-u) f_1(t,v)\mathrm{d}v - c_{13}u^2 f_1(t,u) f_3(t) \\
&\quad + p_{12}\, f_1(t,u)\int_0^1 f_2(t,w)\mathrm{d}w - d_{13}\, f_1(t,u) f_3(t), \qquad (11) \\
\frac{\partial f_2}{\partial t}(t,u) &= 2c_{21}\int_0^u (u-v) f_2(t,v) dv \int_{w^\star}^1 f_1(t,w) dw - c_{21}(u-1)^2 f_2(t,u) \\
&\quad \int_{w^*}^1 f_1(t,w) dw + 2c_{23} f_3(t) \int_u^1 (v-u) f_2(t,v) dv - c_{23}u^2 f_2(t,u) f_3(t) \\
&\quad + p_{21} f_2(t,u)\int_0^1 f_1(t,w) dw - d_{23} f_2(t,u) f_3(t), \qquad (12) \\
\frac{df_3}{dt}(t) &= p_{31} f_3(t)\int_0^1 f_1(t,v) dv + p_{34} f_3(t) f_4(t), \qquad (13) \\
\frac{df_4}{dt}(t) &= x(t) - d_4 f_4(t), \qquad (14)
\end{aligned}$$

where the parameters p_{ij}, d_{ij} and c_{ij} indicate, as before, constant rates of proliferative, destructive and conservative interactions.

The initial conditions for system (11)–(14) are given by

$$f_1(0,u) = f_1^0(u), \quad f_2(0,u) = f_2^0(u), \quad f_3(0) = f_3^0, \quad f_4(0) = f_4^0. \qquad (15)$$

The description obtained with the kinetic system (11)–(14) reflects how the cellular interactions among cells affect the activity of the various populations and how they contribute to the evolution of the distribution functions $f_i,\ i = 1, 2, 3, 4$.

The Macroscopic Model

Integration of the kinetic equations (11)–(14) over the biological activity variable $u \in [0, 1]$ leads to the corresponding macroscopic balance equations. The resulting system describes the time evolution of the cellular density of each population and is represented by the following ODE system,

$$\frac{dn_1}{dt}(t) = p_{12}n_1(t)n_2(t) - d_{13}n_1(t)n_3(t), \tag{16}$$

$$\frac{dn_2}{dt}(t) = p_{21}n_2(t)n_1(t) - d_{23}n_2(t)n_3(t), \tag{17}$$

$$\frac{dn_3}{dt}(t) = p_{31}n_3(t)n_1(t) + p_{34}n_3(t)n_4(t), \tag{18}$$

$$\frac{dn_4}{dt}(t) = x(t) - d_4n_4(t), \tag{19}$$

where $n_4(t)$ is the number density of the IL-2 population. The initial conditions for the ODE system (16)–(19) are

$$n_i(0) = n_i^0 > 0, \quad \text{for } i = 1, 2, 3, 4. \tag{20}$$

4.2 Mathematical Analysis and Optimal Control

The macroscopic system shows good consistency properties for what concerns the qualitative behaviour of its solution. An optimal control problem relative to this system can be formulated in view of simultaneously minimizing the quantity of both the SRTCs that are produced in the body and the IL-2 cytokines that are administrated. See paper [2] for the complete analysis.

The Wellposedness
The Cauchy problem for system (16)–(19) and (20) is studied in detail in paper [2]. Here we state the results concerning the wellposedness of the system.

Theorem 4 (Positivity) *If $(n_1(t), n_2(t), n_3(t), n_4(t))$ is a solution to the Cauchy problem (16)–(19) and (20) defined on the time interval $[0, T]$, with $0 < T < \infty$, then this solution is positive, that is $n_1(t) > 0$, $n_2(t) > 0$, $n_3(t) > 0$ and $n_4(t) > 0$, for $t \in [0, T]$.*

Proof The proof of positivity of $n_1(t)$, $n_2(t)$ and $n_3(t)$ can be carried out in a similar way as the one presented in paper [1] for an analogous result. On the other hand, equation (19) can be solved analytically and the proof of the positivity of $n_4(t)$ is straightforward, since $x(t)$ is described by a sectionally continuous positive branch function.

Theorem 5 (Global solution and asymptotic behaviour) *Suppose that the proliferative rates p_{21} and p_{31} are such that $p_{21} < p_{31}$. Then the Cauchy problem (16)–(19) and (20) has a unique solution $\big(n_1(t), n_2(t), n_3(t), n_4(t)\big)$ defined on all $\mathbb{R}^+$. This solution is bounded and satisfies the conditions*

$$\lim_{t\to\infty} n_1(t) = 0, \quad \lim_{t\to\infty} n_2(t) = 0, \quad \lim_{t\to\infty} n_4(t) = 0, \tag{21}$$

$$\lim_{t\to\infty} n_3(t) = \sigma < +\infty, \tag{22}$$

whatever are the corresponding initial conditions (20).

Proof Condition (21) on $n_4(t)$ is easy to prove from the analytical solution to the uncoupled equation (19). Furthermore, the proof of the other results for $n_1(t)$, $n_2(t)$ and $n_3(t)$ can be obtained following the same rationale as the one used in [1] for an analogous result.

Once again, under the assumption of constant proliferation and destruction rates, it can be proven that the boundedness of the solution to the macroscopic system (16)–(19) implies the boundedness of the local solution to the kinetic system (11)–(14). Therefore, also for this model, the basic information on the behaviour of the solution to the kinetic system (11)–(14) can be "extracted" from the information concerning the solution to the corresponding macroscopic system (16)–(19).

The Optimal Control Problem

We study the control problem of deriving the optimal policy for IL-2 immunotherapeutic treatment for autoimmune diseases, in view of determining an optimal external influx of the IL-2 drug, $x^\star(t)$, for the macroscopic system (16)–(19) with initial conditions (20). The optimality criteria consists in minimizing the total number of SRTCs over the complete treatment and, at the same time, minimizing the IL-2 drug administration. We consider the following objective functional

$$J(t_f; x) = \int_0^{t_f} \Big(\beta\, n_2(t) + \alpha\, x(t)\Big) dt, \tag{23}$$

where t_f is the given final time of the complete treatment and α, $\beta > 0$ are the weight parameters of the SRTCs and IL-2 drug administration, respectively.

The goal is to find an optimal control function $x^\star(t)$, representing the optimal treatment with IL-2, so that

$$J(t_f; x^\star) = \min\Big\{J(t_f; x):\ x \in X\Big\}, \tag{24}$$

where X is the set of admissible control functions,

$$X = \Big\{x(t):\ 0 \le x(t) \le 1, \quad x \text{ is piecewise continuous, } t \in [0, t_f]\Big\}. \tag{25}$$

In paper [2], first we have proven the existence of a linear optimal control solution for our problem starting from the boundedness of the solution to the macroscopic system stated in Theorem 5. Then, we have characterized the optimal solution. The results are as follows. See paper [2] for the proofs and other details.

Theorem 6 (Existence of the optimal control) *Consider the objective functional* $J(t_f; x)$ *given in (23) with control set* X *defined in (25), subject to system* (16)–(19) *with initial conditions* (20)*. There exists an optimal control* $x^\star \in X$*, such that*

$$\min_{0 \le x \le 1} J(t_f; x) = J(t_f; x^\star),$$

if the following conditions are satisfied:

(a) the set consisting of the controls $x \in X$ *and corresponding state variable solutions of the Cauchy problem* (16)–(19) *and* (20) *is non empty;*
(b) the control set X *is convex and closed;*
(c) each function on the right hand side of the equations that constitute system (16)–(19) *is continuous and bounded from above by a linear function of* x *and of the state variables;*
(d) the integrand function of the objective functional $J(t_f; x)$ *is convex on* X *and bounded from below by a linear function of* x *of the form* $c_1 x - c_2$*, with* c_1, c_2 *positive constants.*

Proof Statements *(a)* through *(d)* are sufficient conditions for the existence of solution to the optimal control problem, see [20]. Therefore, it is enough to prove conditions *(a)* through *(d)*. Condition *(a)* results from the boundedness of the solution to the Cauchy problem (16)–(20) combined with a result by Lukes [21]. Condition *(b)* results from the definition (25) of the control set X. Concerning condition *(c)*, the continuity is obvious. Then, we prove that

$$\left| \mathscr{F}\Big(N(t), x(t)\Big) \right| \le C\Big(|N(t)| + |x(t)|\Big),$$

where $N(t) = \big(n_1(t), n_2(t), n_3(t), n_4(t)\big)^T$, $\mathscr{F}\big(N(t), x(t)\big)$ is the vector formed by the functions on the right hand side of equations (16)–(19), and C is a positive constant that depends on the parameters p_{ij} and on the maximum values of the state variables. Finally, concerning condition *(d)*, the convexity follows from the equality

$$J\Big(t_f; (1-p)x + py\Big) = (1-p)J\big(t_f; x\big) - pJ\big(t_f; y\big),$$

which can be easily obtained. Additionally, we have

$$\beta n_2(t) + \alpha x(t) \ge \alpha x(t) \ge \alpha x(t) - c,$$

for any positive constant c, so that the boundedness condition is also verified.

Theorem 7 (Characterization of the optimal control) *Given an optimal control* $x^\star$ *and a solution* (n_1, n_2, n_3, n_4) *to the corresponding state system* (16)–(19)*, that minimizes the functional (23), there exist adjoint variables* $\psi_i(t)$*,* $i = 1, \ldots, 4$*, satisfying the following equations*

$$\frac{d\psi_1}{dt}(t) = -\big[p_{12}n_2(t) - d_{13}n_3(t)\big]\psi_1(t) - p_{21}n_2(t)\psi_2(t) - p_{31}n_3(t)\psi_3(t), \tag{26a}$$

$$\frac{d\psi_2}{dt}(t) = -\beta - p_{12}n_1(t)\psi_1(t) - \big[p_{21}n_1(t) - d_{23}n_3(t)\big]\psi_2(t), \tag{26b}$$

$$\frac{d\psi_3}{dt}(t) = d_{13}n_1(t)\psi_1(t) + d_{23}n_2(t)\psi_2(t) - \big[p_{31}n_1(t) + p_{34}I(t)\big]\psi_3(t), \tag{26c}$$

$$\frac{d\psi_4}{dt}(t) = -p_{34}n_3(t)\psi_3(t) + d_4\psi_4(t), \tag{26d}$$

and verifying the terminal conditions, $\psi_j(t_f) = 0$*, for* $j = 1, \ldots, 4$*. Furthermore, the optimal control is characterized as follows:*

(i) If $d_{13} \neq d_{23}$ *and* $\beta p_{34} d_{13} p_{21} \neq \alpha\, d_4\, p_{31}\, d_{23}\, p_{12}$ *then*

$$x^\star(t) = \begin{cases} 0, & \text{if } \alpha + \psi_4(t) > 0, \\ 1, & \text{if } \alpha + \psi_4(t) < 0. \end{cases}$$

(ii) If $\alpha^2 p_{12} d_4^2 p_{31}^2 A(t) = \beta^2 p_{21} p_{34}^2$ *and* $\beta p_{34} d_{13} p_{21} = \alpha\, d_4\, p_{31}\, d_{23}\, p_{12}$ *then*

$$x^\star(t) = \begin{cases} 0, & \text{if } \alpha + \psi_4(t) > 0, \\ 1, & \text{if } \alpha + \psi_4(t) < 0, \\ f\big(n_2(t), n_3(t), n_4(t), \psi_1(t), \psi_2(t)\big), & \text{if } \alpha + \psi_4(t) = 0, \end{cases} \tag{27}$$

where $f\big(n_2(t), n_3(t), n_4(t), \psi_1(t), \psi_2(t)\big)$ *is defined by a rather long expression that is given in Appendix A of paper [2].*

Proof The proof of this theorem is rather intricate and will not be reported here. It is given in detail in paper [2] and results from a rather careful manipulation of the optimality conditions as well as of the switch function and its successive derivatives.

4.3 Numerical Solutions of the Model with Immunotherapy

We perform some numerical simulations for the model with immunotherapy.

The Optimal Immunotherapy

First, we determine the optimal control $x^*(t)$ that describes the optimal treatment protocol. With this in mind, we solve numerically the optimal control problem of minimizing the functional (24) over the set (25), when subjected to the state equations (16)–(19) with initial conditions (20). We consider $\alpha = \beta = 1$ for the weight parameters of the objective functional $J(t_f; x)$ given in (23). Moreover, we assume the terminal time to be $t_f = 30$, in appropriate time units, and take $d_4 = 1$.

The optimal control problem is solved numerically by a direct sequential method. The control problem is discretized and the resulting problem is solved using nonlinear programming (NLP) techniques. When a direct sequential method is used, only

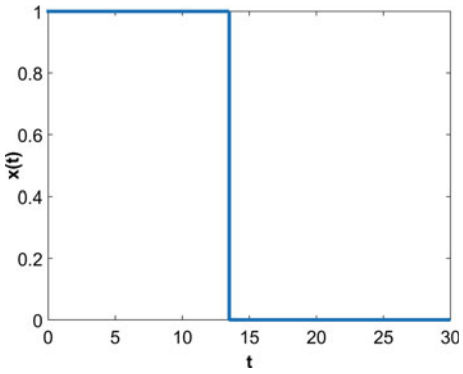


Fig. 3 The optimal control $x^\star(t)$, representing the optimal treatment protocol as given in (24)

the controls are discretized whereas the ODE system of state equations is embedded in the NLP problem and solved by an ODE solver in order to obtain the state values for the optimization. More in detail, the control $x(t)$ is discretized using the simplest piecewise polynomial approximations, defined by a a piecewise function with constant branches,

$$x(t) = c_i \quad \text{for} \quad t \in [t_{i-1}, t_i] \quad \text{and} \quad i = 1, \ldots, n,$$

so that $x(t)$ only depends on the control parameters $c_1, c_2, \ldots, c_n$. Above, $[t_{i-1}, t_i]$ represents a generic subinterval of the time interval $[0, t_f]$ introduced by the discretization process. We use the Matlab® function ode15s to solve the ODE system that is embedded in the discrete NLP problem.

The optimal control $x^\star(t)$ obtained in our simulations is represented in Fig. 3, and is of bang-bang type, since the values for the parameters used in our calculations satisfy $d_{13} \neq d_{23}$ and $\beta p_{34} d_{13} p_{21} - \alpha\, d_4\, p_{31}\, d_{23}\, p_{12} \neq 0$, see Theorem 7. We show numerically that the bang-bang control have at most one switching time at $t_s = 13$, from maximum control to no control and the switch occurs before the peak of the infection, $t_i = 20$. The behaviour of $x^\star(t)$ is in accordance with the administration of the IL-2 drug given in the clinical trial described in paper [2], that can be found in the medical literature. It corresponds to a situation where the IL-2 drug is administered during a certain consecutive period of time after which the administration of the drug is suspended.

The Immunoregulatory Effect at the Macroscopic Level

The optimal therapeutic protocol represented in Fig. 3 is shown to be effective in controlling the proliferation of SRTCs and consequent evolution of an autoimmune reaction. This behaviour can be observed when comparing Fig. 4b with Fig. 4a, and is due to a more prompt response of these cells to the immunosuppressive cells that receive an external boost from the IL-2 drug therapy.

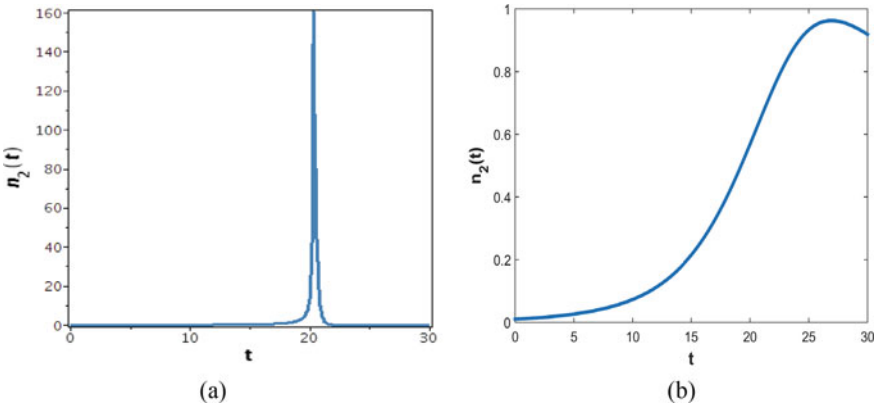


Fig. 4 Time evolution of SRTCs density determined by the macroscopic system (16)–(19), in the absence of immunotherapy (**a**) and in presence of immunotherapy (**b**)

Thus, we can conclude that the optimal immunotherapy prevents the SRTCs mass proliferation and possible autoimmune episode.

The Immunoregulatory Effect at the Cellular Level

We can observe the effect of the optimal immunotherapy at the cellular level, if we solve numerically the kinetic system (11)–(14) when the optimal drug therapy $x^\star$ of Fig. 3 is prescribed. The description obtained in this way gives a more detailed representation of the immunoregulatory effect than the one of Fig. 4b, because the conservative interactions participate in the evolution showing the influence of the cellular activity on the dynamics.

The numerical method used in the simulations is the same as the one proposed in [1]. As initial data, we assume that the distribution functions f_i^0, $i = 1, 2, 3$, are of the order 10^{-2}, as before, and f_4^0 is of the order 10^{-3}. The input data for the conservative, proliferative and destructive parameters are those given in (10), that were used to obtain Figs. 3 and 4.

In view of estimating the effects of the conservative interactions in the evolution, we start with the description of Fig. 5, when all conservative terms are taken to be null.

The graph of Fig. 5 for the distribution function of the SRTCs, $f_2(t, u)$, behaves in the same way as the graph of Fig. 4b for the number density of the SRTCs, $n_2(t)$, which is what would be expected for this particular model, see Eq. (12).

In Fig. 6, conservative terms are included in the model, reflecting the influence of the cell interactions on the activity of SRTCs. We are interested in analysing the decreasing effect of the activity of the SRTCs caused by the conservative interactions with ISCs. Therefore we vary the value of the corresponding conservative rate, by considering $c_{23} = 0.01$ in diagram (a), $c_{23} = 0.03$ in diagram (b) and $c_{23} = 0.2$ in diagram (c). We can observe that the mass production of SRTCs with high activity decreases when c_{23} increases, and becomes residual when c_{23} takes the highest value.

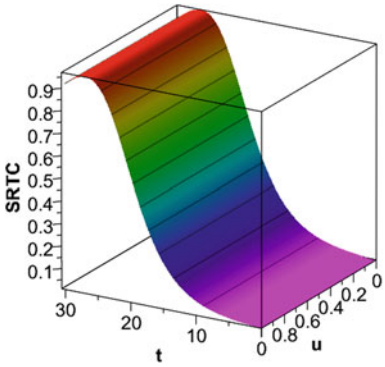


Fig. 5 Dynamic response of self-reactive T cells to the optimal control of non-conservative interactions. Evolution determined by the kinetic system (11)–(14) without conservative interactions

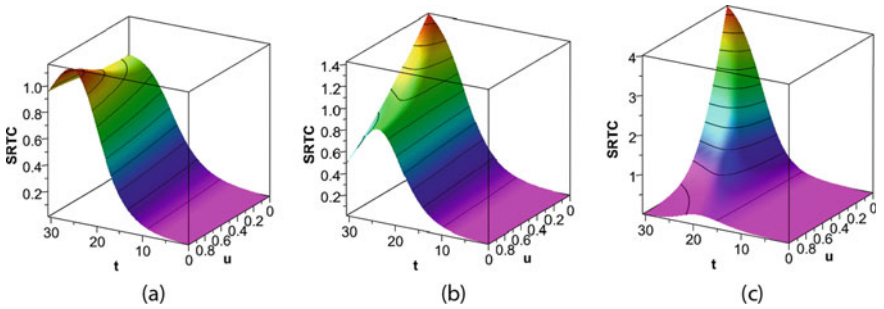


Fig. 6 Conservative dynamic response of self-reactive T cells to the optimal control, varying the conservative rate c_{23}. Evolution determined by the kinetic system (11)–(14), with **(a)** $c_{23} = 0.01$, **(b)** $c_{23} = 0.03$, **(c)** $c_{23} = 0.2$

In fact, the peak in the graph of SRTCs moves from a region of high activity in (a) to a region of almost vanishing activity in (c).

5 Conclusion and Future Projects

A new mathematical model, based on the Boltzman-like kinetic theory, describing an autoimmune response against self-antigens, was developed in [1]. In this model three of the main cell populations involved in the development of an autoimmune reaction are considered, namely, self-antigen presenting cells, self-reactive T cells and immunosupressive cells, such as Tregs and NKCs. The interactions between these cell populations are constructed in the model based on biological considerations appearing in the literature. The model is characterized by a system of integro-differential

equations. The mathematical analysis showing existence, uniqueness, positivity and boundedness of the solution of this system was performed in [1].

This analysis is fundamental for the task of generating numerical simulations of the model that translate, as realistically as possible, the behaviour of the cells involved in autoimmunity and that are considered in this work. Consequently, it is possible to study the sensitivity of the model to certain parameters appearing in the equations. The effect of such parameters on the model can be interpreted as the effect of the behaviour and characteristics of the cells involved on the evolution of the autoimmune reaction.

The model proposed in [1] is reviewed in these proceedings and some numerical simulations, different from those performed in [1], are also described and interpreted here, in line with the objectives of the present work.

In paper [2], the macroscopic analogue of the kinetic model given in [1] is extended to include a fourth population of IL-2 cytokines and an artificial inlet of these cytokines representing an external drug therapy. Again, an analytical analysis showing existence, uniqueness, positivity and boundedness of the solution to this system was performed [2]. This analysis allows us to proceed in determining the optimal policy for IL-2 immunotherapeutic treatment for autoimmune disease, which reduces the number of self-reactive T cells while at the same time minimizing the artificial inlet of IL-2. We can then perform numerical simulations for the model and explicitly determine the optimal drug therapy.

In the work presented here, we have gone a little further in the study of our model by presenting a kinetic system whose macroscopic analogue is the model given in [2]. This kinetic system allows us to observe the result of the optimal drug therapy with IL-2 at the cellular level. This is our main new contribution in these proceedings.

The models given in [1, 2] describe the cellular interactions and their consequences when a single autoimmune reaction occurs. However, since most autoimmune diseases are chronic conditions, the next step in our study is to introduce recurrence in the mathematical model. We have, in fact, in a more recent work, introduced recurrency in our macroscopic model described by an oscillatory behaviour of the solution and illustrating the relapse-remission pattern that is typical of some autoimmune diseases.

In this new mathematical model, the macroscopic system of ODEs admits Hopf bifurcations and therefore shows the desired oscillatory pattern. This is the topic of recently developed work whose results can be found in [19].

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References

1. M.P. Ramos, C. Ribeiro, A.J. Soares, A kinetic model of T cell autoreactivity in autoimmune diseases. J. Math. Biol. **79**, 2005–2031 (2019)

2. M.F. Costa, M.P. Ramos, C. Ribeiro, A.J. Soares, Mathematical modeling and optimal control of immunotherapy for autoimmune disease (submitted)
3. N. Bellomo, G. Forni, Dynamics of tumor interaction with the host immune system. Mathl. Comput. Model. **20**, 107–122 (1994)
4. L. Arlotti, N. Bellomo, K. Latrach, From the Jager and Segel model to kinetic population dynamics nonlinear evolution problems and applications. Mathl. Comput. Model. **30**, 15–40 (1999)
5. L. Arlotti, M. Lachowicz, Qualitative analysis of a nonlinear integrodifferential equation modeling tumor-host dynamics. Mathl. Comput. Model. **23**, 11–29 (1996)
6. M. Delitala, U. Dianzani, T. Lorenzi, M. Melensi, A mathematical model for immune and autoimmune response mediated by T-cells. Comput. Math. Appl. **66**, 1010–1023 (2013)
7. M. Kolev, I. Nikolova, Dynamical properties of autoimmune disease models: tolerance, flare-up, dormancy. J. Theor. Biol. **246**, 646–659 (2007)
8. G. Ajmone Marsan, N. Bellomo, L. Gibelli, Stochastic evolutionary differential games toward a systems theory of behavioral social dynamics. Math. Mod. Meth. App. Sci. **26**, 1051–1093 (2016)
9. M. Kolev, I. Nikolova, A mathematical model of some viral-induced autoimmune diseases. Math. Appl. **46**, 97–108 (2018)
10. R. Eftimie, L. Gibelli, A kinetic theory approach for modelling tumour and macrophages heterogeneity and plasticity during cancer progression. Math. Mod. Meth. App. Sci. **30**, 659–683 (2020)
11. B. Akkaya, Y. Oya, M. Akkaya, J.A. Souz, A.H. Holstein, O. Kamenyeva, J. Kabat, R. Matsumura, D.W. Dorward, D.D. Glass, E.M. Shevach, Regulatory T cells mediate specific suppression by depleting peptide MHC class II from dendritic cells. Nat. Immunol. **20**, 218–231 (2019)
12. T.M. Brusco, A.L. Putnam, J.A. Bluestone, Human regulatory T cells: role in autoimmune disease and therapeutic opportunities. Immun. Rev. **223**, 371–390 (2008)
13. R. Liberal, C.R. Grant, M.S. Longhi, G. Mieli-Vergani, D. Vergani, Regulatory T cells: mechanisms of suppression and impairment in autoimmune liver disease. Int. Union Biochem. Mol. Biol. **67**, 88–97 (2015)
14. A. Sharabi, M.G. Tsokos, Y. Ding, T.R. Malek, D. Klatzmann, G.C. Tsokos, Regulatory T cells in the treatment of disease. Nat. Rev. Drug Discov. **17**, 823–844 (2018)
15. A.L. Zozulya, H. Wiendl, The role of regulatory T cells in multiple sclerosis. Nat. Clin. Pract. Neurol. **4**, 384–398 (2008)
16. A. Poggi, M.R. Zocchi, NK cell autoreactivity and autoimmune diseases. Front. Immunol. **5**, 1–15 (2014)
17. Z. Tian, M.E. Gershwin, C. Zhang, Regulatory NK cells in autoimmune disease. J. Autoimmun **39**, 206–215 (2012)
18. F. Shi, L.V. Kaer, Reciprocal regulation between natural killer cells and autoreactive T cells. Nat. Rev. Immunol. **6**, 751–760 (2006)
19. R. Della Marca, M.P. Ramos, C. Ribeiro, A.J. Soares, Mathematical modelling of oscillating patterns for chronic autoimmune diseases (work in progress)
20. W.H. Fleming, R.W. Rishel, *Deterministic and Stochastic Optimal Control* (Springer, Berlin, 1975)
21. D.L. Lukes, *Differential Equations: Classical to Controlled*, vol. 162 (Academic, New York, 1982)

Geometrical Structures of the Instantaneous Current and Their Macroscopic Effects: Vortices and Perspectives in Non-gradient Models

Leonardo De Carlo

Abstract First we discuss the definition of the instantaneous current in interacting particle systems, in particular in mass-energy systems and we point out its role in the derivation of the hydrodynamics. Later we present some geometrical structures of the instantaneous current when the rates of stochastic models satisfy a very common symmetry. This structures give some new ideas in non-gradient models and show new phenomenology in diffusive interacting particle systems. Specifically, we introduce models with vorticity and present some new perspectives on the link between the Green-Kubo's formula and the hydrodynamics of non-gradient models.

Keywords Stochastic lattice gases · Non-gradient models · Discrete Hodge decomposition

AMS 2010 Subject Classification: 60K35 · 82C22 · 82C20

1 Introduction and Results

When many interacting particles are modelled by Newton's equations the rigorous derivation of hydrodynamics equations, consisting in some PDEs and describing the evolution of thermodynamic quantities, is often a too optimistic programme, mainly because of the lack of good ergodic property of the system. To overcome the mathematical problem two assumptions are traditionally made: or modelling the problem with a stochastic microscopic evolution or assuming a low density of particles. In the present framework we are interested in the first assumption and we are not having a complete rigorous point of view. For a rigorous and didactic treatment traditional references are [14, 18]. The microscopic dynamics consists of random walks of particles on a lattice V_N that are constrained to some rule expressing

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the local interaction, these are the so-called *interacting particle systems* introduced by Spitzer [17].

In this paper we focus on the instantaneous current which is the bridge from the microscopic description to the macroscopic description of interacting particle systems. In Sect. 2 we give some definitions that we will use trough all the paper. In Sects. 3 and 4 we present the models and describe the instantaneous current, in particular its definitions it is clarified in in mass-energy systems like KMP [6, 13]. In Sect. 5 we recall the functional Hodge decomposition obtained in [5] in dimension one and two and we apply it to some interacting particle models. The expert reader can skip the first four sections and Sect. 6, where well known notions of the literature are presented with a general flavour, and refer these sections just for notation if necessary.

In the work the attention is on diffusive models. Some new models with vorticity are introduced in Sect. 8. After reviewing the qualitative theory of scaling limits in diffusive systems in Sect. 7, in Sect. 8, for the first time we study the macroscopic consequences of this decomposition. This leads us to some new phenomenology in particle systems, that is we show in a non-rigorous way that the hydrodynamics of the macroscopic current can present zero divergence terms that are not observed in the hydrodynamics of the density. This extend the usual Fick's law (58) to the a new picture (68) where the diffusion matrix is a positive non-symmetric matrix.

In diffusive non gradient systems a derivation of the hydrodynamics with an explicit diffusion coefficient is an open problem. The relative PDEs are in term of a variational expression of the diffusion coefficient equivalent to the Green-Kubo's formula, see [15, 18]. In the last Sect. 9, we try to give some perspectives coming from our Hodge decomposition. We give a possible explicit description of the minimizer of Green-Kubo's formula using our functional Hodge decomposition and describe a scheme that connects this minimizer with an explicit hydrodynamics.

2 Definitions

Interacting particle systems are stochastic models evolving on a lattice along a continuous time Markov dynamics. For the purposes of the paper, we are going to consider only periodic boundary conditions for the lattice where particles move, i.e. the set of vertices V_N of the lattice will be the n-dimensional discrete torus $\mathbb{T}_N^n = \mathbb{Z}^n/N\mathbb{Z}^n$ or $\mathbb{T}_\varepsilon^n = \varepsilon\mathbb{Z}^n/N\mathbb{Z}^n$, where $\varepsilon = 1/N$ along the space scale we want to consider. We denote with $\mathscr{E}_N$ the set of all couples of vertices $\{x, y\}$ of V_N such that $y = x \pm \delta\, e_i$ where e_i is the canonical versor in $\mathbb{Z}^n$ along the direction i and δ is equals to 1 on $\mathbb{T}_N^n$ and to $1/N$ on $\mathbb{T}_\varepsilon^n$. The elements of $\mathscr{E}_N$ are named non-oriented edges or simply edges. In this way we have an non-oriented graph $(V_N, \mathscr{E}_N)$. To every non-oriented graph $(V_N, \mathscr{E}_N)$ we associate canonically an oriented graph (V_N, E_N) such that the set of oriented edges E_N contains all the ordered pairs (x, y) such that $\{x, y\} \in \mathscr{E}_N$. Note that if $(x, y) \in E_N$ then also $(y, x) \in E_N$. If $e = (x, y) \in E_N$ we denote $e^- := x$ and $e^+ := y$ and we call $\mathfrak{e} := \{x, y\}$ the non-oriented edge.

The microscopic configurations of our particle models are given by the collection of variables $\eta(x)$ representing the number of particles, the energy or mass at $x \in V_N$ along the model. When the variables $\eta(x)$ are discrete we interpret them as number particles and when continuous as mass-energy. Calling Σ the state space at x we define the configuration state space as $\Sigma_N := \Sigma^{V_N}$. The microscopic dynamics is a Markov process $\{\eta_t\}_{t\in\mathbb{R}}$ where particles or masses interact along rules encoded in the generator $\mathscr{L}_N$, i.e.

$$\mathscr{L}_N f(\eta) = \sum_{\eta' \in \Sigma_N} c(\eta, \eta')[f(\eta') - f(\eta)], \tag{1}$$

where f is an observable and $c(\eta, \eta')$ the transition rates from η to η'.

Let τ_z be the shift by z on $\mathbb{Z}^n$ defined by the relation $\tau_z \eta(x) := \eta(x - z)$ with $z \in \mathbb{Z}^n$ and for a function $h : \eta \to h(\eta) \in \mathbb{R}$ we define $\tau_z h(\eta) := h(\tau_{-z}\eta)$, moreover for a domain $B \subseteq V_N$ we define $\tau_z B := B + z$. A function $h : \Sigma_N \to \mathbb{R}$ is called *local* if it depends only trough the configuration in a finite domain $B \subset V_N$ denoted $D(f)$. Let $[\cdot]_+$ be the positive part function.

3 Particle Models and Instantaneous Current

We treat only nearest neighbour conservative dynamics, that is (1) becomes

$$\mathscr{L}_N f(\eta) = \sum_{(x,y)\in E_N} c_{x,y}(\eta)\left(f(\eta^{x,y}) - f(\eta)\right), \quad \eta^{x,y}(z) := \begin{cases} \eta(x) - 1 & \text{if } z = x \\ \eta(y) + 1 & \text{if } z = y \\ \eta(z) & \text{if } z \neq x, y \end{cases}. \tag{2}$$

We study *translational covariant models*, i.e. $c_{x,x\pm e^{(i)}}(\eta) = \tau_x c_{0,\pm e^{(i)}}(\eta) \;\; \forall x \in V_N$.

3.1 Exclusion Process and the 2-SEP

In an *exclusion process* particles move according to a conservative dynamics of independent random walks with the exclusion rule that there cannot be more than one particle in a single lattice site (hard core interaction). The rates of (2) have the general form

$$c_{x,y}(\eta) = \eta(x)(1 - \eta(y))\widetilde{c}_{x,y}(\eta), \tag{3}$$

where $\widetilde{c}_{x,y}(\eta)$ is the jump rates when η has a particle in x and an empty site in y.

The next example of (2) is the *2-SEP* (2-simple exclusion process), in this model the interaction is simply hardcore but in every site there can be at most 2 particles. The state space is $\Sigma_N = \{0, 1, 2\}$ and the dynamics is defined by

$$\mathscr{L}_N^{\text{2-SEP}} f(\eta) = \sum_{(x,y)\in E_N} c_{x,y}(\eta)\left(f(\eta^{x,y}) - f(\eta)\right), \quad c_{x,y}(\eta) = \chi^+(\eta(x))\chi^-(\eta(y)), \tag{4}$$

where $\chi^+(\alpha) = 1$ if $\alpha > 0$ and zero otherwise while $\chi^-(\alpha) = 1$ if $\alpha < 2$ and zero otherwise.

3.2 Instantaneous Current in Particle Systems

In interacting particle systems there are deep underlying geometrical structures that reflects in the hydrodynamics of lattice models as we will discuss later, see also [5]. The basis is the fact that the instantaneous current is a discrete vector field and closely related to a microscopic mass conservation law leading to the hydrodynamics.

Definition 1 A discrete vector field is a function $\varphi : E_N \to \mathbb{R}$ that is *antisymmetric*, i.e. $\varphi(x, y) = -\varphi(y, x)$ for any $(x, y) \in E_N$.

The *instantaneous current* for our particle models is defined as

$$j_\eta(x, y) := c_{x,y}(\eta) - c_{y,x}(\eta)\,, \tag{5}$$

which is a discrete vector field for each fixed configuration η. The intuitive interpretation of the instantaneous current is the rate at which particles cross the bond (x, y). Let $\mathscr{N}_t(x, y)$ be the number of particles that jumped from site x to site y up to time t. The *current flow* across the bond (x, y) up to time t is defined as

$$J_t(x, y) := \mathscr{N}_t(x, y) - \mathscr{N}_t(y, x)\,. \tag{6}$$

This is a discrete vector field ($J_t(x, y) = -J_t(y, x)$) depending on the trajectory $\{\eta_t\}_t$. Between the instantaneous current $j_\eta(x, y)$ and the current flow $J_t(x, y)$ there is a strict connection given by the key observation (see for example [18] Sect. 2.3 in part II) that

$$M_t(x, y) = J_t(x, y) - \int_0^t j_{\eta(s)}(x, y)ds \tag{7}$$

is a martingale. This allows to treat the difference between $J_t(x, y)$ and the integral $\int_0^t ds\, j_{\eta(s)}(x, y)$ as a microscopic fluctuation term. It also gives a more physical definition of $j_\eta(x, y)$ as follows. Consider an initial configuration $\eta_0 = \eta$, the explicit expression of the instantaneous current can be defined as

$$j_\eta(x, y) := \lim_{t\to 0} \frac{\mathbb{E}^\eta(J_t(x, y))}{t}. \tag{8}$$

The expectation is $\mathbb{E}^\eta(J_t(x, y)) = \int \mathbb{P}^\eta(d\{\eta_t\}_t) J_t(x, y)$, where the integration is over all trajectories $\{\eta_t\}_t$ starting from η at time 0 and $\mathbb{P}^\eta$ the probability induced by the Markov process. For a trajectory $\{\eta_t\}_t$ the probability to observe more than one jump goes like $O(t^2)$, then it is negligible since we are interested in an infinitesimal time interval. Since $c(\eta, \eta') = \lim_{t\to 0} \frac{\mathbb{P}^\eta(\eta_t=\eta')}{t} = \lim_{t\to 0} \frac{p_t(\eta,\eta')}{t}$, where $p_t(\eta, \eta')$ are the transition probability, when t goes to zero $J_t(x, y)$ takes value $+1$ if a jump from x to y happens, -1 in the opposite case and 0 in the other cases. So the current defined in (8) becomes $j_\eta(x, y) = c_{x,y}(\eta) - c_{y,x}(\eta)$ as in (5).

The discrete divergence for a discrete vector field φ on E_N is $\nabla \cdot \varphi(x) := \sum_{y\sim x} \varphi(x, y)$, where the sum is on the nearest neighbours $y \sim x$ of x. For convenience of notation, we will use the symbol $\nabla\cdot$ both for the discrete case and the continuous one, therefore we recommend to the reader to pay attention about this. The local microscopic conservation law of the number of particles is then given by

$$\eta_t(x) - \eta_0(x) + \nabla \cdot J_t(x) = 0. \tag{9}$$

Using (7) in (9) we get

$$\eta_t(x) - \eta_0(x) + \int_0^t ds\, \nabla \cdot j_s(x) + \nabla \cdot M_t(x) = 0. \tag{10}$$

We can deduce that at the equilibrium, that is when for a measure μ_N on Σ_N the *detailed balance condition* is true, i.e. $\mu_N(\eta)c(\eta, \eta^{x,y}) = \mu_N(\eta^{x,y})c(\eta^{x,y}, \eta)$ for all $(x, y) \in E_N$, the average flow $\mathbb{E}^\eta_{\mu_N}(J_t(x, y))$ is constantly zero, where the subscript μ_N indicates the average respect to the equilibrium measure μ_N. For a small time interval Δt from (7), (8) and the detailed balance we have $\mathbb{E}^\eta_{\mu_N}(J_{\Delta t}(x, y)) \sim \mathbb{E}_{\mu_N}(j_\eta(x, y))\Delta t = 0$. Since this is true for any time interval Δt and the current flow $J_t(x, y)$ is additive we conclude that $\mathbb{E}^\eta_{\mu_N}(J_t(x, y)) = 0$. More generally for a *stationary measure* μ_N, that is $\mu_N(\mathscr{L}_N f) = 0$ for any f, we have that

$$\mathbb{E}^\eta_{\mu_N}(J_t(x, y)) = \mathbb{E}_{\mu_N}(j_\eta(x, y))t. \tag{11}$$

Remark 1 For a *translational covariant model*, i.e. $c_{x,y}(\eta) = c_{x+z,y+z}(\tau_z\eta)$ for any $z \in V_N$, then the instantaneous current is translational covariant too, namely it satisfies the symmetry relation

$$j_\eta(x, y) = j_{\tau_z\eta}(x + z, y + z). \tag{12}$$

4 Energy-Mass Models

In this section we adapt the concepts of the previous section to the continuous case, where we consider models that exchange continuous quantity between sites. The lattice variables are interpreted as energy or mass along the context and the configuration is denoted with $\xi = \{\xi(x)\}_{x\in V_N}$. The first model to be described is the most famous model of this class, namely the Kipnis-Marchioro-Presutti (KMP) model [13].

4.1 KMP Model and Generalization, Dual KMP, Gaussian Model

The *KMP dynamics* is a generalized stochastic lattice gas on which energies or masses are associated to oscillators at the vertices V_N . The stochastic evolution is of the type

$$\mathscr{L}_N f(\xi) = \sum_{\{x,y\}\in\mathscr{E}_N} \mathscr{L}_{\{x,y\}} f(\xi)\,, \text{ with} \tag{13}$$

$$\mathscr{L}_{\{x,y\}} f(\xi) := \int_{-\xi(y)}^{\xi(x)} \frac{dq}{\xi(x)+\xi(y)} \left[f\left(\xi - q\left(\varepsilon^x - \varepsilon^y\right)\right) - f(\xi)\right]. \tag{14}$$

where $\varepsilon^x = \{\varepsilon^x(y)\}_{y\in V_N}$ is the configuration of mass with all the sites different from x empty and having unitary mass at site x, this means that $\varepsilon^x(y) = \delta_{x,y}$ where δ is the Kronecker symbol. Formula (14) define the model as a uniform distributed random current model.

The dynamics (14) can be generalized substituting the uniform distribution on $[-\xi(y), \xi(x)]$ for a different probability measure (or just positive measure) $\Gamma^{\xi}_{x,y}(dq)$, i.e.

$$\mathscr{L}_{\{x,y\}} f(\xi) := \int \Gamma^{\xi}_{x,y}(dq) \left[f\left(\xi - q\left(\varepsilon^x - \varepsilon^y\right)\right) - f(\xi)\right] \tag{15}$$

with the symmetry $\Gamma^{\xi}_{x,y}(q) = \Gamma^{\xi}_{y,x}(-q)$ so that (13) is a sum over unordered edges. When considering a discrete state space, a natural choice for $\Gamma^{\xi}_{x,y}(dq)$ in (15) is the discrete uniform distribution on the integer points in $[-\xi(y), \xi(x)]$. This means that if ξ is a configuration of mass assuming only integer values then

$$\Gamma^{\xi}_{x,y}(dq) = \frac{1}{\xi(x)+\xi(y)+1} \sum_{i\in[-\xi(y),\xi(x)]} \delta_i(dq) \tag{16}$$

where $\delta_i(dq)$ is the delta measure at i and the sum is over the integer values belonging to the interval. This is exactly the dual model of KMP [13] called also *KMPd*.

Another interesting model could be the following *Gaussian model*. In this case the interpretation in terms of mass is missing since the variables can assume also negative values and it could be interpreted as a charge model. The bulk dynamics is defined by a distribution of current having support on all the real line

$$\Gamma^{\xi}_{x,y}(dq) = \frac{1}{\sqrt{2\pi\gamma^2}} e^{-\frac{\left(q-\frac{(\xi(x)-\xi(y))}{2}\right)^2}{2\gamma^2}} dq\,. \tag{17}$$

4.2 Weakly Asymmetric Energy-Mass Models

We consider dynamics perturbed by a space and time dependent discrete external field $\mathbb{F}$ defined as follows. Let $F : \mathbb{T}^n \to \mathbb{R}^n$ be a smooth vector field with components $F(x) = (F_1, \ldots, F_n)$, describing the force acting on the masses of the systems. We associate to F a discrete vector field $\mathbb{F}(x, y)$ defined by

$$\mathbb{F}(x, y) = \int_{(x,y)} F(z) \cdot dz, \tag{18}$$

(x, y) is an oriented edge and the integral is a line integral that corresponds to the work done by the vector field F when a particle moves from x to y. So we think about $\mathbb{F}(x, y)$ as work done per particle. We want to change the random distribution (15) of the current on each bond according to a perturbed measure $\Gamma^{\mathbb{F}}$, that is

$$\mathscr{L}^{\mathbb{F}}_{\{x,y\}} f(\xi) := \int \Gamma^{\xi,\mathbb{F}}_{x,y}(dq)\big[f(\xi - q\left(\varepsilon^x - \varepsilon^y\right)) - f(\xi)\big], \quad \Gamma^{\xi,\mathbb{F}}_{x,y}(dq) = \Gamma^{\xi}_{x,y}(dq) e^{\frac{\mathbb{F}(x,y)}{2}q}\,. \tag{19}$$

The effect of an external field is modelled by perturbing the rates and giving a net drift toward a specified direction. When the size of $|y - x|$ is of order $1/N$ we obtain a *weakly asymmetric model*, the discrete vector field (18) is of order $1/N$ too and the hydrodynamics is studied considering a perturbative expansion of $\Gamma^{\xi,\mathbb{F}}_{x,y}(dq)$ for the orders that will give a macroscopic effect. We will see that for weakly asymmetric diffusive models this expansion is necessary up to the order two. If $F = -\nabla H$ is a gradient vector field, then $\mathbb{F}(x, y) = H(x) - H(y)$ and $\Gamma^{\xi,\mathbb{F}}_{x,y}(dq) = \Gamma^{\xi}_{x,y}(dq) e^{(H(x)-H(y))q}$.

By the symmetry of the measure Γ and the antisymmetry of the discrete vector field $\mathbb{F}$ we have that $\Gamma^{\xi,\mathbb{F}}_{x,y}(q) = \Gamma^{\xi,\mathbb{F}}_{y,x}(-q)$ and we can define the generator considering sums over unordered bonds

$$\mathscr{L}_N f(\xi) = \sum_{\{x,y\}\in\mathscr{E}_N} \mathscr{L}^{\mathbb{F}}_{\{x,y\}} f(\xi). \tag{20}$$

4.3 Instantaneous Current of Energy-Mass Systems

Here we adapt the definition of instantaneous current to the formalism of the interacting nearest neighbour energy-mass models. The generator is (19), the case $\mathbb{F} = 0$ is treated as a subcase and we omit the index when the external field is zero. The *instantaneous current* for the bulk dynamics is defined as

$$j_\xi^{\mathbb{F}}(x, y) := \int \Gamma_{x,y}^{\xi,\mathbb{F}}(dq)q \,. \tag{21}$$

Its interpretation is the rate at which masses-energies cross the bond (x, y) and it is still a discrete vector field. The *current flow* now is indicated with $\mathscr{J}_t(x, y)$ and it is the net total amount of mass-energy that has flown from x to y in the time window $[0, t]$. It can be defined as sum of all the differences between the mass-energy measured in x before and after of every jump on the bond $\{x, y\}$. Let τ_i be the time of the ith jump on the bond $\{x, y\}$ for some i, we write the current flow as follows

$$\mathscr{J}_t(x, y) := \sum_{\tau_i : \tau_i \in [0,t]} J_{\tau_i}(x, y)\,, \tag{22}$$

where $J_\tau(x, y)$ is the *present flow* defined as the current flowing from x to y jump time τ

$$J_\tau(x, y) := \lim_{h \downarrow 0} \xi_{\tau-h}(x) - \lim_{h \downarrow 0} \xi_{\tau+h}(x). \tag{23}$$

Defining $J_\tau(y, x) := \lim_{h\downarrow 0} \xi_{\tau-h}(y) - \lim_{h\downarrow 0} \xi_{\tau+h}(y)$, the flow $\mathscr{J}_t(x, y)$ is still an anti-symmetric vector field depending on the trajectory $\{\xi_t\}$, i.e. $J_\tau(y, x) := -J_\tau(x, y)$. As in the particles case $\mathscr{J}_t(x, y)$ is a function on the path space, while the instantaneous current $j_\xi^{\mathbb{F}}(x, y)$ is a function on the configuration space and the difference

$$M_t(x, y) = \mathscr{J}_t(x, y) - \int_0^t ds\, j_{\xi(s)}^{\mathbb{F}}(x, y). \tag{24}$$

is a martingale. Repeating what we did in Sect. 3.2 (with a formalism suitable to energy-mass models) the instantaneous current (21) can be obtained as

$$j_\xi^{\mathbb{F}}(x, y) := \lim_{t \to 0} \frac{\mathbb{E}^\xi(\mathscr{J}_t(x, y))}{t}. \tag{25}$$

As we did in Sect. 3.2 from the local discrete conservation of the mass-energy $\xi_t(x) - \xi_0(x) + \nabla \cdot \mathscr{J}_t(x) = 0$ we have

$$\xi_t(x) - \xi_0(x) + \int_0^t ds\, \nabla \cdot j_{\xi(s)}^{\mathbb{F}}(x) + \nabla \cdot M_t(x) = 0. \tag{26}$$

The microscopic fluctuation (24) has mean zero and (11) can be obtained similarly to conclude that the average currents are zero in the equilibrium case, i.e. when detailed balance conditions (DBC) hold.

The natural scaling limit for this class of processes is the diffusive one, where the rates have to be multiplied by N^2 to get a non trivial scaling limit. So, instead of (24), we will consider in the macroscopic theory the speeded up martingale $M_t(x, y) = \mathscr{J}_t(x, y) - N^2 \int_0^t ds\, j^{\mathbb{F}}_{\xi(s)}(x, y)$.

Example 1 For example the instantaneous current across the edge (x, y) for the KMP process is given by

$$\int_{-\xi(y)}^{\xi(x)} \frac{q dq}{\xi(x) + \xi(y)} = \frac{1}{2}\left(\xi(x) - \xi(y)\right) . \tag{27}$$

This computation shows that the KMP model is of gradient type, see definition (35), with $h(\xi) = -\frac{\xi(0)}{2}$. Also the KMPd is gradient with respect to the same function h.

Example 2 For the weakly asymmetric KMP in the case of a constant external field $F = E$ in the direction from x to y the discrete field $\mathbb{F}(x, y)$ is given by E/N on $\mathbb{T}^n_\varepsilon$ and

$$\Gamma^{\xi,E}_{x,y}(q) = \frac{1 + \frac{E}{N} q}{\xi(x) + \xi(y)} + o(N)$$

Then the instantaneous current is

$$\begin{aligned} j^E_\xi(x, y) &= \int_{-\xi(y)}^{\xi(x)} \Gamma^{\xi,E}_{x,y}(q) q dq = \\ &\frac{2N}{E(\xi(x) + \xi(y))}\left[e^{\frac{E}{2N}\xi(x)} \xi(x) + e^{-\frac{E}{2N}\xi(y)} \xi(y) - 2\frac{e^{\frac{E}{2N}\xi(x)} - e^{-\frac{E}{2N}\xi(y)}}{E} \right] = \\ &= \frac{1}{2}\big(\xi(x) - \xi(y)\big) + \frac{E}{N} 6\big[\xi(x)^2 + \xi(y)^2 - \xi(x)\xi(y)\big] + o(N) . \end{aligned} \tag{28}$$

The hydrodynamic behavior of the model under the action of an external field in the weakly asymmetric regime, i.e. when the external field E is of order $1/N$, is determined by the first two orders in the expansion (28). In particular any perturbed KMP model having the same expansion as in (28) will have the same hydrodynamics.

While for the KMPd model we get

$$j^E_\xi(x, y) = \frac{1}{2}\big(\xi(x) - \xi(y)\big) + \frac{E}{N} 12\big[2\xi(x)^2 + 2\xi(y)^2 - 2\xi(x)\xi(y) + 3\xi(x) + 3\xi(y)\big] + o(N) . \tag{29}$$

5 Discrete Hodge Decomposition in Interacting Particle Systems

In the first section we defined the graph $(V_N, \mathscr{E}_N)$. Now we enter into the detail of the discrete mathematics we need to study the geometrical structures of the current. We consider the case when the graph $(V_N, \mathscr{E}_N)$ is on $\mathbb{T}_N^2$.

A sequence $(z_0, z_1, \dots, z_k)$ of elements of V_N such that $(z_i, z_{i+1}) \in E_N$, $i = 0, \dots k-1$, is called an oriented path, or simply a *path*. A *cycle* $C = (z_0, z_1, \dots, z_k)$ is a path with distinct vertices except $z_0 = z_k$ and it is defined as an equivalence class modulo cyclic permutations. If C is a cycle and there exists an i such that $(x, y) = (z_i, z_{i+1})$ we write $(x, y) \in C$. Likewise if there exists an i such that $x = z_i$ we write $x \in C$. A *discrete vector field* φ on (V_N, E_N) is a map $\varphi : E_N \to \mathbb{R}$ such that $\varphi(x, y) = -\varphi(y, x)$. A discrete vector field is of *gradient type* if there exists a function $h : V_N \to \mathbb{R}$ such that $\varphi(x, y) = [\nabla h](x, y) := h(y) - h(x)$. The divergence of a discrete vector field φ at $x \in V_N$ is defined by

$$\nabla \cdot \varphi(x) := \sum_{y\,:\,\{x,y\}\in\mathscr{E}_N} \varphi(x, y)\,. \tag{30}$$

We call Λ^1 the $|\mathscr{E}_N|$-dimensional vector space of discrete vector fields. We endow Λ^1 with the scalar product

$$\langle \varphi, \psi \rangle := \frac{1}{2} \sum_{(x,y)\in E_N} \varphi(x, y)\psi(x, y)\,, \qquad \varphi, \psi \in \Lambda^1\,. \tag{31}$$

We recall briefly the Hodge decomposition for discrete vector fields. We call Λ^0 the collection of real valued function defined on the set of vertices $\Lambda^0 := \{g : V_N \to \mathbb{R}\}$. Finally we call Λ^2 the vector space of *2-forms* defined on the faces of the lattice $\mathbb{Z}_N^2$. Let us define this precisely. An oriented face is for example an elementary cycle in the graph of the type $(x, x + e^{(1)}, x + e^{(1)} + e^{(2)}, x + e^{(2)}, x)$. In this case we have an *anticlockwise oriented face*. This corresponds geometrically to a square having vertices $x, x + e^{(1)}, x + e^{(1)} + e^{(2)}, x + e^{(2)}$ plus an orientation in the anticlockwise sense. The same elementary face can be oriented *clockwise* and this corresponds to the elementary cycle $(x, x + e^{(2)}, x + e^{(1)} + e^{(2)}, x + e^{(1)}, x)$. If f is a given oriented face we denote by $-f$ the oriented face corresponding to the same geometric square but having opposite orientation. A 2-form is a map ψ from the set of oriented faces F_N to $\mathbb{R}$ that is antisymmetric with respect to the change of orientation, i.e. such that $\psi(-f) = -\psi(f)$. The boundary $\delta\psi$ of ψ is a discrete vector field defined by

$$\delta\psi(e) := \sum_{f\,:\,e\in f} \psi(f)\,. \tag{32}$$

Since a face is a cycle the meaning of $e \in f$ has been just discussed above. Note that (32) is a discrete orthogonal gradient, the orthogonal gradient $\nabla^{\perp} f$ of a smooth function f is defined as $(-\partial_y f, \partial_x f)$. In higher dimension this a discrete curl.

By construction $\nabla \cdot \delta\psi = 0$ for any ψ. The 2-dimensional *discrete Hodge decomposition* is written as the direct sum

$$\Lambda^1 = \nabla\Lambda^0 \oplus \delta\Lambda^2 \oplus \Lambda^1_H \,, \tag{33}$$

where the orthogonality is with respect to the scalar product (31). The discrete vector fields on $\nabla\Lambda^0$ are the gradient ones. The dimension of $\nabla\Lambda^0$ is $N^2 - 1$. The vector subspace $\delta\Lambda^2$ contains all the discrete vector fields that can be obtained by (32) from a given 2-form ψ. The dimension of $\delta\Lambda^2$ is $N^2 - 1$. Elements of $\delta\Lambda^2$ are called *circulations*. The dimension of Λ^1_H is simply 2. Discrete vector fields in Λ^1_H are called *harmonic*. A basis in Λ^1_H is given by the vector fields $\varphi^{(1)}$ and $\varphi^{(2)}$ defined by

$$\varphi^{(i)}\left(x, x + e^{(j)}\right) := \delta_{i,j} \,, \qquad i, j = 1, 2 \,. \tag{34}$$

Given a vector field $\varphi \in \Lambda^1$, we write $\varphi = \varphi^{\nabla} + \varphi^{\delta} + \varphi^{H}$ to denote the unique splitting in the three orthogonal components. This decomposition can be computed as follows. The harmonic part is determined writing $\varphi^H = c_1\varphi^{(1)} + c_2\varphi^{(2)}$ with The coefficients c_i determined by $c_i = \frac{1}{N^2}\sum_{x \in V_N} \varphi\left(x, x + e^{(i)}\right)$. To determine the gradient component φ^{∇} we need to determine a function h for which $\varphi^{\nabla}(x, y) = [\nabla h](x, y) = h(y) - h(x)$. This is done by taking the divergence on both side of $\varphi = \varphi^{\nabla} + \varphi^{\delta} + \varphi^{H}$ and obtaining the h solving the discrete Poisson equation $\nabla \cdot \nabla h = \nabla \cdot \varphi$. The remaining component φ^{δ} is computed just by difference $\varphi^{\delta} = \varphi - \varphi^{\nabla} - \varphi^{H}$. We refer to [4, 10] for a version of discrete calculus with cubic cells and to [8] for a version of discrete calculus with simplexes.

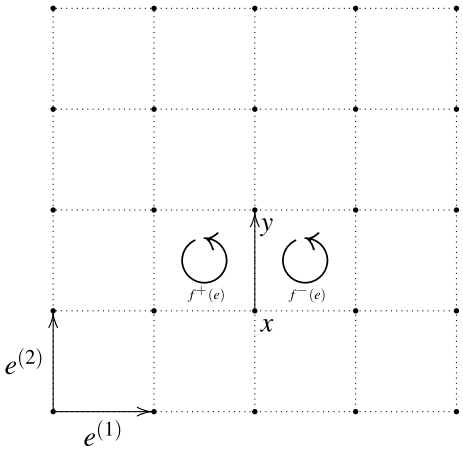

Fig. 1 On discrete two dimensional torus, given $(x, y) = e$ we draw the faces $f^-(e)$ and $f^+(e)$

Given an oriented edge e or an oriented face f we denote respectively by $\mathfrak{e}$, $\mathfrak{f}$ the corresponding un-oriented edge and face. Note that both f and $-f$ are associated with the same un-oriented face $\mathfrak{f}$. Given an oriented edge $e \in E_N$ of the lattice there is only one anticlockwise oriented face to which e belongs that we call it $f^+(e)$. There is also an unique anticlockwise face, that we call $f^-(e)$, such that $e \in -f^-(e)$ (see Fig. 1).

It is useful to define $\tau_{\mathfrak{f}}$ for an un-oriented face $\mathfrak{f}$. If $\mathfrak{f} = \{x, x + e^{(1)}, x + e^{(2)}, x + e^{(1)} + e^{(2)}\}$ then we define $\tau_{\mathfrak{f}} := \tau_x$. For $\mathfrak{e} = \{x, x + e^{(i)}\}$ we define $\tau_{\mathfrak{e}} := \tau_x$. We use also the notation $f^{\circlearrowleft}$ for an anticlockwise face and $f^{\circlearrowright}$ for a clockwise one.

5.1 Functional Discrete Hodge Decomposition and Lattice Gases

A relevant notion in the derivation of the hydrodynamic behavior for diffusive particle systems is the definition of gradient particle system. A particle system is called of *gradient type* if there exists a local function h such that

$$j_\eta(x, y) = \tau_y h(\eta) - \tau_x h(\eta) \text{ for all } (\eta, (x, y)) \in (\Sigma_N, E_N). \tag{35}$$

The relevance of this notion is on the fact that the proof of the hydrodynamic limit for gradient systems is extremely simplified. Moreover for gradient and reversible models it is possible to obtain explicit expressions of the transport coefficients.

Here we show that (35) is a subcase of general geometrical structures for the instantaneous current. In next sections, we will try to understand the consequences of these structures in the hydrodynamic limits and how it could be useful in understanding the hydrodynamics of non-gradient models. We present a functional Hodge decomposition of *translational covariant discrete vector fields*. This means vector fields $j_\eta(x, y)$ depending on the configuration $\eta \in \Sigma_N$ and satisfying (12). Vector fields of the form (35) play the role of the gradient vector fields. Circulations will also be suitably defined in the context of particle systems.

5.2 The One Dimensional Case

On the one dimensional torus V_N, we have the following theorem.

Theorem 1 *Let j_η be a translational covariant discrete vector field. Then there exists a function $h(\eta)$ and a translational invariant function $C(\eta)$ such that*

$$j_\eta(x, x + 1) = \tau_{x+1} h(\eta) - \tau_x h(\eta) + C(\eta)\,. \tag{36}$$

The function C is uniquely identified and coincides with

$$C(\eta) = \frac{1}{N} \sum_{x \in V_N} j_\eta(x, x+1)\,. \tag{37}$$

The function h is uniquely identified up to an arbitrary additive translational invariant function and coincides with

$$h(\eta) = \sum_{x=1}^{N-1} \frac{x}{N} j_\eta(x, x+1)\,. \tag{38}$$

Proof The basic idea of the theorem is the usual strategy to construct the potential of a gradient discrete vector field plus a subtle use of the translational covariance of the model. For the details of the proof see [5].

Observe that a one dimensional system of particles is of gradient type (with a possibly not local h) if and only if $C(\eta) = 0$. This corresponds to say that for any fixed configuration η then $j_\eta(x, y)$ is a gradient vector field. This was already observed in [2, 15]. Now we compute the decomposition (36) in some examples. Later we will discuss how it can be related to the hydrodynamics of non-gradient systems.

Example 3 On the one-dimensional discrete torus, the symmetric exclusion process with rates $c_{x,x+1}(\eta) = \eta(x)(1 - \eta(x+1))[1 + \alpha\eta(x-1)]$ and $c_{x+1,x}(\eta) = \eta(x+1)(1 - \eta(x))[1 + \alpha\eta(x-1)]$, with the constant $\alpha \in (0, 1)$, is reversible with respect to the Bernoulli measure. This is a non-gradient systems, expected to have a diffusive scaling limits, where the instantaneous current is given by

$$j_\eta(x, x+1) = (\eta(x) - \eta(x+1)) + (\eta(x) - \eta(x+1))\alpha\eta(x-1). \tag{39}$$

Therefore its functional Hodge decomposition (36) is

$$h(\eta) = -\eta(0) + \sum_{x=1}^{N-1} \frac{x}{N}(\eta(x) - \eta(x+1))\alpha\eta(x-1), \quad C(\eta) = \sum_{x \in V_N} \frac{x}{N}(\eta(x) - \eta(x+1))\alpha\eta(x-1). \tag{40}$$

Example 4 (*The 2-SEP*) The model we are considering is the 2-SEP, see its definition in Sect. 3.1. We denote by $D_\eta^{\pm}(x, x+1)$ the local functions associated with the presence on the bond $(x, x+1)$ of what we call respectively a positive or negative discrepancy. More precisely $D_\eta^{+}(x, x+1) = 1$ if $\eta(x) = 2$ and $\eta(x+1) = 1$ and zero otherwise. We have instead $D_\eta^{-}(x, x+1) = 1$ if $\eta(x+1) = 2$ and $\eta(x) = 1$ and zero otherwise. We define also $D_\eta := D_\eta^{+} - D_\eta^{-}$. The instantaneous current across the edge $(x, x+1)$ associated with the configuration η is

$$j_\eta(x, x+1) := \chi^{+}(\eta(x)) - \chi^{+}(\eta(x+1)) + D_\eta(x, x+1). \tag{41}$$

For this specific model formulas (37) and (38) become

$$h(\eta) = -\chi^+(\eta(0)) + \sum_{x=1}^{N-1} \frac{x}{N} D_\eta(x, x+1), \quad C(\eta) = \frac{1}{N} \sum_{x \in V_N} D_\eta(x, x+1). \quad (42)$$

Remark 2 Both formulas (39) and (41) are written in the form $j_\eta(x, y) = j^h_\eta(x, y) + j^a_\eta(x, y)$, namely they are given by the sum of a local gradient current $j^h_\eta(x, y) = \tau_y h(\eta) - \tau_x h(\eta)$ and a single net contribution $j^a_\eta(x, y)$ to the harmonic function $C(\eta)$. We will refer to $j^a_\eta(x, y)$ as *single harmonic contribution* on $(x.y)$. In Sect. 9, we will discuss that we think from this way of rewriting the current it has to start both the study of an explicit hydrodynamics for the case of non-gradient diffusive model and the computation of Green-Kubo's formula.

Our decomposition is motivated by the study of diffusive models where the current can not be written in the gradient form (35), but it can be computed also in not diffusive models when the hypothesis of theorem (1) hold. For example for the asymmetric simple exclusion process it is as follows.

Example 5 (*ASEP*) The asymmetric simple exclusion process is characterized by the rates $c_{x,x+1}(\eta) = p\eta(x)(1 - \eta(x+1))$ and $c_{x,x-1}(\eta) = q\eta(x)(1 - \eta(x-1))$. Given a configuration of particles $\eta \in \Sigma$, we call $\mathfrak{C}(\eta)$ the collection of clusters of particles that is induced on V_N. A cluster $c \in \mathfrak{C}(\eta)$ is a subgraph of $(V_N, \mathscr{E}_N)$. Two sites $x, y \in V_N$ belong to the same cluster c if $\eta(x) = \eta(y) = 1$ and there exists an un-oriented path $(z_0, z_1, \dots, z_k)$ such that $\eta(z_i) = 1$ and $(z_i, z_{i+1}) \in \mathscr{E}_N$. Given a cluster $c \in \mathfrak{C}$ we call $\partial^l c$ and $\partial^r c \in V_N$ respectively the first element on the left of the leftmost site of c and the rightmost one. The decomposition (36) holds with

$$h(\eta) = \frac{1}{N} \sum_{c \in \mathfrak{C}(\eta)} \left[p\partial^r c - q\partial^l c \right], \quad C(\eta) = \frac{(p-q)\,|\mathfrak{C}(\eta)|}{N}. \quad (43)$$

where $|\mathfrak{C}(\eta)|$ denotes the number of clusters.

5.3 The Two Dimensional Case

On the two dimensional torus V_N the decomposition is as follows.

Theorem 2 *Let j_η be a covariant discrete vector field. Then there exist four functions $h, g, C^{(1)}, C^{(2)}$ on configurations of particles such that for an edge of the type $e = (x, x \pm e^{(i)})$ we have*

$$j_\eta(e) = \left[\tau_{e^+} h(\eta) - \tau_{e^-} h(\eta)\right] + \left[\tau_{\mathfrak{f}^+(e)} g(\eta) - \tau_{\mathfrak{f}^-(e)} g(\eta)\right] \pm C^{(i)}(\eta)\,. \quad (44)$$

The functions $C^{(i)} = \frac{1}{N^2} \sum_{x \in V_N} j_\eta(x, x + e^{(i)})$ are translational invariant and uniquely identified. The functions h and g are uniquely identified up to additive arbitrary translational invariant functions.

Proof see [5].

We remark that the proof in [5] is constructive, that is the function $h(\eta)$, $g(\eta)$ and $C^{(i)}(\eta)$ have explicit expressions. In analogy to gradient systems we can say a particle system is of *circulation type* when there exist a local function g such that

$$j_\eta(e) = \tau_{\mathfrak{f}^+(e)} g(\eta) - \tau_{\mathfrak{f}^-(e)} g(\eta), \tag{45}$$

for all edges $e \in E_N$ and $\eta \in \Sigma_N$. We will see that for these systems the hydrodynamics can be treated with the same method of gradient systems. In particular later in Sect. 8 we study the scaling limits of systems where gradient and circulation dynamics are superposed. Now we introduce some examples of this kind.

Example 6 (*A non gradient lattice gas with local decomposition*) We construct a model of particles satisfying an exclusion rule, with jumps only trough nearest neighbour sites and having a non trivial decomposition of the instantaneous current (44) with $C^{(i)} = 0$ and h and g local functions. The functions h and g have to be chosen suitably in such a way that the instantaneous current is always zero inside cluster of particles and empty clusters and has to be always such that $j_\eta(x, y) \geq 0$ when $\eta(x) = 1$ and $\eta(y) = 0$. A possible choice is the following perturbation of the SEP. We fix $h(\eta) = -\eta(0)$ and $g(\eta)$ with $D(g) = \{0, e^{(1)}, e^{(2)}, e^{(1)} + e^{(2)}\}$ (we denote by 0 the vertex $(0, 0)$) defined as follows. We have $g(\eta) = \alpha$ if $\eta(0) = \eta(e^{(1)} + e^{(2)}) = 1$ and $\eta(e^{(1)}) = \eta(e^{(2)}) = 0$. We have also $g(\eta) = \beta$ if $\eta(0) = \eta(e^{(1)} + e^{(2)}) = 0$ and $\eta(e^{(1)}) = \eta(e^{(2)}) = 1$. The real numbers α, β are such that $|\alpha| + |\beta| < 1$. For all the remaining configurations we have $g(\eta) = 0$. Since $\Sigma = \{0, 1\}$ the rates of jump are uniquely determined by $c_{x,y}(\eta) = \big[j_\eta(x, y)\big]_+$.

Example 7 (*A perturbed zero range dynamics*) A face $\mathfrak{f} = \{0, e^{(1)}, e^{(2)}, e^{(1)} + e^{(2)}\}$ is occupied in the configuration $\eta \in \mathbb{N}^{V_N}$ if $\eta(x) \neq 0$ for some $x \in \mathfrak{f}$. Consider two non negative functions $w^\pm$ that are identically zero when the face $\mathfrak{f}$ is not occupied. Given a positive function $\widetilde{h} : \mathbb{N} \to \mathbb{R}^+$, we define the rates of jump as

$$c_{e^-,e^+}(\eta) = \widetilde{h}(\eta(e^-)) + \tau_{\mathfrak{f}^+(e)} w^+ + \tau_{\mathfrak{f}^-(e)} w^- . \tag{46}$$

This corresponds to a perturbation of a zero range dynamics such that one particle jumps from one site with k particles with a rate $\widetilde{h}(k)$. The perturbation increases the rates of jump if the jump is on the edge of a full face. The gain depends on the orientation and the effect of different faces is additive. For such a model the instantaneous current has a local decomposition (44) with $h(\eta) = -\widetilde{h}(\eta(0))$ and $g(\eta) = w^+(\eta) - w^-(\eta)$.

The decomposition can be extended to higher dimensions. For the three dimensional case we refer to [3].

6 Interacting Particle Systems with Vorticity

The models presented in Examples 6 and 7 are superposition of a gradient system and a circulation one, see definition (45). This kind of models are not gradient along the classical definition. Here we want to study them from the microscopic point of view and giving some physical motivation why we talk about them as *interacting particle systems with vorticity*, this will become more clear at the end of Sect. 7. A better discussion with graphical examples will appear in [7].

Let us consider the instantaneous current (5) with a decomposition (44) as

$$j_\eta(x,y) = [\tau_y h(\eta) - \tau_x h(\eta)] + [\tau_{f^+(x,y)} g(\eta) - \tau_{f^-(x,y)} g(\eta)] = j_\eta^h(x,y) + j_\eta^g(x,y), \tag{47}$$

with h and g local functions. We are defining $j_\eta^h(x,y) := \tau_y h(\eta) - \tau_x h(\eta)$ and $j_\eta^g(x,y) := \tau_{f^+(x,y)} g(\eta) - \tau_{f^-(x,y)} g(\eta)$. For example, taking an exclusion process with rates

$$c_{x,y}(\eta) = \eta(x)(1-\eta(y)) + \eta(x)[\tau_{f^+(x,y)} g(\eta) - \tau_{f^-(x,y)} g(\eta)], \tag{48}$$

we have $j_\eta(x,y)$ as in (47) with $h(\eta) = -\eta(0)$, note that example 6 is of this form.

Models with $j_\eta(x,y)$ as in (47) can be thought as a generalization of the gradient case $j_\eta(x,y) = [\tau_y h(\eta) - \tau_x h(\eta)]$, indeed the current is a gradient part plus an *orthogonal gradient part* (discrete bidimensional curl). Because of the presence of this discrete curl we use the terminology of "*exclusion process with vorticity*".

When the rates satisfies (47), we will see that the hydrodynamics for the empirical measure (50) works exactly as if only the gradient part was present because

$$\nabla \cdot j_\eta^g(x) = 0, \quad \forall\, x \in V_N, \tag{49}$$

that is the part of the dynamics related to the current $j_\eta^g(x,y)$ does not give any macroscopic effect to the hydrodynamics of the particles density because its contribution to the microscopic conservation law (9) is already zero. To observe macroscopically the effect of the discrete curl we have to consider the scaling limits of the current flow $J_t(x,y)$ of formula (6). In Sect. 8 we derive the macroscopic current $J(\rho)$ that will appear in the hydrodynamics $\partial_t \rho = \nabla \cdot (-J(\rho))$. Another physical phenomena of this kind of dynamics (48) is that they are diffusive even if in general they are not reversible on the torus $\mathbb{T}_N^n$, namely this means that at the stationary state there is a non-zero macroscopic current (11). For an explicit example see [7].

7 Scaling Limits and Transport Coefficients of Diffusive Models

To derive the hydrodynamics of diffusive systems the rates are multiplied by a factor N^2 (diffusive time scale) and the space scale $\varepsilon = 1/N$ is considered. The particles jump on the discrete torus $\mathbb{T}^n_\varepsilon := \varepsilon\mathbb{Z}/\mathbb{Z}$ with mesh of size ε. When N goes to infinity $\mathbb{T}^n_\varepsilon$ approximates the continuous torus $\mathbb{T}^n = [0, 1)^n$. A very general class of diffusive systems are models that are reversible with respect to a Gibbs measure when no boundary conditions are imposed. Reversibility with respect to a measure μ_N means $\langle f, \mathscr{L}_N g\rangle_{\mu_N} = \langle \mathscr{L}_N f, g\rangle_{\mu_N}$ for all functions f, g while stationarity means$\langle \mathscr{L}_N f\rangle_{\mu_N} = 0$. $\langle\cdot\rangle$ is the expectation on Σ_N respect to μ_N and $\langle\cdot,\cdot\rangle_{\mu_N}$ is the scalar product respect to μ_N. We assume μ_N to be a grand-canonical measure parametrized by the density ρ, i.e. $\mathbb{E}_{\mu_N}(\eta(x)) = \rho$. For this reason instead of μ_N we are going to use the notation μ^ρ_N.

The macroscopic evolution of the mass is described by the *empirical measure*. This is a positive measure on the continuous torus $\mathbb{T}^n$ associated to any fixed microscopic configuration η, defined as a convex combination of delta measures

$$\pi_N(\eta) := \frac{1}{N}\sum_{x\in V_N} \eta(x)\delta_x\,. \tag{50}$$

It represents a mass density or an energy density along the interpretation of the model. Integrating a continuous function $f : \mathbb{T}^n \to \mathbb{R}$ with respect to $\pi_N(\eta)$ we get $\int_{\mathbb{T}^n} f\, d\pi_N(\eta) = \frac{1}{N}\sum_{x\in V_N} f(x)\eta(x)$. In the hydrodynamic scaling limit the empirical measure becomes deterministic and absolutely continuous for suitable initial conditions ξ_0 associated to a given density profile $\gamma(x)dx$, in the sense that in probability

$$\lim_{N\to+\infty}\int_{\mathbb{T}^n} f\, d\pi_N(\xi_0) = \int_{\mathbb{T}^n} f(x)\gamma(x)dx. \tag{51}$$

Let P^γ_N be the distribution of the Markov chain of the energy-mass/particle interacting model with initial condition associated to γ as in (51) . On $D([0, T]; \mathscr{M}^1(\mathbb{T}^n))$ the space of trajectories from $[0, T]$ to the space of positive measure $\mathscr{M}^1(\mathbb{T}^n)$, $\mathbb{P}^\gamma_N := P^\gamma_N \circ \pi_N^{-1}$ is the measure induced by the empirical measure. We have that $\pi_N(\eta_t)$ is associated to the density profile $\rho(x, t)dx$ where ρ is the weak solution to a diffusive equation with initial condition γ, i.e. $\mathbb{P}^\gamma_N \xrightarrow[N]{d} \delta_\rho$ where and δ_ρ is the distribution concentrated on the unique weak solution of a Cauchy problem

$$\begin{cases} \partial_t\rho = \nabla\cdot(D(\rho)\nabla\rho) \\ \rho(x, 0) = \gamma(x). \end{cases} \tag{52}$$

This is a space-time law of large numbers, where $D(\sigma)$ is a positive symmetric matrix called *diffusion matrix*.

7.1 Qualitative Derivation of Hydrodynamics

In this subsection we illustrate the general structure of the proof of the hydrodynamic limit for reversible gradient models on the torus $\mathbb{T}^n_\varepsilon$. We use the notion ξ of Sect. 4 of energy-mass models because for them we gave some example of weakly asymmetric model and we want to emphasize that the KMP model is gradient. But the whole scheme apply to particle models in the same way.

The starting point for the hydrodynamic description is the continuity equation

$$\xi_t(x) - \xi_0(x) = -\nabla \cdot \mathscr{J}_t(x)\,, \tag{53}$$

where $\mathscr{J}_t$ has been defined in Sect. 4.3 and $\nabla\cdot$ denotes the discrete divergence defined in (30). Using (24) we can rewrite (53) as (26) with $\mathbb{F} = 0$. Multiplying (26) by a test function ψ, dividing by N and summing over x we obtain

$$\int_{\mathbb{T}^n} \psi\, d\pi_N(\xi_t) - \int_{\mathbb{T}^n} \psi\, d\pi_N(\xi_0) = -N \int_0^t \sum_{x\in V_N} \nabla \cdot j_{\xi_s}(x)\, \psi\,(x)\, ds + o(1)\,. \tag{54}$$

The infinitesimal term $o(1)$ comes from the martingale term. The idea is that the martingales $M_t(x, y)$ in (7) describe some microscopic fluctuations whose additive macroscopic contributions vanishes as $N \to \infty$ as they are mean zero martingales and are almost independent for different bonds. This contribution can be shown to be negligible (in probability) in the limit of large N with the methods of [11, 14]. Using the gradient condition $j_\xi(x, y) = \tau_x h(\xi) - \tau_y h(\xi)$, for example for the KMP (14) and KMPd (16) we have $h(\xi) = \frac{\xi(0)}{2}$, and performing a double discrete integration by part, up to the infinitesimal term, one has that the right hand side of (54) is $\frac{1}{N}\sum_{x\in V_N}\int_0^t \tau_x h(\xi_s)\left[N^2\left(\psi\left(x+\frac{1}{N}\right)+\psi\left(x-\frac{1}{N}\right)-2\psi\Big(x\Big)\right)\right] ds$. Considering a C^2 test function ψ, the term inside squared parenthesis coincides with $\Delta\psi\,(x)$ up to an uniformly infinitesimal term.

At this point the main issue in proving hydrodynamic behavior is to prove the validity of a local equilibrium property. Let us define

$$A(\rho) = \mathbb{E}_{\mu_N^\rho}\,(h(\xi))\,, \tag{55}$$

where μ_N^ρ is the invariant measure characterized by a density profile ρ, that is $\mathbb{E}_{\mu_N^\rho}(\xi(x)) = \rho$. The local equilibrium property is explicitly stated through a replacement lemma that shows that (in probability)

$$\frac{1}{N}\sum_{x\in V_N}\int_0^t \tau_x h(\xi_s)\Delta\psi\,(x)\, ds \simeq \frac{1}{N}\sum_{x\in V_N}\int_0^t A\left(\frac{\int_{B_x} d\pi_N(\xi_s)}{|B_x|}\right)\Delta\psi\,(x)\, ds \tag{56}$$

where B_x is a microscopically large but macroscopically small volume around the point $x \in V_N$. For a precise formulation of (56) see Lemma 1.10 and Corollary 1.3

respectively in Chap. 5 and in Chap. 6 of [14] or Chap. 2 in [11]. This allows to write (up to infinitesimal corrections) Eq. (54) in terms only of the empirical measure. Substituting the r.h.s. of (56) in the place of the r.h.s. of (54), we obtain that in the limit of large N the empirical measure $\pi_N(\eta_t)$ converges in weak sense to $\rho(x,t)dx$ satisfying for any C^2 test function ψ

$$\int_{\mathbb{T}^n} \psi(x)\rho(x,t)\,dx - \int_{\mathbb{T}^n} \psi(x)\rho(x,0)\,dx = \int_0^t ds \int_{\mathbb{T}^n} A(\rho(x,s))\Delta\psi(x)\,dx\,. \tag{57}$$

Equation (57) is a weak form of (52) with diagonal diffusion matrix $D(\rho)$ with each term in the diagonal equal to $D(\rho) = \frac{dA(\rho)}{d\rho}$. We are calling $D(\rho)$ both the number and the diagonal matrix $D(\rho)\mathbb{I}$. For $h(\xi) = \frac{\xi(0)}{2}$ it is $A(\rho) = \frac{\rho}{2}$. To have an unitary diffusion matrix we multiply all the rates of transition by a factor of 2 and correspondingly the diffusion matrix is the identity matrix. Equation (52) can be written in the form

$$\partial_t \rho + \nabla \cdot (J(\rho)) = 0, \text{ with } J(\rho) = -D(\rho)\nabla\rho, \tag{58}$$

where the macroscopic current $J(\rho)$ associated to ρ satisfies the *Fick's law*.The hydrodynamics for weakly asymmetric diffusive models of Sect. 4.2 is

$$\partial_t \rho = \nabla \cdot (-J_E(\rho)) \text{ with } J_E(\rho) := D(\rho)\nabla\rho - \sigma(\rho)E. \tag{59}$$

The positive definite matrix σ is called the *mobility*. For the weakly asymmetric versions of the KMP and the KMPd, in Sect. 4.2 it is respectively $\sigma(\rho) = 2\mathbb{E}_{\mu_N^\rho}[g(\eta)] = \rho^2$ and $\rho + \rho^2$, where respectively $g(\xi) = \frac{1}{6}\big(\xi(0)^2 + \xi(1/N)^2 - \xi(0)\xi(1/N)\big)$ and $g(\xi) = 12\big(2\xi(x)^2 + 2\xi(y)^2 - 2\xi(x)\xi(y) + 3\xi(x) + 3\xi(y)\big)$. For a discussion on the computations of these kind of expectations see [1].

The hydrodynamics was derived with periodic boundary conditions but in the bulk it is still the same for a boundary driven version of the system, see [9].

8 Scaling Limit of an Exclusion Process with Vorticity

In this section we want to show how to compute the scaling limit of the macroscopic current $J(\rho)$ for diffusive models with vorticity of Sect. 6, namely having the instantaneous current with an expression like (47). Here for the purpose of the paper the treatment will be qualitative. It is the first time that the hydrodynamics of this kind of models is discussed. A complete rigorous treatment of the problem is now being developed in the work in progress [7], where a generalized picture of the Fick's law is under construction. Here we will discuss its main ideas. We consider a discrete torus of mesh $\varepsilon = 1/N$ but specifically in dimension 2, i.e. $V_N = \mathbb{T}^2_\varepsilon$.

If the current has an Hodge decomposition (44) only the gradient part contributes to the hydrodynamics (54), indeed $\nabla \cdot j_\eta(x) = \nabla \cdot j^h_\eta(x)$ since $\nabla \cdot j^g_\eta(x) = \nabla \cdot j^H_\eta(x) = 0$ with $j^H_\eta(x,y) = C^1(\eta)\varphi^1(x,y) + C^2(\eta)\varphi^2(x,y)$. So if the gradient part of the current $j^h_\eta(x)$ is diffusive with respect to a local gradient function $h(\cdot)$, the hydrodynamics of $\pi_N(\eta)$ works exactly as if we considered a model with $j_\eta(x,y) = j^h_\eta(x,y)$ along the scheme in Sect. 7.

Now we want to study the scaling limits of the current $J(\rho)$ appearing in (58), as model of reference for what we are going to present, the reader should keep in mind the exclusion process of Example 6 but with $\alpha = \beta$. More precisely the model has the rates (48) with the local function $g(\eta)$ defined as

$$g(\eta) := \begin{cases} \alpha \text{ if } \eta(0) = \eta(\frac{e^{(1)}}{N} + \frac{e^{(2)}}{N}) = 1 \text{ and } \eta(\frac{e^{(1)}}{N}) = \eta(\frac{e^{(2)}}{N}) = 0\,, \\ \alpha \text{ if } \eta(\frac{e^{(1)}}{N}) = \eta(\frac{e^{(2)}}{N}) = 1 \text{ and } \eta(0) = \eta(\frac{e^{(1)}}{N} + \frac{e^{(2)}}{N}) = 0\,, \\ 0 \text{ otherwise}\,, \end{cases} \tag{60}$$

where α is a real parameter such that $|\alpha| < 1$. The informal and intuitive description of the dynamics associated to the rates (48) is the following. Particles perform a simple exclusion process, but the faces containing exactly 2 particles located at sites which are not nearest neighbors let the particles rotate anticlockwise when $\alpha > 0$ and clockwise when $\alpha < 0$ with a rate equal to $|\alpha|$. For this choice of the parameters, the model of example 6 can be proven to be a non-reversible stationary dynamics with respect to Bernoulli measures of density parameter ρ. In this section, the language will be general for a model that is invariant with respect to a measure μ^ρ_N parametrized by a density ρ, having the decomposition (47) and hydrodynamics for the empirical measure of the form (58), while the results will be made explicit for the toy model (60).

The scaling limits for the current $J(\rho)$ it is obtained from the *empirical current measure* $\mathbb{J}_N$ in the space of the vector signed measure $\mathscr{M}(\mathbb{T}^2, \mathbb{R}^2)$ defined as

$$\int_{\mathbb{T}^2} H \cdot d\mathbb{J}_N := \frac{1}{N^2} \sum_{\{x,y\} \in \mathscr{E}_N} J_t(x,y)\mathbb{H}(x,y) \text{ where } \mathbb{H}(x,y) = \int_x^y H(z) \cdot dz. \tag{61}$$

The family $(\mathbb{J}_N(t))_{t\in[0,T]}$ belongs to the space $D([0,T], \mathscr{M}(\mathbb{T}^2, \mathbb{R}^2))$ of trajectories from $[0,T]$ to $\mathscr{M}(\mathbb{T}^2, \mathbb{R}^2)$. Calling $\mathbb{P}_{\mathbb{J}_N} := P^\gamma_N \circ \mathbb{J}^{-1}_N$ the measure induced by empirical current measure on $D([0,T], \mathscr{M}(\mathbb{T}^2, \mathbb{R}^2))$, we have that $\mathbb{J}_N(t)$ is associated to a vector signed measure $J(\rho)dx$ in weak sense, that is in probability for any C^1 vector field on $\mathbb{T}^2$ we will have

$$\begin{gathered} \lim_{N\to+\infty} \textstyle\int_\Lambda H \cdot d\mathbb{J}_N(t) = \int_\Lambda dx \int_0^T dt\, J(\rho_t(x)) \cdot H(x), \\ J(\rho) = -D(\rho) \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix} \nabla\rho - D^\perp(\rho) \begin{pmatrix} 0 & -1 \\ 1 & 0 \end{pmatrix} \nabla\rho\,, \end{gathered} \tag{62}$$

where $D(\rho)$ and $D^{\perp}(\rho)$ are two real coefficients depending on ρ, $\rho_t(x)$ is the solution of the Cauchy problem (52) and $J(\rho(0))$ is equal 0 by definition. This means that $\mathbb{P}_{\mathbb{J}_N} \xrightarrow[N]{d} \delta_{J(\rho)}$ where $\delta_{J(\rho)}$ is the distribution concentrated on the measure $J(\rho)dx$ that we have just described. For the model (60) we will show that $D(\rho) = 1$ and $D^{\perp}(\rho) = \frac{d}{d\rho}(2\alpha(\rho - \rho^2)^2)$. The derivation of the hydrodynamics starts from the martingale

$$M(t) = \frac{1}{N^d} \sum_{\{x,y\} \in \mathscr{E}_N} J_t(x, y)\mathbb{H}(x, y) - N^{2-d} \int_0^t ds \sum_{\{x,y\} \in \mathscr{E}_N} j_{\eta_s}(x, y)\mathbb{H}(x, y), \tag{63}$$

where N^2 is the diffusive scaling and the factor N^{-d} it is a normalization. By the anti-symmetry of the discrete vector fields there is no ambiguity in this definition. Therefore $\frac{1}{N^d} \sum_{\{x,y\} \in \mathscr{E}_N} J_t(x, y)\mathbb{H}(x, y) = N^{2-d} \int_0^t ds \sum_{\{x,y\} \in \mathscr{E}_N} j_{\eta_s}(x, y)\mathbb{H}(x, y) + o(1)$, where $o(1)$ is a negligible (in probability) martingale term for large N, for which holds a discussion like that one about the martingale in (54). From (47)

$$\sum_{\{x,y\} \in \mathscr{E}_N} j_{\eta_s}(x, y)\mathbb{H}(x, y) = \int_0^t \left[\sum_{x \in V_N} \tau_x h(\eta)(x) \nabla \cdot \mathbb{H}(x) + \sum_{\mathfrak{f} \in \mathscr{F}_N} \tau_{\mathfrak{f}} g(\eta_s) \sum_{(x,y) \in f^{\circlearrowleft}} \mathbb{H}(x, y) \right], \tag{64}$$

where $N^2 \nabla \cdot \mathbb{H}(x) = \nabla \cdot H(x) + o(1/N)$ and $N^2 \sum_{(x,y) \in f^{\circlearrowleft}} \mathbb{H}(x, y) = \nabla^{\perp} \cdot H(z) + o(1/N)$. In the above formula z is any point belonging to the face, while given a C^1 vector field $H = (H_1, H_2)$ we used the notation $\nabla^{\perp} \cdot H(z) := -\partial_y H_1(z) + \partial_x H_2(z)$. When N is diverging, we assume the local equilibrium hypothesis with respect to the grand-canonical measure μ_N^{ρ} to prove with a replacement lemma as discussed in section7, this means that (64) converges (in probability) to

$$\int_0^t ds \int_{\mathbb{T}^2} dx \left[a(\rho(x, s)) \nabla \cdot H(x) + a^{\perp}(\rho(x, s)) \nabla^{\perp} \cdot H(x) \right], \tag{65}$$

applying the replacement lemmas $a(\rho) = \mathbb{E}_{\mu_N^{\rho}}[h(\eta)]$ and $a^{\perp}(\rho) = \mathbb{E}_{\mu_N^{\rho}}[g(\eta)]$, for the model of reference (60) its $a(\rho) = \rho$ and $a^{\perp}(\rho) = 2\alpha[\rho(1 - \rho)]^2$. Formula (65) is a weak form of $\int_0^t ds \int_{\Lambda} J(\rho) \cdot H \, dx$ with

$$J(\rho) = -\nabla a(\rho) - \nabla^{\perp} a^{\perp}(\rho) = -D(\rho)\nabla\rho - D^{\perp}(\rho)\nabla^{\perp}\rho, \tag{66}$$

where $D(\rho) = d(a(\rho))/d\rho$, $D^{\perp}(\rho) = d(a^{\perp}(\rho))/d\rho$ and $\nabla^{\perp} f := (-\partial_y f, \partial_x f)$. As we expected from the microscopic argument (49) we have $\nabla \cdot (-D(\rho)\nabla\rho - D^{\perp}(\rho)\nabla^{\perp}\rho) = \nabla \cdot (-D(\rho)\nabla\rho)$, hence the hydrodynamics is left unchanged with respect to the usual gradient case. For the model (60) we obtain $D(\rho) = 1$ and $D^{\perp}(\rho) = \frac{d}{d\rho}(2\alpha(\rho - \rho^2)^2)$ as anticipated above. Hence formula (66) can be rewritten in the form

$$J(\rho) = -\left[D(\rho) \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix} + D^{\perp}(\rho) \begin{pmatrix} 0 & -1 \\ 1 & 0 \end{pmatrix} \right] \nabla\rho. \tag{67}$$

From the computations presented here and other considerations in [7] we think that the Fick's law (58) for particle models has to be replaced by the general picture

$$J(\rho) = -\mathscr{D}(\rho)\nabla\rho, \tag{68}$$

where the diffusion matrix $\mathscr{D}(\rho)$ is positive but not necessarily symmetric and in general with respect to (67) the terms on the same diagonal can have different coefficients.

Remark 3 An important question is to understand if there exist models with vorticity that are also reversible. At the present stage, we are not able neither to find reversible models of this kind neither to prove that this property is a genuine microscopic non equilibrium property, if this is case, it looks that typically they will be diffusive models with a non-zero average microscopic current at the stationary state.

9 Green-Kubo's Formula and Perspectives in Non-gradient Particles Systems

Scaling limits of non gradient particles systems can be proved to be diffusive with the methods developed in [16, 19] if the spectral gap of the generator satisfies suitable conditions [14], but even in one dimension when the instantaneous current is not gradient there are no explicit PDEs. For what we know, the only case where there is an explicit PDE is [20], where the author consider a spatial inhomogeneous simple symmetric exclusion process where particles jump with two different constant along an edge is even or odd. The model of Wick is translational covariant, see (36), with respect to translations on two sites instead of one. To look at Wick model into the context of this paper and in particular of this section, one has to generalize the decomposition (36) for translational covariant models on two sites, this is done considering a renormalized current on two sites and rewriting the decomposition for it. Then, taking a lattice with a even number of sites, the discrete hydrodynamics (54) can be written with respect to this current.

We start to explore if the decompositions (36) and (44) can tell something about this problem. Let us consider exclusion processes in one dimension on the torus with nearest neighbours interaction, reversible with respect to μ_N^ρ and non gradient, a case is Example 3. For these models the hydrodynamics is expected to be diffusive with the diffusion coefficient having the following variational expression

$$D(\rho) = \frac{1}{2\chi(\rho)} \inf_f \mathbb{E}_{\mu_N^\rho}\Big[c_{0,1}(\eta)\big((\eta(0) - \eta^{0,1}(0)) + \sum_{x\in V_N}(S_{0,1}\tau_x)f(\eta)\big)^2\Big], \tag{69}$$

where $\chi(\rho)$ is the mobility $\mathbb{E}_{\mu_N^\rho}(\eta^2(0)) - \rho^2$, $(S_{x,y}f) = f(\eta^{x,y}) - f(\eta)$ and the inf is over all functions $f : \Sigma_N \to \mathbb{R}$. This is discussed in Chap. 2 of part 2 in [18] and has been proved for the 2-SEP in chapter 7 of [14]. The variational formula (69) is

proved to be equal to the *Green-Kubo's* formula for interacting particles systems

$$D(\rho) = \frac{1}{2\chi(\rho)}\Big[\mathbb{E}_{\mu_N}(c_{0,1}(\eta)) - 2\int_0^{+\infty} \mathbb{E}_{\mu_N}(j_\eta(0,1)e^{\mathscr{L}_N t}\tau_x j_\eta(0,1))\Big], \tag{70}$$

where $e^{\mathscr{L}_N t}$ is the evolution operator of the Markov process. We consider translational covariant rates (Remark 1) to have the decomposition (36), plugging this one in (70) we find

$$D(\rho) = \frac{1}{2\chi(\rho)}\Big[\mathbb{E}_{\mu_N}(c_{0,1}(\eta)) - 2N\,\mathbb{E}_{\mu_N}(C(\eta)\mathscr{L}_N^{-1}C(\eta))\Big], \tag{71}$$

where $\mathscr{L}_N^{-1}$ is the generalized inverse operator of $\mathscr{L}_N$ (for $f(\eta)$ constant function $\mathscr{L}_N f(\eta) = 0$), for this definition see [12]. Formula (71) tells us that just the harmonic part of the current $C(\eta)$ contributes to the second term of the Green-Kubo's formula and for gradient systems we have $D(\rho) = \frac{1}{2\chi(\rho)}\mathbb{E}_{\mu_N}(c_{0,1}(\eta))$ even if the h is not local, admitting that such models exist. Expression (71) has an equivalent variational formulation with a minimizer that is computable in principle. The term $\mathbb{E}_{\mu_N^\rho}(C(\eta)\mathscr{L}_N^{-1}C(\eta))$ can be seen as the scalar product $\langle C(\eta), \mathscr{L}_N^{-1}C(\eta)\rangle_{\mu_N^\rho}$, where $\langle f, g\rangle_{\mu_N^\rho} = \sum_\eta f(\eta)g(\eta)\mu_N^\rho(\eta)$. Since $\mathscr{L}_N$ is symmetric with respect to this scalar product we have

$$\langle C(\eta), \mathscr{L}_N^{-1}C(\eta)\rangle_{\mu_N^\rho} = \inf_f \Big\{-\langle f, \mathscr{L}_N f\rangle_{\mu_N^\rho} - 2\langle C(\eta), f\rangle_{\mu_N^\rho}\Big\} \tag{72}$$

where the minimizer is over all function $f : \Sigma_N \to \mathbb{R}$ and a solution is given by

$$\mathscr{L}_N f(\eta) = -C(\eta) \text{ for all } \eta \in \Sigma_N. \tag{73}$$

The solution (73) is well posed since $C(\eta)$ is orthogonal to the eigenspace of eigenvalue zero. This minimizer looks to us more simple to solve than the one of the expression in [18], for example interpreting the model of Wick as explained at the beginning of the section this minimum can be solved within the framework we are going to explain in next paragraphs. We think that the solution of this minimizer is equivalent to rewrite the discrete hydrodynamics in a form such that the only macroscopic relevant terms are reduced to the usual case of Sect. 7 of gradient systems. In some special non-gradient cases (as Wick [20]) we expect a simplified scheme, that is an exact case of a more general scheme briefly described at the end.

The idea starts from the observation that a natural attempt to solve (73) is to look for a $f(\eta)$ of the form

$$f(\eta) = \sum_{x\in V_N} \tau_x g(\eta), \tag{74}$$

where $g(\eta)$ is a local function. Note that the left-hand side of (73) is invariant by translation as it has to be. Remark 2 gives a connection between the minimizer and the conservation law leading to the hydrodynamics, there we discussed

that in reversible non-gradient model the current can be rewritten in the form $j_\eta(x,y) = j^h_\eta(x,y) + j^a_\eta(x,y)$, where the single harmonic contributions are such that $C(\eta) = \frac{1}{N}\sum_{x\in V_N} j_\eta(x,x+1) = \frac{1}{N}\sum_{x\in V_N} j^a_\eta(x,x+1)$. So to the part of the current denoted $j^h_\eta(x,y)$ we can apply the scheme of Sect. 7 with respect to a gradient function $h(\eta)$, while it is not possible for the part $j^a_\eta(x,y)$. But if we are able to find a local function $\widetilde{g}(\eta)$ such that

$$\mathscr{L}_N \widetilde{g}(\eta) = j^a_\eta(0,1) + \tau\widetilde{h}(\eta) - \widetilde{h}(\eta), \tag{75}$$

where $\widetilde{h}(\eta)$ is another local function, then we are done both with the solution (74) and the discrete form of the hydrodynamics (54). Indeed respectively taking $f(\eta) = \sum_{x\in V_N} \tau_x g(\eta)$ with $g(\eta) = -\widetilde{g}(\eta)$ we solve (73) and with the replacements (75) of the harmonic contributions we will be able to treat the hydrodynamics. This is because considering the translations of relation (75), in the discrete hydrodynamics (54) will contribute only the local function $h'(\eta) = -\widetilde{h}(\eta)$ since with the local equilibrium hypothesis (55) the terms $\mathbb{E}_{\mu^\rho_N}(\mathscr{L}_\mathscr{N}\tau_x g(\eta_t))$ will be negligible in the scaling limit as they are time derivatives and from the time integral they will give a contribution of order $O(1/N^2)$ each one. At the end, the hydrodynamics will follow Sect. 7 with respect to the local function $H(\eta) := h(\eta) + h'(\eta)$.

In the non-local decomposition (36) the part $C(\eta)$ is divergence free and therefore will not appear in the hydrodynamics (54). We expect that writing this last one with respect to the non-local $h^a(\eta)$ of the Hodge decomposition $j^a_\eta(x,y) = \tau_y h^a(\eta) - \tau_x h^a(\eta) + C(\eta)$, doing the substitution (75) in $h^a = \sum_{x=1}^{N-1} \frac{x}{N} j^a_\eta(x,x+1)$, with proper cancellations the hydrodynamics will still reduce to the one related to $H(\eta)$.

In general solving (73) with an $f(\eta)$ of the form (74) with the property (75) will be not possible. But for models like Example 3, we expect a generalization of this case where (73) is solved unless of (non-local) gradients (which will not contribute in the computation of the scalar products in (72)) with a solution as (74) where $g(\eta)$ satisfies (75) unless extra terms on the right-hand side that in probabilistic sense will be of order $o(1/N)$ and will not contribute to hydrodynamics.

Similarly to (71), in dimension higher than one, the extra terms for non gradient systems will come only from the harmonic part, i.e. $C^1(\eta)\varphi^1(x,y)$ and $C^1(\eta)\varphi^1(x,y)$ in dimension two.

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References

1. L. Bertini, D. Gabrielli, J.L. Lebowitz, Large deviations for a stochastic model of heat flow. J. Stat. Phys. **121**, 843–885 (2005)
2. L. Bertini, A. De Sole, D. Gabrielli, G. Jona-Lasinio, C. Landim, Stochastic inter- acting particle systems out of equilibrium. J. Stat. Mech **P07014** (2007)
3. L. De Carlo, *Microscopic and Macroscopic Perspectives on Stationary Nonequilibrium States* (2019), arXiv:1906.05763
4. L. De Carlo, *Discrete Calculus with Cubic Cells on Discrete Manifolds* (2019), arXiv:1906.07054
5. L. De Carlo, D. Gabrielli, Gibbsian stationary nonequilibrium states. J. Stat. Phys. **168**(2017), 1191–1222 (2017)
6. L. De Carlo, D. Gabrielli, Totally asymmetric limit for models of heat conduction. J. Stat. Phys. **168**, 508–534 (2017)
7. L. De Carlo, D. Gabrielli, P. Gonçalves, *Scaling Limit of an Exclusion Process with Vorticity*, in preparation
8. M. Desbrun, E. Kanso, Y. Tong, Discrete differential forms for computational modeling, in *Discrete Differential Geometry. Oberwolfach Seminars*, ed. by A.I. Bobenko, J.M. Sullivan, P. Schröder, G.M. Ziegler (eds.), vol. 38 (Birkhäuser, Basel, 2008)
9. G.L. Eyink, J.L. Lebowitz, H. Spohn, Hydrodynamics and fluctuations outside of local equili6brium: driven diffusive systems J. Statist. Phys. **83**(3–4), 385–472 (1986)
10. D. Gabrielli, C. Valente, Which random walks are cyclic? ALEA, Lat. Am. J. Probab. Math. Stat. **9**, 231–267 (2012)
11. P. Gonçalves, *Equilibrium Fluctuations for Totally Asymmetric Particle Systems: exclusion and zero-range processes* (VDM Verlag Dr, Müller, 2010)
12. J. Hunter, Generalized inverses of Markovian kernels in terms of properties of the Markov chain. Linear Algebra Appl. **447**, 38–55 (2014)
13. C. Kipnis, C. Marchioro, E. Presutti, Heat flow in an exactly solvable modelJ. Stat. Phys. **27**, 65 (1982)
14. C. Kipnis, C. Landim, *Scaling Limits of Interacting Particle Systems* (Springer, New York, 1999)
15. Y. Nagahata, Regularity of the diffusion coefficient matrix for generalized exclusion process. Stochast. Process. Their Appl. **116**, 957–982 (2016)
16. J. Quastel, Diffusion of color in the simple exclusion process. Comm. Pure Appl. Math. **XLV**, 623–679 (1992)
17. F. Spitzer, Interaction of Markov processes. Adv. Math. **5**, 246–290 (1970)
18. H. Spohn, *Large Scale Dynamics of Interacting Particles* (Springer, New York, 1991)
19. S.R.S. Varadhan, Nonlinear diffusion limit for a system with nearest neighbor interactions-II, in *Asymptotic Problems in Probability Theory: Stochastic Models and Diffusion on Fractals*, vol. 283 (1994), pp. 75–128
20. W.D. Wick, Hydrodynamic limit of a nongradient interacting particle process. J. Stat. Phys. **54**, 873–892 (1989)

Porous Medium Model: An Algebraic Perspective and the Fick's Law

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Abstract In this work, we study the porous medium model (PMM), an interacting particle system with nearest neighbor interactions of particles under some constraints. First, we consider the discrete space $\{1, \ldots, n-1\}$ with additional Glauber dynamics acting respectively on sites 0 and n. We assume the hydrodynamic limit (proved in a companion paper [4]) and we prove that the Fick's law holds. Moreover, we review how to construct a self-duality relation starting from the reversible measure of the process. Following this method, we show a self-duality result for the process without reservoirs, which is found inspired by its description via the Lie algebra $\mathfrak{su}(2)$.

Keywords Porous medium model · Hydrodynamic limit · Fick's law · Porous medium equation · Boundary conditions · Stochastic duality · Lie algebra $\mathfrak{su}(2)$

1 Introduction

One of the major problems in non-equilibrium Statistical Mechanics is the study of scaling limits of interacting particle systems (IPS). In particular, the derivation of macroscopic partial differential equations (PDE's) from microscopic systems, known in the literature as hydrodynamic limit, see [7] for a review. In recent years, a lot of attention has been devoted to the study of the asymptotic behavior of microscopic systems coupled with reservoirs, which bring up boundary conditions to the associated hydrodynamic equation. In the case of microscopic systems with independent particles, we usually have linear hydrodynamic equations, as in [1]. Otherwise, which is the case of the PMM, we usually have nonlinear hydrodynamic equations, as in [13].

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The PMM is a special case of the KLS model introduced by Katz, Lebowitz, and Spohn [18] where particles only hope randomly with no bias to nearest neighbors sites with rates depending on the occupation of the nearest and next-nearest-neighbor sites. See also [16], where, using their notation the PMM corresponds to the case which has hopping rates given by $\delta = -1$ and $\varepsilon = 0$. More recently in [13] the authors derived for the first time the porous medium equation (PME) considering discrete occupational variables. In addition, in [1], the authors studied the simple symmetric exclusion process (SSEP) combined with a Glauber dynamics, that they called "slow reservoirs", which has the heat equation with Dirichlet, Neumann, and Robin boundary conditions as hydrodynamic equations. In [4], in order to study non-linear versions of the hydrodynamic equations obtained in [1], the authors considered the PMM with a microscopic perturbation and slow reservoirs. Thus, they derived for the first time the PME with similar boundary conditions as [1].

In this paper, we will work with two versions of the PMM. In the first part of the paper, our microscopic system of interest will be the perturbed PMM with slow reservoirs evolving in the discrete space $\{1, \dots, n-1\}$, as in [4]. The perturbation is necessary in order to assume the validity of the hydrodynamic limit through the Entropy method of Guo, Papanicolau, and Varadhan [15]. The name "slow" comes from the fact that we have a parameter $\theta \in [0, +\infty)$ which regulates the reservoirs' strength. In the second part, our microscopic system will be the PMM without perturbations and without reservoirs, evolving in the one-dimensional discrete torus $\mathbb{T}_n = \{0, 1, \dots, n-1\}$. The aforementioned open models belong to the class of diffusive systems. To illustrate, consider a finite volume containing interacting particles coupled with opposite reservoirs, one at the left boundary and another at the right boundary, both having a different density of particles. In this situation, one predicts a net flux of particles from the reservoir with a higher density to the reservoir with a lower density. Therefore, after some initial transitions, we expect a non-equilibrium steady state to arise in the system, i.e., a state with a nonzero flux of particles that is constant in space and time.

The aim of this paper is to examine some questions that arise when studying diffusive systems out of equilibrium. We focus on Fick's law of diffusion, and on the self-duality for the generator of the PMM in the one-dimensional discrete torus.

The first result of this paper regards the Fick's law of diffusion, derived by Adolf Fick in [10], that says that the rate of the flux of particles is proportional to the density gradient. Although the authors in [4] studied scaling limits for the empirical density of the perturbed PMM with slow reservoirs, in the first part of this paper we study scaling limits for the empirical currents of this model. The motivation comes from [3], in which the authors derived the large deviation principle for the empirical currents of the SSEP in the domain $\{-n, n\}$ with creation and annihilation of particles in the bulk and a Glauber dynamics at the boundaries.

As mentioned above the PMM has the porous medium equation as hydrodynamic equation. It is a partial differential equation that can be seen in dimension one as

$$\partial_t \rho = \Delta \rho^M, \quad M > 1. \tag{1}$$

It is a nonlinear diffusion equation that can be written in the divergence form as

$$\partial_t \rho = \nabla(D(\rho)\nabla\rho),$$

where $\rho = \rho(t, u)$ is a scalar function, which in this paper, denotes the macroscopic density of particles in $u \in [0, 1]$ at time $t > 0$, and $D(\rho) = M\rho^{M-1}$ is the diffusion coefficient. The equation is parabolic at the points where $\rho \neq 0$, but it changes its character at the level $\rho = 0$, since $D(\rho)$ vanishes as $\rho \to 0$. See [23] for more details.

In this work, for simplicity of the presentation, we will consider the case $M = 2$, so that the hydrodynamic equations studied here are the same that the ones in [4]. These equations will be the PME with boundary conditions depending on the parameter θ, which, as mentioned above, regulates the reservoirs' strengths. For $0 \leq \theta < 1$, we have the PME with Dirichlet boundary conditions (19); For $\theta = 1$, the boundary dynamics is slowed enough so the boundary conditions of Dirichlet type are replaced by a type of Robin boundary conditions (20); Finally, for $\theta > 1$, the boundary is sufficiently slowed so that the Robin boundary conditions are replaced by Neumann boundary conditions.

Therefore, with the notations above, we can write the Fick's law in dimension one as

$$J = -D(\rho)\nabla\rho,$$

where J is the diffusion flux. We stress that throughout the first part of the paper we are assuming the validity of the hydrodynamic limit for the perturbed PMM with slow reservoirs, which was proved in [4]. Thus, for the convenience of the reader, we repeat the relevant material from [4] without proofs, thus making our exposition self-contained.

The second result of this paper regards self-duality for the generator of the PMM whose dynamics take place in the discrete one-dimensional torus, $\mathbb{T}_n = \{0, 1, \ldots, n-1\}$. Duality, first introduced by Liggett in [21], is a powerful and rare tool to deal with Markov processes and, in particular, interacting particle systems.

Duality relations allow us to connect two Markov processes via a duality function; such functions are observables in terms of both processes whose expectations satisfy a specific relation. We speak of self-duality if the two Markov processes are two independent copies of the same process. The usefulness of (self-)duality is due to the fact that the dual process may be easier to deal with than the initial process. Duality plays a role in non-equilibrium statistical mechanics: a microscopic knowledge of particle systems can only be reached for a particular class of model - known as exactly solvable models.

Unfortunately, these models, for which we can analytically compute profiles and covariances in non-equilibrium settings, are rare and it turns out that they exhibit a self-duality property. Two examples are the SSEP and the KMP model, which describes a system of one-dimensional oscillators that redistribute energy among nearest neighbors [20]. In this context, the self-duality relations can be used to infer information regarding the $n-$point correlation functions using information (when available) on n dual particles. The literature so far has been concentrated on several

IPS and diffusion processes (see e.g. [6]): among the others the SSEP, of which the PMM share several aspects but it is, however, more complicated.

It is not hard to see that from the PMM one can always retrieve results regarding the SSEP: this is done by setting $M = 1$ in the hydrodynamic equation above and microscopically by setting the exchange rate by 1. For the SSEP a meaningful duality relation is well-known to exist and it is related to the fact that the stationary correlation functions satisfy linear difference equations not involving correlation of higher orders [22], see also Remark 11 below. In this case, an explicit expression of such correlations is known and can be used in the study, for example, of the hydrostatic equation for which an upper bound on the two-points correlation function is needed with the aim of knowing the decreasing rate of convergence to zero. This preliminary study of duality for PMM is motivated by the fact that the hydrostatic limit is still an open problem. As mentioned above, at the microscopic level, PMM has kinetic constraints given by the configuration while macroscopically one derives a nonlinear PDE as hydrodynamic limit. One of the main issues is that the equations given by the (same time) correlations are not closed in the sense that at each step the degree is increased by one; for this reason, finding a meaningful duality relation is far from trivial. On these grounds, this second part has a more investigative approach as, so far, no duality relations are known, for systems with such features.

1.1 Organization of the Paper

Our presentation is divided into two sections: one to derive the Fick's law for our model under the hypothesis of hydrodynamic limit and another to provide an algebraic perspective of the model. We have divided them in such a way that the reader can read Sects. 2 and 3 separately. In Sects. 2.1 and 2.2, we look more closely at the instantaneous and integrated currents of the model. In Sect. 2.3, we defined the empirical measures associated with these currents. In Sect. 2.4, we present the notion of weak solution of the PME with different boundary conditions, to finally prove, in Sect. 2.5, that the Fick's law holds. Sect. 3 starts with a review of duality theory in the context of interacting particle systems. In Sect. 3.1, we explain the algebraic approach to duality by introducing the Lie algebra $\mathfrak{su}(2)$ and we describe how, starting from the reversible measure of the process one can find some duality relations. In Sect. 3.2, we describe the bulk of our model via the generators of the $\mathfrak{su}(2)$ algebra and, lastly, in Sect. 3.3 we show how two different self-duality functions can be constructed. We end this first section by describing the model in two different settings: first,we illustrate its bulk dynamics, which is common to both Sects. 2 and 3; then, we have a subsection to develop the perturbed dynamics in an open setting, by superposing it with a SSEP dynamics and adding two external reservoirs at the boundary, needed for Sect. 2 only.

1.2 The Model

The bulk of the PMM is a continuous time Markov process where particles jump under the exclusion rule to nearest neighbor sites according to the state of the process. However, there are some constraints to take into consideration. Our discrete space is $\Sigma_n := \{1, \ldots, n-1\}$. Suppose that a particle at the site x wants to perform a jump to the site $x+1$: the jump with rate 1 is allowed only if there is a particle at the site $x-1$ or at the site $x+2$. If these sites are empty, then the particle at site x cannot jump and we called it blocked; if both the aforementioned sites are occupied, then the particle performs the jump with rate 2. Due to the constraints of the model's rates, the PMM has configurations that do not evolve under the dynamics of the model, the so-called blocked configurations. The construction of the process is done in the following way. For each $x \in \Sigma_n$, the occupation variable $\eta(x)$ denotes the number of particles at site x, where $\eta(x) = 0$ (resp. $\eta(x) = 1$) stands for empty (resp. occupied) site, which makes our state space $\Omega_n := \{0, 1\}^{\Sigma_n}$. We denote by $\eta \in \Omega_n$ the configuration of particles. To each bond of the bulk $\{x, x+1\}$ with $x = 1 \ldots, n-2$, we associate three Poisson clocks with a parameter depending on the exclusion rule and on the constraints of the process, which are represented by the following Poisson processes: $N^{x-1}_{x,x+1}(t)$ and $N^{x-2}_{x,x+1}(t)$ with parameter 1, while $N_{x,x+1}(t)$ with parameter 2. The PMM generator describes the evolution of the process and it acts on functions $f : \Omega_n \to \mathbb{R}$ as

$$L_P f(\eta) = \sum_{x=1}^{n-2} c_{x,x+1}(\eta) \left\{ a_{x,x+1}(\eta) + a_{x+1,x}(\eta) \right\} \left(f(\eta^{x,x+1}) - f(\eta) \right) \tag{2}$$

where

$$c_{x,x+1}(\eta) = \eta(x-1) + \eta(x+2), \tag{3}$$

$$a_{x,x+1}(\eta) = \eta(x)(1 - \eta(x+1)), \tag{4}$$

are the exchange rates, while the exchange configuration $\eta^{x,y}$ is given by

$$\eta^{x,y}(z) = \begin{cases} \eta(z), & z \neq x, y, \\ \eta(y), & z = x, \\ \eta(x), & z = y. \end{cases}$$

Notice that L_P conserves the total number of particles.

1.2.1 The Open PMM

Let us now describe the open dynamics of the perturbed PMM with slow reservoirs. Fix the following real numbers: $1 < a < 2$, $\theta \geq 0$, $m > 0$, and $\alpha, \beta \in (0, 1)$. Let

$n \geq 1$ be a scaling parameter. The particles are distributed on the points of the discrete space Σ_n. We artificially add two external sites 0 and n where particles can be inserted or removed from the bulk with some rates defined below. We associate two Poisson clocks at the bonds $\{0, 1\}$ and $\{n-1, n\}$ in the following way: $N_{0,1}(t)$ (resp. $N_{n,n-1}(t)$) with parameter $m\alpha n^{-\theta}$ (resp. $m\beta n^{-\theta}$) and $N_{1,0}(t)$ (resp. $N_{n-1,n}(t)$) with parameter $m(1-\alpha)n^{-\theta}$ (resp. $m(1-\beta)n^{-\theta}$). The Poisson processes associated to a bulk bond are now affected by the superposed SSEP dynamics, thus we need to add a factor of n^{a-2} to their parameters. We stress that all of these Poisson processes are independent and throughout the text we use the convention

$$\eta(0) = \alpha, \quad \eta(n) = \beta.$$

For a description of the dynamics of the model, see Fig. 1.

The perturbed PMM with slow reservoirs is a continuous time Markov process $\{\eta_t\}_{t\geq 0}$ on $\Omega_n = \{0, 1\}^{\Sigma_n}$. It can be fully characterized by the infinitesimal generator L_n given by

$$L_n = L_P + n^{a-2}L_S + L_\alpha + L_\beta, \tag{5}$$

where L_P is the bulk generator of the PMM defined in Eq. (2), while L_S is the generator of the SSEP. L_α and L_β are the generators of the Glauber dynamics which act at sites 1 and $n-1$. Their actions on functions $f : \Omega_n \to \mathbb{R}$ are

$$\begin{aligned}
L_S f(\eta) &= \sum_{x=1}^{n-2} \left\{a_{x,x+1}(\eta) + a_{x+1,x}(\eta)\right\} (f(\eta^{x,x+1}) - f(\eta)),\\
L_\alpha f(\eta) &= \frac{m}{n^\theta} \{\alpha(1-\eta(1)) + (1-\alpha)\eta(1)\} (f(\eta^1) - f(\eta)),\\
L_\beta f(\eta) &= \frac{m}{n^\theta} \{\beta(1-\eta(n-1)) + (1-\beta)\eta(n-1)\} (f(\eta^{n-1}) - f(\eta)),
\end{aligned} \tag{6}$$

where the flip configuration η^x is given by

$$\eta^x(z) = \begin{cases} \eta(z), & z \neq x, \\ 1-\eta(x), & z = x. \end{cases}$$

Remark 1 Recall that the diffusion coefficient of the PME is given by $D(\rho) = M\rho^{M-1}$, for $M > 1$. We note that the exchange rate in (3) is related to the diffusion coefficient of the PME when $M = 2$. Considering different values of M (including $M = 1$), we have to consider different exchange rates, for example:

M	$D(\rho)$	$c_{x,x+1}(\eta)$
1	1	1
2	2ρ	$\eta(x-1) + \eta(x+2)$
3	$3\rho^2$	$\eta(x-2)\eta(x-1) + \eta(x-1)\eta(x+2) + \eta(x+2)\eta(x+3)$

Remark 2 Throughout the text we denote by $\{\eta_{tn^2}\}_{t\geq 0}$ the Markov process sped up in the diffusive time scale tn^2.

Remark 3 The results presented here are also valid for any integer number $M > 2$. For a deeper discussion about the model we refer the reader to [4].

Remark 4 The dynamics of the PMM is degenerate (due to the constraints of the jump rates) and do not conserve the total number of particles (due to the Glauber dynamics). However, since the PMM is superposed with a SSEP dynamics, it becomes an irreducible Markov process and therefore only one invariant measure exists. In the equilibrium state ($\alpha = \beta$), it is not difficult to see that the Bernoulli product measure with a constant parameter ($\rho = \alpha = \beta$) is a reversible measure, and in particular, it is invariant. But in the non-equilibrium state ($\alpha \neq \beta$), we have no information about the invariant measure of the process. We stress that we have been trying different approaches in order to have some information about it but without success. One of them was to use the matrix ansatz, introduced in [9], which we could not apply due to the complicated action of the bulk dynamics. Another one is to use duality theory for IPS [12], we start the work here via a description of the PMM which uses algebra representation theory; nevertheless this is still a work in progress.

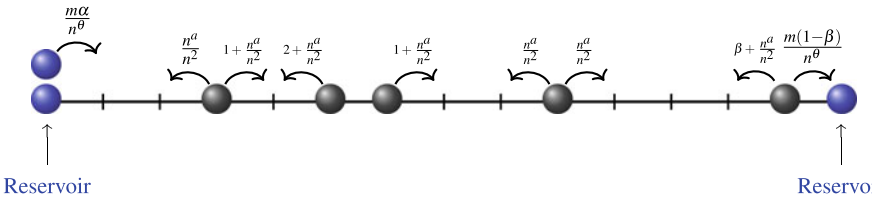

Fig. 1 Allowed jumps for the perturbed porous medium model with slow reservoirs (with $M = 2$)

2 Fick's Law for the PMM with Slow Reservoirs

Throughout this section we will work with the open PMM, introduced in the previous subsection. Moreover, since we are assuming the validity of the hydrodynamic limit proved in [4] using the Entropy method of [15], we need to avoid blocked configurations in order to have an irreducible Markov process. For this reason we superposed the PMM dynamics with a SSEP dynamics with a time scale slower than the diffusive one. This guarantees that, when scaling the time diffusively, we can see the impact of the SSEP at the microscopic level, but we cannot see it at the macroscopic level.

2.1 Currents

Let $\eta \in \Omega_n$. We denote by $j_{x,x+1}(\eta)$ the instantaneous current of particles over the bond $\{x, x+1\}$. In other words, it is the rate at which the particle jumps from the site x to $x+1$, minus the rate at which the particle jumps from the site $x+1$ to x. Thus, for $x \in \Sigma_{n-1}$, the current in the bulk is given by

$$j_{x,x+1}(\eta) = (\eta(x) - \eta(x+1))(\eta(x-1) + \eta(x+2) + n^{a-2}). \tag{7}$$

In the same manner, the current over the bond in the left (resp. right) boundary is given by

$$j_{0,1}(\eta) = \tfrac{m}{n^\theta}(\alpha - \eta(1)) \quad \text{and} \quad j_{n-1,n}(\eta) = \tfrac{m}{n^\theta}(\eta(n-1) - \beta).$$

Now, we look for a local function $h : \Omega_n \to \mathbb{R}$, such that for every $x \in \Sigma_{n-1}$ the current can be written as $j_{x,x+1}(\eta) = \tau_x h(\eta) - \tau_{x+1} h(\eta)$, where $\tau_x h(\eta) = h(\tau_x \eta)$. The function τ_x being the translation by x in the configuration η. If such a function exists, the Dynkin martingale will be much easier to compute (see (23)), since we can sum by parts and transfer the gradient to the test function. Models for which the current is the gradient of a local function are called gradient models, see for instance [19]. Hence, summing and subtracting $\eta(x)\eta(x+1)$ in (7), we can write it as

$$j_{x,x+1}(\eta) = \tau_x h(\eta) - \tau_{x+1} h(\eta), \tag{8}$$

where

$$\tau_x h(\eta) = \eta(x-1)\eta(x) + \eta(x)\eta(x+1) - \eta(x-1)\eta(x+1) + n^{a-2}\eta(x). \tag{9}$$

Therefore, the PMM is a gradient model.

2.2 Integrated Currents

Let $t \in [0, T]$, for $T > 0$. For any $x \in \Sigma_n \cup \{0\}$, we denote by $N_t^n(x)$ the total number of particles that jumped from site x to $x+1$ in an interval of time $[0, tn^2]$, and by $\tilde{N}_t^n(x)$ the total number of particles that jumped from site $x+1$ to x in the same time interval. Thus, we define the integrated current at time t and location x by

$$J_t^n(x) := N_t(x) - \tilde{N}_t(x), \quad \text{for } x \in \Sigma_n \cup \{0\}. \tag{10}$$

In other words, $J_t^n(x)$ denotes the flux of particles through the bond $\{x, x+1\}$ in an interval of time $[0, tn^2]$. The integrated current (10) can be written in terms of its conservative and non-conservative parts. We denote by $Q_t^n(x)$ the conservative

integrated current at time t and location x, which records the particle jumps from the diffusive part of the dynamics (PMM and SSEP)

$$Q_t^n(x) := J_t^n(x), \quad \text{for } x \in \Sigma_{n-1}. \tag{11}$$

We denote by $K_t^n(x)$ the non-conservative integrated current at time t and location x, which records the particles inserted and removed from the system at sites 1 or $n-1$ (Glauber dynamics)

$$K_t^n(x) := J_t^n(x), \quad \text{for } x = 0, n-1. \tag{12}$$

Having disposed of this preliminary step, we can now define the infinitesimal generator of the joint process $\{\eta_t, J_t^n(x)\}_{t\geq 0}$ as

$$\begin{aligned}\tilde{L}_n f(\eta, J^n(x)) = \tilde{L}_P f(\eta, J^n(x)) + n^{a-2}\tilde{L}_S f(\eta, J^n(x)) \\ + \tilde{L}_\alpha f(\eta, J^n(x)) + \tilde{L}_\beta f(\eta, J^n(x)),\end{aligned} \tag{13}$$

for $x \in \Sigma_n \cup \{0\}$. To simplify the notation, let $p_{x,x+1}(\eta) = a_{x,x+1}(\eta)(c_{x,x+1}(\eta) + n^{a-2})$. For each $x \in \Sigma_{n-1}$, we define the part of (13) corresponding to the jumps in the bulk as

$$\begin{aligned}\left(\tilde{L}_P + n^{a-2}\tilde{L}_S\right) f(\eta, J^n(x)) &= p_{x,x+1}(\eta)\left(f(\eta^{x,x+1}, J^n(x)+1) - f(\eta, J^n(x))\right) \\ &+ p_{x+1,x}(\eta)\left(f(\eta^{x,x+1}, J^n(x)-1) - f(\eta, J^n(x))\right) \\ &+ \sum_{\substack{y\in\Sigma_{n-1}\\ y\neq x}} (p_{y,y+1}(\eta) + p_{y+1,y}(\eta))\left(f(\eta^{y,y+1}, J^n(y)) - f(\eta, J^n(y))\right),\end{aligned} \tag{14}$$

and the part of (13) corresponding to the jumps in the boundaries as

$$\begin{aligned}\tilde{L}_\alpha f(\eta, J^n(0)) &= \frac{m}{n^\theta}\Big(\alpha(1-\eta(1))\left(f(\eta^1, J^n(0)+1) - f(\eta, J^n(0))\right)\Big) \\ &+ \frac{m}{n^\theta}\Big((1-\alpha)\eta(1)\left(f(\eta^1, J^n(0)-1) - f(\eta, J^n(0))\right)\Big), \\ \tilde{L}_\beta f(\eta, J^n(n-1)) &= \frac{m}{n^\theta}\Big(\beta(1-\eta(n-1))\left(f(\eta^{n-1}, J^n(n-1)-1) - f(\eta, J^n(n-1))\right) \\ &+ (1-\beta)\eta(n-1)\left(f(\eta^{n-1}, J^n(n-1)+1) - f(\eta, J^n(n-1))\right)\Big).\end{aligned} \tag{15}$$

Remark 5 Throughout this section the process is sped up in the diffusive time scale tn^2.

Remark 6 If we take $f(\eta, J) = f(\eta)$ in (14) and (15), we recover the infinitesimal generator of $\{\eta_t\}_{t\geq 0}$, which is defined in (5). Moreover, if we take f being the projection in the second variable, that is, $f(\eta, J) = J$ in (14) and (15), we recover the instantaneous current through the bond $\{x, x+1\}$ as we can see below.

For $x \in \Sigma_{n-1}$, we have

$$\begin{aligned}\left(\tilde{L}_P + n^{a-2}\tilde{L}_S\right) J^n(x) &= a_{x,x+1}(\eta)(c_{x,x+1}(\eta) + n^{a-2})\left(J^n(x) + 1 - J^n(x)\right) \\ &\quad + a_{x+1,x}(\eta)(c_{x+1,x}(\eta) + n^{a-2})\left(J^n(x) - 1 - J^n(x)\right) \\ &= j_{x,x+1}(\eta).\end{aligned}$$

For the left (resp. right) boundary, we have

$$\begin{aligned}\tilde{L}_\alpha J^n(0) &= \frac{m}{n^\theta}\Big(\alpha(1-\eta(1))\left(J^n(0) + 1 - J^n(0)\right)\Big) \\ &\quad + \frac{m}{n^\theta}\Big(((1-\alpha)\eta(1))\left(J^n(0) - 1 - J^n(0)\right)\Big) \\ &= j_{0,1}(\eta),\end{aligned}$$

$$\begin{aligned}\tilde{L}_\beta J^n(n-1) &= \frac{m}{n^\theta}\Big(\beta(1-\eta(n-1))\left(J^n(n-1) - 1 - J^n(n-1)\right)\Big) \\ &\quad + \frac{m}{n^\theta}\Big(((1-\beta)\eta(n-1))\left(J^n(n-1) + 1 - J^n(n-1)\right)\Big) \\ &= j_{n-1,n}(\eta).\end{aligned}$$

2.3 Empirical Measures

Fix $t \in [0, T]$. For $\eta \in \Omega_n$, we define the empirical measure π_t^n on $[0, 1]$ as

$$\pi_t^n := \frac{1}{n}\sum_{x\in\Sigma_n} \eta_t(x)\delta_{x/n}, \tag{16}$$

where δ_u is the Dirac measure concentrated on $u \in [0, 1]$. Recall the definition of the conservative current (11). The empirical measure associated with this current is defined as the signed measure on $[0, 1]$

$$Q_t^n := \frac{1}{n^2}\sum_{x=1}^{n-2} Q_t^n(x)\delta_{x/n}. \tag{17}$$

Note that the renormalization factor of order n^2 arises in (17) because we need to take into account the space renormalization and the diffusive scaling of the PMM and SSEP dynamics. Now, recall the definition of (12). The empirical measure associated with this boundary current is defined as

$$K_t^n := \frac{1}{n}K_t^n(0)\delta_{0/n} + \frac{1}{n}K_t^n(n-1)\delta_{n-1/n}. \tag{18}$$

Since expression (18) is related to the Glauber part of the process, we only need to take into account the space renormalization factor of order n.

Let $f \in C^1([0,1])$ be a test function. We define the empirical density of particles at time t, that is, the integral of f with respect to the empirical measure π_t^n, as

$$\pi_t^n(f) = \frac{1}{n} \sum_{x \in \Sigma_n} f\left(\tfrac{x}{n}\right) \eta_t(x).$$

In the same manner, the current field J_t^n is defined as

$$J_t^n(f) := Q_t^n(f) + K_t^n(f),$$

where Q_t^n is the conservative current field

$$Q_t^n(f) := \frac{1}{n^2} \sum_{x=1}^{n-2} f\left(\tfrac{x}{n}\right) Q_t^n(x),$$

and K_t^n is the non-conservative current field

$$K_t^n(f) := \frac{1}{n} \left(f(0) K_t^n(0) - f\left(\tfrac{n-1}{n}\right) K_t^n(n-1) \right).$$

2.4 Fick's Law

In this section, we define the notion of weak solution of the PME with Dirichlet, Robin, and Neumann boundary conditions, and we state the Fick's law for the PMM with slow reservoirs. Before we start, let us fix some notations. We denote by:

- $C_c^\infty(0,1)$, the set of all real-valued functions $G \in C^\infty(0,1)$ with compact support;
- $C_0^{1,2}([0,T] \times [0,1])$, the set of all real-valued functions $G \in C^{1,2}([0,T] \times [0,1])$ such that $G_s(0) = G_s(1) = 0$, for all $s \in [0,T]$;
- $\langle \cdot, \cdot \rangle$, the inner product in $L^2([0,1])$ with corresponding norm $\| \cdot \|_2$.

Definition 1 Let $\mathscr{H}^1$ be the set of all locally summable functions $\zeta : [0,1] \to \mathbb{R}$ such that there exists a function $\partial_u \zeta \in L^2([0,1])$ satisfying

$$\langle \partial_u G, \zeta \rangle = \langle G, \partial_u \zeta \rangle,$$

for all $G \in C_c^\infty(0,1)$. For $\zeta \in \mathscr{H}^1$, we define the norm

$$\| \zeta \|_{\mathscr{H}^1} := \left(\| \zeta \|_2^2 + \| \partial_u \zeta \|_2^2 \right)^{1/2}.$$

Let $L^2(0,T;\mathscr{H}^1)$ be the set of all measurable functions $\xi : [0,T] \to \mathscr{H}^1$ such that

$$\|\xi\|^2_{L^2(0,T;\mathscr{H}^1)} := \int_0^T \|\xi_t\|^2_{\mathscr{H}^1}\, dt < \infty.$$

Definition 2 Let $T > 0, \alpha, \beta \in (0,1)$ and $g : [0,1] \to [0,1]$ a measurable function. We say that $\rho : [0,T] \times [0,1] \to [0,1]$ is a weak solution of the PME with Dirichlet boundary conditions

$$\begin{cases} \partial_t \rho_t(u) = \Delta\,(\rho_t(u))^2, \quad (t,u) \in (0,T] \times (0,1), \\ \rho_t(0) = \alpha, \quad \rho_t(1) = \beta, \quad t \in (0,T], \\ \rho_0(u) = g(u), \quad u \in [0,1], \end{cases} \tag{19}$$

if the following conditions hold:

1. $\rho^2 \in L^2(0,T;\mathscr{H}^1)$;
2. ρ satisfies the integral equation:

$$\int_0^1 \left\{\rho_t(u)G_t(u) - g(u)G_0(u)\right\} du - \int_0^t \int_0^1 \left\{\rho_s(u)\partial_s G_s(u) + (\rho_s)^2(u)\Delta G_s(u)\right\} du\, ds + \int_0^t \left\{\beta^2 \partial_u G_s(1) - \alpha^2 \partial_u G_s(0)\right\} ds = 0,$$

   for all $t \in [0,T]$ and any function $G \in C_0^{1,2}([0,T] \times [0,1])$;
3. $\rho_t(0) = \alpha$ and $\rho_t(1) = \beta$ for all $t \in (0,T]$.

Definition 3 Let $T > 0, \kappa \geq 0, \alpha, \beta \in (0,1)$ and $g : [0,1] \to [0,1]$ a measurable function. We say that $\rho : [0,T] \times [0,1] \to [0,1]$ is a weak solution of the PME with Robin boundary conditions

$$\begin{cases} \partial_t \rho_t(u) = \Delta\,(\rho_t(u))^2, \quad (t,u) \in (0,T] \times (0,1), \\ \partial_u(\rho_t(0))^2 = \kappa(\rho_t(0) - \alpha), \quad t \in (0,T], \\ \partial_u(\rho_t(1))^2 = \kappa(\beta - \rho_t(1)), \quad t \in (0,T], \\ \rho_0(u) = g(u), \quad u \in [0,1], \end{cases} \tag{20}$$

if the following conditions hold:

1. $\rho^2 \in L^2(0,T;\mathscr{H}^1)$;
2. ρ satisfies the integral equation:

$$\int_0^1 \left\{\rho_t(u)G_t(u) - g(u)G_0(u)\right\} du - \int_0^t \int_0^1 \left\{\rho_s(u)\partial_s G_s(u) + \rho_s^2(u)\Delta G_s(u)\right\} du\, ds + \int_0^t \left\{(\rho_s(1))^2 \partial_u G_s(1) - (\rho_s(0))^2 \partial_u G_s(0)\right\} ds - \kappa \int_0^t \left\{G_s(0)(\alpha - \rho_s(0)) + G_s(1)(\beta - \rho_s(1))\right\} ds = 0,$$

   for all $t \in [0,T]$ and any function $G \in C^{1,2}([0,T] \times [0,1])$.

Before stating the Fick's law let us fix some notations. Let $\mathscr{M}_+$ be the space of positive measures on $[0, 1]$ with total mass bounded by 1 equipped with the weak topology. Let μ_n be measure on Ω_n. We denote by $\mathbb{P}_{\mu_n}$ the probability measure in the Skorokhod space $\mathscr{D}([0, T], \Omega_n)$, induced by the accelerated Markov process $\{\eta_{tn^2}\}_{t\geq 0}$ and the initial measure μ_n. We denote by $\mathbb{E}_{\mu_n}$ the expectation with respect to $\mathbb{P}_{\mu_n}$.

Let $g : [0, 1] \to [0, 1]$ be a measurable function. For each $n \in \mathbb{N}$, we say that $\{\mu_n\}_{n\in\mathbb{N}}$ is associated with $g(\cdot)$, if for any continuous function $H : [0, 1] \to \mathbb{R}$ and any $\delta > 0$:

$$\lim_{n\to+\infty} \mu_n \left(\eta \in \Omega_n : \left| \frac{1}{n} \sum_{x\in\Sigma_n} H(\tfrac{x}{n})\eta(x) - \int_0^1 H(u)g(u)\,du \right| > \delta \right) = 0. \tag{21}$$

Theorem 1 (Fick's law) *Fix $\theta \in [0, +\infty)$. Let $g : [0, 1] \to [0, 1]$ be a measurable function, $H : [0, 1] \to \mathbb{R}$ a continuous function, and $\{\mu_n\}_{n\in\mathbb{N}}$ a sequence of probability measures on Ω_n associated with $g(\cdot)$, as in (21). Then, for any $t \in [0, T]$ and any $\delta > 0$, we have*

$$\lim_{n\to+\infty} \mathbb{P}_{\mu_n}\left(\eta_\cdot \in \mathscr{D}([0, T], \Omega_n) : \left|\frac{1}{n^2}\sum_{x=1}^{n-2} Q_t^n(x)H\left(\tfrac{x}{n}\right) - \int_0^1 H(u)\nabla\rho_t^2(u)\,du\right| > \delta\right) = 0,$$

$$\lim_{n\to+\infty} \mathbb{P}_{\mu_n}\left(\eta_\cdot \in \mathscr{D}([0, T], \Omega_n) : \left|\frac{1}{n}\left(H(0)K_t^n(0) - H\left(\tfrac{n-1}{n}\right)K_t^n(n-1)\right)\right.\right.$$
$$\left.\left. - \mathbb{1}_{\{\theta=1\}}\kappa\int_0^t H(0)(\alpha - \rho_s(0)) + H(1)(\beta - \rho_s(1))ds\right| > \delta\right) = 0,$$

where

- *$\rho_t(u)$ is a weak solution of (19), for $0 \leq \theta < 1$;*
- *$\rho_t(u)$ is a weak solution of (20) ($\kappa = m$), for $\theta = 1$;*
- *$\rho_t(u)$ is a weak solution of (20) (with $\kappa = 0$), for $\theta > 1$.*

Remark 7 Note that $J_t^n = Q_t^n + K_t^n$. From the previous theorem we have that J^n converges weakly to $J\,du$, where J is the weak solution of

$$J = -D(\rho)\nabla\rho = -\nabla\rho^2.$$

The result stated in Theorem 1, that we will prove in the next section, is the Law of large numbers for the empirical measures defined in (17) and (18). It is the analog of the Law of large numbers for the empirical measure (16), known in the literature as hydrodynamic limit.

2.5 *Proof of Theorem 1*

In this section, we prove Theorem 1, that is, the validity of Fick's law: the currents which enter and exit from the system are at all times equal to the local density gradient at 0 and 1. In order to prove it we need to assume the validity of the hydrodynamic limit and some technical results, known as replacement lemmas, which are stated in the appendix. These results and the hydrodynamic limit are proved in [4]. The theorems we refer to in the proof are stated in the first and second sections of the Appendix.

Proof Let us prove the first identity of the theorem. Our proof starts with the observation that by Dynkin's formula, see Lemma A1.5.1 of [19], for a fixed test function $H \in C^1([0,1])$, we have that

$$M_t^n(H) = Q_t^n(H) - Q_0^n(H) - \int_0^t n^2 \tilde{L}_n Q_s^n(H)\, ds, \tag{22}$$

is a martingale with respect to the natural filtration $\{\mathscr{F}_t\}_{t\geq 0}$, which vanishes as $n \to \infty$ in $L^2(\mathbb{P}_{\mu_n})$ (see fist section of the Appendix). Note that $Q_0^n(H) = 0$. Hence, we can write (22) as

$$Q_t^n(H) - \int_0^t \sum_{x=1}^{n-2} H\left(\tfrac{x}{n}\right) j_{x,x+1}(\eta_{sn^2})\, ds.$$

Since the PMM is a gradient model, performing a summation by parts in the previous expression, we can write (22) as

$$Q_t^n(H) - \int_0^t \frac{1}{n} \sum_{x=1}^{n-2} \nabla_n^- H\left(\tfrac{x}{n}\right) \tau_x h(\eta_{sn^2}) + H\left(\tfrac{0}{n}\right) \tau_1 h(\eta_{sn^2}) - H\left(\tfrac{n-1}{n}\right) \tau_{n-1} h(\eta_{sn^2})\, ds, \tag{23}$$

where $\tau_x h(\eta_{sn^2})$ is defined in (9) and

$$\nabla_n^+ H\left(\tfrac{x}{n}\right) = n\left(H\left(\tfrac{x+1}{n}\right) - H\left(\tfrac{x}{n}\right)\right), \quad \nabla_n^- H\left(\tfrac{x}{n}\right) = n\left(H\left(\tfrac{x}{n}\right) - H\left(\tfrac{x-1}{n}\right)\right). \tag{24}$$

Thus, we want to examine the convergence of (23) for each value of $\theta \in [0, +\infty)$.

If $\theta < 1$, the test function vanishes at the boundary. From the hydrodynamic limit and Theorem 3, we have that the integral term of (23) converges in $\mathbb{P}_{\mu_n}$, as $n \to \infty$ to

$$\int_0^t \int_0^1 \nabla H(u) \rho_s^2(u)\, du\, ds = \int_0^t H(1)\rho_s^2(1) - H(0)\rho_s^2(0)\, ds - \int_0^t \int_0^1 H(u) \nabla \rho_s^2(u)\, du\, ds,$$

which is equal to $-\int_0^t \int_0^1 H(u) \nabla \rho_s^2(u)\, du\, ds$.

If $\theta \geq 1$, the test function does not necessarily vanishes at the boundary. From the hydrodynamic limit, Theorems 3 and 4 it follows that the integral term of (23) converges in $\mathbb{P}_{\mu_n}$, as $n \to \infty$ to

$$\int_0^t \int_0^1 \nabla H(u) \rho_s^2(u)\, du\, ds + \int_0^t H(0)\rho_s^2(0) - H(1)\rho_s^2(1)\, ds,$$

which is also equal to $-\int_0^t \int_0^1 H(u) \nabla \rho_s^2(u)\, du\, ds$.

In the same manner, for $H \in C^1([0,1])$ we have that

$$\tilde{M}_t^n(H) = K_t^n(H) + \kappa \int_0^t \frac{n}{n^\theta} \left(H(\tfrac{1}{n})(\alpha - \eta_{sn^2}(1)) + H(\tfrac{n-1}{n})(\beta - \eta_{sn^2}(n-1)) \right) ds, \tag{25}$$

is also a martingale that vanishes in $L^2(\mathbb{P}_{\mu_n})$ as $n \to \infty$, see first section of the Appendix. Let us now examine the convergence of the integral term of (25), for each value of $\theta \in [0, +\infty)$.

If $0 < \theta < 1$, the test function vanishes at the boundary, and by a Taylor expansion on H we get

$$\frac{\kappa}{n^\theta} \int_0^t -\nabla_n^+ H(0)(\alpha - \eta_{sn^2}(1)) - \nabla_n^- H\,(1)\,(\beta - \eta_{sn^2}(n-1))\, ds,$$

where $\nabla_n^{\pm} H\left(\frac{x}{n}\right)$ are defined in (24). The previous expression is bounded from above by

$$\frac{\kappa}{n^\theta} \|\nabla H\|_\infty \int_0^t |\alpha - \eta_{sn^2}(1)| + |\beta - \eta_{sn^2}(n-1)|\, ds,$$

which vanishes as $n \to \infty$. If $\theta = 0$, the test function vanishes at the boundary, and by Theorem 5 we have that the integral term of (25) vanishes. If $\theta = 1$, the test function does not vanishes at the boundary, and from Theorem 6 we have that the integral term of (25) converges in $\mathbb{P}_{\mu_n}$, as $n \to \infty$ to

$$\kappa \int_0^t H(0)(\alpha - \rho(s,0)) + H(1)(\beta - \rho(s,1))\, ds.$$

Finally, if $\theta > 1$, we have that the integral term of (25) is bounded from above by

$$\frac{\kappa}{n^{\theta-1}} \|H\|_\infty \int_0^t |\alpha - \eta_{sn^2}(1)| + |\beta - \eta_{sn^2}(n-1)|\, ds,$$

which vanishes as $n \to \infty$, concluding the proof.

3 Stochastic Duality Relations for the PMM

In order to show our self-duality result for the PMM, we first need to give some context regarding stochastic duality theory for Markov jumping processes. The idea behind duality is to get information on a given process from another process, its *dual*. The link between these two processes is provided by a set of so-called *duality functions*, i.e. a set of observables that are functions of both processes and whose expectations satisfy the following definition.

Definition 4 (*Duality of processes*) For $t \geq 0$, let η_t and ξ_t be two continuous time Markov processes with state spaces Ω and Ω^{dual} , respectively. We say that ξ_t is *dual* to η_t with duality function $D : \Omega \times \Omega^{dual} \to \mathbb{R}$ if

$$\mathbb{E}_\eta[D(\eta_t, \xi)] = \mathbb{E}_\xi[D(\eta, \xi_t)] \,, \tag{26}$$

for all $(\eta, \xi) \in \Omega \times \Omega^{dual}$ and $t \geq 0$. In (26) $\mathbb{E}_\eta$ (respectively $\mathbb{E}_\xi$) is the expectation with respect to the law of the η_t process initialized at η (respectively the ξ_t process initialized at ξ).

If η_t and ξ_t are two independent copies of the same process, we say that η_t is *self-dual* with self-duality function D. We will see that this is the case for the bulk dynamics of the PMM. Indeed, self-duality can always be thought as a special case of duality where the dual process is an independent copy of the first one. The simplification of self-duality typically arises from the fact that in the copy process only a small number of particles are considered. Given the one-to-one correspondence between Markov processes and their semigroups, then one sees that a duality relation between two Markov processes is equivalent to a duality relation between their Markov semigroups, i.e.

$$\left(T_t D\left(\cdot, \xi\right)\right)(\eta) = \left(T_t^{dual} D\left(\eta, \cdot\right)\right)(\xi) \,, \text{ for } t \geq 0, \tag{27}$$

where T_t denotes the semigroup of the original process η and T_t^{dual} the semigroup of the dual process ξ. In the context of IPS duality can be defined at the level of their Markov generator, this is usually a definition easier to work with and the equivalence of these two definitions has been proved in [17].

Definition 5 (*Duality of generators*) For $t \geq 0$, let L and L^{dual} be generators of the two Markov processes η_t and ξ_t, respectively. We say that L^{dual} is *dual* to L with duality function $D : \Omega \times \Omega^{dual} \longrightarrow \mathbb{R}$ if

$$[L D(\cdot, \xi)](\eta) = [L^{dual} D(\eta, \cdot)](\xi) \tag{28}$$

where we assume that both sides are well defined.

In case $L = L^{dual}$ we shall say that the process is *self-dual* and the self-duality relation becomes

$$[L D(\cdot, \xi)](\eta) = [L D(\eta, \cdot)](\xi) \,. \tag{29}$$

In Eq. (28) (respectively (29)) it is understood that L on the left hand side acts on D as a function of the first variable η, while L^{dual} (resp. L) on the right hand side acts on D as a function of the second variable ξ. Definition 5 is easier to prove, so we will usually work under the assumption that the notion of duality (respectively self-duality) is the one in Eq. (28) (respectively (29)).

If the original process η_t and the dual process ξ_t are Markov processes with countable state space Ω and Ω^{dual} respectively, then the duality relation is equivalent to

$$\sum_{\eta' \in \Omega} L(\eta, \eta') D(\eta', \xi) = \sum_{\xi' \in \Omega^{dual}} (L^{dual})^T(\xi', \xi) D(\eta, \xi') \ , \tag{30}$$

where L^T denotes the transposition of the generator L. In matrix notation (30) becomes

$$LD = D(L^{dual})^T \ . \tag{31}$$

Once more, if $L^{dual} = L$ we obtain the corresponding definition for self-duality. In this context, the generator L is given by a matrix known as *rate matrix* such that

$$L(\eta, \eta') \geq 0 \qquad \text{and} \qquad \sum_{\eta'} L(\eta, \eta') = 0 \ .$$

For $\eta \neq \eta'$, we say that the process jumps from η to η' with *rate* $L(\eta, \eta')$.

Remark 8 Given that the PMM has a finite state space, the self-duality relations, which will be characterized in the following two sections, read as in Eq. (31).

Our goal is to frame and find a self-duality relation for the PMM. This is achieved via an algebraic approach, first proposed in [12] and further developed in [5, 11, 14], which relies on the following idea. It starts from the hypothesis that the Markov generator is an element of the universal enveloping algebra of a Lie algebra. Then the derivation of a (self-)duality relation is based on two structural ideas:

(i) duality can be seen as a change of representation of a Lie algebra: more precisely one moves between two equivalent representations and the *intertwiner* of those representations yields the duality function.
(ii) self-duality is related to the reversibility of the process and the existence of an algebra element that commutes with the generator of the process.

We will make use of item (ii) to find a self-duality function for the bulk generator of the PMM in Eq. (2).

In what follows, classical theorems and propositions are taken from [11, 12].

3.1 Algebraic Approach to Duality

In this section, we briefly recall the idea to find self-duality relation for an IPS with a reversible measure, see [12]. For the PMM the existence of a reversible measure can be found by the detailed balance equations and it is the starting point of our analysis. As stated in Remark 4, the reversible measure is known for the open system only in case the reservoirs are tuned with the same parameter. In the case of a closed system, the reversible measure has the same form, namely the product of Bernoulli distribution, with a free constant parameter.

3.1.1 Symmetries and Self-Duality

In this subsection, we review the general techniques to exhibit a self-duality relation for an IPS.

Definition 6 Let A and B be two matrices having the same dimension. We say that A is a symmetry of B if A commutes with B, i.e.

$$[A, B] := AB - BA = 0 .$$

Clearly the identity matrix is always a symmetry and it is easy to verify that $[AB, CD] = A[B, C]D + CA[B, D] + [A, C]BD + C[A, D]B$. The main idea is that self-duality (in the context of Markov processes with countable state space) can be recovered starting from a *trivial duality* which is based on the reversible measures of the corresponding process. One then can act with a symmetry of the model on this trivial self-duality and turn it into a non-trivial one. The following theorem formalizes this last idea.

Proposition 1 (Symmetries and self-duality) *Let d be a self-duality function of the generator L and let S be a symmetry of L, then $D = Sd$ is again a self-duality function for L.*

Proof The proof follows from a straightforward computation and in matrix notation it reads

$$LD = LSd = SLd = SdL^T = DL^T ,$$

where the second identity follows from the fact that S and L commutes, while the third one is due to the self-duality of the generator L with self-duality function d.

If there is a description of the process generator in terms of a Lie algebra, then symmetries can be constructed using this algebraic structure. Notice that the two main elements of the theorem above are the initial self-duality d and the symmetry operator S. We explain now how these two objects can easily be found whenever reversibility and an algebraic description of the process are available. In general, if the process has a reversible measure, the self-duality d can be easily found starting from the reversibility, as the following proposition shows.

Proposition 2 *If the process associated with the generator L has reversible measure μ, then the function $d : \Omega \times \Omega \to \mathbb{R}$*

$$d(\eta, \xi) = \frac{\delta_{\eta,\xi}}{\mu(\eta)} \tag{32}$$

is a self-duality function.

Proof The proof follows from the reversibility of the measure μ. Since we are on a countable state space, we can use the notion of self-duality via the matrix notation in Eq. (31). Namely,

$$Ld = dL^T$$

which reads

$$\sum_{\eta' \in \Omega} L(\eta, \eta') d(\eta', \xi) = \sum_{\xi' \in \Omega} d(\eta, \xi') L^T(\xi', \xi) \ ,$$

once we substitute the expression of d as in Eq. (32) we get

$$\sum_{\eta' \in \Omega} L(\eta, \eta') \frac{\delta_{\eta',\xi}}{\mu(\xi)} = \sum_{\xi' \in \Omega} \frac{\delta_{\eta,\xi'}}{\mu(\eta)} L^T(\xi', \xi) \ .$$

The sum on the left-hand side only survives for $\eta' = \xi$ while the one on the right-hand side only survives for $\xi' = \eta$, i.e,

$$L(\eta, \xi) \frac{1}{\mu(\xi)} = L(\xi, \eta) \frac{1}{\mu(\eta)},$$

which is exactly the detailed balance condition.

We refer to this diagonal self-duality function in Eq. (32) as trivial or cheap self-duality function. At this point one may now wonder how the operator S is found; here it is where the properties of the algebra help. If the algebra admits the Casimir element $\mathscr{C}$ then it is not hard to find symmetries for the process generator. Indeed, since the Casimir element commutes with all the other elements of the algebra, then any element of the algebra is potentially a good candidate as a symmetry of $\mathscr{C}$. Moreover, whenever the process generator L can be written as the coproduct of the Casimir element, then a symmetry of the Casimir can be extended using its coproduct to a symmetry of the generator as shown in the proposition below. It will also be useful to recall that the coproduct of a Lie algebra generator X, denoted by $\Delta(X)$ is defined via the tensor product $\otimes$, as

$$\Delta(X) = 1 \otimes X + X \otimes 1 \tag{33}$$

and that it can be extended as an algebra homomorphism to the universal enveloping algebra.

Proposition 3 *If S is a symmetry of the central element $\mathscr{C}$, then $\Delta(S)$ is a symmetry for $\Delta(\mathscr{C})$.*

Proof Starting from $[\mathscr{C}, S] = 0$, we want to show that $[\Delta(\mathscr{C}), \Delta(S)] = 0$. This follows from the fact that the coproduct is an algebra homomorphism, i.e.

$$[\Delta(\mathscr{C}), \Delta(S)] = \Delta(\mathscr{C})\Delta(S) - \Delta(S)\Delta(\mathscr{C}) = \Delta(\mathscr{C}S) - \Delta(S\mathscr{C}) = \Delta(\mathscr{C}S - S\mathscr{C}) = 0\,.$$

3.1.2 The Lie Algebra $\mathfrak{su}(2)$

In this subsection, we link our process to the Lie algebra $\mathfrak{su}(2)$, for which the Casimir element exists. The $\mathfrak{su}(2)$ Lie algebra is generated by three abstract operators, namely J^0, J^+ and J^-, which satisfy the following commutation relations

$$[J^0, J^\pm] = \pm J^\pm \qquad \text{and} \qquad [J^+, J^-] = 2J^0\,, \tag{34}$$

while the adjoint are given by $(J^0)^* = J^0$, $(J^+)^* = J^-$ and $(J^-)^* = J^+$. The Casimir element is

$$\mathscr{C} = 2(J^0)^2 + J^+J^- + J^-J^+\,. \tag{35}$$

It is easy to check that $\mathscr{C}$ is self-adjoint, i.e. $\mathscr{C} = \mathscr{C}^*$ and it commutes with any generators of the algebra. We propose here two different notations that satisfy the rules of the $\mathfrak{su}(2)$ algebra. The first one is defined by the action of the three matrices on vectors of the natural basis of $\mathbb{R}^2$, $\left\{\begin{pmatrix}1\\0\end{pmatrix}, \begin{pmatrix}0\\1\end{pmatrix}\right\}$. In bra-ket notation, it becomes

$$\begin{cases} J^+ \mid \eta_x\rangle = (1-\eta_x) \mid \eta_x + 1\rangle, \\ J^- \mid \eta_x\rangle = \eta_x \mid \eta_x - 1\rangle, \\ J^0 \mid \eta_x\rangle = (\eta_x - 1/2) \mid \eta_x\rangle, \end{cases}$$

where the $\mid n\rangle$ here is a column vector that represents the nth element of the canonical basis of $\mathbb{R}^2$. Explicitly this means that we can think of the $\mathfrak{su}(2)$ generators as three 2×2 matrices

$$J^+ = \begin{pmatrix}0&0\\1&0\end{pmatrix} \qquad J^- = \begin{pmatrix}0&1\\0&0\end{pmatrix} \qquad J^0 = \begin{pmatrix}-1/2&0\\0&1/2\end{pmatrix}\,.$$

The second representation, equivalent, acts of functions $f : \{0, 1\} \to \mathbb{R}$ and is given by

$$\begin{cases} (J^+ f)(\eta_x) = \eta_x f(\eta_x - 1), \\ (J^- f)(\eta_x) = (1-\eta_x) f(\eta_x + 1), \\ (J^0 f)(\eta_x) = (\eta_x - 1/2) f(\eta_x), \end{cases}$$

where $f(-1) = f(2) = 0$. In the next section, we use these two representations to show how the PMM can be described using the algebra's generators J^+, J^-, and J^0. From the first representation the rate matrix will arise, while the second one is used to find the generators of Sect. 1.2

3.2 Porous Medium Model Described with the $\mathfrak{su}(2)$ Algebra

We now link together the previous two Sects. 3.1 and 3.2: we will show that it is possible to describe the PMM generator, L_P, using the three algebra generators J^+, J^- and J^0. This is inspired by the algebraic description of the SSEP which we recall here. We start by considering two sites, labeled by 1 and 2, then the SSEP generator is

$$\begin{aligned} L_S f(\eta) = &[\eta_1(1-\eta_2)][f(\eta_1 - 1, \eta_2 + 1) - f(\eta_1, \eta_2)] \\ &+ (\eta_2(1-\eta_1)][f(\eta_1 + 1, \eta_2 - 1) - f(\eta_1, \eta_2)] \ , \end{aligned} \tag{36}$$

for $\eta = (\eta_1, \eta_2)$. We will see that L_S can be described via the two representations of the $\mathfrak{su}(2)$ algebra introduced above.

Remark 9 In principle L_S is found by summing all over the lattice site Σ_n. However, with abuse of notation, but without loss of generality since the coproduct structure introduced in Eq. (33) can be generalized to any lattice size, we will refer to the SSEP generator for two sites only. Conversely, the minimum number of sites to describe the PMM is 4. At this stage, it is still not clear how to treat the duality relations for the Glauber dynamics, namely for the generators L_α and L_β defined in Eq. (6). For this reason, it will be convenient to expand the space Σ_n into the one dimensional discrete torus with n points, $\mathbb{T}_n$.

The theorem below is saying that the SSEP bulk generator of equation (36) and the Casimir of the $\mathfrak{su}(2)$ of equation (35) are deeply related. An analog result holds for the PMM.

Theorem 2 *Given the structure of the $\mathfrak{su}(2)$ algebra described in the previous section, we can write the SSEP generator in terms of the coproduct of the Casimir element of the algebra in the following way*

$$L_S = \frac{1}{2}\Delta(\mathscr{C}) - \frac{1}{2} \otimes \mathscr{C} - \mathscr{C} \otimes \frac{1}{2} - \frac{1}{2} \ .$$

Moreover, the term $-\frac{1}{2} \otimes \mathscr{C} - \mathscr{C} \otimes \frac{1}{2} - \frac{1}{2}$ on the right hand side of the previous display represents the identity times a constant.

Proof First we substitute the expression of the coproduct of the Casimir $\Delta(\mathscr{C})$, so that we get

$$L_S = J^+ \otimes J^- + J^- \otimes J^+ + 2J^0 \otimes J^0 - 1/2 \, .$$

Using the first representation via matrices, we can write the rate matrix of the SSEP (for two sites) as

$$L_S = \begin{pmatrix} 0 & 0 & 0 & 0 \\ 0 & -1 & 1 & 0 \\ 0 & 1 & -1 & 0 \\ 0 & 0 & 0 & 0 \end{pmatrix} .$$

In this case, the expression $-\frac{1}{2} \otimes \mathscr{C} - \mathscr{C} \otimes \frac{1}{2} - \frac{1}{2}$ is the diagonal matrix with element -2. Equivalently, using the second notation, i.e. acting on the function of two variables we recover the well-known expression of equation (36). In this representation one can check that the action of the Casimir on function is $\mathscr{C} f(\eta) = \frac{3}{2} f(\eta)$, so that the expression $-\frac{1}{2} \otimes \mathscr{C} - \mathscr{C} \otimes \frac{1}{2} - \frac{1}{2}$ on functions of two variables just gives $-2 f(\eta_1, \eta_2)$.

We now go back to the PMM. The first observation is that it works on 4 sites because even if the jumps only contemplate two central sites, there are two extra sites to be taken into account. For this reason, we start by considering the action on 4 sites only and so we restrict the analysis to the finite one-dimensional lattice Σ_5. Here we observe jumps between sites 2 and 3. In this setting the PMM generator acts on functions $f : \{0, 1\}^{\Sigma_5} \to \mathbb{R}$. The key observation is that

$$\begin{aligned} L_P &= (J_1^0 + J_4^0 + 1) L_S \\ &= \left(J_1^0 + J_4^0 + 1\right) \left(J_2^+ J_3^- + J_2^- J_3^+ + 2J_2^0 J_3^0 - 1/2\right) \, . \end{aligned} \tag{37}$$

Here the notation J_x^a means that J^a is acting on sites $x \in \Sigma_5$ for $a \in \{0, +, -\}$. Indeed, since the algebra generator J^0 does not increase or decrease the degree of the functions, we can use them to describe the extra constraint for the PMM. Here L_S has to be thought as the SSEP generator acting on sites 2 and 3.

In the same spirit of Theorem 2 one can check that using the first representation we get the PMM rate matrix for 4 sites, namely

$$\begin{aligned} L_P = &\left(J^0 \otimes 1 \otimes 1 \otimes 1 + 1 \otimes 1 \otimes 1 \otimes J^0 + 1\right) \\ &\cdot \left(1 \otimes J^+ \otimes J^- \otimes 1 + 1 \otimes J^- \otimes J^+ \otimes 1 + 21 \otimes J^0 \otimes J^0 \otimes 1 - \frac{1}{2} 1\right) \, , \end{aligned} \tag{38}$$

here $1 = 1 \otimes 1 \otimes 1 \otimes 1$, is shorthand for the identity matrix of dimension 16. Using the second representation we get L_P, the PMM generator of equation (2) on 4 sites only.

3.3 Duality Relations for the Porous Medium Model

We now show how to use the above algebraic approach to find a self-duality relation. In general, it is simpler to have a duality function in a factorized and space homogeneous form, i.e. which can be written in the following way

$$D(\eta, \xi) = \prod_x d(\eta_x, \xi_x) \ , \tag{39}$$

so that one can focus on finding the single site self-duality function $d(\eta_x, \xi_x)$. However, unlike all the other IPS for which self-dualities have been established, in this model the jump rates depend not only on the state of the two sites involved but also on neighboring sites. This will lead the analysis to two different self-duality functions, one that cannot be factorized unless losing some information, while the other one has a factorized structure but it is non-homogeneous over the lattice site.

3.3.1 Duality Function I

It is easy to check that on $\mathbb{T}_n$ the PMM has the same reversible measure than the SSEP, i.e. homogeneous product of Bernoulli with free parameter $\rho \in (0, 1)$:

$$\mu(\eta : \eta(x) = 1) = \rho = 1 - \mu(\eta : \eta(x) = 0).$$

Therefore, by Proposition 2 a cheap self-duality function is guaranteed to exist. In virtue of the fact that the total number of particles is conserved by the dynamic of the model (recall Remark 9, the state space of the process is $\Omega_n = \{0, 1\}^{\mathbb{T}_n}$), then duality functions that differ by constants or quantities that are kept constant by the dynamics (e.g. the total number of particles) are equivalent (see Lemma 3 of [5]). In our case, this means that any term that depends only on ρ can be neglected for the self-duality function, and so we have that the cheap self-duality function is

$$D^{cheap}(\eta, \xi) = \prod_{x \in \mathbb{T}_n} d^{cheap}(\eta_x, \xi_x) = \prod_{x \in \mathbb{T}_n} \delta_{\eta_x, \xi_x} \ . \tag{40}$$

We now look for our symmetry S, acting on D^{cheap}, to find a non-trivial self-duality function. To do this we start with the result for the SSEP and extend it for the PMM. For the SSEP it is known that the $\mathfrak{su}(2)$ algebra generator J^+ is a symmetry of the Casimir by definition of the Casimir element. By Theorem 3 its coproduct is a symmetry of the coproduct of the Casimir which means that we have a symmetry for the SSEP generator. In order to have self-duality in a factorized form, we will consider its exponential, e^{J^+}. By inspection of the PMM generator one then sees that for sites 2 and 3, the same symmetry must hold. However, the generator used in sites

1 and 4 do not commute with J^+, and so we extend the symmetry using the identity operator. This is formalized in the following lemma.

Lemma 1 *In the context of the Lie algebra* $\mathfrak{su}(2)$*, the following operator*

$$S = 1_1 \otimes e^{J_2^+} \otimes e^{J_3^+} \otimes 1_4$$

is a symmetry of the generator L_P.

Proof One way to verify this is, for example, to show that $[L_P^{2,3}, S] = 0$. On the other hand, from the expression of L_P in Eq. (37) the second parenthesis only involves sites 2 and 3 and it commutes with $e^{J_2^+} \otimes e^{J_3^+}$, while for the first parenthesis we just use the fact that the identity operator is always a symmetry.

Remark 10 At this point, it is important to stress the following observation. One would expect that, given that the PMM and the SSEP are described via the same algebra, with the only difference of the operator J^0 (which does not increase nor decrease the degree of the functions), then a duality relation for the PMM would be close to the SSEP one. However, we can already see from the space non-homogeneity expression of the symmetry S that this cannot be the case.

Following Theorem 1 we now have to act with S on D^{cheap} in order to construct a new non-trivial self-duality function, namely

$$D(\eta, \xi) = SD^{cheap}(\cdot, \xi)(\eta)$$

in operator notation or $D = SD^{cheap}$ in matrix notation. The matrix S can be written as $S = \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix} \otimes \begin{pmatrix} 1 & 0 \\ 1 & 1 \end{pmatrix} \otimes \begin{pmatrix} 1 & 0 \\ 1 & 1 \end{pmatrix} \otimes \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix}$ which leads to

$$S = \left(\begin{array}{c|c} A & \mathbf{0} \\ \hline \mathbf{0} & A \end{array}\right),$$

where A is the following lower triangular block:

$$A = \begin{pmatrix} 1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 & 0 & 0 & 0 & 0 \\ 1 & 0 & 1 & 0 & 0 & 0 & 0 & 0 \\ 0 & 1 & 0 & 1 & 0 & 0 & 0 & 0 \\ 1 & 0 & 0 & 0 & 1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 & 0 & 1 & 0 & 0 \\ 1 & 0 & 1 & 0 & 1 & 0 & 1 & 0 \\ 0 & 1 & 0 & 1 & 0 & 1 & 0 & 1 \end{pmatrix}.$$

Since D^{cheap} is just the identity matrix, we have that the above matrix is also our new non-trivial self-duality matrix. As a function, we can see that the matrix D above can be written in a factorized form as

$$D(\eta,\xi)=\mathbf{1}_{\{\eta_1=\xi_1\}}\mathbf{1}_{\{\eta_2\geq\xi_2\}}\mathbf{1}_{\{\eta_3\geq\xi_3\}}\mathbf{1}_{\{\eta_4=\xi_4\}}\ . \tag{41}$$

For the first and the last factors above no computations are needed, while for the second and third it is enough to see that, for the single site self-duality function we have

$$\begin{aligned} d(\eta,\xi)=e^{J^+}d^{cheap}(\cdot,\xi)(\eta)&=\sum_{i=0}^{\infty}\frac{(J^+)^i}{i!}\delta_{\eta,\xi}=\sum_{i=0}^{\infty}\frac{1}{i!}\frac{\eta!}{(\eta-i)!}\mathbf{1}_{\{i\leq\eta\}}\delta_{\eta-i,\xi}\\ &=\binom{\eta}{\xi}\mathbf{1}_{\{0\leq\xi\leq\eta\}}=\mathbf{1}_{\{\xi\leq\eta\}}\ . \end{aligned}$$

The last equality follows from the fact that we are only dealing with 0 or 1, whose factorial is always 1. As expected, given the observation in Remark 10, the self-duality function of equation (41) is non-homogeneous. If we want to write this in a homogeneous form the only possibility is to "lose" some information in the two central sites. Namely, to impose that the single-site duality function for sites 2 and 3 matches the one for sites 1 and 4 and so losing the choice $\{\eta<\xi\}$. This allows to retrieve a duality function on the torus, which matches the cheap duality function, i.e.

$$D(\eta,\xi)=\prod_{x\in\mathbb{T}_n}\mathbf{1}_{\{\eta_x=\xi_x\}}\ .$$

It is a bit counter-intuitive that diagonal operators such as the J^0, which is morally a multiplicative operator actually do change profoundly the form of the self-duality function compared to the self-duality of the SSEP, see Remark 11 below. We could claim that duality relations are not robustness when kinetically constrains of the microscopic model are taken into consideration.

Remark 11 A similar strategy for the SSEP leads to the self-duality function

$$D(\eta,\xi)=\prod_{x\in\mathbb{T}_n}\mathbf{1}_{\{\eta_x\geq\xi_x\}}\ , \tag{42}$$

which is useful because one can write it in terms of the η process. For example assuming $\xi=\delta_x$, the dual configuration with just one particle at site $x\in\mathbb{T}_n$, the expression of the self-duality function in Eq. (42) reads for all $y\in\mathbb{T}_n-\{x\}$ as $\mathbf{1}_{\{\eta_y\geq 0\}}$ which is always one. While for site x we have

$$\mathbf{1}_{\{\eta_x\geq 1\}}=\begin{cases}0 & \text{if } \eta_x=0\\ 1 & \text{if } \eta_x=1\end{cases}=\eta_x$$

leading to $D(\eta,\delta_x)=\eta_x$. A similar reasoning leads to $D(\eta,\delta_x+\delta_y)=\eta_x\eta_y$ and so on. This is how duality relates n dual walkers with the $n-$point correlation function of the original process.

3.3.2 Duality Function II

We conclude this overview of self-duality for IPS with a different, more direct approach that produces a distinct, far from trivial self-duality function. The idea is to take advantage of the self-duality relation of the SSEP with the self-duality function in Eq. (42). We have seen that, thanks to the algebraic approach, the PMM and the SSEP generators are connected by

$$L_P = (J_1^0 + J_4^0 - 1)L_S. \tag{43}$$

Looking for a self-duality relation introduced in Eq. (29), it means that

$$(\eta_1 + \eta_4)L_S D(\cdot, \xi)(\eta) = (\xi_1 + \xi_4)L_S D(\eta, \cdot)(\xi) \ .$$

Now the key observation is that $L_S D(\cdot, \xi)(\eta) = L_S D(\eta, \cdot)(\xi)$ holds for every D of the form we are interested in as in Eq. (39). Indeed, for two neighboring sites (say 2 and 3 to be consistent) we assume that

$$D(\eta, \xi) = d_2(\eta_2, \xi_2)d_3(\eta_3, \xi_3) \ .$$

Since we are working with the hard-core exclusion we have that for $x = 2, 3$ the possible choices for d are

$$d(\eta_x, \xi_x) = A + B\eta_x + C\xi_x + D\eta_x\xi_x \ ,$$

for A, B, C and D arbitrary constant where $\eta_x, \xi_x \in \{0, 1\}$. At this point, it is not hard to verify via an explicit, long but trivial computation that the duality relation in Definition 5 holds independently from the choices of A, B, C or D. This means that we have the freedom to choose D such that it just has to satisfy the identity $\eta_1 + \eta_4 = \xi_1 + \xi_4$. In other words, we are saying that a self-duality function requires to have the same number of particles in the original and dual process for sites that have distance 2, i.e.

$$D(\eta, \xi) = \prod_{x \in \mathbb{T}_n} \mathbf{1}_{\{\eta_{x-1} + \eta_{x+2} = \xi_{x-1} + \xi_{x+2}\}} \ .$$

If the self-duality function above can be of any interest, it is not clear at this stage. We were able to have a product form which, unluckily, is inhomogeneous; in a symmetric context, all useful applications, as far as we know only deal with space homogeneous self-duality functions.

We conclude here the section regarding self-duality for the PMM. A question, still open, would be to figure out if we can also have an algebraic description of the generators L_α and L_β of equation (6). This would give more insight in the form of the dual process at the boundaries. Moreover, we believe that, if the Glauber dynamic

allows an algebraic description, one would have hope to infer the one or two points correlation functions using the dual – possibly only absorbing – process.

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Appendix

Finally, we write some auxiliary results for the work to be consistent. We start by showing that the quadratic variation vanishes in $L^2(\mathbb{P}_{\mu_n})$, as n goes to infinity, and we then recall the replacement lemmas needed to prove the Fick's law.

Quadratic Variation

In this section we will prove that the quadratic variation of (22) vanishes in $L^2(\mathbb{P}_{\mu_n})$, as n goes to infinity.

Fix $f \in C^1(0,1)$. From Dynkin's formula (see Lemma A1.5.1 of [19]) we have that

$$M_t^n(f) = J_t^n(f) - J_0^n(f) - \int_0^t n^2 \tilde{L}_n J_s^n(f)\, ds,$$

is a martingale with respect to the natural filtration $\{\mathscr{F}_t\}_{t\geq 0}$. The quadratic variation of M_t^n is given by $\langle M^n(f)\rangle_t = \int_0^t B_s^n(f)\, ds$, where

$$B_s^n(f) := n^2 \left(\tilde{L}_n J_s^n(f)^2 - 2 J_s^n(f) \tilde{L}_n J_s^n(f) \right).$$

Recalling the definition of $\tilde{L}_n$ in (13), we can write $B_s^n(f)$ in the following form

$$B_s^n(f) = B_{s,\alpha}^n(f) + B_{s,P}^n(f) + n^{a-2} B_{s,S}^n(f) + B_{s,\beta}^n(f). \tag{44}$$

Let us examine the conservative part of (44). Note that

$$\left(B_{s,P}^n + n^{a-2} B_{s,S}^n\right)(f) = n^2 \left(\left(\tilde{L}_P + n^{a-2}\tilde{L}_S\right) Q_s^n(f)^2 - 2 Q_s^n(f) \left(\tilde{L}_P + n^{a-2}\tilde{L}_S\right) Q_s^n(f) \right). \tag{45}$$

To simplify notation, take $Q_s^n(f) = F(\eta_{sn^2}, Q_s^n(x))$. Now, we can write (45) as

$$\left(B_{s,P}^n + n^{a-2} B_{s,S}^n\right)(f) = n^2 \sum_{x=1}^{n-1} \left(B_{s,P}^n + n^{a-2} B_{s,S}^n\right)(x),$$

where

$$\left(B^n_{s,P} + n^{a-2}B^n_{s,S}\right)(x) = \left(\tilde{L}_P + n^{a-2}\tilde{L}_S\right)F(\eta_{sn^2}, Q^n_s(x))^2 \\ - 2F(\eta_{sn^2}, Q^n_s(x))\left(\tilde{L}_P + n^{a-2}\tilde{L}_S\right)F(\eta_{sn^2}, Q^n_s(x)).$$

The previous expression is equal to

$$a_{x,x+1}(\eta_{sn^2})(c_{x,x+1}(\eta_{sn^2}) + n^{a-2})\left(F\left(\eta^{x,x+1}_{sn^2}, Q^n_s(x)+1\right) - F\left(\eta_{sn^2}, Q^n_s(x)\right)\right)^2$$
$$+a_{x+1,x}(\eta_{sn^2})(c_{x,x+1}(\eta_{sn^2}) + n^{a-2})\left(F\left(\eta^{x,x+1}_{sn^2}, Q^n_s(x)-1\right) - F\left(\eta_{sn^2}, Q^n_s(x)\right)\right)^2$$
$$+\sum_{\substack{y=1\\ y\neq x}}^{n-2}\left(\eta_{sn^2}(x) - \eta_{sn^2}(x+1)\right)^2(c_{x,x+1}(\eta_{sn^2}) + n^{a-2})\left(F\left(\eta^{y,y+1}_{sn^2}, Q^n_s(y)\right) - F(\eta_{sn^2}, Q^n_s(y))\right)^2.$$

Thus, since $Q^n_s(f) = F(\eta_{sn^2}, Q^n_s(x))$, we get

$$a_{x,x+1}(\eta_{sn^2})(c_{x,x+1}(\eta_{sn^2}) + n^{a-2})\left(\frac{1}{n^2}\sum_{y=1}^{n-2} f\left(\tfrac{y}{n}\right)Q^{n,x+1}_s(y) - \frac{1}{n^2}\sum_{y=1}^{n-2} f\left(\tfrac{y}{n}\right)Q^n_s(y)\right)^2$$
$$+a_{x+1,x}(\eta_{sn^2})(c_{x,x+1}(\eta_{sn^2}) + n^{a-2})\left(\frac{1}{n^2}\sum_{y=1}^{n-2} f\left(\tfrac{y}{n}\right)Q^{n,x-1}_s(y) - \frac{1}{n^2}\sum_{y=1}^{n-2} f\left(\tfrac{y}{n}\right)Q^n_s(y)\right)^2,$$

which is equal to

$$a_{x,x+1}(\eta_{sn^2})(c_{x,x+1}(\eta_{sn^2}) + n^{a-2})\left(\frac{1}{n^2}f\left(\tfrac{x}{n}\right)\left(Q^n_s(x)+1\right) - \frac{1}{n^2}f\left(\tfrac{x}{n}\right)Q^n_s(x)\right)^2$$
$$+a_{x+1,x}(\eta_{sn^2})(c_{x,x+1}(\eta_{sn^2}) + n^{a-2})\left(\frac{1}{n^2}f\left(\tfrac{x}{n}\right)\left(Q^n_s(x)-1\right) - \frac{1}{n^2}f\left(\tfrac{x}{n}\right)Q^n_s(x)\right)^2.$$

Hence,

$$\left(B^n_{s,P} + n^{a-2}B^n_{s,S}\right)(x) = \frac{1}{n^4}f\left(\tfrac{x}{n}\right)^2(a_{x,x+1}(\eta_{sn^2}) + a_{x+1,x}(\eta_{sn^2}))(c_{x,x+1}(\eta_{sn^2}) + n^{a-2}).$$

Therefore,

$$\left(B^n_{s,P} + n^{a-2}B^n_{s,S}\right)(f) = \frac{1}{n^2}\sum_{x=1}^{n-2} f\left(\tfrac{x}{n}\right)^2(a_{x,x+1}(\eta_{sn^2}) + a_{x+1,x}(\eta_{sn^2}))(c_{x,x+1}(\eta_{sn^2}) + n^{a-2})$$
$$\leq 2\frac{\|f^2\|_\infty}{n} + \frac{\|f^2\|_\infty}{n^{3-a}},$$

which vanishes when n goes to infinity since $1 < a < 2$.

Let us now examine the non-conservative part of the quadratic variation. Note that

$$\left(B^n_{s,\alpha} + B^n_{s,\beta}\right)(f) = n^2\left(\left(\tilde{L}_\alpha + \tilde{L}_\beta\right)K^n_s(f)^2 - 2K^n_s(f)\left(\tilde{L}_\alpha + \tilde{L}_\beta\right)K^n_s(f)\right).$$

We will examine only $B^n_{s,\alpha}(f)$ since the computations for $B^n_{s,\beta}(f)$ are the same. Take $K^n_s(f) = F(\eta_{sn^2}, K^n_s(0))$. Repeating the same arguments used above, we have that

$$B^n_{s,\alpha}(f) = n^2\frac{m}{n^\theta}\Big\{\alpha(1-\eta_{sn^2}(1))\left(F\left((\eta^1_{sn^2}, K^n_s(0)+1\right) - F(\eta_{sn^2}, K^n_s(0))\right)^2$$
$$+ (1-\alpha)(\eta_{sn^2}(1))\left(F\left((\eta^1_{sn^2}, K^n_s(0)-1\right) - F(\eta_{sn^2}, K^n_s(0))\right)^2\Big\}.$$

Since $K^n_s(f) = F(\eta_{sn^2}, K^n_s(0))$, we get

$$n^2\frac{m}{n^\theta}\left\{\alpha(1-\eta_{sn^2}(1))\left(\frac{1}{n}f(0)(K^n_s(0)+1) - \frac{1}{n}f(0)K^n_s(0)\right)^2\right.$$
$$\left.+(1-\alpha)(\eta_{sn^2}(1))\left(\frac{1}{n}f(0)(K^n_s(0)-1) - \frac{1}{n}f(0)K^n_s(0)\right)^2\right\}.$$

Hence,

$$B^n_{s,\alpha}(f) = \frac{m}{n^\theta}f(0)^2(\alpha - \eta_{sn^2}(1))^2.$$

In the same manner, we also have

$$B^n_{s,\beta}(f) = \frac{m}{n^\theta}f\left(\tfrac{n-1}{n}\right)^2(\beta - \eta_{sn^2}(n-1))^2.$$

Therefore,

$$B^n_{s,\alpha}(f) + B^n_{s,\beta}(f) \le C(\alpha,\beta)\frac{m}{n^\theta}\|f^2\|_\infty, \tag{46}$$

which vanishes as n goes to infinity for any $\theta > 0$. In order to conclude the proof we need to show that (46) vanishes for $\theta = 0$. This case is proved in Proposition 4.1 of [8] and we refer the interested reader to see the proof there.

Replacement Lemmas

In this section, we state all the replacement lemmas used along the paper. For the proofs, we refer the reader to [4]. Before stating the results let us fix some notation.

Fix $n, \ell \in \mathbb{N}$, $x \in \Sigma_n$ and $\varepsilon > 0$. Let $\Sigma^\varepsilon_n = \{1+\varepsilon n, \ldots, n-1-\varepsilon n\}$, where εn denotes $\lfloor \varepsilon n \rfloor$,

$$\overleftarrow{\Lambda}_x^\ell := \{x-\ell+1,\dots,x\} \quad \text{and} \quad \overrightarrow{\Lambda}_x^\ell := \{x,\dots,x+\ell-1\},$$

be the boxes of size ℓ to the left and to the right of site x, respectively. We denote by

$$\overleftarrow{\eta}^\ell(x) = \frac{1}{\ell}\sum_{y\in\overleftarrow{\Lambda}_x^\ell}\eta(y) \quad \text{and} \quad \overrightarrow{\eta}^\ell(x) = \frac{1}{\ell}\sum_{y\in\overrightarrow{\Lambda}_x^\ell}\eta(y)$$

the empirical densities in the boxes $\overleftarrow{\Lambda}_x^\ell$ and $\overrightarrow{\Lambda}_x^\ell$.

Theorem 3 *Let $H:[0,1]\to\mathbb{R}$ be such that $\|H\|_\infty \le M < \infty$. For any $t\in[0,T]$, we have that*

$$\lim_{\varepsilon\to 0}\overline{\lim_{n\to+\infty}}\,\mathbb{E}_{\mu_n}\left(\int_0^t \frac{1}{n}\sum_{x\in\Sigma_n^\varepsilon} H\left(\tfrac{x}{n}\right)\left(\eta_{sn^2}(x)\eta_{sn^2}(x+1) - \overleftarrow{\eta}^{\varepsilon n}_{sn^2}(x)\overrightarrow{\eta}^{\varepsilon n}_{sn^2}(x+1)\right) ds\right) = 0.$$

Theorem 4 *For any $t\in[0,T]$, we have*

$$\lim_{\varepsilon\to 0}\overline{\lim_{n\to+\infty}}\,\mathbb{E}_{\mu_n}\left(\left|\int_0^t \eta_{sn^2}(1)\eta_{sn^2}(2) - \overrightarrow{\eta}^{\varepsilon n}_{sn^2}(1)\overrightarrow{\eta}^{\varepsilon n}_{sn^2}(\varepsilon n+1)\,ds\right|\right) = 0$$

and

$$\lim_{\varepsilon\to 0}\overline{\lim_{n\to+\infty}}\,\mathbb{E}_{\mu_n}\left(\left|\int_0^t \eta_{sn^2}(n-1)\eta_{sn^2}(n-2) - \overleftarrow{\eta}^{\varepsilon n}_{sn^2}(n-1)\overleftarrow{\eta}^{\varepsilon n}_{sn^2}(n-1-\varepsilon n)\,ds\right|\right) = 0.$$

Theorem 5 *Fix $\theta<1$. Let $\varphi:\Omega_n\to\Omega_n$ be a positive and bounded function which does not depend on the value of the configuration η at site 1. For any $t\in[0,T]$, we have that*

$$\lim_{\varepsilon\to 0}\overline{\lim_{n\to+\infty}}\,\mathbb{E}_{\mu_n}\left(\left|\int_0^t \varphi(\eta_{sn^2})(\alpha-\eta_{sn^2}(1))\,ds\right|\right) = 0.$$

The same is true for β if place of α, $n-1$ in place of 1 and requiring φ not to depend on η at site $n-1$.

Theorem 6 *For any $t\in[0,T]$, we have*

$$\lim_{\varepsilon\to 0}\overline{\lim_{n\to+\infty}}\,\mathbb{E}_{\mu_n}\left(\left|\int_0^t \eta_{sn^2}(1) - \overrightarrow{\eta}^{\varepsilon n}_{sn^2}(1)\,ds\right|\right) = 0,$$

The same is true for $\eta_{sn^2}(n-1)$ if place of $\eta_{sn^2}(1)$ and $\overleftarrow{\eta}^{\varepsilon n}_{sn^2}(n-1)$ in place of $\overrightarrow{\eta}^{\varepsilon n}_{sn^2}(1)$.

References

1. R. Baldasso, O. Menezes, A. Neumann, R. Souza, Exclusion process with slow boundary. J. Stat. Phys. **167**(5), 1112–1142 (2017)
2. O. Blondel, P. Gonçalves, M. Simon, Convergence to the stochastic Burgers equation from a degenerate microscopic dynamics. Electron. J. Probab. **2**(69), 1–25 (2016)
3. T. Bodinou, M. Lagouge, Large deviations of the empirical currents for a boundary driven reaction diffusion model. Ann. Appl. Prob. **22**(6), 2282–2319 (2012)
4. L. Bonorino, R. De Paula, P. Gonçalves, A. Neumann, Hydrodynamics for porous medium model with slow reservoirs (2019)
5. G. Carinci, C. Franceschini, C. Giardinà, F. Redig, W. Groenevelt, Orthogonal dualities of Markov processes and unitary symmetries, symmetry. Integr. Geometry: Methods Appl. **15**(53) (2019)
6. G. Carinci, C. Giardinà, C. Giberti, F. Redig, Duality for stochastic models of transport. J. Stat. Phys. **152**(4), 657–697 (2013)
7. A. De Masi, E. Presutti, *Mathematical Methods for Hydrodynamic Limits*, vol. 1501, Lecture Notes in Mathematics (Springer, Berlin, 1991)
8. R. De Paula, P. Gonçalves, A. Neumann, Porous medium model in contact with slow reservoirs. In: From Particle Systems to Partial Differential Equations, pp. 123–147. Springer International Publishing, Berlin (2018)
9. B. Derrida, M. Evans, V. Hakim, V. Pasquier, Exact solution of a 1D asymmetric exclusion model using a matrix formulation. J. Phys. A: Math. Gen. **26**(7), 1493 (1993)
10. A. Fick, Ueber Diffusion. Annalen der Physik. **94**(1), 59–86 (1855)
11. C. Franceschini, C. Giardinà, W. Groenevelt, Self-duality of Markov processes and intertwining functions. Math. Phys., Anal. Geometry **21**(4), 29 (2018)
12. C. Giardinà, J. Kurchan, F. Redig, K. Vafayi, Duality and hidden symmetries in interacting particle systems. J. Stat. Phys. **135**(1), 25–55 (2009)
13. P. Gonçalves, C. Landim, C. Toninelli, Hydrodynamic limit for a particle system with degenerate rates. Ann. Inst. H. Poincar: Probab. Stat. **45**(4), 887–909 (2009)
14. W. Groenevelt, Orthogonal stochastic duality functions from Lie algebra representations. J. Stat. Phys. **174**(1), 97–119 (2019)
15. M.Z. Guo, G.C. Papanicolaou, S.R.S. Varadhan, Nonlinear diffusion limit for a system with nearest neighbor interactions. Commun. Math. Phys. **118**, 31–59 (1988)
16. J.S. Hager, J. Krug, V. Popkov, G.M. Schütz, Minimal current phase and universal boundary layers in driven diffusive systems. Phys. Rev. E **63**(5), 056110 (2001)
17. S. Jansen, N. Kurt, On the notion(s) of duality for Markov processes. Prob. Surv. **11**, 59–120 (2014)
18. S. Katz, J.L. Lebowitz, H. Spohn, Nonequilibrium steady states of stochastic lattice gas models of fast ionic conductors. J. Stat. Phys. **34**(3–4), 497–537 (1984)
19. C. Kipnis, C. Landim, *Scaling Limits of Interacting Particle Systems. Grundlehrender Mathematischen Wissenschaften [Fundamental Principles of Mathematical Sciences]*, vol. 320. Springer, Berlin (1999)
20. C. Kipnis, C. Marchioro, E. Presutti, Heat flow in an exactly solvable model. J. Stat. Phys. **27**(1), 65–74 (1982)
21. T.M. Liggett, *Interacting Particles Systems* (Springer, Berlin, 1985)
22. G.M. Schütz, Reaction-diffusion processes of hard-core particles. J. Stat. Phys. **79**(1–2), 243–264 (1995)
23. J. Vazquez, *The Porous Medium Equation: Mathematical Theory* (Oxford University Press, Oxford, 2007)

Forward Utilities and Mean-Field Games Under Relative Performance Concerns

Gonçalo dos Reis and Vadim Platonov

Abstract We introduce the concept of mean field games for agents using Forward utilities of CARA type to study a family of portfolio management problems under relative performance concerns. Under asset specialization of the fund managers, we solve the forward-utility finite player game and the forward-utility mean-field game. We study best response and equilibrium strategies in the single common stock asset and the asset specialization with common noise. As an application, we draw on the core features of the forward utility paradigm and discuss a problem of time-consistent mean-field dynamic model selection in sequential time-horizons.

Keywords Forward utility · Mean-field games · Social interactions · Performance concerns

1 Introduction

This work brings together the concept of forward utilities to the mean-field game setting in the limelight of competitive optimal portfolio management of agents under relative performance criteria and the analysis of the associated finite-player game.

There exists a very rich literature on portfolio management for agents with utility preferences and under performance concerns to which this short introduction cannot possibly due justice. For a literature perspective of the financial setting including an in-depth discussion of agents with performance concerns and its impact in the

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utility maximization framework we refer to [4, 8, 14, 15] and references therein. Additionally, we point the reader to the beautiful introductions of [20, 21] where those concepts are brought to the framework of mean-field games. Further, those works also make for an excellent review of mean-field games in the context of the Merton problem which is the framework underlying our work.

In short, mean-field games (MFG), stochastic or not, gained renewed interest due to their modelling power in crucially reducing the dimensionality of the underlying problem under the assumption of statistically equivalent populations [5, 6, 19]. In other words, as long as the actions of a single agent do not affect the average interaction of the agents in their whole, then, in principle, the MFG framework stands to be more tractable than the n-agent games. See [20, 21].

The novelty of our work is the conceptualization and analysis, simplified here, of the formulation of mean-field games within the so-called *forward utilities* framework. Further, we juxtapose our construction to the related finite-player game.

The classical and ubiquitous approach of *utility preferences*, found throughout the literature [4, 8, 14, 15], is that each agent, at an initial-time, specifies their risk-preferences to some future time T and proceeds to optimize their investment to that initial-time. This *backward* approach lacks flexibility to handle mid-time changes of risk-preferences by the agents, or, to allow an update of the underlying model: having in mind Covid-19, if the fund manager made investments in early 2019 to mature in the later part of 2020, how would one update the underlying model stock model to the change of parameters?

These problems feature an inherently *forward-in-time* nature of investment. A view that is particularly clear for (competitive) fund managers updating their investment preferences frequently depending on market behavior. To cope with the limitation of the backward-in-time view induced by the classical utility optimization formulation, and, to better address this forward view, the mathematical tool of *forward utilities* was developed. It was initially introduced for the analysis of the portfolio management problems in [22–24] and subsequently expanded [1, 7, 27] and [11–13]. The latter dealing with general forward utility Itô random fields and with applications to longevity risk. Our approach builds from [16] where the first forward-utility definition under competition appeared (for finite-player games); we additionally refer the reader to the forthcoming works [2, 10] (who also build from [16]).

In essence, the concept of forward utility reflects that the utility map must be adaptive and adjusted to the information flow. The forward *dynamic* utility map is built to be consistent with respect to the given investment universe and the approach we discuss here is based on the martingale optimality principle (see Sect. 2.1).

To the MFG context, the closest to our work we have found is the concept of Forward-Forward MFG concept of [18].

Organization of the paper. In Sect. 2 we introduce the financial market. In Sects. 3 and 4 we study the finite-agent and mean-field game respectively. We study forward utilities of time-monotone type. In Sect. 4.4 we discuss the mean-field investment problem with dynamic model selection in large time-horizons. We conclude in Sect. 5 with a discussion of open questions and future research.

2 Asset Specialization, Forward Utilities and CARA Preferences

The market. We consider a market environment with one riskless asset and n risky securities which serve as proxies for two distinct asset classes. We assume their prices to be of log-normal type, each driven by two independent Brownian motions. More precisely the price $(S_t^i)_{t\geqslant 0}$ of the stock i traded exclusively by the ith agent solves

$$\frac{dS_t^i}{S_t^i} = \mu_i dt + \nu_i dW_t^i + \sigma_i dB_t, \tag{1}$$

with constant parameters $\mu^i > 0$, $\sigma_i \geqslant 0$ and $\nu_i \geqslant 0$ with $\sigma_i + \nu_i > 0$. We refer the reader to [20, 21] for an in-depth motivation of the model. The one-dimensional standard Brownian motions $B, W^1, \ldots, W^n$ are independent. When $\sigma_i > 0$, the process B induces a correlation between the stocks, and thus we call B the *common noise* and W^i an *idiosyncratic noise*. The independent Brownian motions $B, W^1, \ldots, W^n$ are defined on a probability space $(\Omega, \mathbb{F}, \mathscr{F}, \mathbb{P})$ endowed with the natural filtration $\mathbb{F} = (\mathscr{F}_t)_{t\geqslant 0}$ generated by them and satisfies the usual conditions.

We recall the case of *single common stock*, where for any $i = 1, \ldots, n$, $(\mu_i, \sigma_i) = (\mu, \sigma)$, $\nu_i = 0$, for some $\mu, \sigma > 0$ and independent of i. The single common stock case has been explored in great generality in [4, 14, 15] incorporating portfolio constraints, general stock price dynamics and risk-sharing mechanisms.

We aim to contribute to the literature on mean field games and forward utilities by providing an explicitly solvable example. As argued by [20], outside linear-quadratic structures such is very rare, and it is one of these rarities we bring here. We work with the very tractable model (1) and include common noise, heterogeneous of agents, a mean field interaction through the controls in addition to the state processes and forward utilities.

Agents' wealth. Each agent $i = 1, \ldots, n$ trades using a self-financing strategy, $(\pi_t^i)_{t\geqslant 0}$, which represent the (discounted by the bond) amount invested in the ith stock. The i^{th} agent's wealth $(X_t^i)_{t\geqslant 0}$ then solves

$$dX_t^i = \pi_t^i\Big(\mu_i dt + \nu_i dW_t^i + \sigma_i dB_t\Big), \quad \text{with} \quad X_0^i = x_0^i \in \mathbb{R}. \tag{2}$$

We recall that the strategy is self-financing, when the agent wealth evolve from the starting capital only by agent's investment decisions in the market without any external sources of income and this evolution is described by respective SDE (2).

A portfolio strategy is said admissible if it belongs to the set $\mathscr{A}^i$, which consists of

$$\mathscr{A}^i = \Big\{\pi^i : \mathbb{F} - \text{progressively measurable } \mathbb{R} - \text{valued processes } (\pi_t^i)_{t\geqslant 0}, \\ \text{and self-financing such that } \mathbb{E}[\int_0^t |\pi_s|^2 ds] < \infty, \text{ for all } t \geqslant 0\Big\}.$$

The Agents' social interaction. Each manager measures the performance of her strategy taking into account the policy of the other. Each agent engages in a form of social interaction that affects the agent's perception of wealth, all in an additive fashion modelled through the arithmetic average wealth of all agents (this model is largely inspired in [4, 14, 15, 21]). The way the agent assesses and optimizes his relative performance is explored through Definition 2 in the latter Sect. 3. So far we introduce the *relative performance metric* of manager $i \in \{1, \dots, n\}$, denoted $\widetilde{X}^i$ is defined to be

$$\widetilde{X}^i = X^i - \theta_i \overline{X}, \quad \text{where} \quad \overline{X} := \frac{1}{n}\sum_{k=1}^{n} X^k \quad \text{and} \quad \theta_i \in [0,1], \tag{3}$$

where deterministic θ_i stands for the competition weight for agent i.

We easily obtain a dynamics for $\overline{X}$ and $\widetilde{X}^i$, namely

$$\begin{aligned}
d\overline{X}_t &= \Big(\frac{1}{n}\sum_{k=1}^{n}\pi_t^k\mu_k\Big)dt + \Big(\frac{1}{n}\sum_{k=1}^{n}\pi_t^k\nu_k dW_t^k\Big) + \Big(\frac{1}{n}\sum_{k=1}^{n}\pi_t^k\sigma_k\Big)dB_t \\
&= \overline{(\pi\mu)}_t dt + \Big(\frac{1}{n}\sum_{k=1}^{n}\pi_t^k\nu_k dW_t^k\Big) + \overline{(\pi\sigma)}_t dB_t, \quad \overline{X}_0 = \overline{x}_0 = \frac{1}{n}\sum_{k=1}^{n} x_0^k \\
d\widetilde{X}_t^i &= \big(\pi_t^i\mu_i - \theta_i\overline{(\pi\mu)}_t\big)dt + \Big(\pi_t^i\nu_i dW_t^i - \theta_i\big(\frac{1}{n}\sum_{k=1}^{n}\pi_t^k\nu_k dW_t^k\big)\Big) \\
&\quad + \big(\pi_t^i\sigma_i - \theta_i\overline{(\pi\sigma)}_t\big)dB_t, \quad \widetilde{X}_0^i = x_0^i - \theta_i\overline{x}_0,
\end{aligned} \tag{4}$$

where $\overline{x}_0$, $\overline{\pi\mu}$ and $\overline{\pi\sigma}$ are identified as averages (as seen from the 1st equation to the 2nd). Similarly to [21, Remark 2.5], it is natural to replace the average wealth $\overline{X}$ in (3) by the average over all other agents. With that in mind we define for convenience $\overline{X}^{(-i)} = \frac{1}{n-1}\sum_{k\neq i} X^k$ and $Y^{(-i)} = \frac{n}{n-1}\overline{X}^{(-i)}$. This leads us to recast (3) as

$$\widehat{X}^i = X^i - \theta_i\overline{X}^{(-i)}, \qquad \text{where} \qquad \overline{X}^{(-i)} = \frac{1}{n-1}\sum_{k\neq i} X^k. \tag{5}$$

We easily obtain a dynamics for $\widehat{X}$ and $\overline{X}^{(-i)}$, namely

$$\begin{aligned}
d\overline{X}_t^{(-i)} &= \overline{(\pi\mu)}_t^{(-i)}dt + \Big(\frac{1}{n-1}\sum_{k\neq i}\pi_t^k\nu_k dW_t^k\Big) + \overline{(\pi\sigma)}_t^{(-i)}dB_t, \quad \overline{X}_0^{(-i)} = \overline{x}_0^{(-i)} \\
d\widehat{X}_t^i &= \big(\pi_t^i\mu_i - \theta_i\overline{(\pi\mu)}_t^{(-i)}\big)dt + \Big(\pi_t^i\nu_i dW_t^i - \theta_i\big(\frac{1}{n-1}\sum_{k\neq i}^{n}\pi_t^k\nu_k dW_t^k\big)\Big) \\
&\quad + \big(\pi_t^i\sigma_i - \theta_i\overline{(\pi\sigma)}_t^{(-i)}\big)dB_t, \quad \widehat{X}_t^i = x_0^i - \theta_i\overline{x}_0^{(-i)}.
\end{aligned} \tag{6}$$

We also define the quantities

$$\widehat{\pi\sigma}^{(-i)} := \frac{1}{n}\sum_{k\neq i}\pi^k\sigma_k, \quad \overline{(\pi\mu)}^{(-i)} := \frac{1}{n}\sum_{k\neq i}\pi^k\mu_k \text{ and } \overline{(\pi\nu)^2}^{(-i)} := \frac{1}{n}\sum_{k\neq i}(\pi^k\nu_k)^2,$$

where we have the following relations between $\widehat{\pi\sigma}^{(-i)}$, $\overline{\pi\sigma}^{(-i)}$ and $\overline{\pi\sigma}$:

$$\overline{\pi\sigma}^{(-i)} = \frac{n}{n-1}\overline{\pi\sigma} - \frac{1}{n-1}\pi^i\sigma_i, \quad \overline{\pi\sigma}^{(-i)} = \frac{n}{n-1}\widehat{\pi\sigma}^{(-i)}, \tag{7}$$

and $\widehat{\pi\sigma}^{(-i)} = \overline{\pi\sigma} - \frac{1}{n}\pi^i\sigma_i$. We do not write it explicitly but we extend the same notation and relations to $\widehat{\pi\mu}^{(-i)}$, $\overline{\pi\mu}^{(-i)}$ and $\overline{\pi\mu}$.

2.1 Forward Dynamic Utilities (Classic)

We recall, for reference, the classic *forward utility* formulation. We define a *forward dynamic utilities* in the context of the probability space $(\Omega, \mathbb{F}, \mathscr{F}, \mathbb{P})$. We denote by $u_0 : \mathbb{R} \to \mathbb{R}$ the initial data. The forward utility is constructed based on the martingale optimality principle.

Definition 1 (*Forward dynamic utilities*) Let $U : \Omega \times \mathbb{R} \times [0, \infty) \to \mathbb{R}$ be an $\mathbb{F}$-progressively measurable random field. U is a *forward dynamic utility* if

(i) For all $t \geqslant 0$ the map $x \mapsto U(x, t)$ is $\mathbb{P}$-a.s. increasing and concave;
(ii) It satisfies $U(x, 0) = u_0(x)$;
(iii) For all $T \geqslant t$ and each self-financing strategy, represented by π, the associated discounted wealth process X^π satisfies a supermartingale property

$$\mathbb{E}[U(X_T^\pi, T)|\mathscr{F}_t] \leqslant U(X_t^\pi, t) \quad \mathbb{P}\text{-a.s.};$$

(iv) For all $T \geqslant t$ there exists a self financing strategy, represented by π^*, for which the associated discounted wealth X^* satisfies a martingale property

$$\mathbb{E}[U(X_T^*, T)|\mathscr{F}_t] = U(X_t^*, t) \quad \mathbb{P}\text{-a.s.}$$

The above definition assumes the optimizer is attained. This is a somewhat strong assumption which is discussed in [1, 27]. There it is argued that such constraint is not necessary for the forward utility construction in certain contexts.

Following e.g. [24, Sect. 5], we say a utility map U is of *Constant Absolute Risk Aversion* (CARA) type if the *local risk tolerance function* $r^i : \Omega \times \mathbb{R} \times [0, \infty) \to \mathbb{R}$, given by the quotient $r^i(x, t) := -U_x^i(x, t)/U_{xx}^i(x, t)$, is constant uniformly. This is the case for the classical exponential utility function, see Example 1 below.

3 Forward Relative Performance Criteria

3.1 Forward Relative Performance Criteria

Each manager measures the output of her relative performance metric using a forward relative one as modelled by an $\mathscr{F}_t$-progressively measurable random field $U^i : \mathbb{R} \times [0, \infty) \to \mathbb{R}$ for $i \in \{1, \dots, n\}$. The below criteria follows those proposed in [16].

The main idea here being a formulation inspired in the first step in the usual strategy of solving a Nash game, namely the best response of an agent to the actions of all other agents. Take manager i and assume all other agents $j \neq i$ have acted with an investment policy π^j then for any strategy $\pi^i \in \mathscr{A}^i$, the process $U^i(\widehat{X}^i_t, t)$ is a (local) supermartingale, and there exists $\pi^{i,*} \in \mathscr{A}^i$ such that $U^i(\widehat{X}^{i,*}_t, t)$ is a (local) martingale where $\widehat{X}^i$ and $\widehat{X}^{i,*}$ solves (5) with strategies π^i and $\pi^{i,*}$ respectively.

This version of a relative criterion is (implicitly and) exogenously parametrized by the policies of all other managers $j \neq i$ over which there is no assumption on their optimality. In Nash-game language, we solve the so-called best response.

Definition 2 (*Forward relative performance for the manager*) Each manager $i \in \{1, \dots, n\}$ satisfies the following. Let $\pi^j \in \mathscr{A}^j$, for any $j \neq i$ be arbitrary but fixed admissible policies, in other words, the other managers have fixed their admissible strategies.

An $\mathbb{F}$-progressively measurable random field $U^i(x, t)$ is a *forward relative performance* for manager i if, for all $t \geqslant 0$, the following conditions hold:

(i) The mapping $x \mapsto U^i(x, t)$, is $\mathbb{P}$-a.s. strictly increasing and strictly concave;
(ii) For any $\pi^i \in \mathscr{A}^i$, $U^i(\widehat{X}^i_t, t)$ is a (local) supermartingale and $\widehat{X}^i$ is the relative performance metric given in (5);
(iii) There exists $\pi^{i,*} \in \mathscr{A}^i$ such that $U^i(\widehat{X}^{i,*}_t, t)$ is a (local) martingale where $\widehat{X}^{i,*}$ solves (5) with strategies $\pi^{i,*}$ being used.

In the above definition, we do not make explicit references to the initial conditions $U^i(x, 0)$ but we assume that admissible initial data exists such that the above definition is viable. Contrary to the classical expected utility case, the forward utility process is an investor-specific input. Once it is chosen, the supermartingale and martingale properties impose conditions on the drift of the process. Under enough regularity, these conditions lead to the forward performance SPDE (see [26]).

Since we are working in a log-normal market, it suffices to study smooth relative performance criteria of zero volatility (of the forward utility map). Such processes are extensively analysed in [25] in the absence of relative performance concerns. There, a concise characterization of the forward criteria is given along necessary and sufficient conditions for their existence and uniqueness. In that setting, the zero-volatility forward processes are always time-decreasing processes. We point to the reader that this does not have to be case if relative performance concerns are present (see also [16]). Before proving the main result of the subsection, we make a standing assumption regarding the regularity of the forward utility maps.

Assumption 1 *Assume that the derivatives $U_t^i(x,t)$, $U_x^i(x,t)$ and $U_{xx}^i(x,t)$ exists for $t \geqslant 0,\ x \in \mathbb{R}$, $\mathbb{P}$-a.s.*

From Assumption 1, the Itô decomposition of the forward utility map is

$$dU^i(x,t) = U_t^i(x,t)dt, \quad \text{for } i \in \{1,\dots,n\}. \tag{8}$$

We next derive a PDE with random coefficients and an optimal investment strategy for a smooth relative performance criteria of zero volatility of some agent i assuming that all other agents $j \neq i$ have made their investment decisions.

Proposition 1 (Best responses) *Fix $i \in \{1,\dots,n\}$ and the agent's initial preference u_0^i. Assume that each manager $j \neq i$ follows $\pi^j \in \mathscr{A}^j$. Consider the PDE with stochastic coefficients for $(x,t) \in \mathbb{R} \times [0,\infty)$*

$$\begin{aligned} U_t^i = &\Big(\theta_i \overline{(\pi\mu)}_t^{(-i)} - \frac{\mu_i\theta_i\sigma_i\overline{(\pi\sigma)}_t^{(-i)}}{\nu_i^2+\sigma_i^2}\Big)U_x^i + \frac{\mu_i^2}{2(\nu_i^2+\sigma_i^2)}\frac{(U_x^i)^2}{U_{xx}^i} \\ &+ \frac{1}{2}U_{xx}^i\Big[\Big(\theta_i\overline{(\pi\sigma)}_t^{(-i)}\Big)^2\Big(\frac{\sigma_i^2}{\nu_i^2+\sigma_i^2}-1\Big) - \frac{\theta_i^2}{n-1}\overline{(\pi\nu)^2}^{(-i)}\Big], \end{aligned} \tag{9}$$

and assume that for an admissible initial condition $U(\cdot,0) = u_0^i(\cdot)$, the PDE has a smooth solution U^i satisfying Assumption 1, such that $x \mapsto U^i(x,t)$ is strictly increasing ($U_x > 0$) and strictly concave ($U_{xx} < 0$) for each $t > 0$, $\mathbb{P}$-a.s.

Define the strategy $\pi^{i,*}$

$$\pi_t^{i,*} = \frac{1}{\nu_i^2+\sigma_i^2}\Big(\theta_i\sigma_i\overline{(\pi\sigma)}_t^{(-i)} - \mu_i\frac{U_x^i(\widehat{X}_t^{i,*},t)}{U_{xx}^i(\widehat{X}_t^{i,*},t)}\Big), \quad t > 0,$$

where $\widehat{X}^{i,*}$ solves (6) with $\pi^{i,*}$ being used.

If $\pi^{i,*} \in \mathscr{A}^i$ and $\widehat{X}^{i,*}$ are well-defined, then $U^i(x,t)$ is a forward utility performance process. Moreover, the policy $\pi^{i,*}$ is optimal (in the sense of Definition 2).

Remark 1 Note that the randomness in PDE (9) is coming from $\pi^{\cdot}$ only.

By direct inspection of the expression for $\pi^{i,*}$ one sees that if the *local risk tolerance function* $r^i(x,t) = r^i = Const$, for all $t > 0$ (e.g. the utility is of *Constant Absolute Risk Aversion (CARA)* type – see Sect. 2.1) then the optimal strategy will be constant throughout time if additionally all other agents also choose a constant strategy.

Corollary 1 (Constant strategies under CARA) *Assume that all agents $j \neq i$ invest according to constant strategies $\pi^j \in \mathbb{R}$ and that the* local risk tolerance function r^i *is constant. Then $\pi^{i,*}$ is constant.*

We now prove the previous "best responses" proposition above.

Proof (*of Proposition* 1) From (5) we have the dynamics of $d\widehat{X}^i$ (and hence that of $d(X^i - \theta_i \overline{X}^{(-i)})$). We now apply the Itô formula to $U^i(\widehat{X}^i_t, t) = U^i(X^i_t - \theta_i \overline{X}^{(-i)}_t, t)$,

$$\begin{aligned}
dU^i(\widehat{X}^i_t, t) &= U^i_t(\widehat{X}^i_t, t)dt + U^i_x(\widehat{X}^i_t, t)d\widehat{X}^i_t + \frac{1}{2}U^i_{xx}(\widehat{X}^i_t, t)d\langle \widehat{X}^i_t\rangle \\
&= U^i_t(\widehat{X}^i_t, t)dt + U^i_x(\widehat{X}^i_t, t)\big(\pi^i_t \mu_i - \theta_i \overline{(\pi\mu)}^{(-i)}_t\big)dt \\
&\quad + U^i_x(\widehat{X}^i_t, t)\Big(\pi^i_t \nu_i dW^i_t - \theta_i\big(\frac{1}{n-1}\sum_{k\neq i}^{n} \pi^k_t \nu_k dW^k_t\big)\Big) \\
&\quad + U^i_x(\widehat{X}^i_t, t)\big(\pi^i_t \sigma_i - \theta_i \overline{(\pi\sigma)}^{(-i)}_t\big)dB_t \\
&\quad + \frac{1}{2}U^i_{xx}(\widehat{X}^i_t, t)\Big[(\pi^i_t \nu_i)^2 + \frac{\theta_i^2}{n-1}\overline{(\pi\nu)^2}^{(-i)} + \big(\pi^i_t \sigma_i - \theta_i \overline{(\pi\sigma)}^{(-i)}_t\big)^2\Big]dt,
\end{aligned} \tag{10}$$

with $U^i(\widehat{X}^i_0, 0) = U^i(x^i_0 - \theta_i \overline{x}^{(-i)}_0, 0)$ and we used that the B, W^j are all i.i.d.

By Definition 2, the process $U^i(\widehat{X}^i_t, t)$ becomes a Martingale at the optimum π. Direct computations using first order conditions (∂_{π^i}"drift" $= 0$) yield

$$\begin{aligned}
&0 + U^i_x\big(\mu_i - 0\big) + \frac{1}{2}U^i_{xx}\Big[2\pi^i \nu_i^2 + 0 + 2\big(\pi^i_t \sigma_i - \theta_i \overline{(\pi\sigma)}^{(-i)}_t\big)\sigma_i\Big] = 0 \\
\Leftrightarrow\quad & U^i_{xx}\pi^i(\nu_i^2 + \sigma_i^2) = -U^i_x \mu_i + U^i_{xx}\theta_i \sigma_i \overline{(\pi\sigma)}^{(-i)}_t \\
\Rightarrow\quad & \pi^i_t = \frac{1}{\nu_i^2 + \sigma_i^2}\Big(\theta_i \sigma_i \overline{(\pi\sigma)}^{(-i)}_t - \mu_i \frac{U^i_x(\widehat{X}^i_t, t)}{U^i_{xx}(\widehat{X}^i_t, t)}\Big).
\end{aligned} \tag{11}$$

Injecting the expression of π^i_t in the drift term of (10) and simplifying we arrive at the consistency condition (9), we do not carry out this step explicitly, nonetheless, using that U^i solves (9), Eq. (10) simplifies to (exact calculations are carried out in the Sect. 6),

$$\begin{aligned}
&dU^i(\widehat{X}^i_t, t) \\
&= U^i_x(\widehat{X}^i_t, t)\Big(\pi^i_t \nu_i dW^i_t - \theta_i\big(\frac{1}{n-1}\sum_{k\neq i}^{n} \pi^k_t \nu_k dW^k_t\big)\Big) \\
&\quad + U^i_x(\widehat{X}^i_t, t)\Big(\pi^i_t \sigma_i - \theta_i \overline{(\pi\sigma)}^{(-i)}_t\Big)dB_t \\
&\quad + \frac{1}{2}U^i_{xx}(\widehat{X}^i_t, t)\frac{1}{\nu_i^2 + \sigma_i^2}\Big|\pi^i(\nu_i^2 + \sigma_i^2) - \Big(\theta_i \sigma_i \overline{(\pi\sigma)}^{(-i)}_t - \mu_i \frac{U^i_x(\widehat{X}^i_t, t)}{U^i_{xx}(\widehat{X}^i_t, t)}\Big)\Big|^2 dt.
\end{aligned} \tag{12}$$

The concavity assumption of $U^i(x, t)$ implies that the drift term above is non-positive and vanishes when (11) holds. We can conclude that, if $\pi^{i,*}_t = \pi^i_t \in \mathscr{A}^i$ and the associated process $\widehat{X}^{i,*}$ is well-defined (solution to (6) with $\pi^{i,*}$), the process $U^i(\widehat{X}^{i,*}_t, t)$ is a local-martingale, otherwise it is a local supermartingale.

3.1.1 Examples: CARA Case

Example 1 (*The classic CARA case—exponential case*) The exponential criterion takes as initial condition the map $U(x,0)$ $(x \in \mathbb{R})$ defined as

$$U^i(x,0) = -e^{-x/\delta}, \quad \text{with} \quad \delta > 0. \tag{13}$$

In this case, the *local risk tolerance function* $r = -U^i_x/U^i_{xx} = \delta$.

In our case accounting for social interaction between agents in the form of performance concerns, the ith agent's utility is a function $U^i : \Omega \times \mathbb{R} \times \mathbb{R} \times [0,\infty) \to \mathbb{R}$ of both her individual wealth x and the average wealth wealth of all agents, m. The initial/starting utility map is of the form

$$U^i(x,m,0) = -\exp\Big\{-\frac{1}{\delta_i}(x-\theta_i m)\Big\},$$

where we refer to the constants $\delta_i > 0$ and $\theta_i \in [0,1]$ as *personal risk tolerance* and *competition weight* parameters, respectively.

Example 2 (*The time-monotone forward utility with starting exponential*) For $i \in \{1,\dots,n\}$, let the dynamics of U^i be given by (8) and assume $U^i(x,0) = -e^{-x/\delta_i}$ with $\delta_i > 0$. Then the solution to the PDE (9) is given by

$$U^i(x,t) = -e^{-\frac{x}{\delta_i}+f_i(t)}, \qquad \text{with} \quad \delta_i > 0, \tag{14}$$

where $(f_i(t))_{t\geqslant 0}$ is the random map given below independent of x satisfying $f_i(0) = 0$, sufficiently integrable and $t \mapsto f_i(t)$ is differentiable. Note that in this case, the *local risk tolerance function* satisfies $r^i = -U^i_x/U^i_{xx} = \delta_i$.

Injecting $U^i(x,t)$ above in (9) yields an ODE for f_i (we omit the time variable),

$$\begin{aligned} f_i' &= -\frac{\theta_i}{\delta_i}\Big(\overline{(\pi\mu)}^{(-i)} - \frac{\mu_i\sigma_i\overline{(\pi\sigma)}^{(-i)}}{\nu_i^2+\sigma_i^2}\Big) + \frac{\mu_i^2}{2(\nu_i^2+\sigma_i^2)} \\ &\quad + \frac{\theta_i^2}{2\delta_i^2}\Big[\Big(\overline{(\pi\sigma)}^{(-i)}\Big)^2\Big(\frac{\sigma_i^2}{\nu_i^2+\sigma_i^2}-1\Big) - \frac{1}{n-1}\overline{(\pi\nu)^2}^{(-i)}\Big] \\ &= -\frac{\theta_i}{\delta_i}\overline{(\pi\mu)}^{(-i)} + \frac{1}{2(\nu_i^2+\sigma_i^2)}\Big(\mu_i + \frac{\theta_i}{\delta_i}\sigma_i\overline{(\pi\sigma)}^{(-i)}\Big)^2 \\ &\quad - \frac{\theta_i^2}{2\delta_i^2}\Big[\Big(\overline{(\pi\sigma)}_t^{(-i)}\Big)^2 + \frac{1}{n-1}\overline{(\pi\nu)^2}^{(-i)}\Big] =: \lambda_i. \end{aligned}$$

Hence, $f_i(t) = \int_0^t \lambda_i(s)ds$. In particular, if all coefficients and strategies are constant, then (with a slight abuse of notation) $f_i(t) = t\lambda_i$ for a constant λ_i given by the RHS of the above ODE.

Example 3 (*No performance concerns:* $\theta^i = 0$) We continue to work under the time-monotone forward utility case of the previous example. Without performance concerns, i.e. $\theta_i = 0$, then $\lambda_i = \frac{\mu_i^2}{2(\nu_i^2+\sigma_i^2)}$ and we recover well-known results. We have from Proposition 1 that

$$\pi_\cdot^{i,*} = \frac{\mu_i \delta_i}{\nu_i^2 + \sigma_i^2} \quad \text{and} \quad U^i(x,t) = -\exp\Big\{ -\frac{x}{\delta_i} + t\lambda_i^{(\theta_i=0)} \Big\},$$

with the constant $\lambda_i^{(\theta_i=0)} = \frac{\mu_i^2}{2(\nu_i^2+\sigma_i^2)}$.

3.2 The Forward Nash Equilibrium

In view of the *best responses* discussed in Proposition 1 we now investigate the *simultaneous best responses* as to establish the existence of a Nash equilibrium.

Definition 3 (*Forward Nash equilibrium*) A forward Nash equilibrium consists of n-pairs of $\mathbb{F}$-adapted maps $(U^i, \pi^{i,*})$ such that for any $t \geqslant 0$ the following conditions hold.

(i) For any $i \in \{1, \dots, n\}$, $\pi^{i,*} \in \mathscr{A}^i$;
(ii) For each player $i \in \{1, \dots, n\}$ the following holds: given the strategies $\pi^{j,*} \in \mathscr{A}^j$ (any $j \neq i$) the processes $U^i(\widehat{X}_t^i(\pi^{*,-i}), t)$ is a (local) supermartingale where $\widehat{X}^i(\pi^{*,-i})$ solves (6) with all managers $j \neq i$ acting according to $\pi^{j,*}$;
(iii) For each player $i \in \{1, \dots, n\}$ the following holds: the process $U^i(\widehat{X}_t^{i,*}(\pi^{*,-i}), t)$ is a (local) martingale where $\widehat{X}^i(\pi^{*,-i})$ solves (6) with *all* managers j acting according to $\pi^{j,*}$.

If all the optimal strategies are constant we say we have a *constant forward Nash equilibrium*.

Under appropriate integrability conditions plus the martingale/supermartingale characterizations, we have for some agent i for any $\pi^i \in \mathscr{A}^i$

$$\begin{aligned}\mathbb{E}[U^i(\widehat{X}_t^{i,*}(\pi^{*,-i}), t)] &= \mathbb{E}[U^i(\widehat{X}_0^{i,*}(\pi^{*,-i}), 0)] = \mathbb{E}[U^i(x_0^i - \theta_i \overline{x}_0^{(-i)}, 0)] \\ &= U^i(x_0^i - \theta_i \overline{x}_0^{(-i)}, 0) \geqslant \mathbb{E}[U^i(\widehat{X}_t^i(\pi^{*,-i}), t)].\end{aligned}$$

As expected, no manager can increase the expected utility of her relative performance metric by unilateral decision.

The solvability of the general forward Nash equilibrium seems very difficult for a general forward criteria as one needs to solve the following system for the $\pi^{i,*}$ (see Proposition 1, in particular (11)) and the corresponding PDEs for the U^i, $i \in \{1, \dots, n\}$:

$$\pi_t^{i,*}(\nu_i^2+\sigma_i^2)=\theta_i\sigma_i\Big(\frac{1}{n-1}\sum_{k=1,k\neq i}^{n}\pi_t^{k,*}\sigma_k\Big)-\mu_i\frac{U_x^i\big(\widehat{X}_t^{i,*}(\pi^{*,-i}),t\big)}{U_{xx}^i\big(\widehat{X}_t^{i,*}(\pi^{*,-i}),t\big)}. \tag{15}$$

3.2.1 Equilibrium with Time-Monotone Forward Utilities and Exponential Initial Condition

In order to obtain explicit results we focus on the time-monotone case presented in Example 2 for which $U_x^i/U_{xx}^i=-\delta_i$. More notably, at the level at which we have formulated our problem we can easily recover the results of [21, Theorem 2.3] for which one has $U_x^i/U_{xx}^i=-\delta_i$, for any t (note their Remark 2.5).

Theorem 1 *Assume the conditions of Proposition 1 hold for all agents $i\in\{1,\dots,n\}$. Assume furthermore that agents have time-monotone forward utility U^i with initial condition (13).*

Define the quantities φ_n^σ and ψ_n^σ by

$$\varphi_n^\sigma:=\frac{1}{n}\sum_{i=1}^{n}\delta_i\frac{\mu_i\sigma_i}{\nu_i^2+\sigma_i^2\big(1+\frac{\theta_i}{n-1}\big)}\quad\text{and}\quad\psi_n^\sigma:=\frac{1}{n-1}\sum_{i=1}^{n}\theta_i\frac{\sigma_i^2}{\nu_i^2+\sigma_i^2\big(1+\frac{\theta_i}{n-1}\big)}. \tag{16}$$

If $\psi_n^\sigma\neq 1$, then a constant forward Nash equilibrium *exists and is unique, with the constant optimal strategies $\pi^{i,*}$ given by*

$$\pi_\cdot^{i,*}=\frac{1}{\nu_i^2+\sigma_i^2\big(1+\frac{\theta_i}{n-1}\big)}\Big(\theta_i\sigma_i\Big(1+\frac{1}{n-1}\Big)\frac{\varphi_n^\sigma}{1-\psi_n^\sigma}+\mu_i\delta_i\Big). \tag{17}$$

The forward Nash equilibria is given by the n-pairs $\{(U^{i,*},\pi^{i,*})\}_{i=1,\dots,n}$ where the $U^{i,*}$ is the solution of (9) (see Example 2) under the optimal constant strategies $\pi^{\cdot,*}$.

The term λ_i (see Example 2), at equilibrium, is given by

$$\begin{aligned}\lambda_i=&-\frac{\theta_i}{\delta_i}\Big(\Big\{\frac{n}{n-1}\overline{\pi\mu}-\frac{1}{n-1}\pi^i\mu_i\Big\}-\frac{\mu_i\sigma_i}{\nu_i^2+\sigma_i^2}\Big\{\frac{n}{n-1}\overline{\pi\sigma}-\frac{1}{n-1}\pi^i\sigma_i\Big\}\Big)\\&+\frac{\mu_i^2}{2(\nu_i^2+\sigma_i^2)}+\frac{\theta_i^2}{2\delta_i^2}\Big[\Big\{\frac{n}{n-1}\overline{\pi\sigma}-\frac{1}{n-1}\pi^i\sigma_i\Big\}^2\Big(\frac{\sigma_i^2}{\nu_i^2+\sigma_i^2}-1\Big)\\&-\Big\{\frac{n}{(n-1)^2}\overline{(\pi\nu)^2}-\frac{1}{(n-1)^2}(\pi^i\nu_i)^2\Big\}\Big],\end{aligned} \tag{18}$$

where the relevant expressions for $\overline{\pi\sigma}$, $\overline{\pi\mu}$ and $\overline{(\pi\nu)^2}$ are given below in (19), (20) and (21).

Remark 2 We note that we do not solve the same problem studied at [21] but an equivalent one. However, imposing the scaling factor given by [21, Remark 2.5] we recover the same results as in [21, Theorem 2.3].

Proof Injecting the condition $U_x/U_{xx} = -\delta_i$ in (15), the system to be solved in order to ascertain the Nash equilibrium is, across $i \in \{1, \dots, n\}$,

$$\begin{aligned}\pi_t^{i,*}(\nu_i^2 + \sigma_i^2) &= \theta_i\sigma_i\Big(\frac{1}{n-1}\sum_{k=1,k\neq i}^{n}\pi_t^{k,*}\sigma_k\Big) + \mu_i\delta_i \\ &= \theta_i\sigma_i\Big(\frac{n}{n-1}\overline{(\pi\sigma)}_t - \frac{1}{n-1}\pi^{i,*}\sigma_i\Big) + \mu_i\delta_i \\ \Leftrightarrow\quad \pi_t^{i,*} &= \frac{1}{\nu_i^2 + \sigma_i^2\big(1+\frac{\theta_i}{n-1}\big)}\Big(\theta_i\sigma_i\frac{n}{n-1}\overline{(\pi\sigma)}_t + \mu_i\delta_i\Big).\end{aligned}$$

The final line yields the expression for $\pi^{i,*}$ as a function of the unknown $\overline{\pi\sigma}$. To determine the latter, multiply both sides by σ_i and average over $i \in \{1, \dots, n\}$, this yields a solvability condition

$$\overline{(\pi\sigma)}_t = \overline{(\pi\sigma)}_t\psi_n^\sigma + \varphi_n^\sigma \quad\Leftrightarrow\quad \overline{\pi\sigma} = \frac{\varphi_n^\sigma}{1-\psi_n^\sigma} \quad \text{as long as} \quad \psi_n^\sigma \neq 1. \tag{19}$$

Plugging the expression $\overline{(\pi\sigma)}$ in that for $\pi^{i,*}$ yields the result. That the optimal strategies are constant is now obvious.

It remains to derive the expression for the λ_i's. Just like for $\overline{\pi\sigma}$, we obtain an expression for $\overline{\pi\mu}$ by multiplying $\pi^{i,*}$ by μ_i and averaging on both sides, we have

$$\overline{\pi\mu} = \frac{n}{n-1}\cdot\frac{\varphi_n^\sigma}{1-\psi_n^\sigma}\cdot\psi_n^\mu + \phi_n^\mu \quad\text{and}\quad \overline{\pi\mu}^{(-i)} = \frac{n}{n-1}\overline{\pi\mu} - \frac{1}{n-1}\pi^i\mu_i, \tag{20}$$

where we used (7) and the quantities φ_n^μ, ψ_n^μ are defined as

$$\varphi_n^\mu := \frac{1}{n}\sum_{k=1}^{n}\delta_k\frac{\mu_k^2}{\nu_k^2 + \sigma_k^2(1+\frac{\theta_k}{n-1})} \quad\text{and}\quad \psi_n^\mu := \frac{1}{n}\sum_{k=1}^{n}\theta_k\frac{\mu_k\sigma_k}{\nu_k^2 + \sigma_k^2(1+\frac{\theta_k}{n-1})}.$$

Similarly, defining $\overline{(\pi\nu)^2} := \frac{1}{n-1}\sum_{k\neq i}(\pi_t^k\nu_k)^2$ we have

$$\overline{(\pi\nu)^2} = \frac{1}{n}\sum_{i=1}^{n}\Big(\frac{\nu_i\theta_i\sigma_i\cdot\frac{n}{n-1}\cdot\frac{\varphi_n^\sigma}{1-\psi_n^\sigma} + \nu_i\mu_i\delta_i}{\nu_i^2 + \sigma_i^2\big(1+\frac{\theta_i}{n-1}\big)}\Big)^2. \tag{21}$$

Similarly to (7), we have $\overline{(\pi\nu)^2}^{(-i)} = \frac{n}{n-1}\overline{(\pi\nu)^2} - \frac{1}{n-1}(\pi^i\nu_i)^2$. Replacing these expressions in that for λ_i in Example 2 the expression in the result's statement follows.

From the forward utility machinery one can easily recover the classical case of utility optimization where one prescribes the utility map for the horizon time T then proceeds to optimize.

Example 4 (*Recovering the classical utility problem from the forward one.*) If one would start the forward utility with (for some $0 < T < \infty$)

$$u_0^i(x) := -e^{-x/\delta_i - T\lambda_i},$$

then computations like those presented yield the forward utility map $U(x,t)$ as

$$U^i(x,t) = -e^{-x/\delta_i + (t-T)\lambda_i}, \quad t \in [0,T]$$

and in particular $U(x,T) = -e^{-x/\delta_i}$. In other words, our forward utility recovers as a particular case the classical exponential utility maximization problem (discussed in [21]).

Corollary 2 (Single stock) *Let* $\mu_i = \mu > 0$, $\sigma_i = \sigma > 0$ *and* $\nu_i = 0$, *for any* $i = 1, \ldots, n$. *Let the constants*

$$\varphi_n^\sigma := \frac{1}{n}\sum_{i=1}^n \frac{\delta_i}{1+\frac{\theta_i}{n-1}} \quad \textit{and} \quad \psi_n^\sigma := \frac{1}{n-1}\sum_{i=1}^n \frac{\theta_i}{1+\frac{\theta_i}{n-1}}. \tag{22}$$

If $\psi_n^\sigma \neq 1$, *then a* constant forward Nash equilibrium *exists, with the constant optimal strategies* $\pi^{i,*}$ *given by*

$$\pi_\cdot^{i,*} = \frac{\mu}{\sigma^2\left(1+\frac{\theta_i}{n-1}\right)}\left(\theta_i\left(1+\frac{1}{n-1}\right)\frac{\varphi_n^\sigma}{1-\psi_n^\sigma} + \delta_i\right).$$

4 The Mean Field Game

By inspection of Theorem 1 one sees that the optimal strategy and forward utility map for some agent depend on that agent's specific parameters (model parameters, initial wealth, risk tolerance and performance concern) and on certain averages of the parameters of all agents. This makes a case for a MFG approach to the game.

In this section and inspired by the results in the previous one, we formalize the concept of forward mean-field Nash game. We use the concept of *type distributions* introduced in [19–21]. We follow the construction presented in the latter.

We focus on initial forward utilities at time $t = 0$ that are of exponential type,

$$U^i(x,m,0) = -\exp\left\{-\frac{1}{\delta_i}(x-\theta_i m)\right\},$$

where we refer to the constants $\delta_i > 0$ and $\theta_i \in [0, 1]$ as *personal risk tolerance* and *competition weight* parameters, respectively.

For the n-agent game, we define for each agent $i = 1, \ldots, n$ the *type vector*

$$\zeta_i := (x_0^i, \delta_i, \theta_i, \mu_i, \nu_i, \sigma_i),$$

which characterizes perfectly each agent i. These *type vectors* induce an empirical measure, called the *type distribution*, which is the probability measure on the *type space*

$$\mathscr{Z}^e := \mathbb{R} \times (0, \infty) \times [0, 1] \times (0, \infty) \times [0, \infty) \times [0, \infty), \tag{23}$$

given by

$$m_n(A) = \frac{1}{n} \sum_{i=1}^{n} 1_A(\zeta_i), \quad \text{for Borel sets } A \subset \mathscr{Z}^e.$$

Assume now that as the number of agents becomes large, $n \to \infty$, the above empirical measure m_n has a weak limit m, in the sense that $\int_{\mathscr{Z}^e} f \, dm_n \to \int_{\mathscr{Z}^e} f \, dm$ for every bounded continuous function f on $\mathscr{Z}^e$. For example, this holds almost surely if the ζ_i's are i.i.d. samples from m. Let $\zeta = (\xi, \delta, \theta, \mu, \nu, \sigma)$ denote an $\mathscr{Z}^e$-valued random variable with this limiting distribution m.

The *mean field game* (MFG) defined next allows us to derive the limiting strategy as the outcome of a self-contained equilibrium problem, which intuitively represents a game with a continuum of agents with type distribution m. Rather than directly modelling a continuum of agents, we follow the MFG paradigm of modelling a single *generic agent*, who we view as randomly selected from the population. The probability measure m represents the distribution of type parameters among the continuum of agents; equivalently, the generic agent's type vector is a random variable with law m. Heuristically, each agent in the continuum trades in a single stock driven by two Brownian motions, one of which is unique to this agent and one of which is common to all agents. We extend the Forward Nash equilibrium of Definition 3 to the MFG setting below.

4.1 Agents Through Type-Distribution and the Market

Let $(\Omega, \mathscr{F}, \mathbb{F} = (\mathscr{F})_{t \geqslant 0}, \mathbb{P})$ be a stochastic basis supporting two independent Brownian motions $W = (W_t)_{t \geqslant 0}$ and $B = (B_t)_{t \geqslant 0}$ together with a random vector ζ having distribution m and given by

$$\zeta = (\xi, \delta, \theta, \mu, \nu, \sigma),$$

with values in the space $\mathscr{Z}^e$ defined in (23) and independent of W and B. Let $\mathbb{F} = (\mathscr{F}_t)_{t\in[0,T]}$ denote the smallest filtration satisfying the usual assumptions for which ζ is $\mathscr{F}_0$-measurable and both W and B are adapted. Let also $\mathbb{F}^B = (\mathscr{F}_t^B)_{t\in[0,T]}$ denote the natural filtration generated by the Brownian motion B.

The *generic agent's* wealth process solves

$$dX_t = \pi_t(\mu dt + \nu dW_t + \sigma dB_t), \quad X_0 = \xi, \tag{24}$$

where the portfolio strategy must belong to the admissible set $\mathscr{A}_{\mathrm{MF}}$ of self-financing $\mathbb{F}$-progressively measurable real-valued processes $(\pi_t)_{t\geqslant 0}$ satisfying the square-integrability condition $\mathbb{E}[\int_0^T |\pi_t|^2 dt] < \infty$ for any $T \in [0, \infty)$. The generic agent's initial wealth is given by ξ, whereas (μ, ν, σ) are the market parameters. In the sequel, the parameters δ and θ will affect the risk preferences of the generic agent. Each agent among the continuum will have different preference parameters and hence these six parameters are $\mathscr{F}_0$-random, and each has the exact same interpretation an in the n-player game of the earlier section.

4.2 The Equilibrium

The formulation of the forward Nash game of Sect. 3 drives the formulation of the Mean-field game we discuss here. Recall that in the MFG-formulation the *generic agent* has no influence on the average wealth of the continuum of agents, as but one agent amid a continuum of agents. We next introduce the concept of the main object of interest the *MF-Forward relative performance equilibrium*.

We introduce the regularity requirements for the utility.

Assumption 2 *Assume that the derivatives $U_t(x,t)$, $U_x(x,t)$ and $U_{xx}(x,t)$ exists for $t \geqslant 0$, $x \in \mathbb{R}$, $\mathbb{P}$-a.s.*

As in Sect. 3.1, Assumption 2 implies the Itô decomposition of map U

$$dU(x,t) = U_t(x,t)dt.$$

Given this market setup we next define our concept of equilibrium.

Definition 4 (*MF-Forward CARA relative performance equilibrium (for the generic manager)*) Let $(\overline{X}_t)_{t\geqslant 0}$ be the $\mathbb{F}^B$-adapted square integrable stochastic process representing the average wealth of the continuum of agents. Let $\pi \in \mathscr{A}^{\mathrm{MF}}$ and X^π solve (24) with π.

The $\mathbb{F}^{\mathrm{MF}}$-progressively measurable random field $(U(x,t))_{t\geqslant 0}$ is an *MF-forward relative performance* for the *generic manager* if, for all $t \geqslant 0$, the following conditions hold:

(i) The mapping $x \mapsto U(x,t)$, is $\mathbb{P}$-a.s. strictly increasing and strictly concave;

(ii) For any $\pi \in \mathscr{A}^{\mathrm{MF}}$, $U(X_t^\pi - \theta\overline{X}_t, t)$ is a (local) supermartingale and X^π is the *generic agent's* wealth process solving (24) for the strategy π;
(iii) There exists $\pi^* \in \mathscr{A}^{\mathrm{MF}}$ such that $U(X_t^* - \theta\overline{X}_t, t)$ is a (local) martingale where X^* solves (24) with π^* plugged in as the strategy;
(iv) We call π^* of point (iii) a *MF-equilibrium* if $\overline{X}_t = \mathbb{E}[X_t^*|\mathscr{F}_t^B]$ for all $t \geqslant 0$ where where X^* solves (24) with π^* plugged in as the strategy.

We denote the triplet $(U, \pi^*, \overline{X},)$ satisfying (i)–(iv) the *MF-Forward relative performance equilibrium*. An MF-equilibrium is *constant* if there exists an $\mathscr{F}_0^{\mathrm{MF}}$-measurable RV π^* such that $\pi_t = \pi^*$, for all $t \geqslant 0$.

The last point can be understood as a fixed point argument which creates a compatibility condition between the generic agent within the continuum of agents. In fact, conditionally on the BM B each agent faces an independent noise W and an independent type vector ζ. As in Mean-field games [20, 21], conditionally on B, all agents faces i.i.d. copies of the same optimization problem. The law of large numbers suggests that the average terminal wealth of the whole population should be $\mathbb{E}[X_t^*|\mathscr{F}_t^B]$.

Our construction allows us to identify $\mathbb{E}[X_t^*|\mathscr{F}_t^B]$ with a certain dynamics and, in turn, treat this component as an additional uncontrolled state process. This avoids altogether the conceptualization of the master equation for models with different types of agents. The latter is left for future research.

4.3 Solving the Optimization Problem

We now present the main result of this section which is the existence of a *MF-Forward CARA relative performance equilibrium* for the generic manager according to Definition 4 within the context of time-monotone forward utilities.

From the methodological point of view, the problem is solved as before. Apply Itô formula to $U(Z_t^\pi, t)$, determine the optimal strategy π^* and the consistency condition (the PDE) for U such that the first three conditions of Definition 4 hold. The last condition, to show that π^* is indeed the MFG Forward equilibrium follows by construction as we will see.

Theorem 2 *Take a generic agent* $\zeta = (\xi, \delta, \theta, \mu, \nu, \sigma)$ *and assume that* $\delta > 0$, $\theta \in [0, 1]$, $\mu > 0$, $\sigma \geqslant 0$, $\nu \geqslant 0$ *such that* $\sigma^2 + \nu^2 > 0$.

Assume the following constants are finite

$$\psi^\sigma := \mathbb{E}\Big[\theta \frac{\sigma^2}{\nu^2 + \sigma^2}\Big], \quad \varphi^\sigma := \mathbb{E}\Big[\delta \frac{\mu\sigma}{\nu^2 + \sigma^2}\Big],$$
$$\psi^\mu := \mathbb{E}\Big[\theta \frac{\mu\sigma}{\nu^2 + \sigma^2}\Big], \quad \textit{and} \quad \varphi^\mu := \mathbb{E}\Big[\delta \frac{\mu^2}{\nu^2 + \sigma^2}\Big].$$

Assume that $\psi^\sigma \neq 1$. Then there exists a unique constant MF-Forward CARA relative performance equilibrium in the sense of Definition 4.

The constant MF-equilibrium strategy is unique and is given by

$$\pi^* = \frac{1}{\nu^2+\sigma^2}\Big(\theta\sigma\frac{\varphi^\sigma}{1-\psi^\sigma} + \mu\delta\Big), \tag{25}$$

constrained to the identity

$$\mathbb{E}[\sigma\pi^*] = \frac{\varphi^\sigma}{1-\psi^\sigma} < \infty.$$

The MF-forward CARA relative performance utility map under Assumption 2 is the unique solution of the PDE with stochastic coefficients

$$\begin{aligned} U_t = \theta\Big(\frac{\varphi^\sigma}{1-\psi^\sigma}\cdot\psi^\mu + \varphi^\mu - \mu\frac{\sigma}{\nu^2+\sigma^2}\cdot\frac{\varphi^\sigma}{1-\psi^\sigma}\Big)U_x \\ + \frac{\mu^2}{2(\nu^2+\sigma^2)}\frac{(U_x)^2}{U_{xx}} + \frac{1}{2}U_{xx}\cdot\theta^2\Big(\frac{\varphi^\sigma}{1-\psi^\sigma}\Big)^2\Big(\frac{\sigma^2}{\nu^2+\sigma^2}-1\Big). \end{aligned} \tag{26}$$

When the initial condition is $U(x,0) = u_0(x) = -e^{-x/\delta}$, i.e. the exponential preferences, U is given explicitly by $U(x,t) = u_0(x)e^{t\lambda}$ with λ given by

$$\lambda = -\frac{\theta}{\delta}\overline{\mu\pi} + \frac{1}{2(\nu^2+\sigma^2)}\Big(\mu + \frac{\theta}{\delta}\sigma\overline{\sigma\pi}\Big)^2 - \frac{\theta^2}{2\delta^2}\Big(\overline{\sigma\pi}\Big)^2, \tag{27}$$

where $\overline{\sigma\pi}$ and $\overline{\mu\pi}$ are given by (31) and (32) respectively. If $\psi^\sigma = 1$, then there exists no constant MF-equilibrium.

By comparing the statements of Theorem 1 and Theorem 2 (and same happens for the respective Single (common) Stock Corollaries) one easily sees that as $n \to \infty$ the strategies, weights ($\phi_n^{\cdot}$ and $\psi_n^{\cdot}$) and forward-utility map in Theorem 1 converge to the respective quantities appearing in Theorem 2.

Remark 3 We point out that the interaction of the generic agent with the continuum is only performed through the common noise B. That can be seen by the term $\frac{n}{(n-1)^2}\overline{(\pi\nu)^2} - \frac{1}{(n-1)^2}(\pi^i\nu_i)^2$ from λ_i's in (18) converging to zero as $n \to \infty$, as we have by (34) (compare with (27)). We can interpret it via the standard mean-field approximation, the individual's impact on the others is negligible for the infinite system.

Remark 4 In contrast with Remark 2, here we recover the result from [21, Theorem 2.10] as the scaling factors converge to 1 (as $n \to \infty$). Hence, due to space constraints we defer the reader to [21, Sect. 2.3] for the discussion of the equilibria.

Proof We proceed in several steps in order to construct the constant MF-equilibrium. To that end we must solve (ii)–(iii) in Definition 4 for a given $\overline{X}$ process associated to

$\pi \in \mathscr{A}_{\mathrm{MF}}$. Condition iv), for MF-equilibrium allows us to focus only on processes of the form $\overline{X}_t = \mathbb{E}[X_t^\pi | \mathscr{F}_t^B]$ where X^π solves (24) for a constant strategy π (i.e. $\mathscr{F}_0^{\mathrm{MF}}$-measurable) satisfying $\mathbb{E}[\pi^2] < \infty$.

Step 0. The dynamics of the average wealth process. To solve the above problem given $(\overline{X}_t)_{t\geqslant 0}$ it suffices to restrict ourselves to processes $(\overline{X}_t)_{t\geqslant 0}$ satisfying $\overline{X}_t = \mathbb{E}[X_t^\pi | \mathscr{F}_t^B]$ $\mathbb{P}$-a.s.. We then have

$$\begin{aligned}\overline{X}_t = \mathbb{E}[X_t^\pi | \mathscr{F}_t^B] &= \mathbb{E}\Big[\xi + \int_0^t \mu\pi\, ds + \int_0^t \nu\pi\, dW_s + \int_0^t \sigma\pi\, dB_s \Big| \mathscr{F}_t^B\Big] \\ &= \bar{\xi} + \int_0^t \overline{\mu\pi_s} ds + \int_0^t \overline{\sigma\pi_s} dB_s, \end{aligned} \tag{28}$$

where, for consistency of notation with the previous section, we denote

$$\bar{\xi} := \mathbb{E}[\xi], \quad \overline{\mu\pi} := \mathbb{E}[\mu\pi] \quad \text{and} \quad \overline{\sigma\pi} := \mathbb{E}[\sigma\pi].$$

Hence for $\pi \in \mathscr{A}^{\mathrm{MF}}$ and as in the previous section we can define the dynamics of the process $Z^\pi = X^\pi - \theta\overline{X}$

$$dZ_t^\pi = \big(\mu\pi_t - \theta\overline{\mu\pi}\big)dt + \nu\pi_t dW_t + \big(\sigma\pi_t - \theta\overline{\sigma\pi}\big)dB_t, \quad Z_0^\pi = \xi - \theta\bar{\xi},$$

and solve the MFG Forward utility problem in Definition 4 with its help.

Hence applying Itô's formula to $U(Z_t^\pi, t)$ yields

$$\begin{aligned} dU(Z_t^\pi, t) &= U_t(Z_t^\pi, t)dt + U_x(Z_t^\pi, t)dZ_t^\pi + \frac{1}{2}U_{xx}(Z_t^\pi, t)d\langle Z_t^\pi\rangle \\ &= \Big[U_t(Z_t^\pi, t) + U_x(Z_t^\pi, t)\big(\mu\pi_t - \theta\overline{\mu\pi}\big) \\ &\quad + \frac{1}{2}U_{xx}(Z_t^\pi, t)\Big((\nu\pi_t)^2 + \big(\sigma\pi_t - \theta\overline{\sigma\pi}\big)^2\Big)\Big]dt, \\ &\quad + U_x(Z_t^\pi, t)\nu\pi_t dW_t + U_x(Z_t^\pi, t)\big(\sigma\pi_t - \theta\overline{\sigma\pi}\big)dB_t, \end{aligned} \tag{29}$$

with $U(Z_0^\pi, 0) = U(\xi - \theta\bar{\xi}, 0) = -\exp\{-(\xi - \theta\bar{\xi})/\delta\}$ and we used that the B, W are all i.i.d. Exact calculations on deriving (29) are presented in the Sect. 6.

Step 1. Finding the candidate optimal strategy π^*. As before, the process $U(Z_t^\pi, t)$ becomes a Martingale at the optimum π. Direct computations using first order conditions (∂_π"drift" $= 0$) yield

$$\begin{aligned} &0 + U_x \cdot \big(\mu - 0\big) + \frac{1}{2}U_{xx}\Big[2\pi\nu^2 + 2\big(\sigma\pi_t - \theta\overline{\sigma\pi}\big)\sigma\Big] = 0 \\ \Rightarrow \quad &\pi_t^*(\nu^2 + \sigma^2) = \theta\sigma\overline{\sigma\pi} - \mu\frac{U_x(Z_t^\pi, t)}{U_{xx}(Z_t^\pi, t)} = \theta\sigma\overline{\sigma\pi} + \mu\delta, \end{aligned} \tag{30}$$

where we injected the CARA constraint $U_x/U_{xx} = -\delta$, for all t. By inspection it is clear that π^* is a $\mathscr{F}_0^{\mathrm{MF}}$-measurable RV which is independent of time and is well-defined as long as $\overline{\sigma\pi}$ is finite.

Step 2. The optimality of the strategy. The argument is similar to that in [21]. The original constant strategy π if a MF-equilibrium if and only if for all $t \geqslant 0$

$$\begin{aligned}\mathbb{E}[X_t^{\pi}|\mathscr{F}_t^B] = \mathbb{E}[X_t^{\pi^*}|\mathscr{F}_t^B] \quad a.s.\\ \Leftrightarrow \quad \bar{\xi} + \overline{\mu\pi}\, t + \overline{\sigma\pi} B_t = \bar{\xi} + \overline{\mu\pi^*}\, t + \overline{\sigma\pi^*} B_t \quad a.s.\end{aligned}$$

Taking expectations on both sides implies that π is a MG-equilibrium if and only if the following two conditions holds

$$\overline{\mu\pi} = \overline{\mu\pi^*} \quad \text{and} \quad \overline{\sigma\pi} = \overline{\sigma\pi^*}.$$

Using (30) with $U_x/U_{xx} = -\delta$ and the expressions for φ^σ, ψ^σ one derives that

$$\sigma\pi^* = \theta\frac{\sigma^2}{\nu^2+\sigma^2}\overline{\sigma\pi} + \delta\frac{\mu\sigma}{\nu^2+\sigma^2} \quad \Rightarrow \quad \overline{\sigma\pi^*} = \overline{\sigma\pi}\psi^\sigma + \varphi^\sigma,$$

using that $\overline{\sigma\pi} = \overline{\sigma\pi^*}$ yields solvability if $\psi^\sigma = \mathbb{E}\big[\theta\frac{\sigma^2}{\nu^2+\sigma^2}\big] \neq 1$. The same procedure deals with the condition $\overline{\mu\pi} = \overline{\mu\pi^*}$. We then have

$$\overline{\sigma\pi^*} = \overline{\sigma\pi} = \frac{\varphi^\sigma}{1-\psi^\sigma} = \text{Const}, \tag{31}$$

$$\overline{\mu\pi^*} = \overline{\mu\pi} = \frac{\varphi^\sigma}{1-\psi^\sigma}\cdot\psi^\mu + \varphi^\mu = \text{Const}. \tag{32}$$

Injecting these identities in the expression for π^* we find (25).

For the non-solvability statement, if the Eq. (32) has $\psi^\sigma = 1$ and $\varphi^\sigma \neq 0$ then the equation has no solution and hence no constant MF-equilibrium exists. The case $\psi^\sigma = 1$ and $\varphi^\sigma = 0$ is impossible. Since $\mu > 0$ and $\delta > 0$ by assumption, it implies that $\sigma = 0$ and hence that $\psi^\sigma = 0$ contradicting the condition $\psi^\sigma = 1$.

Step 3. Finding the consistency PDE and the Utility map. We do not carry out this step explicitly, nonetheless, injecting the expression of π^*, $\overline{\sigma\pi}$ and $\overline{\mu\pi}$ in the drift term of (29) and simplifying, we find the necessary Eq. (26), i.e. the consistency condition the random field U must satisfy to that the required properties in Definition 4 hold.

Just like in Example 2, the time-monotone forward utility Eq. (26) can be solved and indeed one has a simplified version. We have

$$U(x,t) = -e^{-x/\delta + t\lambda}, \tag{33}$$

where the $\mathscr{F}_0^{\mathrm{MF}}$-measurable RV λ is given by (using (31) and (32))

$$\begin{aligned}\lambda &= -\frac{\theta}{\delta}\overline{\mu\pi} + \frac{1}{2(\nu^2+\sigma^2)}\Big(\mu + \frac{\theta}{\delta}\sigma\overline{\sigma\pi}\Big)^2 - \frac{\theta^2}{2\delta^2}\Big(\overline{\sigma\pi}\Big)^2 \\ &= -\frac{\theta}{\delta}\Big(\frac{\varphi^\sigma}{1-\psi^\sigma}\cdot\psi^\mu + \varphi^\mu - \mu\frac{\sigma}{\nu^2+\sigma^2}\cdot\frac{\varphi^\sigma}{1-\psi^\sigma}\Big) \\ &\quad + \frac{\mu^2}{2(\nu^2+\sigma^2)} + \frac{\theta^2}{2\delta^2}\Big(\frac{\varphi^\sigma}{1-\psi^\sigma}\Big)^2\Big(\frac{\sigma^2}{\nu^2+\sigma^2}-1\Big).\end{aligned} \tag{34}$$

Step 4. The MFG forward utility dynamics. Injecting the consistency PDE (26) in the expression for $dU(Z_t^\pi, t)$ given in (29) yields,

$$\begin{aligned}dU(Z_t^\pi,t) = \frac{1}{2}\frac{U_{xx}(Z_t^\pi,t)}{(\nu^2+\sigma^2)}\Big|\pi_t(\nu^2+\sigma^2) - \Big(\theta\sigma\cdot\frac{\varphi^\sigma}{1-\psi^\sigma} + \mu\delta\Big)\Big|^2 dt \\ + U_x(Z_t^\pi,t)\nu\pi_t dW_t + U_x(Z_t^\pi,t)\Big(\sigma\pi_t - \theta\cdot\frac{\varphi^\sigma}{1-\psi^\sigma}\Big)dB_t.\end{aligned}$$

We close with a corollary regarding the common stock case.

Corollary 3 (Single stock) *Let μ, σ, ν be deterministic with $\nu = 0, \mu, \sigma > 0$. Let the constants*

$$\varphi := \mathbb{E}[\delta] \quad \textit{and} \quad \psi := \mathbb{E}[\theta]. \tag{35}$$

Then, if $\psi \neq 1$ then a constant MF-equilibrium *exists, with the constant optimal strategy π^* given by*

$$\pi_\cdot^* = \frac{\mu}{\sigma^2}\Big(\theta\frac{\varphi}{1-\psi} + \delta\Big).$$

4.4 Mean-Field Dynamic Model Selection with Large Horizons

Over the time interval $[0, \infty)$ our generic agent selects a sequence of horizon time $(T_j)_{j\in\mathbb{N}_0}$ (such that $T_0 = 0$, $T_{j+1} - T_j > 0$ and $\lim_j T_j = \infty$) on which the agent assesses and updates the market model by adjusting the model's coefficients. Comparing with (24) the agent models the stock as

$$\frac{dS_t^j}{S_t^j} = \mu_j dt + \nu_j dW_t + \sigma_j dB_t, \quad S_{T_j} = s_j, \ \ t \in [T_j, T_{j+1}], \tag{36}$$

where the index j represents the model specification at time T_j. The associated wealth process of the *generic agent* is

$$dX_t^j = \pi_t(\mu_j dt + \nu_j dW_t + \sigma_j dB_t), \quad X_{T_j} = \xi_j, \ \ t \in [T_j, T_{j+1}].$$

Following the earlier constructions of this section, assume that at time $T_0 = 0$ the agent starts with initial utility $u_0(x) = -e^{-x/\delta}$. Then using the results of Theorem 2, the agent's forward utility map is given by

$$U(x,t) = -e^{x/\delta}e^{t\lambda_0} = u_0(x)e^{t\lambda_0}, \quad t \in [T_0, T_1] = [0, T_1],$$

where λ_0 is the version of (34) for the type of the agent over the time interval $[T_0, T_1]$ and all the coefficients correspond to a type ζ_0, i.e. $\lambda(\zeta_0) = \lambda_0$, with

$$\lambda_0 = \lambda(\zeta_0) := -\frac{\theta}{\delta}\overline{\mu\pi} + \frac{1}{2(\nu^2+\sigma^2)}\Big(\mu + \frac{\theta}{\delta}\sigma\overline{\sigma\pi}\Big)^2 - \frac{\theta^2}{2\delta^2}\Big(\overline{\sigma\pi}\Big)^2. \tag{37}$$

At time T_1, the generic agent assesses the previous model specification and chooses new coefficients (leading to a change in type, say from ζ_0 to ζ_1). The agent then carries out the optimization program over $t \in [T_1, T_2]$ but starting from initial utility $U(x, T_1)$. Under the assumption of constant coefficients Theorem 2, yields,

$$U(x,t) = \Big(u_0(x)e^{T_1\lambda_0}\Big)e^{(t-T_1)\lambda_1}, \quad t \in [T_1, T_2],$$

where $\lambda_1 = \lambda(\zeta_1)$ (given by (37)) depends only on information at time T_1. Quick calculations generalize to any time horizon T_j. Assume we work on the time interval $[T_j, T_{j+1}]$. Stemming from previous calculations, it is easy to see that the initial condition for the forward utility problem is

$$U(x, T_j) = u_0(x)\prod_{k=1}^{j} e^{(T_k - T_{k-1})\lambda_{k-1}}$$

(with the convention that if $j < 1$ then $\prod_{k=1}^{j} \cdots = 0$) and the MFG forward utility is for all $t \in [T_j, T_{j+1}]$, $j > 1$ and using that $\lambda_j = \lambda(\zeta_j)$.

$$\begin{aligned} U(x,t) = U(x,T_j)e^{(t-T_j)\lambda_j} &= u_0(x)\prod_{k=1}^{j} e^{(T_k-T_{k-1})\lambda_{k-1}} \cdot e^{(t-T_j)\lambda_j}, \\ &= u_0(x)\exp\Big\{T_1(\lambda_0-\lambda_1) + T_2(\lambda_1-\lambda_2) + \cdots + T_j(\lambda_{j-1}-\lambda_j)\Big\}e^{t\lambda_j}. \end{aligned}$$

There are two points to highlight. Firstly, the agent needs to carry information of what happened in the past in order to have time-consistency at present time. Secondly, this construction also allows the agents to change not just the model specification (μ, ν, σ) but also their type including risk parameter δ and performance-concern level θ. The initial wealth is fixed from the previous time interval.

5 Outlook and Open Questions

In this work we considered two optimal portfolio management problems under forward utility performance concerns. We presented a simplified setting allowing for explicit calculations of the optimal control value function, strategies and an intuitive validation that the finite-play game reaches the mean-field game in the limit.

This work provides a proof-of-concept for the forward mean-field utility construction leaving open many questions. Generalizing the dynamics of the forward utility (8) to a fully Itô-dynamics and stochastic strategies is also open. A crucial tool for such would be a general Itô-Wentzell-Lions chain rule as developed in [9]. Such an approach would require [13, 27].

Here we addressed only the exponential-utilities (CARA) and left the power-case (CRRA) open. Even within (8), one can build towards the CRRA case in [21] or include the consumption problem [20], on the latter see [10] for recent developments; for the general forward utility case see [11]. Also open is the so-called mean-field aggregation problem where different agents use utility maps from different families, e.g. CRRA and CARA: [12] would be a starting point for the finite-player case while the mean-field case would requires the multi-class approach of [3, Sect. 8] with the parameterization technique of from our Sect. 4. Many other questions can be posed in this context of mean-field forward utilities, ranging from possible non-solvability [15], to risk-sharing [4], ergodic problems [7] and associated numerics [17].

6 Supplementary Calculations

Proof (*of Proposition* 1) We recall the optimal strategy is given by (11), where we define

$$\widehat{\sigma} := \overline{(\pi\sigma)}_t^{(-i)}, \quad B_t^{\nu} := \theta_i^2 \frac{1}{(n-1)^2} \sum_{k\neq i} (\pi_t^k \nu_k)^2, \quad M_t^{\mu} := \theta_i \overline{(\pi\mu)}_t^{(-i)} = \frac{\theta_i}{n-1} \sum_{k\neq i} \pi_t^k \mu_k.$$

The drift of (10) becomes (we omit the argument in U_t, U_x, U_{xx} and use $\widehat{\sigma} := \overline{(\pi\sigma)}_t^{(-i)}$)

$$\begin{aligned}
&U_t^i + U_x^i\big(\pi_t^i\mu_i - M_t^{\mu}\big) + \frac{1}{2}U_{xx}^i\Big[(\pi_t^i\nu_i)^2 + B_t^{\nu} + \big(\pi_t^i\sigma_i - \theta_i\overline{(\pi\sigma)}_t^{(-i)}\big)^2\Big] \\
&\quad = \Big(U_t^i - M_t^{\mu}U_x^i + \frac{1}{2}U_{xx}^i B_t^{\nu}\Big) + \frac{1}{2}U_{xx}^i\Big[\big(\theta_i\widehat{\sigma}\big)^2 - (\pi_t^i)^2(\nu_i^2+\sigma_i^2)\Big] \\
&\quad = U_t^i + U_x^i\Big[\theta_i\sigma_i\widehat{\sigma}\mu_i\frac{1}{\nu_i^2+\sigma_i^2} - M_t^{\mu}\Big] - \frac{\mu_i^2}{2}\frac{1}{\nu_i^2+\sigma_i^2}\frac{(U_x^i)^2}{U_{xx}^i} \\
&\qquad + \frac{1}{2}U_{xx}^i\Big\{B_t^{\nu} + \big(\theta_i\widehat{\sigma}\big)^2 - \frac{1}{\nu_i^2+\sigma_i^2}\big(\theta_i\sigma_i\widehat{\sigma}\big)^2\Big\}
\end{aligned}$$

$$
\begin{aligned}
&= U_t^i + U_x^i\Big[\frac{\mu_i\theta_i\sigma_i\widehat{\sigma}}{\nu_i^2+\sigma_i^2} - \theta_i\overline{(\pi\mu)}_t^{(-i)}\Big] - \frac{\mu_i^2}{2(\nu_i^2+\sigma_i^2)}\frac{(U_x^i)^2}{U_{xx}^i} \\
&\quad + \frac{1}{2}U_{xx}^i\Big\{\theta_i^2\frac{1}{(n-1)^2}\sum_{k\neq i}(\pi_t^k\nu_k)^2 + \big(\theta_i\widehat{\sigma}\big)^2\Big[1-\frac{\sigma_i^2}{\nu_i^2+\sigma_i^2}\Big]\Big\}.
\end{aligned}
$$

Equation (9) now follows as U_t^i needs to be chosen such that the equation is zero. We inject in the drift of (10) the expression (9) and obtain a simplified version

$$
\begin{aligned}
&- \Big\{U_x^i\Big[\theta_i\sigma_i\widehat{\sigma}\mu_i\frac{1}{\nu_i^2+\sigma_i^2} - M_t^\mu\Big] - \frac{\mu_i^2}{2}\frac{1}{\nu_i^2+\sigma_i^2}\frac{(U_x^i)^2}{U_{xx}^i} + \frac{1}{2}U_{xx}^i\Big\{B_t^\nu + \big(\theta_i\widehat{\sigma}\big)^2 \\
&- \frac{1}{\nu_i^2+\sigma_i^2}\big(\theta_i\sigma_i\widehat{\sigma}\big)^2\Big\}\Big\} + U_x^i\big(\pi_t^i\mu_i - M_t^\mu\big) \\
&+ \frac{1}{2}U_{xx}^i\Big[(\pi_t^i\nu_i)^2 + B_t^\nu + \big(\pi_t^i\sigma_i\big)^2 - 2\pi_t^i\sigma_i\theta_i\widehat{\sigma} + \big(\theta_i\widehat{\sigma}\big)^2\Big] \\
&= \frac{U_{xx}^i}{2}\frac{1}{\nu_i^2+\sigma_i^2}\Big(\big(\pi_t^i\big)^2(\nu_i^2+\sigma_i^2)^2 - 2\big(\pi_t^i(\nu_i^2+\sigma_i^2)\big)\Big(\sigma_i\theta_i\widehat{\sigma} - \mu_i\frac{U_x^i}{U_{xx}^i}\Big)\Big) \\
&+ -\frac{1}{\nu_i^2+\sigma_i^2}\frac{U_{xx}^i}{2}\frac{2}{U_{xx}^i}\Big\{U_x^i\Big[\theta_i\sigma_i\widehat{\sigma}\mu_i\Big] - \frac{\mu_i^2}{2}\frac{(U_x^i)^2}{U_{xx}^i} + \frac{1}{2}U_{xx}^i\Big\{-\big(\theta_i\sigma_i\widehat{\sigma}\big)^2\Big\}\Big\} \\
&= \frac{U_{xx}^i}{2}\frac{1}{\nu_i^2+\sigma_i^2}\Big|\pi_t^i(\nu_i^2+\sigma_i^2) - \Big(\sigma_i\theta_i\widehat{\sigma} - \mu_i\frac{U_x^i}{U_{xx}^i}\Big)\Big|^2,
\end{aligned}
$$

which results in (12).

Proof (*of Equation* (29)) We take up the drift of (29) and we have just by re-organizing the terms

$$
\begin{aligned}
0 &= U_t(Z_t^\pi,t) + U_x(Z_t^\pi,t)\big(\mu\pi_t - \theta\overline{\mu\pi_t}\big) + \frac{1}{2}U_{xx}(Z_t^\pi,t)\Big((\nu\pi_t)^2 + \big(\sigma\pi_t - \theta\overline{\sigma\pi_t}\big)^2\Big) \\
&= \Big(U_t - U_x\theta\overline{\mu\pi_t} + \frac{1}{2}U_{xx}\theta^2(\overline{\sigma\pi_t})^2\Big) \\
&\qquad + \frac{1}{2}\frac{U_{xx}}{(\nu^2+\sigma^2)}\Big(\pi_t^2(\nu^2+\sigma^2)^2 - 2\pi_t(\nu^2+\sigma^2)\Big\{\theta\sigma\overline{\sigma\pi_t} - \mu\frac{U_x}{U_{xx}}\Big\}\Big)
\end{aligned}
$$

We recall the optimal strategy given by (30), where we complete the square inside the U_{xx} term in the SPDE above we have

$$
\begin{aligned}
0 = &\Big\{U_t + U_x\cdot\Big(\mu\frac{\theta\sigma\overline{\sigma\pi_t}}{(\nu^2+\sigma^2)} - \theta\overline{\mu\pi_t}\Big) + \frac{1}{2}U_{xx}\cdot\theta^2(\overline{\sigma\pi_t})^2\Big(1-\frac{\sigma^2}{\nu^2+\sigma^2}\Big) \\
&- \frac{1}{2}\frac{\mu^2}{(\nu^2+\sigma^2)}\frac{(U_x)^2}{U_{xx}}\Big\} + \frac{1}{2}\frac{U_{xx}}{(\nu^2+\sigma^2)}\Big|\pi_t(\nu^2+\sigma^2) - \Big(\theta\sigma\overline{\sigma\pi_t} - \mu\frac{U_x}{U_{xx}}\Big)\Big|^2
\end{aligned}
$$

Under the CARA condition $U_x/U_{xx} = -\delta$ and the choice of the optimal strategy, the remaining drift must zero-out. We then have

$$U_t = -\frac{U_x}{2(\nu^2+\sigma^2)} \cdot \left(\mu\theta\sigma\overline{\sigma\pi_t} + \delta\mu^2\right) + U_{xx}\frac{(\theta\,\sigma\,\overline{\sigma\pi_t})^2}{2(\nu^2+\sigma^2)} - \frac{1}{2}U_{xx}\cdot(\theta\,\overline{\sigma\pi_t})^2 + U_x\left(\theta\overline{\mu\pi_t}\right).$$

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References

1. M. Anthropelos, Forward exponential performances: pricing and optimal risk sharing. SIAM J. Financ. Math. **5**(1), 626–655 (2014)
2. M. Anthropelos, T. Geng, T. Zariphopoulou, Competition in fund management and forward relative performance criteria. Available at SSRN 3723229 (2020)
3. A. Bensoussan, J. Frehse, P. Yam, *Mean Field Games and Mean Field Type Control Theory*, Springer Briefs in Mathematics (Springer, New York, 2013)
4. J. Bielagk, A. Lionnet, G. dos Reis, Equilibrium pricing under relative performance concerns. SIAM J. Financ. Math. **8**(1), 435–482 (2017)
5. P. Cardaliaguet, F. Delarue, J.-M. Lasry, P.-L. Lions, The master equation and the convergence problem in mean field games **201**, x+212 (2019)
6. R. Carmona, F. Delarue, D. Lacker, Mean field games of timing and models for bank runs. Appl. Math. Optim. **76**(1), 217–260 (2017)
7. W.F. Chong, Y. Hu, G. Liang, T. Zariphopoulou, An ergodic BSDE approach to forward entropic risk measures: representation and large-maturity behavior. Finance Stoch. **23**(1), 239–273 (2019)
8. C. Deng, X. Su, C. Zhou, Relative wealth concerns with partial information and heterogeneous priors (2020). arXiv preprint arXiv:2007.11781
9. G. dos Reis, V. Platonov, Itô-Wentzell-Lions formula for measure dependent random fields under full and conditional measure flows (2019). arXiv preprint arXiv:1910.01892
10. G. dos Reis, V. Platonov, Forward utility and market adjustments in relative investment-consumption games of many players (2020). arXiv preprint arXiv: 2012.01235
11. N. El Karoui, C. Hillairet, M. Mrad, Consistent utility of investment and consumption: a forward/backward SPDE viewpoint. Stochastics **90**(6), 927–954 (2018)
12. N. El Karoui, C. Hillairet, M. Mrad, Construction of an aggregate consistent utility, without Pareto optimality. Application to long-term yield curve modeling, in *Frontiers in Stochastic Analysis—BSDEs, SPDEs and Their Applications*. Springer Proceedings in Mathematics and Statistics, vol. 289 (Springer, Cham, 2019), pp. 169–199
13. N. El Karoui, M. Mrad, An exact connection between two solvable SDEs and a nonlinear utility stochastic PDE. SIAM J. Financ. Math. **4**(1), 697–736 (2013)
14. G.-E. Espinosa, N. Touzi, Optimal investment under relative performance concerns. Math. Financ. **25**(2), 221–257 (2015)
15. C. Frei, G. Dos Reis, A financial market with interacting investors: does an equilibrium exist? Math. Financ. Econ. **4**(3), 161–182 (2011)
16. T. Geng, T. Zariphopoulou, Passive and competitive investment strategies under relative forward performance criteria. Available at SSRN 2870040 (2017)
17. E. Gobet, M. Mrad, Convergence rate of strong approximations of compound random maps, application to SPDEs. Discret. Contin. Dyn. Syst. Ser. B **23**(10), 4455–4476 (2018)

18. D.A. Gomes, L. Nurbekyan, M. Sedjro, One-dimensional forward-forward mean-field games. Appl. Math. Optim. **74**(3), 619–642 (2016)
19. M. Huang, R.P. Malhamé, P.E. Caines, Large population stochastic dynamic games: closed-loop McKean-Vlasov systems and the Nash certainty equivalence principle. Commun. Inf. Syst. **6**(3), 221–251 (2006)
20. D. Lacker, A. Soret, Many-player games of optimal consumption and investment under relative performance criteria. Math. Financ. Econ. **14**(2), 263–281 (2020)
21. D. Lacker, T. Zariphopoulou, Mean field and n-agent games for optimal investment under relative performance criteria. Math. Financ. **29**(4), 1003–1038 (2019)
22. M. Musiela, T. Zariphopoulou, Investment and valuation under backward and forward dynamic exponential utilities in a stochastic factor model, in *Advances in Mathematical Finance*, ed. by M.C. Fu, R.A. Jarrow, J.-Y.J. Yen, R.J. Elliott (Birkhäuser, Boston, 2007), pp. 303–334
23. M. Musiela, T. Zariphopoulou, Optimal asset allocation under forward exponential performance criteria, in *Markov Processes and Related Topics: a Festschrift for Thomas G. Kurtz*. Institute of Mathematical Statistics (IMS) Collection, vol. 4 (Institute of Mathematical Statistics, Beachwood, 2008), pp. 285–300
24. M. Musiela, T. Zariphopoulou, Portfolio choice under dynamic investment performance criteria. Quant. Financ. **9**(2), 161–170 (2009)
25. M. Musiela, T. Zariphopoulou, Portfolio choice under space-time monotone performance criteria. SIAM J. Financ. Math. **1**(1), 326–365 (2010)
26. M. Musiela, T. Zariphopoulou, Stochastic partial differential equations and portfolio choice, in *Contemporary Quantitative Finance* (Springer, Berlin, 2010), pp. 195–216
27. G. Zitković, A dual characterization of self-generation and exponential forward performances. Ann. Appl. Probab. **19**(6), 2176–2210 (2009)

The Boundary Driven Zero-Range Process

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Abstract We study the asymptotic behaviour of the symmetric zero-range process in the finite lattice $\{1, \ldots, N-1\}$ with slow boundary, in which particles are created at site 1 or annihilated at site $N-1$ with rate proportional to $N^{-\theta}$, for $\theta \geq 1$. We present the invariant measure for this model and obtain the hydrostatic limit. In order to understand the asymptotic behaviour of the spatial-temporal evolution of this model under the diffusive scaling, we start to analyze the hydrodynamic limit, exploiting attractiveness as an essential ingredient. We obtain, through some heuristic arguments, the hydrodynamic equation, whose boundary conditions depend on θ.

Keywords Zero-range process · Slow boundary · Invariant measure · Hydrostatic limit · Hydrodynamic limit · Boundary conditions

1 Introduction

The zero-range process, originally introduced in 1970 by Spitzer [27], is a model that describes the behaviour of interacting particles moving on a lattice without restriction on the total number of particles per site. In this model, a particle leaves a site according to a jump rate $g(k)$ that only depends on the number of particles, k, in that site. The zero-range process has been mostly studied in infinite lattices (see [2, 3, 18, 19, 26]) and in discrete torus (see [4, 9, 20–22] and the references therein). In the present work we consider the process defined in the finite lattice $I_N = \{1, \ldots, N-1\}$ with creation and annihilation of particles at the boundary.

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One of the main interest in the study of interacting particle systems is the derivation of partial differential equations (PDE) to describe the time evolution of the macroscopic density of particles as the lattice is rescaled to the continuum. Such classical scaling limit is called *hydrodynamic limit* and the associated PDE is called *hydrodynamic equation*. In recent years there has been an increasing interest in models that leads to hydrodynamic equations with boundary conditions (see [8, 12, 13, 17]). This has been done, for example, for the exclusion process in [5] and for the porous medium model in [10]. In both cases, the lattice I_N is connected to reservoirs so that particles can be inserted into or removed from the system with rate proportional to $N^{-\theta}$, and the obtained hydrodynamic equations have boundary conditions that depend on the value of θ. One common characteristic of the models in [5, 10] is that the exclusion rule only allows one particle per site, which provides a natural control for the number of particles in the system.

For the classical zero-range process in the discrete torus, see [22, Chap. 5], conservation of particles is an extensively used property in the proof of hydrodynamic limit, together with a hypothesis that controls the relative entropy of the initial distribution with respect to some invariant measure. In the open zero-range process, considered in the present work, the number of particles in the system is not conserved as it was in the process in the discrete torus and neither bounded as it was in the exclusion process and porous medium model. To overcome this difficulty, instead of assuming a relative entropy hypothesis, we exploit the attractiveness present in our model under the assumption that the jump rate function g is non decreasing and that the initial distribution is bounded above by the invariant measure. Attractiveness was also an essential ingredient in [3], where the authors obtained the hydrodynamic limit through preservation of local equilibrium for the asymmetric zero-range process on $\mathbb{Z}$ under Euler scaling. The same was done, for example, for the symmetric zero-range process in the discrete torus under the diffusive scaling, see [22, Chap. 9].

In this work we consider a symmetric nearest-neighbour zero-range process in I_N with the following dynamics at the boundary: a particle is inserted into the system at site 1 with rate α/N^θ and removed from the system through site $N-1$ with rate $g(k)/N^\theta$, if there are k particles at site $N-1$[1], where $\alpha \geq 0$, $\theta \geq 1$ and g is same jump rate function used in I_N. Computing analytically the stationary distribution of a non-equilibrium stochastic model is usually a very challenging task, see [7, 14–16]. However, an important general aspect of the zero-range process, that is not present in the models considered in [5, 10], is that its invariant distribution is a product measure that can be explicitly computed, see [1, 27]. This is also true in our case, despite of the boundary conditions, as already considered in [6, 11, 23], and the resulting steady-state, when it exists, is a product measure imitating the periodic case, but now it is characterized by a non homogeneous space-dependent fugacity which is a function of the boundary rates. In Sect. 3, we present the invariant measure for our model obtained through elementary computations involving the jump rates. Having

[1] See Remark 4 for a more general dynamics allowing creation and annihilation of particles at both sides of the boundary.

the explicit form of the invariant measure, we obtain the stationary density profile, the so called *hydrostatic limit*.

Our main goal is to describe the asymptotic behaviour for the time evolution of the spacial density of particles for zero-range process with slow boundary introduced above. More precisely, we want to prove that, if we start our evolution with an initial configuration of particles that converges to a macroscopic density profile $\gamma : [0, 1] \to \mathbb{R}_+$, as $N \to \infty$, then, under the diffusive scaling, and in a fixed time interval $[0, T]$, the time trajectory of the spatial density of particles, $\{\pi_t^N : t \in [0, T]\}$, converges to a deterministic limit, $\{\pi_t : t \in [0, T]\}$. In the present work we prove relative compactness for the sequence $\{\pi_t^N : t \in [0, T]\}$ and that the limit points, $\{\pi_t : t \in [0, T]\}$, are trajectories of absolutely continuous measures on $[0, 1]$, that is, $\pi_t(du) = \rho(t, u)\, du$, for $t \in [0, T]$ and $u \in [0, 1]$. We conjecture, based on some heuristic arguments, that ρ is the weak solution of the following non-linear diffusion equation with boundary conditions:

$$\begin{cases} \partial_t \rho(t, u) = \Delta \Phi(\rho(t, u)), & \text{for } u \in (0, 1) \text{ and } t \in (0, T], \\ \partial_u \Phi(\rho(t, 0)) = -\kappa\, \alpha\,, & \text{for } t \in (0, T], \\ \partial_u \Phi(\rho(t, 1)) = -\kappa\, \Phi(\rho(t, 1))\,, & \text{for } t \in (0, T], \\ \rho(0, u) = \gamma(u), & \text{for } u \in [0, 1], \end{cases}$$

where $\kappa = 1$, if $\theta = 1$, and $\kappa = 0$, if $\theta > 1$. The function Φ will be defined in (15), in terms of the jumps rate g. In Remark 3, we explain what happens in the stationary regime for the case $\theta < 1$.

The paper is organized as follows. In Sect. 2, we introduce some notations and define precisely the zero-range process with the boundary dynamics that we are considering. In Sect. 3, we present the invariant measure and observe the different asymptotic behaviour of the fugacity profile, depending on the value of θ. We also provide the invariant measure for a more general dynamics that allows creation and annihilation of particles in both sides of I_N. In Sect. 4, we define the notion of measures associated to a density profile and present the hydrostatic limit for our model. The small Sect. 5 is devoted to recall the essential property of attractiveness for the zero-range process. In Sect. 6, we prove tightness for the sequence of probabilities of interest. For that, we introduce the related martingales that will be very useful also in the derivation of the hydrodynamic equation. In Sect. 7, we start the characterization of the limit points by showing concentration on absolutely continuous measures. In Sect. 8, we present the hydrodynamic equation that we conjecture for this model, together with the necessary steps for a complete proof the of hydrodynamic limit. In Sect. 9, we show how to obtain the integral form of the hydrodynamic equation from the Dynkin martingales presented in Sect. 6. We use some heuristic arguments that can be formalized through some fundamental replacement lemmas, whose proof is postponed to a future work. Finally, in Sect. 10, we present the hydrodynamic equation obtained if we consider the general model presented in Remark 4, in which particles are created and annihilated in both sides of I_N.

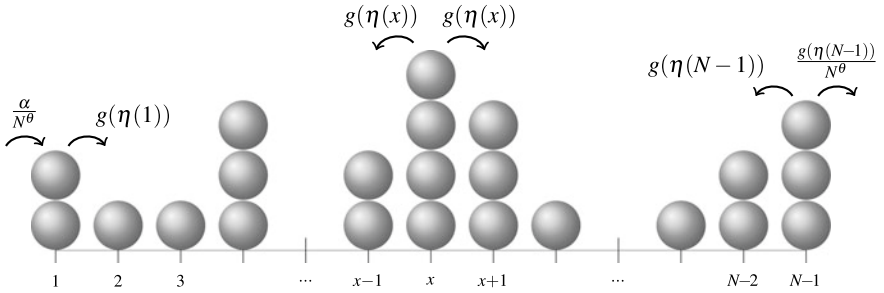

Fig. 1 The boundary driven zero-range process

2 Definition of the Model

Let $I_N = \{1, \ldots, N-1\}$ be the finite lattice where the distinguishable particles will be moving around, we called it by bulk. For $x \in I_N$, the occupation variable $\eta(x)$ stands for the number of particles at site x. The zero-range process is an evolution without restriction on the total number of particles per site, and therefore the state space for the configurations η is the set $\Omega_N = \mathbb{N}^{I_N}$.

The process is defined through a function $g : \mathbb{N} \to \mathbb{R}_+$, with $g(0) = 0$. We assume, throughout this work, that g has bounded variation in the following sense:

$$g^* = \sup_k |g(k+1) - g(k)| < \infty. \tag{1}$$

The bulk dynamics can be described as: a particle leaves a site $x \in \{2, \ldots, N-2\}$ with rate $2g(\eta(x))$, and jumps to one of the neighbouring sites ($x-1$ or $x+1$) chosen uniformly. A particle jumps from the sites $x = 1$ and $x = N-1$ to a neighbour site in I_N with rate $g(\eta(x))$. The boundary dynamics is given by the following birth and death processes at the sites $x = 1$ and $x = N-1$ (see Fig. 1). For fixed non-negative parameters α and θ, a particle is inserted into the system with rate α/N^θ at site 1 and removed with rate $g(\eta(N-1))/N^\theta$ through the site $N-1$.[2]

We can entirely characterize the continuous time Markov process $\{\eta_t : t \geq 0\}$ by its infinitesimal generator L_N given by

$$L_N = L_{N,0} + L_{N,b}, \tag{2}$$

where $L_{N,0}$ and $L_{N,b}$ represent the infinitesimal generators of the bulk dynamics and the boundary dynamics, respectively. The generators act on functions $f : \Omega_N \to \mathbb{R}$ as

[2] See Remark 4 for a more general boundary dynamics.

$$(L_{N,0}f)(\eta) = \sum_{x=1}^{N-1} \sum_{y\in\{x-1,x+1\}\cap I_N} g(\eta(x))\,[f(\eta^{x,y}) - f(\eta)], \tag{3}$$

$$(L_{N,b}f)(\eta) = \frac{\alpha}{N^\theta}[f(\eta^{1+}) - f(\eta)] + \frac{g(\eta(N-1))}{N^\theta}[f(\eta^{(N-1)-}) - f(\eta)], \tag{4}$$

where $\eta^{x,y}$ represents the configuration obtained when, in the configuration η, a particle jumps from site x to y, i.e,

$$\eta^{x,y}(z) = \begin{cases} \eta(z)\,, & \text{if } z \neq x,\, y, \\ \eta(z) - 1\,, & \text{if } z = x, \\ \eta(z) + 1\,, & \text{if } z = y; \end{cases} \tag{5}$$

and $\eta^{\omega\pm}$ represents a configuration obtained from η adding or subtracting one particle at site ω, that is,

$$\eta^{\omega\pm}(z) = \begin{cases} \eta(z)\,, & \text{if } z \neq \omega, \\ \eta(z) \pm 1\,, & \text{if } z = \omega. \end{cases} \tag{6}$$

Remark 1 Contrary to the classical zero-range process on the torus, see for example [22], the process with these boundary conditions is not reversible, and does not conserve the number of particles.

3 Invariant Measure

Since we do not have conservation of particles, the Markov process with generator L_N is irreducible in Ω_N. If the process is non-explosive and has an invariant distribution, then the invariant measure is unique and the process is positive recurrent (see [25, Proposition 3.5.3]). Coupling with a birth and death processes, we can see that if g is such that $\sum_{k=1}^{\infty} \frac{1}{\max_{1\le i\le k} g(i)} = \infty$, then the process is non-explosive. This condition is satisfied, since we are assuming that g has bounded variation, as stated in (1).

A particular aspect of the zero-range process is that its invariant measure can be explicitly computed (see [1, 27]). This can also be done in our case, despite of the boundary conditions, as already considered in [11, 23]. For the convenience of the reader, we will present the calculations in the following.

Inspired by the periodic case, we look for an invariant probability $\bar{\nu}^N$ which is a product measure on Ω_N with marginals given by

$$\bar{\nu}^N\{\eta : \eta(x) = k\} = \frac{1}{Z(\varphi(x))}\frac{(\varphi(x))^k}{g(k)!}, \tag{7}$$

for $x \in I_N$. Here $g(k)!$ stands for $\Pi_{1\le j\le k} g(j)$, and $g(0)! = 1$, $\varphi : I_N \to \mathbb{R}_+$ is a function to be determined, and Z is the normalizing partition function

$$Z(\varphi) = \sum_{k\geq 0} \frac{\varphi^k}{g(k)!}. \tag{8}$$

Denote by φ^* the radius of convergence of the partition function (8).

Lemma 1 *For α, θ and N satisfying $\alpha(\frac{1}{N^{\theta-1}} - \frac{2}{N^\theta} + 1) < \varphi^*$, the measure $\bar{\nu}^N$ defined in (7) with fugacity profile*

$$\varphi(x) = \varphi^N(x) = -\tfrac{\alpha}{N^\theta}(x+1) + \tfrac{\alpha}{N^{\theta-1}} + \alpha\,, \quad x \in I_N\,, \tag{9}$$

is the unique invariant distribution for the Markov process on Ω_N with infinitesimal generator L_N, defined in (2).

Proof Let $\eta \in \Omega_N$ be an arbitrary configuration. We have to prove that

$$\sum_{\tilde{\eta}\neq\eta} \frac{\bar{\nu}^N(\tilde{\eta})}{\bar{\nu}^N(\eta)} R(\tilde{\eta}, \eta) = \lambda(\eta)\,, \tag{10}$$

where $R(\tilde{\eta}, \eta)$ is the rate at which the process jumps from $\tilde{\eta}$ to η and

$$\lambda(\eta) = g(\eta(1)) + 2\sum_{x=2}^{N-2} g(\eta(x)) + g(\eta(N-1)) + \frac{\alpha}{N^\theta} + \frac{g(\eta(N-1))}{N^\theta} \tag{11}$$

is the rate at which the process jumps from the configuration η. In the left-hand side of the equation (10), there are four types of configurations $\tilde{\eta}$ for which $R(\tilde{\eta}, \eta) \neq 0$: $\tilde{\eta} = \eta^{x,x+1}$ and $\tilde{\eta} = \eta^{x+1,x}$, for $x \in \{1, \ldots, N-2\}$, $\tilde{\eta} = \eta^{1-}$ and $\tilde{\eta} = \eta^{(N-1)+}$. Decomposing the summation in these types of configurations, using the definition of $\bar{\nu}^N$ in (7) and the jump rates in (3) and (4), we can rewrite the left-hand side of (10) as

$$\sum_{x=1}^{N-2} \frac{\varphi(x+1)}{\varphi(x)} g(\eta(x)) + \sum_{x=1}^{N-2} \frac{\varphi(x)}{\varphi(x+1)} g(\eta(x+1)) + \frac{\alpha g(\eta(1))}{N^\theta \varphi(1)} + \frac{\varphi(N-1)}{N^\theta}.$$

Thus, changing the index in the second sum above, the last expression becomes

$$\begin{aligned} &\sum_{x=2}^{N-2} \frac{\varphi(x+1)+\varphi(x-1)}{\varphi(x)}\, g(\eta(x)) + \frac{\varphi(2)+\frac{\alpha}{N^\theta}}{\varphi(1)}\, g(\eta(1)) \\ &\qquad + \frac{\varphi(N-2)}{\varphi(N-1)}\, g(\eta(N-1)) + \frac{\varphi(N-1)}{N^\theta}. \end{aligned} \tag{12}$$

In order to (12) be equal to (11) we must require $\frac{\varphi(x+1)+\varphi(x-1)}{\varphi(x)} = 2$, for all $x \in \{2, \ldots, N-2\}$. To get that, choose φ a linear function, let us say $\varphi(x) = ax + b$.

The other required conditions: $\frac{\varphi(2)+\frac{\alpha}{N^\theta}}{\varphi(1)} = 1$, $\frac{\varphi(N-2)}{\varphi(N-1)} = 1 + \frac{1}{N^\theta}$ and $\varphi(N-1) = \alpha$, are satisfied with the choice $a = -\frac{\alpha}{N^\theta}$ and $b = \frac{\alpha}{N^\theta}(N-1) + \alpha$, which leads to (9).

Remark 2 The condition $\alpha(\frac{1}{N^{\theta-1}} - \frac{2}{N^\theta} + 1) < \varphi^*$ imposed in Lemma 1 ensures that the fugacity function satisfies $\varphi(x) < \varphi^*$ for all $x \in I_N$. Note that if φ^* is finite (which occurs, for instance, when g is bounded), then the probability measure $\bar{\nu}^N$ is not well defined if α is too big. This is quite intuitive, since large α (many particles entering the system) and small g (few particles leaving the system) would imply transience of the process.

A simple computation shows that $E_{\bar{\nu}^N}[g(\eta(x))] = \varphi^N(x)$, for $x \in I_N$, where $E_{\bar{\nu}^N}$ denotes expectation with respect to the measure $\bar{\nu}^N$. That is why $\varphi^N(x)$ is called the fugacity at the site x.

Remark 3 We observe that, depending on the value of $\theta \in [0, \infty)$, we have different asymptotic behaviours of the fugacity, see Fig. 2:

- For $\theta = 1$, for $x \in I_N$, $\varphi^N(x) = \bar{\varphi}(\frac{x+1}{N})$, where the asymptotic fugacity profile $\bar{\varphi} : [0, 1] \to \mathbb{R}$ is given by $\bar{\varphi}(u) = \alpha(2 - u)$.
- For $\theta > 1$, $\varphi^N(x) = \alpha + r_N(x)$, where $\lim_{N\to\infty} \sup_{x\in I_N} |r_N(x)| = 0$. In this case, the asymptotic fugacity profile $\bar{\varphi}$ is equal to the constant α.
- For $\theta < 1$, we must look at the two different situations: $\varphi^* < \infty$ and $\varphi^* = \infty$. If $\varphi^* < \infty$, the partition function will not be defined for large values of N. If $\varphi^* = \infty$, it would make sense to consider $N \to \infty$, however, we will have $\varphi^N(1) \to \infty$. Thus, as I_N is rescaled to the continuum, φ^N can not be rescaled to a macroscopic profile $\bar{\varphi} : [0, 1] \to \mathbb{R}$, as in the previous cases.

Remark 4 It is possible also to consider a more general model allowing creation and annihilation of particles at both sides of the boundary (see Fig. 3), let us say: at site 1, particles are inserted into the system with rate $\frac{\alpha}{N^\theta}$ and removed from the system with rate $\frac{\lambda}{N^\theta} g(\eta(1))$; at site $N-1$, particles are inserted into the system with rate $\frac{\beta}{N^\theta}$ and removed from the system with rate $\frac{\delta}{N^\theta} g(\eta(N-1))$. Following the lines

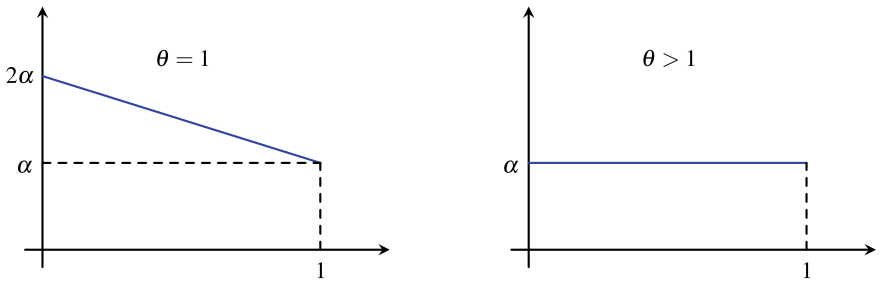

Fig. 2 The asymptotic fugacity profile $\bar{\varphi} : [0, 1] \to \mathbb{R}_+$

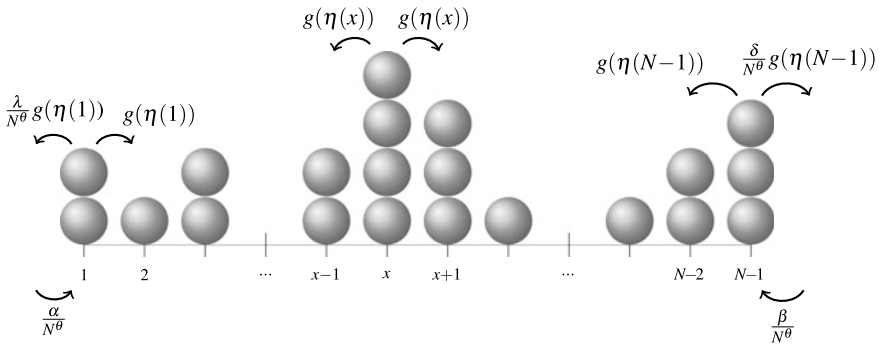

Fig. 3 The general slow boundary driven zero-range process

of Lemma 1 we found that the invariant probability is also a product measure with marginals given by (7) for a linear fugacity profile

$$\varphi(x) = \varphi^N(x) = \frac{-(\alpha\delta - \beta\lambda)(x-1) + \alpha\delta(N-2) + (\alpha+\beta)N^\theta}{\lambda\delta(N-2) + (\lambda+\delta)N^\theta},$$

for $x \in I_N$ and $\alpha, \beta, \delta, \lambda, \theta \geq 0$. In the case $\theta = 0$, this formula coincides with the one presented in [23]. All results obtained in the present work, including the deduction of the hydrodynamic limit (see Sect. 10), can be straightforward adapted to this general case. Nevertheless, in order to avoid too much notation, we choose $\delta = 1, \lambda = \beta = 0$. Also, since the creation of particles at one side has an analogous effect to the creation of particles at the other side, and the same holds for annihilation, the case studied in the present paper captures the essence of the macroscopic effect of the boundary dynamics. Moreover, the dynamic presented in this work has a natural interpretation as a flux of particles from a reservoir at the left-hand side of the bulk toward the one at the right-hand side.

4 Hydrostatic Limit

Definition 1 A sequence $\{\mu^N\}_{N\in\mathbb{N}}$ of probabilities on Ω_N is said to be *associated* to the profile $\rho_0 : [0,1] \to \mathbb{R}_+$ if, for any $\delta > 0$ and any continuous function $H : [0,1] \to \mathbb{R}$ the following limit holds:

$$\lim_{N\to\infty} \mu^N\Big[\,\eta \in \Omega_N : \Big|\frac{1}{N}\sum_{x=1}^{N-1} H(\tfrac{x}{N})\,\eta(x) - \int_0^1 H(u)\,\rho_0(u)\,du\Big| > \delta\,\Big] = 0\,. \quad (13)$$

Recall that φ^* denotes the radius of convergence of the partition function $Z(\varphi) = \sum_{k\geq 0}\frac{\varphi^k}{g(k)!}$. The average particle density corresponding to the fugacity φ is a function $R : [0, \varphi^*) \to \mathbb{R}_+$, given by

$$R(\varphi) = \frac{1}{Z(\varphi)} \sum_{k \geq 0} k \frac{\varphi^k}{g(k)!}. \tag{14}$$

As shown in [22, Sect. 2.3], R is strictly increasing, and, if we assume that

$$\lim_{\varphi \uparrow \varphi^*} Z(\varphi) = \infty,$$

then the range of R is all $\mathbb{R}_+$, i.e, $\lim_{\varphi \uparrow \varphi^*} R(\varphi) = \infty$. Therefore, the inverse of R is well defined.

$$\text{Let } \Phi : \mathbb{R}_+ \to [0, \varphi^*) \text{ be the inverse function of } R. \tag{15}$$

Definition 2 For a continuous function $\rho_0 : [0, 1] \to \mathbb{R}_+$, denote by $\nu^N_{\rho_0(\cdot)}$ the product measure with slowly varying parameter associated to ρ_0, this is the product measure on Ω_N with marginals given by

$$\nu^N_{\rho_0(\cdot)}\{\eta : \eta(x) = k\} = \frac{1}{Z(\Phi(\rho_0(\frac{x}{N})))} \frac{\Phi(\rho_0(\frac{x}{N}))^k}{g(k)!}, \quad \text{for } k \geq 0 \text{ and } x \in I_N. \tag{16}$$

From (14), we have

$$E_{\nu^N_{\rho_0(\cdot)}}[\eta(x)] = \rho_0(\tfrac{x}{N}), \quad \text{for all } x \in I_N. \tag{17}$$

The sequence $\{\nu^N_{\rho_0(\cdot)}\}_{N \in \mathbb{N}}$ is a particular case of a sequence of probabilities associated to the profile ρ_0 in the sense of Definition 1, as stated in Proposition 1. To prove this, we begin with the following lemma.

Lemma 2 *If $\rho_0 : [0, 1] \to \mathbb{R}_+$ is a continuous profile, then for each positive integer ℓ,*

$$\sup_N \sup_{x \in I_N} E_{\nu^N_{\rho_0(\cdot)}}[(\eta(x))^\ell] < \infty.$$

Proof First of all, note that $E_{\nu^N_{\rho_0(\cdot)}}[(\eta(x))^\ell] = R_\ell(\Phi(\rho_0(\frac{x}{N})))$, where R_ℓ is defined for $\varphi \in [0, \varphi^*)$ as $R_\ell(\varphi) = \frac{1}{Z(\varphi)} \sum_{k \geq 0} k^\ell \frac{\varphi^k}{g(k)!}$. The function $\Phi = R^{-1}$ is strictly increasing and $\lim_{v \to \infty} \Phi(v) = \varphi^*$. Denote by $\varphi^{**} = \sup_{u \in [0,1]} \Phi(\rho_0(u))$. Since ρ_0 is bounded, we have $\varphi^{**} < \varphi^*$. Therefore,

$$\sup_N \sup_{x \in I_N} E_{\nu^N_{\rho_0(\cdot)}}[(\eta(x))^\ell] = \sup_N \sup_{x \in I_N} R_\ell(\Phi(\rho_0(x/N))) \leq \sup_{0 \leq \varphi \leq \varphi^{**}} R_\ell(\varphi).$$

In order to conclude that the last expression above is finite we observe that the function R_ℓ is analytic on $[0, \varphi^*)$. To see this, we write $R_\ell(\varphi) = \frac{A_\ell(\varphi)}{Z(\varphi)}$, where A_ℓ is defined inductively by $A_0(\varphi) = Z(\varphi)$ and $A_n(\varphi) = \varphi A'_{n-1}(\varphi)$.

Proposition 1 *If $\rho_0 : [0,1] \to \mathbb{R}_+$ is continuous, then the product measure $\nu^N_{\rho_0(\cdot)}$ defined in (16) is associated to the profile ρ_0 in the sense of Definition 1.*

Proof Fix a continuous test function H. Observing that

$$\frac{1}{N}\sum_{x=1}^{N-1} H(\tfrac{x}{N})\,\rho_0(\tfrac{x}{N}) \to \int_0^1 H(u)\rho_0(u)du,$$

it is enough to show that, for each $\delta > 0$,

$$\nu^N_{\rho_0(\cdot)}\left[\eta : \left|\frac{1}{N}\sum_{x=1}^{N-1} H(\tfrac{x}{N})[\eta(x) - \rho_0(\tfrac{x}{N})]\right| > \delta\right] \tag{18}$$

goes to zero as $N \to \infty$. By Chebyshev's inequality, (17) and independence, the expression in (18) is bounded above by

$$\frac{1}{\delta^2}\frac{1}{N^2}\sum_{x=1}^{N-1} H^2(\tfrac{x}{N})E_{\nu^N_{\rho_0(\cdot)}}\left[(\eta(x) - \rho_0(\tfrac{x}{N}))^2\right] \le \frac{1}{\delta^2}\frac{1}{N^2}\sum_{x=1}^{N-1} H^2(\tfrac{x}{N})E_{\nu^N_{\rho_0(\cdot)}}\left[\eta(x)^2\right].$$

By Lemma 2 and since H is bounded, there exists some constant C such that $H^2(\frac{x}{N})E_{\nu^N_{\rho_0(\cdot)}}\left[\eta(x)^2\right] < C$ for every N and $x \in I_N$. Therefore, the right-hand side of the last displayed inequality goes to 0 when $N \to \infty$.

Since we have the explicit formula for the fugacity profile of the invariant measure $\bar{\nu}^N$, it is straightforward to obtain, in terms of the function R, an expression for the stationary density profile $\bar{\rho} : [0,1] \to \mathbb{R}_+$. Such result is usually called *hydrostatic limit*. Recalling Remark 3, note that, when $\theta = 1$, the invariant measure $\bar{\nu}^N$ satisfies

$$\bar{\nu}^N\{\eta : \eta(x) = k\} = \nu^N_{\bar{\rho}(\cdot)}\{\eta : \eta(x+1) = k\}, \tag{19}$$

where $\bar{\rho}(u) = R(\alpha(2-u))$. Also, when $\theta > 1$, $\varphi^N(x) - \alpha$ goes to zero uniformly in $x \in I_N$, as $N \to \infty$. Therefore, the next result is derived following the lines of the proof of Proposition 1.

Proposition 2 (Hydrostatic Limit) *Let $\bar{\nu}^N$ be the invariant measure in Ω_N for the Markov process with infinitesimal generator L_N. Then the sequence $\bar{\nu}^N$ is associated to the profile $\bar{\rho} : [0,1] \to \mathbb{R}_+$ given by*

$$\bar{\rho}(u) = \begin{cases} R(\alpha(2-u)), & \text{if } \theta = 1, \\ R(\alpha), & \text{if } \theta > 1, \end{cases} \tag{20}$$

for all $u \in [0,1]$.

Notice that the linear fugacity profile does not imply a linear density profile, except in the special case of non-interacting particles where $g(k) = k$.

5 Attractiveness

This small section is devoted to recall the essential property of attractiveness for the zero-range process.

Consider in Ω_N the partial order: $\eta \leq \xi$ if and only if $\eta(x) \leq \xi(x)$ for every $x \in I_N$. A function $f : \Omega_N \to \mathbb{R}$ is called monotone if $f(\eta) \leq f(\xi)$ for all $\eta \leq \xi$. This partial order extends to measures on Ω_N. We say that

$$\mu_1 \leq \mu_2, \quad \text{if} \quad \int f d\mu_1 \leq \int f d\mu_2, \tag{21}$$

for all monotone functions $f : \Omega_N \to \mathbb{R}$.

An interacting particle system $\{\eta_t\}_{t\geq 0}$ is said to be attractive if its semigroup $S(t)$, defined by $S(t)f(\eta) = \mathbb{E}_\eta [f(\eta_t)]$, preserves the partial order:

$$\mu_1 \leq \mu_2 \quad \Rightarrow \quad \mu_1 S(t) \leq \mu_2 S(t),$$

for all $t \geq 0$. Here $\mathbb{E}_\eta [f(\eta_t)]$ stands for the expectation of $f(\eta_t)$ when the process starts at $\eta(0) = \eta$.

It is well known, see [22, Theorem 2.5.2], that the zero-range process is attractive if g is non decreasing.

6 Tightness

Let us denote by $\{\eta_t = \eta_t^N : t \geq 0\}$ the continuous-time Markov process on Ω_N with generator $N^2 L_N$. Let $\mathscr{M}_+$ be the space of positive measures on $[0, 1]$ endowed with the weak topology, and denote by $\pi^N : \Omega_N \to \mathscr{M}_+$ the function that associates to each configuration η the measure obtained by assigning mass $1/N$ to each particle:

$$\pi^N(\eta, du) = \frac{1}{N} \sum_{x=1}^{N-1} \eta(x) \delta_{\frac{x}{N}}(du),$$

where δ_u denotes the Dirac mass at u. Thus, the empirical process $\pi^N(\eta_t)$ is a Markov process in the space $\mathscr{M}_+$. By abuse of notation, in this section we will simply write π_t^N instead of $\pi^N(\eta_t)$. For a function $G : [0, 1] \to \mathbb{R}$, we denote by $\langle \pi_t^N, G \rangle$ the integral of G with respect to the measure π_t^N:

$$\langle \pi_t^N, G \rangle = \frac{1}{N} \sum_{x \in I_N} G(\tfrac{x}{N}) \eta_t(x).$$

For a measure μ^N on Ω^N we denote by $\mathbb{P}_{\mu^N}$ the probability on $\mathscr{D}([0,T],\Omega_N)$, the Skorohod space of càdlàg trajectories, corresponding to the jump process $\{\eta_t : t \geq 0\}$ with generator $N^2 L_N$ and initial distribution μ^N. Expectations with respect to $\mathbb{P}_{\mu^N}$ will be denoted by $\mathbb{E}_{\mu^N}$. We denote by Q^N the probability on $\mathscr{D}([0,T],\mathscr{M}_+)$ defined by $Q^N = \mathbb{P}_{\mu^N}(\pi^N)^{-1}$.

In the next proposition we state the tightness of the sequence $\{Q^N\}_{N\geq 0}$ under the hypothesis

$$g(\cdot) \text{ is non decreasing,} \tag{22}$$

which implies attractiveness of the process.

The conservation of particles is an extensively used property in the proof of tightness for the classical zero-range process in the torus, together with a hypothesis that controls the relative entropy of the initial distribution μ^N with respect to the invariant measure; see [22, Lemma 5.1.5]. Since we do not have conservation in our case, a different approach is necessary. Instead of a relative entropy hypothesis, we assume

$$\mu^N \leq \bar{\nu}^N, \tag{23}$$

in the sense of (21), where $\bar{\nu}^N$ is the invariant measure. Hypothesis (23), along with attractiveness, provide us a way to control the number of particles in the system, as time evolves.

As a consequence of [22, Lemma 2.3.5] the limitation (23) holds if, for instance, μ^N is a product measure of the form (7) associated to a fugacity function bounded above by the fugacity of the stationary measure obtained in (9).

Tightness of the sequence $\{Q^N\}_{N\geq 0}$ is also true if we require that the function g is bounded, instead of the hypothesis (22) and (23). See Remark 6 for more details.

Proposition 3 *Let us consider $\theta \geq 1$. Suppose that the rate function g satisfies (22). Assume that the sequence $\{\mu^N\}_{N\in\mathbb{N}}$ is associated to an integrable initial profile $\rho_0 : [0,1] \to \mathbb{R}_+$, in the sense of (13) and satisfies (23). Then the sequence of measures $\{Q^N\}_{N\geq 0}$ is tight.*

Remark 5 Because of assumption (23), the profile ρ_0 in the above proposition needs to be bounded above by the profile $\bar{\rho}$ given in (20). A natural sequence $\{\mu^N\}_{N\in\mathbb{N}}$ satisfying the hypothesis is the sequence $\nu^N_{\rho_0(\cdot)}$ of product measures with slowly varying parameter associated to a profile $\rho_0 : [0,1] \to \mathbb{R}_+$, such that $\rho_0(u) + \varepsilon \leq \bar{\rho}(u)$ for all $u \in [0,1]$, for some $\varepsilon > 0$.

Proof of Proposition 3 will be postponed to Sect. 6.2. We will introduce now the related martingales of the process studied in this work, which will be very important not only in tightness as in the whole proof of hydrodynamic limit as well.

6.1 Related Martingales

For $G \in C^2[0,1]$, the set of twice continuously differentiable functions in $[0,1]$, the process M_t^G, defined as

$$M_t^G = \langle \pi_t^N, G \rangle - \langle \pi_0^N, G \rangle - \int_0^t N^2 L_N \langle \pi_s^N, G \rangle ds, \tag{24}$$

is a martingale. Recalling the definition of the generator (2), we write

$$\begin{aligned} N^2 L_N \langle \pi_s^N, G \rangle = & \frac{1}{N} \sum_{x=2}^{N-2} g(\eta_s(x)) \Delta_N G\left(\tfrac{x}{N}\right) \\ & + g(\eta_s(1)) \nabla_N^+ G\left(\tfrac{1}{N}\right) - g(\eta_s(N-1)) \nabla_N^- G\left(\tfrac{N-1}{N}\right) \\ & + \frac{\alpha}{N^{\theta-1}} G\left(\tfrac{1}{N}\right) - \frac{g(\eta_s(N-1))}{N^{\theta-1}} G\left(\tfrac{N-1}{N}\right), \end{aligned} \tag{25}$$

where

$$\begin{aligned} \Delta_N G\left(\tfrac{x}{N}\right) &= N^2 \left[G\left(\tfrac{x+1}{N}\right) + G\left(\tfrac{x-1}{N}\right) - 2G\left(\tfrac{x}{N}\right) \right], \\ \nabla_N^+ G(\tfrac{x}{N}) &= N \left[G(\tfrac{x+1}{N}) - G(\tfrac{x}{N}) \right], \\ \nabla_N^- G(\tfrac{x}{N}) &= N \left[G(\tfrac{x}{N}) - G(\tfrac{x-1}{N}) \right]. \end{aligned} \tag{26}$$

The quadratic variation of the martingale M_t^G is

$$\langle M^G \rangle_t = \int_0^t \left[N^2 L_N \langle \pi_s^N, G \rangle^2 - 2N^2 \langle \pi_s^N, G \rangle L_N \langle \pi_s^N, G \rangle \right] ds. \tag{27}$$

After standard calculations we can see that $\langle M^G \rangle_t = \int_0^t B^N(s) ds$, where

$$\begin{aligned} B^N(s) = & \sum_{x=1}^{N-1} \sum_{y \in \{x-1, x+1\} \cap I_N} g(\eta_s(x)) [G(\tfrac{y}{N}) - G(\tfrac{x}{N})]^2 \\ & + \tfrac{\alpha}{N^\theta} G^2(\tfrac{1}{N}) + \tfrac{g(\eta_s(N-1))}{N^\theta} G^2(\tfrac{N-1}{N}). \end{aligned} \tag{28}$$

6.2 Proof of Tightness

By [22, Proposition 4.1.7], to prove Proposition 3 it is sufficient to show the tightness of the measures corresponding to the real processes $\langle \pi_t^N, G \rangle$ for every G in $C^2([0,1])$. By Aldous criterion, is therefore sufficient to show that the following conditions are satisfied:

Condition 1 For every $t \in [0, T]$,

$$\lim_{A\to\infty} \limsup_{N\to\infty} \mathbb{P}_{\mu^N} \left[\frac{1}{N} \sum_{x=1}^{N-1} \eta_t(x) \geq A \right] = 0.$$

Condition 2 For every $\delta > 0$,

$$\lim_{\gamma\to 0} \limsup_{N\to\infty} \sup_{\substack{\tau\in\mathfrak{T}_T \\ \omega\leq\gamma}} \mathbb{P}_{\mu^N} \left[\left| \frac{1}{N} \sum_{x=1}^{N-1} G(\tfrac{x}{N})\eta_{\tau+\omega}(x) - \frac{1}{N} \sum_{x=1}^{N-1} G(\tfrac{x}{N})\eta_\tau(x) \right| > \delta \right] = 0,$$

where $\mathfrak{T}_T$ is the family of all stopping times bounded by T.

Proof of Condition 1

For $\eta \in \mathscr{D}([0, T], \Omega_N)$ define

$$Y_t(\eta) = \text{number of particles created up to time } t. \tag{29}$$

We have the following natural bound

$$\sum_{x=1}^{N-1} \eta_t(x) \leq \sum_{x=1}^{N-1} \eta_0(x) + Y_t, \tag{30}$$

and then

$$\begin{aligned} \mathbb{P}_{\mu^N} \left[\frac{1}{N} \sum_{x=1}^{N-1} \eta_t(x) \geq A \right] &\leq \mathbb{P}_{\mu^N} \left[\frac{1}{N} \sum_{x=1}^{N-1} \eta_0(x) \geq \frac{A}{2} \right] + \mathbb{P}_{\mu^N} \left[\frac{1}{N} Y_t \geq \frac{A}{2} \right] \\ &=: A_N + B_N. \end{aligned}$$

Not that $\lim_{A\to\infty} \limsup_{N\to\infty} A_N = 0$, since μ^N is associated to and integrable profile ρ_0. On the other hand, since the process is accelerated by N^2, under $\mathbb{P}_{\mu^N}$, Y_t is a Poisson process with intensity $N^{2-\theta}\alpha$, and then

$$B_N \leq \frac{2}{AN} \mathbb{E}_{\mu^N}[Y_t] = \frac{2}{AN} \cdot N^{2-\theta}\alpha t \leq \frac{2\alpha t}{A},$$

which goes to zero when $A \to \infty$.

Proof of Condition 2

By (24), it is enough to show that

Condition 2.1 For every $\delta > 0$,

$$\lim_{\gamma\to 0}\limsup_{N\to\infty}\sup_{\substack{\tau\in\mathfrak{T}_T\\ \omega\le\gamma}}\mathbb{P}_{\mu^N}\left[\left|\int_\tau^{\tau+\omega} N^2 L_N\langle\pi_s^N, G\rangle ds\right| > \delta\right] = 0.$$

Condition 2.2 For every $\delta > 0$,

$$\lim_{\gamma\to 0}\limsup_{N\to\infty}\sup_{\substack{\tau\in\mathfrak{T}_T\\ \omega\le\gamma}}\mathbb{P}_{\mu^N}\left[\left|M_{\tau+\omega}^G - M_\tau^G\right| > \delta\right] = 0.$$

By (25), to show Condition 2.1 it is sufficient to show that, for all $\delta > 0$

$$\lim_{\gamma\to 0}\limsup_{N\to\infty}\sup_{\substack{\tau\in\mathfrak{T}_T\\ \omega\le\gamma}}\mathbb{P}_{\mu^N}\left[\left|\int_\tau^{\tau+\omega}\frac{1}{N}\sum_{x=2}^{N-2} g(\eta_s(x))\Delta_N G(\tfrac{x}{N})ds\right| > \delta\right] = 0 \tag{31}$$

$$\lim_{\gamma\to 0}\limsup_{N\to\infty}\sup_{\substack{\tau\in\mathfrak{T}_T\\ \omega\le\gamma}}\mathbb{P}_{\mu^N}\left[\left|\int_\tau^{\tau+\omega} g(\eta_s(1))\nabla_N^+ G(\tfrac{1}{N})ds\right| > \delta\right] = 0 \tag{32}$$

$$\lim_{\gamma\to 0}\limsup_{N\to\infty}\sup_{\substack{\tau\in\mathfrak{T}_T\\ \omega\le\gamma}}\mathbb{P}_{\mu^N}\left[\left|\int_\tau^{\tau+\omega} g(\eta_s(N-1))\nabla_N^- G(\tfrac{N-1}{N})ds\right| > \delta\right] = 0 \tag{33}$$

$$\lim_{\gamma\to 0}\limsup_{N\to\infty}\sup_{\substack{\tau\in\mathfrak{T}_T\\ \omega\le\gamma}}\mathbb{P}_{\mu^N}\left[\left|\int_\tau^{\tau+\omega}\frac{\alpha}{N^{\theta-1}} G(\tfrac{1}{N})ds\right| > \delta\right] = 0 \tag{34}$$

$$\lim_{\gamma\to 0}\limsup_{N\to\infty}\sup_{\substack{\tau\in\mathfrak{T}_T\\ \omega\le\gamma}}\mathbb{P}_{\mu^N}\left[\left|\int_\tau^{\tau+\omega}\frac{g(\eta_s(N-1))}{N^{\theta-1}} G(\tfrac{N-1}{N})ds\right| > \delta\right] = 0 \tag{35}$$

Condition (34) is immediate, since $G \in C^2([0,1])$, and then it is bounded.

Proof (*Proof of* (31)) Since G is of class C^2 and g increases at most linearly (recall hypothesis (1)), the integral in (31) is bounded by

$$C(g^*, G)\int_\tau^{\tau+\omega}\frac{1}{N}\sum_{x=2}^{N-2}\eta_s(x)ds.$$

By (30), this is bounded above by

$$C(g^*, G)\left[\frac{\omega}{N}\sum_{x=1}^{N-1}\eta_0(x) + \int_\tau^{\tau+\omega}\frac{1}{N}Y_s ds\right].$$

Then, observing that Y_s is non decreasing, it is enough to show that, for any $\delta > 0$

$$\lim_{\omega\to 0}\limsup_{N\to\infty}\mathbb{P}_{\mu^N}\left[\frac{\omega}{N}\sum_{x=1}^{N-1}\eta_0(x) > \delta\right] = 0 \tag{36}$$

and

$$\lim_{\omega\to 0}\limsup_{N\to\infty}\mathbb{P}_{\mu^N}\left[\frac{\omega}{N}Y_{T+\omega}>\delta\right]=0. \tag{37}$$

As in the proof of Condition 1, (36) holds because μ^N is associated to an integrable profile ρ_0, and (37) follows from

$$\mathbb{P}_{\mu^N}\left[\frac{\omega}{N}Y_{T+\omega}>\delta\right]\leq\frac{\omega}{\delta N}\mathbb{E}_{\mu^N}\left[Y_{T+\omega}\right]=\frac{\omega\alpha(T+\omega)}{\delta N^{\theta-1}}\leq\frac{\omega\alpha(T+\omega)}{\delta},$$

which goes to zero as $\omega\to 0$.

For the proof of (32), (33) and (35) we will use the following lemma.

Lemma 3 *Under the conditions (22) and (23), for every $s\geq 0$ and $x\in I_N$, it holds*

$$\mathbb{E}_{\mu^N}\left[g(\eta_s(x))\right]\leq\varphi^N(x), \tag{38}$$

$$\mathbb{E}_{\mu^N}\left[g(\eta_s(x))^2\right]\leq g^*\varphi^N(x)+(\varphi^N(x))^2. \tag{39}$$

And consequently, for $\ell=1,2$,

$$\mathbb{E}_{\mu^N}\left[g(\eta_s(x))^\ell\right]\leq C(\alpha), \tag{40}$$

where $C(\alpha)$ is a positive constant that only depends on α.

Remark 6 In the proof of Proposition 3, the hypotheses (22) and (23) are only used in Lemma 3 above. Since this result is trivial when g is bounded, in this case such hypotheses are not needed to prove tightness.

Proof For every $x\in I_N$, by (22) the function $h_x:\Omega_N\to\mathbb{R}$, given by $h_x(\eta)=[g(\eta(x))]^\ell$, is monotone. So, by attractiveness and hypothesis (23), we have

$$\mathbb{E}_{\mu^N}\left[g(\eta_s(x))^\ell\right]\leq\mathbb{E}_{\bar{\nu}^N}\left[g(\eta_s(x))^\ell\right]=\mathbb{E}_{\bar{\nu}^N}\left[g(\eta_0(x))^\ell\right]=E_{\bar{\nu}^N}\left[g(\eta(x))^\ell\right].$$

To conclude the proof of (38), we recall that $E_{\bar{\nu}^N}\left[g(\eta(x))\right]=\varphi^N(x)$.

For the proof of (39), we write

$$\begin{aligned}E_{\bar{\nu}^N}\left[g(\eta(x))^2\right]&=\frac{1}{Z(\varphi^N(x))}\sum_{k=0}^{\infty}g(k)^2\frac{\varphi^N(x)^k}{g(k)!}\\&=\frac{\varphi^N(x)}{Z(\varphi^N(x))}\sum_{k=1}^{\infty}g(k)\frac{\varphi^N(x)^{k-1}}{g(k-1)!}.\end{aligned}$$

By (1), we have that

$$g(k)\leq g^*+g(k-1).$$

Then

$$E_{\bar{\nu}^N}\left[g(\eta(x))^2\right] \leq g^*\varphi^N(x) + \frac{\varphi^N(x)}{Z(\varphi^N(x))}\sum_{k=1}^{\infty} g(k-1)\frac{\varphi^N(x)^{k-1}}{g(k-1)!}$$
$$= g^*\varphi^N(x) + \frac{\varphi^N(x)^2}{Z(\varphi^N(x))}\sum_{k=2}^{\infty}\frac{\varphi^N(x)^{k-2}}{g(k-2)!}$$
$$= g^*\varphi^N(x) + \varphi^N(x)^2.$$

Since φ^N is a linear function satisfying $\varphi^N(N-1) = \alpha$ and, for every $\theta \geq 1$, $\varphi^N(1) \leq 2\alpha$, the proof Lemma 3 is concluded.

Proof (*Proof of* (32), (33) *and* (35)) Since G is of class C^2, the integrals in (32), (33) and (35) are bounded above by

$$C(g^*, G)\int_{\tau}^{\tau+\omega} g(\eta_s(x))ds,$$

for $x = 1$ or $x = N-1$.

For all $x \in I_N$, we have

$$\mathbb{P}_{\mu^N}\left[\int_{\tau}^{\tau+\omega} g(\eta_s(x))ds > \delta\right] \leq \frac{1}{\delta}\mathbb{E}_{\mu^N}\left[\int_{\tau}^{\tau+\omega} g(\eta_s(x))ds\right].$$

By Cauchy–Schwarz's inequality

$$\mathbb{E}_{\mu^N}\left[\int_{\tau}^{\tau+\omega} g(\eta_s(x))ds\right] = \mathbb{E}_{\mu^N}\left[\int_0^T \mathbf{1}_{[\tau,\tau+\omega]}(s)g(\eta_s(x))ds\right]$$
$$\leq \sqrt{\omega}\left[\mathbb{E}_{\mu^N}\left[\int_0^T g(\eta_s(x))^2 ds\right]\right]^{1/2}$$
$$= \sqrt{\omega}\left[\int_0^T \mathbb{E}_{\mu^N}\left[g(\eta_s(x))^2\right]ds\right]^{1/2}.$$

Then, using Lemma 3, we obtain

$$\mathbb{E}_{\mu^N}\left[\int_{\tau}^{\tau+\omega} g(\eta_s(x))ds\right] \leq (\omega T C(\alpha))^{1/2}. \tag{41}$$

Sending $\omega \to 0$, we conclude the proof.

Proof (*Proof of Condition 2.2*) Using Chebychev's inequality and the explicit formula for the quadratic variation given in (27), we have

$$\mathbb{P}_{\mu^N}\left[\left|M^G_{\tau+\omega} - M^G_\tau\right| > \delta\right] \leq \frac{1}{\delta^2}\mathbb{E}_{\mu^N}\left[(M^G_{\tau+\omega} - M^G_\tau)^2\right]$$
$$= \frac{1}{\delta^2}\mathbb{E}_{\mu^N}\left[\int_\tau^{\tau+\omega} B^N(s)ds\right], \tag{42}$$

where $B^N(s)$ was defined in (28).

Using that G and its derivative are bounded functions, and then, using (41), we can see that (42) is bounded above by $\frac{C\omega}{N}$, where C is a constant that does not depends on N and ω. Thus the proof is concluded.

Remark 7 Considering a model in which a particle is removed from the system throughout site $N-1$ with rate $g(\eta(N-1))$ instead of the slow boundary assumption $\frac{g(\eta(N-1))}{N^\theta}$ made in this work, our proof can be adapted and tightness will also hold if we assume that particles are inserted into the system at site 1 with rate $\frac{\alpha}{N^\theta}$ with $\theta > 1$. In this case the fugacity profile φ^N goes to zero uniformly as $N \to \infty$.

7 Limit Points are Concentrated on Absolutely Continuous Measures

The next step to characterize the limit points of $\{Q^N\}$ is to show that they are concentrated on trajectories of measures that are absolutely continuous with respect to the Lebesgue measure.

Next lemma states that for any sequence μ^N of probabilities on Ω_N bounded by the invariant measure $\bar{\nu}^N$, the corresponding sequence of empirical measures, obtained via $\pi^N : \Omega^N \to \mathcal{M}_+$, if converges, must converge to an absolutely continuous measure with respect to Lesbegue.

Lemma 4 *Let μ^N be a sequence of probabilities on Ω_N bounded by the invariant measure $\bar{\nu}^N$, i.e., $\mu^N \leq \bar{\nu}^N$. Let R_{μ^N} be the probability measure $\mu^N(\pi^N)^{-1}$ on $\mathcal{M}_+$, defined by $R_{\mu^N}(\mathcal{A}) = \mu^N\{\eta : \pi^N(\eta) \in \mathcal{A}\}$ for every Borel subset $\mathcal{A} \in \mathcal{M}_+$. Then, all limit points R^* of the sequence R_{μ^N} are concentrated on absolutely continuous measures with respect to the Lebesgue measure:*

$$R^*[\pi : \pi(du) = \rho(u)du] = 1.$$

Proof Let R^* be a limit point of the sequence R_{μ^N}. Recall from (20) that we denoted by $\bar{\rho} : [0,1] \to \mathbb{R}_+$ the density profile associated to the sequence of invariant measures $\bar{\nu}^N$. Fix some $\varepsilon > 0$, it is enough to prove that, for every non negative continuous function $G : [0,1] \to \mathbb{R}$,

$$R^*\left[\pi : \langle \pi, G\rangle \leq \int_0^1 G(u)(\bar{\rho}(u) + \varepsilon)du\right] = 1.$$

Let $R_{\mu^{N_k}}$ be a subsequence converging to R^*, then

$$
\begin{aligned}
&R^*\left[\pi : \langle \pi, G\rangle \le \int_0^1 G(u)(\bar\rho(u)+\varepsilon)du\right] \\
&\quad \ge \limsup_{k\to\infty} R_{\mu^{N_k}}\left[\pi : \langle \pi, G\rangle \le \int_0^1 G(u)(\bar\rho(u)+\varepsilon)du\right] \\
&\quad = \limsup_{k\to\infty} \mu^{N_k}\left[\eta : \langle \pi^N(\eta), G\rangle \le \int_0^1 G(u)(\bar\rho(u)+\varepsilon)du\right].
\end{aligned} \tag{43}
$$

Since $\mu^N \le \bar\nu^N$, by [24, Theorem 2.2.4] there exist a coupling $\bar\mu^N$, i.e, a probability measure on $\Omega_N \times \Omega_N$, with marginals μ^N and $\bar\nu^N$ respectively, such that

$$
\bar\mu^N\left[(\eta,\xi) : \eta \le \xi\right] = 1,
$$

and consequently

$$
\bar\mu^N\left[(\eta,\xi) : \langle \pi^N(\eta), G\rangle \le \langle \pi^N(\xi), G\rangle\right] = 1. \tag{44}
$$

By (43) and (44),

$$
\begin{aligned}
&R^*\left[\pi : \langle \pi, G\rangle \le \int_0^1 G(u)(\bar\rho(u)+\varepsilon)du\right] \\
&\quad \ge \limsup_{k\to\infty} \bar\nu^{N_k}\left[\eta : \langle \pi^N(\eta), G\rangle \le \int_0^1 G(u)(\bar\rho(u)+\varepsilon)du\right] = 1,
\end{aligned} \tag{45}
$$

by Proposition 2.

Assuming that the rate function g is non decreasing, by attractiveness, the semigroup $S^N(t)$ associated to the generator $N^2 L_N$ preserves the partial order $\mu^N \le \bar\nu^N$, that is, $\mu^N S^N(t) \le \bar\nu^N S^N(t) = \bar\nu^N$ for each $0 \le t \le T$. Therefore, Lemma 4, when applied to the marginal at time t of the measure $Q^N = \mathbb{P}_{\mu^N}(\pi^N)^{-1}$, which is $\mu^N S^N(t)$, says that for every limit point Q^*, and every $t \in [0,T]$,

$$
Q^*\left[\pi : \pi_t(du) = \rho_t(u)du\right] = 1.
$$

To short notations, we write $\rho_t(u)$ instead of $\rho(t,u)$. Now consider the functional $J : \mathscr{M}^+ \to \mathbb{R}_+ \cup \{\infty\}$ defined by

$$
J(\pi) = \begin{cases} 1, & \text{if } \pi(du) = \rho(u)du, \\ \infty, & \text{otherwise.} \end{cases}
$$

By Fubini's lemma,

$$
E_{Q^*}\left[\int_0^T J(\pi_t)dt\right] = \int_0^T E_{Q^*}\left[J(\pi_t)\right]dt = T.
$$

In particular, changing, if necessary, $\pi_t(du)$ in a time set of measure zero, all limit points Q^* are concentrated on absolutely continuous trajectories:

$$Q^*[\pi_\cdot : \pi_t(du) = \rho_t(u)du, \quad 0 \le t \le T] = 1.$$

8 Hydrodynamic Limit

In this section we will present the hydrodynamic limit that we expect in this model, together with the structure of the proof. Since some elements of the proof are not yet completed, we present it as a conjecture.

Let us recall the hypotheses assumed in Sects. 6 and 7, that is, $\theta \ge 1$ and g is a non decreasing function with bounded variation, as stated in (1). Also recall that, for $T > 0$, $\mathbb{P}_{\mu^N}$ denotes the probability on the space $\mathscr{D}([0,T], \Omega_N)$ corresponding to the process $\{\eta_t : t \in [0,T]\}$ on Ω_N with infinitesimal generator $N^2 L_N$, where L_N is defined in (2).

Conjecture 1 (*Hydrodynamic limit*) Let $\{\mu^N\}_{N\in\mathbb{N}}$ be a sequence of probability measures on Ω_N, bounded by the invariant measure, i.e., $\mu^N \le \bar{\nu}^N$. Assume that the sequence $\{\mu^N\}_{N\in\mathbb{N}}$ is associated to a continuous profile[3] $\gamma : [0,1] \to \mathbb{R}_+$ in the sense of the Definition 1. Then, for all $t \in [0,T]$, for all continuous function $G : [0,1] \to \mathbb{R}$ and $\delta > 0$,

$$\lim_{N\to+\infty} \mathbb{P}_{\mu^N}\left[\eta_\cdot : \left|\frac{1}{N}\sum_{x\in I_N} G\left(\frac{x}{N}\right)\eta_t(x) - \int_0^1 G(u)\,\rho_t(u)\,du\right| > \delta\right] = 0,$$

where

- for $\theta = 1$, $\rho_t(u)$ is a weak solution of (47) with Robin boundary condition ($\kappa = 1$);
- for $\theta > 1$, $\rho_t(u)$ is a weak solution of (47) with Neumann boundary condition ($\kappa = 0$).

Before introducing the hydrodynamic equation (47), we need to define some function spaces. The bracket $\langle \cdot, \cdot \rangle$ means the inner product in $L^2[0,1]$ and $\|F\|_2^2 = \langle F, F\rangle$, for all $F \in L^2[0,1]$.

We advertise that, to short the notation, we write $\rho_t(u)$ and $G_s(u)$ instead of $\rho(t,u)$ and $G(s,u)$, respectively. The reader must not misunderstand this notation with the time derivative, denoted by ∂_s.

Definition 3 Let $\mathscr{H}^1(0,1)$ be the set of all locally summable functions $\xi : [0,1] \to \mathbb{R}$ such that there exists a function $\partial_u \xi \in L^2[0,1]$ satisfying

[3] As discussed in Remark 5. the assumption (23) naturally imposes the initial profile γ to be bounded above by the profile $\bar{\rho}$ of the hydrostatic limit, given in (20).

$$\langle \partial_u G, \xi \rangle = -\langle G, \partial_u \xi \rangle,$$

for all C^∞ function $G : (0, 1) \to \mathbb{R}$ with compact support.

Let $L^2(0, T; \mathscr{H}^1(0, 1))$ be the set of all measurable functions $\bar{\xi} : [0, T] \to L^2[0, 1]$ such that $\bar{\xi}_t \in \mathscr{H}^1(0, 1)$, for almost $t \in [0, T]$, and

$$\|\bar{\xi}\|^2_{L^2(0,T;\mathscr{H}^1(0,1))} := \int_0^T \{\|\bar{\xi}_t\|_2^2 + \|\partial_u \bar{\xi}_t\|_2^2\}\, dt < \infty. \tag{46}$$

Denote by $C^{1,2}([0, T] \times [0, 1])$ the set of real-valued functions defined on $[0, T] \times [0, 1]$ that are differentiable on the first variable and twice differentiable on the second variable.

Recall that the function $\Phi : \mathbb{R}_+ \to [0, \varphi^*)$ is the inverse function of R, defined in (14).

Definition 4 *(Hydrodynamic equation)* Let $\gamma : [0, 1] \to \mathbb{R}_+$ be a continuous function. Consider the parameter κ equal to 0 or 1. We say that a function $\rho : [0, T] \times [0, 1] \to \mathbb{R}_+$ is a weak solution of the equation

$$\begin{cases} \partial_t \rho_t(u) = \Delta \Phi(\rho_t(u)), & \text{for } u \in (0, 1) \text{ and } t \in (0, T], \\ \partial_u \Phi(\rho_t(0)) = -\kappa\, \alpha, & \text{for } t \in (0, T], \\ \partial_u \Phi(\rho_t(1)) = -\kappa\, \Phi(\rho_t(1)), & \text{for } t \in (0, T], \\ \rho_0(u) = \gamma(u), & \text{for } u \in [0, 1], \end{cases} \tag{47}$$

if $\Phi(\rho) \in L^2(0, T; \mathscr{H}^1(0, 1))$ and

$$\begin{aligned} \langle \rho_t, G_0 \rangle - \langle \gamma, G_0 \rangle - \int_0^t \big\{ \langle \rho_s, \partial_s G_s \rangle + \langle \Phi(\rho_s), \Delta G_s \rangle \big\}\, ds \\ - \int_0^t \big\{ \Phi(\rho_s(0)) \partial_u G_s(0) - \Phi(\rho_s(1)) \partial_u G_s(1) \big\}\, ds \\ - \kappa \int_0^t \big\{ \alpha G_s(0) - \Phi(\rho_s(1)) G_s(1) \big\}\, ds \;=\; 0\,, \end{aligned} \tag{48}$$

for all $t \in [0, T]$ and $G \in C^{1,2}([0, T] \times [0, 1])$.

- When $\kappa = 0$, we say that the PDE (47) has Neumann boundary condition;
- When $\kappa = 1$, we say that the PDE (47) has Robin boundary condition.

We consider the PDE (47) with more general boundary conditions in the Sect. 10, see Eq. (60).

Let us recall, from the beginning of Sect. 6, that Q^N denotes the probability on $\mathscr{D}([0, T], \mathscr{M}_+)$, corresponding to the empirical process $\{\pi_t^N : t \in [0, T]\}$.

Conjecture 2 As $N \to \infty$, the sequence of probabilities $\{Q^N\}_{N \in \mathbb{N}}$ converges weakly to Q, the probability measure on $\mathscr{D}([0, T], \mathscr{M}_+)$ that gives mass one to the trajectory $\pi_t(du) = \rho_t(u)du$, where $\rho : [0, T] \times [0, 1] \to \mathbb{R}$ is the weak solution of the

hydrodynamic equation (47), with $\kappa = 1$ if $\theta = 1$, and $\kappa = 0$ if $\theta > 1$. We call $\rho_t(u)$ the hydrodynamic profile.

Conjecture 1 is a consequence of the Conjecture 2. Since the hydrodynamic behaviour is described by Conjecture 1, it is not mandatory to get Conjecture 2 to understand the hydrodynamics. But the second conjecture gives more information about the asymptotic behaviour of the system, because it handles with the whole time-trajectory of the density of particles. Moreover, using the result stated in Conjecture 2 is possible to study the fluctuations and the large deviations of this convergence, completing the asymptotic characterization of the model.

The proof of Conjecture 2 may be divided into three steps.

The first step is to show tightness, which is done in Sect. 6. This implies that the sequence $\{Q^N\}_{N\in\mathbb{N}}$ has limit points.

The second step is the characterization of these limit points, which we split in two parts: The first part is the subject of Sect. 7, where we proved that the limit points of the sequence $\{Q^N\}$ are concentrated on trajectories of measures that are absolutely continuous with respect to the Lebesgue measure, so that for each t, $\pi_t(du) = \rho_t(u)du$ for some function $\rho : [0, T] \times [0, 1] \to \mathbb{R}_+$. The second part is to show that ρ is a solution of the corresponding hydrodynamic equation. This part we postpone to a future work, however, in the Sect. 9, we present some heuristics of this proof.

The third step, which will be also postponed to a future work, is to show the uniqueness of solution for the hydrodynamic equations. This uniqueness would guarantee that the sequence $\{Q^N\}$ has a unique limit point, and thus the proof of Conjecture 2 would be concluded.

9 Heuristics of the Hydrodynamic Equation

Let $\{\mu^N\}_{N\in\mathbb{N}}$ be a sequence of probability measures on Ω_N, bounded by the invariant measure, as stated in (23), and associated with to a continuous profile $\gamma : [0, 1] \to \mathbb{R}_+$ in the sense of Definition 1. Recall that $\{Q^N\}$ is a sequence of probabilities on $\mathscr{D}([0, T], \mathscr{M}_+)$ defined by $Q^N = \mathbb{P}_{\mu^N}(\pi^N)^{-1}$.

Let Q^* be a limit point of $\{Q^N\}$. In Sect. 7, we proved that Q^* is a probability measure on $\mathscr{D}([0, T], \mathscr{M}_+)$ which gives mass one to paths of absolutely continuous measures: $\pi_t(du) = \rho_t(u)du$. In this section we present some heuristics to obtain that $\rho_t(u)$ is a weak solution of the corresponding hydrodynamic equation. For this purpose, we will assume, *heuristically*, that

$$\left\langle \pi_s^N, H \right\rangle \to \int_0^1 H(u)\, \rho_s(u)\, du\,, \tag{49}$$

when $N \to \infty$, for all $s \in [0, T]$ and $H \in C[0, 1]$.

In order to prove that $\rho_t(u)$ satisfies the hydrodynamic equation, we evoke the Dynkin martingale, introduced in Sect. 6.1, M_t^G for $G \in C^2([0,1])$. Using (24) and (25), we rewrite this martingale as

$$\begin{aligned} M_t^G = &\langle \pi_t^N, G\rangle - \langle \pi_0^N, G\rangle - \int_0^t \frac{1}{N}\sum_{x=2}^{N-2} g(\eta_s(x))\Delta_N G\left(\tfrac{x}{N}\right) ds \\ &- \int_0^t \Big(g(\eta_s(1))\nabla_N^+ G\left(\tfrac{1}{N}\right) - g(\eta_s(N-1))\nabla_N^- G\left(\tfrac{N-1}{N}\right)\Big) ds \\ &- \int_0^t \Big(\frac{\alpha}{N^{\theta-1}} G\left(\tfrac{1}{N}\right) - \frac{g(\eta_s(N-1))}{N^{\theta-1}} G\left(\tfrac{N-1}{N}\right)\Big) ds. \end{aligned} \tag{50}$$

By the definition of $\Delta_N G$, $\nabla_N^+ G$ and $\nabla_N^- G$ in (26) and the fact that $G \in C^2([0,1])$, we can rewrite M_t^G as

$$\begin{aligned} &\langle \pi_t^N, G\rangle - \langle \pi_0^N, G\rangle - \int_0^t \frac{1}{N}\sum_{x=2}^{N-2} g(\eta_s(x))\Delta G\left(\tfrac{x}{N}\right) ds \\ &- \int_0^t \Big(g(\eta_s(1))\partial_u G(0) - g(\eta_s(N-1))\partial_u G(1)\Big) ds \\ &- \int_0^t \Big(\frac{\alpha}{N^{\theta-1}} G(0) - \frac{g(\eta_s(N-1))}{N^{\theta-1}} G(1)\Big) ds + \mathscr{R}_N^{1,\theta}(G,t), \end{aligned} \tag{51}$$

where $\mathbb{E}_{\mu^N}[\mathscr{R}_N^{1,\theta}(G,t)]$ goes to zero, as $N \to \infty$, for all $\theta \geq 1$, and uniformly on $t \in [0,T]$, because of Lemma 3 and Taylor's expansion. By (49), as $N \to \infty$,

$$\langle \pi_t^N, G\rangle - \langle \pi_0^N, G\rangle \to \langle \rho_t, G\rangle - \langle \rho_0, G\rangle .$$

Then we need to study the bulk and boundary terms of the expression (51). We start by the bulk term: $\int_0^t \frac{1}{N}\sum_{x=2}^{N-2} g(\eta_s(x))\Delta G\left(\frac{x}{N}\right) ds$. In order to do this, we will introduce some notation.

For $\varepsilon > 0$, consider the set

$$I_N^\varepsilon := \{1 + \varepsilon N, \ldots, N - 1 - \varepsilon N\}. \tag{52}$$

Above and in all text εN must be understood as $\lfloor \varepsilon N \rfloor$.

Then the bulk term becomes

$$\int_0^t \frac{1}{N}\sum_{x \in I_N^\varepsilon} g(\eta_s(x))\Delta G\left(\tfrac{x}{N}\right) ds + \mathscr{R}_{N,\varepsilon}^2(G,t), \tag{53}$$

where

$$\mathscr{R}^2_{N,\varepsilon}(G,t) = \int_0^t \frac{1}{N}\left(\sum_{x=2}^{\varepsilon N} g(\eta_s(x))\Delta G\left(\tfrac{x}{N}\right) + \sum_{x=N-\varepsilon N}^{N-2} g(\eta_s(x))\Delta G\left(\tfrac{x}{N}\right)\right) ds\,.$$

Using (40) from Lemma 3, we have $\mathbb{E}_{\mu^N}[\mathscr{R}^2_{N,\varepsilon}(G,t)] \le 2\varepsilon CT\|\Delta G\|_\infty$. Thus, $\mathbb{E}_{\mu^N}[\mathscr{R}^2_{N,\varepsilon}(G,t)]$ goes to zero, when $N \to \infty$ and $\varepsilon \to 0$. Adding and subtracting suitable terms, we can see that the integral in (53) is equal to

$$\int_0^t \frac{1}{N}\sum_{x\in I_N^\varepsilon} \Delta G\left(\tfrac{x}{N}\right)\frac{1}{\varepsilon N}\sum_{y=x+1}^{x+\varepsilon N} g(\eta_s(y))\,ds + \mathscr{R}^3_{N,\varepsilon}(G,t)\,, \tag{54}$$

where

$$\mathscr{R}^3_{N,\varepsilon}(G,t) = \int_0^t \frac{1}{N}\sum_{x\in I_N^\varepsilon}\left\{g(\eta_s(x)) - \frac{1}{\varepsilon N}\sum_{y=x+1}^{x+\varepsilon N} g(\eta_s(y))\right\}\Delta G\left(\tfrac{x}{N}\right)\,ds\,.$$

Changing variables $\mathscr{R}^3_{N,\varepsilon}(G,t)$ can be rewritten as

$$\begin{aligned}
&\int_0^t \frac{1}{N}\left\{\sum_{x\in I_N^\varepsilon} g(\eta_s(x))\Delta G\left(\tfrac{x}{N}\right) - \sum_{y\in I_N} g(\eta_s(y))\frac{1}{\varepsilon N}\sum_{z=1}^{\varepsilon N}\Delta G\left(\tfrac{y-z}{N}\right)\right\} ds\\
&= \int_0^t \frac{1}{N}\sum_{x\in I_N^\varepsilon} g(\eta_s(x))\left\{\Delta G\left(\tfrac{x}{N}\right) - \frac{1}{\varepsilon N}\sum_{z=1}^{\varepsilon N}\Delta G\left(\tfrac{x-z}{N}\right)\right\} ds\\
&\quad + \int_0^t \frac{1}{N}\sum_{x\in I_N\setminus I_N^\varepsilon} g(\eta_s(x))\frac{1}{\varepsilon N}\sum_{z=1}^{\varepsilon N}\Delta G\left(\tfrac{x-z}{N}\right)\,ds\,.
\end{aligned}$$

Then $\mathbb{E}_{\mu^N}[\mathscr{R}^3_{N,\varepsilon}(G,t)] \to 0$, as $N \to \infty$ and $\varepsilon \to 0$. To handle the integral term in (54), we use the function $\Phi : \mathbb{R}_+ \to [0,\varphi^*)$, which is the inverse function of R, defined in (14). We will need to introduce some more notation. Let $\overrightarrow{\eta}_s^{\varepsilon N}(x)$ be the empirical density in the box of size εN, which is given on, $x \in I_N^\varepsilon$, by

$$\overrightarrow{\eta}_s^{\varepsilon N}(x) = \frac{1}{\varepsilon N}\sum_{y=x+1}^{x+\varepsilon N}\eta_s(y)\,. \tag{55}$$

Then the integral term in (54) is equal to

$$\int_0^t \frac{1}{N}\sum_{x\in I_N^\varepsilon}\Delta G\left(\tfrac{x}{N}\right)\Phi(\overrightarrow{\eta}_s^{\varepsilon N}(x))\,ds + \mathscr{R}^4_{N,\varepsilon}(G,t)\,. \tag{56}$$

The last term above is the important expression:

$$\mathscr{R}^4_{N,\varepsilon}(G,t) = \int_0^t \frac{1}{N} \sum_{x \in I_N^\varepsilon} \Delta G\left(\tfrac{x}{N}\right) \left\{ \frac{1}{\varepsilon N} \sum_{y=x+1}^{x+\varepsilon N} g(\eta_s(y)) - \Phi(\overrightarrow{\eta}_s^{\varepsilon N}(x)) \right\} ds, \tag{57}$$

which to prove that it is negligible we need to evoke the following very important result:

Lemma 5 (Replacement lemma for the bulk)[4] *For every* $\delta > 0$,

$$\overline{\lim_{\varepsilon \to 0}} \, \overline{\lim_{N \to \infty}} \, \mathbb{P}_{\mu^N}\left[\eta_\cdot : \left| \mathscr{R}^4_{N,\varepsilon}(G,T) \right| > \delta \right] = 0,$$

where $\mathscr{R}^4_{N,\varepsilon}(G,t)$ *was defined in* (57).

Note that, $\overrightarrow{\eta}_s^{\varepsilon N}(x) = \langle \pi_s^N, \iota_\varepsilon^{x/N} \rangle$, where

$$\iota_\varepsilon^u(v) = \tfrac{1}{\varepsilon} \mathbf{1}_{(u,u+\varepsilon)}(v),$$

for $u, v \in [0,1]$. Then the integral in (56) can be rewritten as

$$\int_0^t \frac{1}{N} \sum_{x \in I_N^\varepsilon} \Delta G\left(\tfrac{x}{N}\right) \Phi\left(\langle \pi_s^N, \iota_\varepsilon^{x/N} \rangle\right) ds\,.$$

Since the function inside the summation above is integrable, it is possible to prove that the last integral is asymptotically (when $N \to \infty$ and $\varepsilon \to 0$) equal to

$$\int_0^t \int_0^1 \Delta G\,(u)\, \Phi\left(\langle \pi_s^N, \iota_\varepsilon^u \rangle\right) du\, ds\,.$$

By (49), we have that, for $u \in [0,1]$

$$\langle \pi_s^N, \iota_\varepsilon^u \rangle \to \int_0^1 \rho_s(v) \iota_\varepsilon^u(v)\, dv,$$

as $N \to \infty$. Finally, taking $\varepsilon \to 0$, the last integral converges to $\rho_s(u)$. Then the bulk term of the expression (51) converges to

$$\int_0^t \int_0^1 \Delta G(u) \Phi(\rho_s(u))\, du\, ds = \int_0^t \langle \Phi(\rho_s), \Delta G \rangle\, ds,$$

when $N \to \infty$ and $\varepsilon \to 0$.

In order to analyze the boundary terms of (51), we start by observing that the expectation with respect to the probability $\mathbb{P}_{\mu^N}$ of

[4] The proof of this lemma is a future work.

$$\int_0^t \Big(\frac{\alpha}{N^{\theta-1}} G(0) - \frac{g(\eta_s(N-1))}{N^{\theta-1}} G(1) \Big) ds,$$

goes to zero, as $N \to \infty$, in the case $\theta > 1$, because of Lemma 3. Then, when $\theta > 1$, we only need to analyze the term

$$-\int_0^t \Big(g(\eta_s(1)) \partial_u G(0) - g(\eta_s(N-1)) \partial_u G(1) \Big) ds. \tag{58}$$

In the case $\theta = 1$, rewriting the boundary terms of (51), we have

$$-\int_0^t \Big(g(\eta_s(1)) \partial_u G(0) - \alpha G(0) - g(\eta_s(N-1)) (\partial_u G(1) + G(1)) \Big) ds. \tag{59}$$

In both cases we need to replace $g(\eta_s(1))$ and $g(\eta_s(N-1))$ by the average of g in a box of size εN in a neighborhood of $x = 1$ or $x = N-1$ inside I_N, that is $\frac{1}{\varepsilon N} \sum_{y=2}^{1+\varepsilon N} g(\eta_s(y))$ and $\frac{1}{\varepsilon N} \sum_{y=N-1-\varepsilon N}^{N-2} g(\eta_s(y))$, respectively. Note that this is similar to what we did above in (54). The next step is to use the following replacement lemma with a suitable choice of f_1 and f_2.

Lemma 6 (Replacement lemma for the boundary)[5] *For $\theta \geq 1$ and for all continuous functions $f_i : [0,T] \to \mathbb{R}$, with $i = 1, 2$, and every $\delta > 0$, we have*

$$\overline{\lim_{\varepsilon \to 0}} \, \overline{\lim_{N \to \infty}} \, \mathbb{P}_{\mu^N} \Big[\eta. : \Big| \mathscr{R}^b_{N,\varepsilon}(f_1, f_2, T) \Big| > \delta \Big] = 0,$$

where

$$\mathscr{R}^b_{N,\varepsilon}(f_1, f_2, T) = \int_0^T f_1(s) \Big\{ \frac{1}{\varepsilon N} \sum_{y=2}^{1+\varepsilon N} g(\eta_s(y)) - \Phi(\overrightarrow{\eta}_s^{\varepsilon N}(1)) \Big\} ds$$
$$+ \int_0^T f_2(s) \Big\{ \frac{1}{\varepsilon N} \sum_{y=N-1-\varepsilon N}^{N-2} g(\eta_s(y)) - \Phi(\overleftarrow{\eta}_s^{\varepsilon N}(N-1)) \Big\} ds$$

where $\overrightarrow{\eta}_s^{\varepsilon N}(1)$ was defined in (55) and

$$\overleftarrow{\eta}_s^{\varepsilon N}(N-1) = \frac{1}{\varepsilon N} \sum_{y=N-1-\varepsilon N}^{N-2} \eta_s(y).$$

As we said above $\overrightarrow{\eta}_s^{\varepsilon N}(1) \sim \rho_s(0)$ and $\overleftarrow{\eta}_s^{\varepsilon N}(N-1) \sim \rho_s(1)$, then the expressions in (58) and in (59) converge, as $N \to \infty$ and $\varepsilon \to 0$, to

[5] The proof of this lemma is a future work.

$$-\int_0^t \Big(\Phi(\rho_s(0))\,\partial_u G(0) - \Phi(\rho_s(1))\,\partial_u G(1)\Big)\,ds,$$

in case $\theta > 1$, and

$$-\int_0^t \Big(\Phi(\rho_s(0))\,\partial_u G(0) - \Phi(\rho_s(1))\,(\partial_u G(1) + G(1)) - \alpha G(0)\Big)\,ds,$$

in case $\theta = 1$. These expressions are the boundary terms in the integral equations (48), with $\kappa = 0$ and $\kappa = 1$, respectively.

Summarizing, the expression of the Dynkin martingale, in (50), converges to the left-hand side of the integral equation (48) with $\kappa = 0$ and $\kappa = 1$, for $\theta > 1$ and $\theta = 1$, respectively. Since we are only providing an idea of the proof, to make clear the notation, up to this point we have been assuming that the test G does not depends on the time, that is $G \in C^2[0,1]$.

Note that from Condition 2.2, $\mathbb{P}_{\mu^N}[|M_t^G| > \delta]$ vanishes as $N \to \infty$. Recall that Q^* is a limit point of the sequence $\{Q^N\}$, which is defined by $Q^N = \mathbb{P}_{\mu^N}(\pi^N)^{-1}$. Then, using Portmanteau Theorem, we can conclude that, in the case $\theta = 1$, Q^* satisfies

$$\begin{aligned} Q^*\Big[\pi_\cdot : \langle \rho_t, G_0\rangle - \langle \gamma, G_0\rangle - \int_0^t \big\{\langle \rho_s, \partial_s G_s\rangle + \langle \Phi(\rho_s), \Delta G_s\rangle\big\}\,ds \\ - \int_0^t \big\{\Phi(\rho_s(0))\partial_u G_s(0) - \Phi(\rho_s(1))\partial_u G_s(1)\big\}\,ds \\ - \int_0^t \big\{\alpha G_s(0) - \Phi(\rho_s(1)) G_s(1)\big\}\,ds \;=\; 0\,, \\ \forall t \in [0,T],\ \forall G \in C^{1,2}([0,T]\times[0,1])\Big] = 1. \end{aligned}$$

Note that the expression inside the probability above is the integral equation (48) with $\kappa = 1$. In the case $\theta > 1$, using the same argument, we obtain a similar expression as the one above with the integral equation (48) with $\kappa = 0$ instead of $\kappa = 1$.

Remark 8 In order to show that the boundary terms $\Phi(\rho_s(0))$ and $\Phi(\rho_s(1))$ in the integral equation (48) are well defined we need to assure that $\Phi(\rho)$ belongs to $L^2(0,T;\mathscr{H}^1(0,1))$. To obtain it, using Riesz representation theorem, it is enough to prove the Energy Estimate, that is:

$$\mathbb{E}_{Q^*}\left[\sup_H \left\{\int_0^T \langle \Phi(\rho_s), \partial_u H_s\rangle\,ds - c\int_0^T \langle H_s, H_s\rangle\,ds\right\}\right] \le M_0 < \infty,$$

for some constants M_0 and c. As usual, the supremum above is taken over all functions $H \in C^{0,1}([0,T]\times[0,1])$ with compact support. The notation $\mathbb{E}_{Q^*}$ means the expectation with respect to the measure Q^*, which is the limit point of Q^N.

10 Heuristics for Hydrodynamics of the General Model

If we had considered the more general slow boundary introduced in Remark 4, see Fig. 3, the Dynkin martingale (50) would be

$$
\begin{aligned}
M_t^G = &\langle \pi_t^N, G\rangle - \langle \pi_0^N, G\rangle - \int_0^t \frac{1}{N}\sum_{x=2}^{N-2} g(\eta_s(x))\Delta_N G\left(\tfrac{x}{N}\right) ds \\
&- \int_0^t \Big(g(\eta_s(1))\nabla_N^+ G\left(\tfrac{1}{N}\right) - g(\eta_s(N-1))\nabla_N^- G\left(\tfrac{N-1}{N}\right)\Big) ds \\
&- \int_0^t \left\{ \left(\frac{\alpha - \lambda g(\eta_s(1))}{N^{\theta-1}}\right) G\left(\tfrac{1}{N}\right) + \left(\frac{\beta - \delta g(\eta_s(N-1))}{N^{\theta-1}}\right) G\left(\tfrac{N-1}{N}\right)\right\} ds,
\end{aligned}
$$

for $G \in C^2[0,1]$. Using similar ideas as in Sect. 9, we get that the limit point Q^* satisfies

$$
\begin{aligned}
Q^*\Big[\pi_\cdot : \langle \rho_t, G_0\rangle - \langle \gamma, G_0\rangle - &\int_0^t \left\{\langle \rho_s, \partial_s G_s\rangle + \langle \Phi(\rho_s), \Delta G_s\rangle\right\} ds \\
&- \int_0^t \left\{\Phi(\rho_s(0))\partial_u G_s(0) - \Phi(\rho_s(1))\partial_u G_s(1)\right\} ds \\
-\kappa \int_0^t \Big\{\big(\alpha - \lambda\Phi(\rho_s(0))\big) G_s(0) &+ \big(\beta - \delta\Phi(\rho_s(1))\big) G_s(1)\Big\} ds = 0, \\
&\forall t \in [0,T],\ \forall G \in C^{1,2}([0,T]\times[0,1])\Big] = 1.
\end{aligned}
$$

Above, $\kappa = 1$ in the case $\theta = 1$ and $\kappa = 0$ in the case $\theta > 1$. Therefore, the hydrodynamic equation is

$$
\begin{cases}
\partial_t \rho_t(u) = \Delta\Phi(\rho_t(u)), & \text{for } u \in (0,1) \text{ and } t \in (0,T], \\
\partial_u \Phi(\rho_t(0)) = -\kappa\left(\alpha - \lambda\Phi(\rho_t(0))\right), & \text{for } t \in (0,T], \\
\partial_u \Phi(\rho_t(1)) = \kappa\left(\beta - \delta\Phi(\rho_t(1))\right), & \text{for } t \in (0,T], \\
\rho_0(u) = \gamma(u), & \text{for } u \in [0,1].
\end{cases} \tag{60}
$$

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References

1. E. Andjel, Invariant measures for the zero range process. Ann. Probab. **10**, 525–547 (1982)
2. E. Andjel, C. Kipnis, Derivation of the hydrodynamical equation for the zero-range interaction process. Ann. Probab. **12**, 325–334 (1984)

3. E. Andjel, M.E. Vares, Hydrodynamic equations for attractive particle systems on $\mathbb{Z}$. J. Stat. Phys. **47**(1/2) (1987)
4. I. Armendáriz, S. Grosskinsky, M. Loulakis, Metastability in a condensing zero-range process in the thermodynamic limit. Probab. Theory Relat. Fields **169**, 105–175 (2017)
5. R. Baldasso, O. Menezes, A. Neumann, R. Souza, Exclusion process with slow boundary. J. Stat. Phys. **167**(5), 2–1142 (2017)
6. E. Bertin, M. Vanicat, Matrix product representation of state of the open zero range process. J. Phys. A: Math. Theor. **51**, 245001 (2018)
7. R.A. Blythe, M.R. Evans, Nonequilibrium steady states of matrix-product form: a solver's guide. J. Phys. A: Math. Theor. **40**, R333 (2007)
8. T. Bodineau, B. Derrida, J.L. Lebowitz, A diffusive system driven by a battery or by a smoothly varying field. J. Stat. Phys. **140**(4), 648–675 (2010)
9. N.M. Bogoliubov, C. Malyshev, Zero range process and multi-dimensional random walks, SIGMA 13, **056**, 14 (2017)
10. L. de Bonorino, R. Paula, P. Gonçalves, A. Neumann, Hydrodynamics of porous medium model with slow reservoirs. J. Stat. Phys. **179**(3), 748–788 (2020)
11. A. De Masi, P.A. Ferrari, A remark on the hydrodynamics of the zero range processes. J. Stat. Phys. **36**, 81–87 (1984)
12. A. De Masi, E. Presutti, D. Tsagkarogiannis, M.E. Vares, Current reservoirs in the simple exclusion process. J. Stat. Phys. **144**(6), 1151–1170 (2011)
13. A. De Masi, E. Presutti, D. Tsagkarogiannis, M.E. Vares, Truncated correlations in the stirring process with births and deaths. Electron. J. Probab. **17**(6), 1–35 (2012)
14. B. Derrida, M. Evans, V. Hakim, V. Pasquier, Exact solution of a 1D asymmetric exclusion model using a matrix formulation. J. Phys. A **26**(7), 1493 (1993)
15. B. Derrida, J.L. Lebowitz, E.R. Speer, Large deviation of the density profile in the steady state of the open symmetric simple exclusion process. J. Stat. Phys. **107**, 599 (2002)
16. B. Derrida, Non-equilibrium steady states: fluctuations and large deviations of the density and of the current. J. Stat. Mech. Theory Exp. **P07023** (2007)
17. T. Franco, P. Gonçalves, A. Neumann, Hydrodynamical behavior of symmetric exclusion with slow bonds. Ann. Inst. Henri Poincaré: Probab. Stat. **49**(2), 402–427 (2013)
18. P. Gonçalves, Equilibrium fluctuations for the totally asymmetric zero-range process. J. Stat. Phys. **138**(4–5), 645–661 (2010)
19. P. Gonçalves, On the asymmetric zero-range in the rarefaction fan. J. Stat. Phys. **154**(4), 1074–1095 (2014)
20. S. Grosskynsky, G.M. Schutz, H. Spohn, Condensation in the zero range process: stationary and dynamical properties. J. Stat. Phys. **113**, 389–410 (2003)
21. S. Grosskynsky, H. Spohn, Stationary measures and hydrodynamics of zero range processes with several species of particles. Bull. Braz. Math. Soc. **34**, 489–507 (2003)
22. C. Kipnis, C. Landim, *Scaling Limits of Interaction Particle Systems* (Springer, New York, 1999)
23. E. Levine, D. Mukamel, G.M. Schültz, Zero-range process with open boundaries. J. Stat. Phys. **120**(5–6), 759–778 (2005)
24. T.M. Liggett, *Interacting Particle Systems* (Springer, New York, 1985)
25. J.R. Norris, *Markov Chains* (Cambridge University Press, Cambridge, 1997)
26. F. Rezakhanlou, Hydrodynamic limit for attractive particle systems on $\mathbb{Z}^d$. Commun. Math. Phys. **140**, 417–448 (1991)
27. F. Spitzer, Interaction of Markov processes. Adv. Math. **5**, 246–290 (1970)

Partial Regularity in Time for the Landau Equation (with Coulomb Interaction)

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Abstract The present paper gives a simplified presentation of a partial regularity result obtained in a joint work with M. P. Gualdani, C. Imbert and A. Vasseur [arXiv:1906.02841 [math.AP]] for the spatially homogeneous Landau equation with Coulomb interaction in three space dimensions. Specifically, we prove that the procedure used in [C. Villani: Arch. Rational Mech. Anal. **143** (1998), 273–307] to construct H-solutions of the Landau equation leads to a class of weak solutions satisfying a truncated relative entropy estimate for values of the distribution function larger than any arbitrary level $\kappa > 0$. Using the method introduced in [E. De Giorgi: Mem. Accad. Sci. Torino Cl. Sci. Fis. Mat. Nat., **3** (1957), 25–43] for studying the regularity of parabolic equations with bounded diffusion coefficients, we prove that the set of singular times of any such solution has Hausdorff dimension at most $1/2$.

Keywords Landau equation · Partial regularity · DeGiorgi-Nash-Moser regularity theory · Hausdorff dimension

1 The Landau Equation

The Landau equation [14] (see also Sect. 41 in [17]) is a collisional model used in the kinetic theory of charged particles (ionized gases or plasmas). As in the case of the Boltzmann equation of the kinetic theory of gases, the unknown in the Landau equation is the velocity distribution function, that is the phase space number density of particles which, at time t, are at position x and have velocity v. Throughout the present paper, we focus our attention on the Landau collision integral, and forget about the dependence in the position variable x. Thus, the velocity distribution function is $f \equiv f(t, v) \geq 0$, the number density of particles with velocity $v \in \mathbf{R}^3$ at time $t \geq 0$.

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The space-homogeneous Landau equation with Coulomb interaction between identical particles (with the same electric charge) is

$$\partial_t f(t,v) = \nabla_v \cdot \int_{\mathbf{R}^3} a(v-w)(\nabla_v - \nabla_w)(f(t,v)f(t,w))dw\,, \qquad v \in \mathbf{R}^3\,, \quad (1)$$

with the notation:

$$a(z) := \frac{1}{8\pi}\nabla^2|z| = \frac{1}{8\pi|z|}\Pi(z)\,, \qquad \Pi(z) := I - \left(\frac{z}{|z|}\right)^{\otimes 2}\,.$$

Obviously, this equation can also be written as a parabolic equation in nonconservative form:

$$\partial_t f(t,v) = \left(a_{ij} \star_v f(t,v)\right)\partial_{v_i}\partial_{v_j} f(t,v) + f(t,v)^2\,. \quad (2)$$

Whether there is finite-time blow-up, or global existence of smooth solutions of the Cauchy problem for the space homogeneous Landau equation is one of the major open problems in the mathematical theory of kinetic models at the time of this writing (see Villani's comment on this problem in Sect. 1.3 (2) of [25]).

Looking at the nonconservative parabolic form of the Landau equation suggests comparing this equation with the semilinear heat equation

$$\partial_t u = \Delta_x u + \alpha u^2\,, \quad (3)$$

where $\alpha > 0$ is a constant. It is well known that, for each $d \geq 1$, any classical solution $u \equiv u(t,x) > 0$ of this semilinear heat equation with "large" initial data blows up in finite time (the word "large" will be defined below). This is seen by the following elementary argument: for an arbitrary open ball B of $\mathbf{R}^d$, let $\phi \equiv \phi(x)$ be the solution of

$$-\Delta\phi = \lambda_0\phi\,, \qquad \phi > 0 \text{ on } B\,, \qquad \phi\big|_{\partial B} = 0\,,$$

normalized by the condition

$$\int_B \phi(x)dx = 1\,.$$

Then $\lambda_0 \equiv \lambda_0[B] > 0$. (In fact, $\lambda_0[B]$ is the smallest eigenvalue of $-\Delta$ on the ball B with homogeneous Dirichlet boundary condition on ∂B. For each $x_0 \in \mathbf{R}^d$ and each $r > 0$, one has

$$\lambda_0[B(x_0,r)] = \lambda_0[B(0,1)]r^2$$

by an obvious scaling argument.) Define

$$L(t) := \int_B u(t,x)\phi(x)dx\,.$$

Elementary computations involving the Green formula show that

$$\frac{dL}{dt}(t) \geq -\lambda_0 L(t) + \alpha L^2(t)\,.$$

If $L(0) > \lambda_0/\alpha$, then $t \mapsto L(t)$ cannot remain bounded on $[0, \tau]$ with

$$\tau > \int_{L(0)}^{+\infty} \frac{dL}{\alpha L^2 - \lambda_0 L}\,.$$

Hence, any classical solution $u \equiv u(t,x) \geq 0$ of (3) such that, for some open ball $B \in \mathbf{R}^d$,

$$\int_B u(0,x)\phi(x)dx > \frac{\lambda_0}{\alpha}$$

blows up in finite time. This condition is the precise definition of what we called a "large" initial data above. We refer the interested readers to [26] and Sect. 5.4 in [3] for more details on this problem.

However, the Landau equation is not expected to behave as the semilinear heat Eq. (3) for the following reason. While the term $f(t,v)^2$ in the right hand side of (2) promotes blow-up, the diffusion matrix $a \star_v f(t,v)$ grows with $f(t,\cdot)$, and a large diffusion matrix multiplying $\partial_{v_i}\partial_{v_j} f(t,v)$ in the right hand side of (2) is expected to inhibit blow-up. The diffusion coefficient in the semilinear heat Eq. (3) is constant, and therefore cannot offset the effect of the quadratic term $\alpha u(t,x)^2$.

Another simpler model of the space homogeneous Landau equation is the so-called "isotropic" model Landau equation

$$\partial_t u(t,x) = ((-\Delta_x)^{-1}u(t,x))\Delta u(t,x) + \alpha u(t,x)^2\,,$$

for which the global existence of radially symmetric, nonincreasing solutions has been proved [9, 10, 13].

There is however an unpleasant difference between this "isotropic" model Landau equation and the true Landau equation. Maxwellian distribution functions, i.e. distribution functions of the form

$$\mathscr{M}[\rho,u,\theta](v) := \frac{\rho}{(2\pi\theta)^{3/2}} e^{-|v-u|^2/2\theta}$$

are known to be equilibrium (i.e. independent of time) solutions of the true Landau equation, and are not solutions of the "isotropic" model Landau equation. Since Maxwellian distributions are of fundamental importance in physics, the "isotropic" model Landau equation is only of mathematical interest.

Still another approach to the regularity issue for the Landau equation is to prove conditional regularity results. In other words, assuming some bounds in appropriate Lebesgue spaces on weak solutions of the Landau equation, one tries to prove that such weak solutions must be classical solutions, or at least bounded (weak) solutions.

Perhaps the best result in this direction is [20]—see also [11] for similar results obtained with different techniques—which proves that any weak solution of the (space-homogeneous) Landau equation in the space $L^\infty(\mathbf{R}_+; L^p(\mathbf{R}^3; (1+|v|)^k dv))$ with $p > 3/2$ and $k > 5$ belongs to $L^\infty(\mathbf{R}_+ \times \mathbf{R}^3)$—a similar result for radial solutions had been obtained earlier in [10].

Everywhere in this paper, we use the following notation

$$\|g\|_{L^p_k}^p := \int_{\mathbf{R}^3} (1+|v|^2)^{k/2} |g(v)|^p dv$$

with $p \geq 1$ and $k \in \mathbf{R}$, and we call $L^p_k(\mathbf{R}^3)$ the set of (equivalence classes of a.e. equal) measurable functions $g \equiv g(v)$ on $\mathbf{R}^3$ with $\|g\|_{L^p_k}^p < +\infty$.

In the present paper, we explore still another question: we seek to prove that the set of times at which a weak solution of the Landau equation is singular cannot be too large. Specifically, we seek to control the Hausdorff dimension of the set of singular times of some appropriate class of weak solutions to the Landau equation. This approach to the regularity issue for weak solutions of nonlinear partial differential equations has been proposed by Leray in the case of his "turbulent solutions" (now referred to as "Leray solutions") of the three-dimensional incompressible Navier–Stokes equations [15]: see formula (6.5) in Sect. 34 of [15]. (Leray's observation is not explicitly expressed in terms of Hausdorff dimension in [15].) It has been later considerably improved by [2, 16, 18, 22], and is usually referred to as "partial regularity".

2 A Notion of Weak Solutions of the Landau Equation

Our first task is to define precisely the class of weak solutions to which our partial regularity result will apply.

2.1 Villani's H-Solutions

In his article [24], Villani proposed the following notion of weak solution of the Landau equation. Since this notion of weak solution makes critical use Boltzmann's H Theorem, Villani chose to call such solutions "H-solutions".

A H-solution of the Landau equation is a function

$$f \in C([0,T); \mathscr{D}'(\mathbf{R}^3)) \cap L^1((0,T); L^1_{-1}(\mathbf{R}^3)) \quad \text{s.t. } f(t,\cdot) \geq 0 \text{ in } \mathscr{D}'(\mathbf{R}^3)$$

for all $t \in [0,T)$, satisfying the following two properties:
(a) the conservation laws and Boltzmann's H Theorem: for a.e. $t \in [0,T)$:

$$\int_{\mathbf{R}^3} \begin{pmatrix} 1 \\ v \\ |v|^2 \end{pmatrix} f(t,v)dv = \int_{\mathbf{R}^3} \begin{pmatrix} 1 \\ v \\ |v|^2 \end{pmatrix} f_{in}(t,v)dv\,,$$

$$\int_{\mathbf{R}^3} f(t,v)\ln f(t,v)dv \le \int_{\mathbf{R}^3} f_{in}(v)\ln f_{in}(v)dv\,;$$

(b) the following weak formulation of the Landau equation:

$$\int_{\mathbf{R}^3} f_{in}(v)\phi(0,v)dv + \int_0^T \int_{\mathbf{R}^3} f(t,v)\partial_t\phi(t,v)dv$$
$$= \int_0^T \int_{\mathbf{R}^6} (\Phi(t,v)-\Phi(t,w))\cdot \Pi(v-w)\,(F(\nabla_v-\nabla_w)F)\,(t,v,w)dvdw\,,$$

where

$$\Phi(t,v) := \nabla_v\phi(t,v) \quad \text{and} \quad F(t,v,w) := \sqrt{\frac{f(t,v)f(t,w)}{8\pi|v-w|}}\,.$$

Notice the following subtlety in Villani's definition: the right hand side of the identity above depends on the test function ϕ in a *nonlocal* manner. For this reason, this weak formulation differs from the straightforward definition of a solution of (2) in the sense of distributions.

2.2 Suitable Solutions

However, the notion of H-solution is not sufficient for our purpose in the present paper. We shall need more information in order to control the size of the set of singular times in a weak solution of the Landau equation. Specifically, we shall use the following notion of weak solution of the Landau equation.

Definition 1 Let $\mathcal{N} \subset \mathbf{R}_+$ be a set of Lebesgue measure 0, let $q \ge 1$ and $C'_E > 0$. An $(\mathcal{N}, q, C'_E)$-suitable solution on $[0,T)\times\mathbf{R}^3$ of the Landau equation is an H-solution $f \equiv f(t,v)$ such that

$$H_+(f(t_2,\cdot)|\kappa) + C'_E \int_{t_1}^{t_2} \left\| \mathbf{1}_{f(t,v)>\kappa} \nabla_v f(t,v)^{1/q} \right\|^2_{L^q(\mathbf{R}^3)} dt$$
$$\le H_+(f(t_1,\cdot)|\kappa) + 2\kappa \int_{t_1}^{t_2} \int_{\mathbf{R}^3} (f(t,v)-\kappa)_+ dvdt$$

for all $t_1 < t_2 \in [0,T)\setminus\mathcal{N}$ and all $\kappa \ge 1$, where

$$H_+(g|\kappa) := \int_{\mathbf{R}^3} \kappa h_+\left(\frac{g(v)}{\kappa}\right) dv\,, \qquad h_+(z) := z(\ln z)_+ - (z-1)_+\,.$$

It is interesting to compare the inequality for the "truncated relative entropy" $H_+(f(t,\cdot)|\kappa)$ in the definition above, with what one might have expected from the nonconservative form (2) of the Landau equation. Specifically, the inequality for the truncated relative entropy is obtained formally by multiplying both sides of the Landau equation by $\ln(\frac{f(t,v)}{\kappa})_+$ and integrating by parts in the diffusion operator (in the variable v) on the left hand side of (2). One expects this procedure to lead to the truncated entropy production term on the left hand side of the inequality above, while the term $f(t,v)^2$ on the right hand side of (2) is expected to lead to

$$\int_{t_1}^{t_2}\int_{\mathbf{R}^3} f(t,v)^2 \ln\left(\frac{f(t,v)}{\kappa}\right)_+ dvdt\,.$$

Instead of this term, one finds instead the much weaker (in terms of the growth as $f \to +\infty$) source term

$$\kappa \int_{t_1}^{t_2}\int_{\mathbf{R}^3} (f(t,v)-\kappa)_+ dvdt\,.$$

In other words, there is a remarkable cancellation in the Landau collision integral, which significantly depletes the effect of the nonlinearity $f(t,v)^2$. Since this quadratic source term on the right hand side of (2) is responsible for the suspicion of finite time blow-up in classical solutions of the Landau equation, the fact that the truncated relative entropy inequality partially offsets the effect of the quadratic nonlinearity $f(t,v)^2$ in the form (2) of the Landau equation is a good sign and might tip the scales in favor of global regularity.

3 Partial Regularity in t for Suitable Solutions

In spite of the helpful effect of the depleted nonlinear term on the right hand side of the truncated relative entropy inequality, we have not been able to prove the propagation of regularity in time for suitable solutions of the Landau equation. However, we have been able to control the size of the set of singular times for this class of solutions.

We begin with a precise definition of what we call "singular times" for suitable solutions of the Landau equation.

Definition 2 A regular time for a suitable solution f of the Landau equation defined on $I \times \mathbf{R}^3$, where I is an interval included in $(0,+\infty)$, is a time $\tau \in I$ such that $(\tau-\epsilon,\tau) \subset I$ and $f \in L^\infty((\tau-\epsilon,\tau)\times\mathbf{R}^3)$ for some $\epsilon \in (0,\tau)$. A singular time for f is a time $t \in I$ which is not regular. The set of singular times of f on the time interval I is denoted $\mathbf{S}[f,I]$.

With this definition, we can state our main result in the present paper.

Theorem 1 ([6]) *Let f be a suitable solution to the Landau equation on $[0, T) \times \mathbf{R}^3$ for all $T > 0$, with initial data f_{in} satisfying*

$$\int_{\mathbf{R}^3} (1 + |v|^k + |\ln f_{in}(v)|) f_{in}(v) dv < +\infty \quad \text{for all } k > 3 .$$

Then

$$\text{Hausdorff dim } \mathbf{S}[f, (0, +\infty)] \leq \tfrac{1}{2} .$$

(For the definition of Hausdorff measures, and of Hausdorff dimension, see Sect. 2.1 in Chap. 2 of [1].)

This statement is the main result of our joint article with Gualdani et al. [6]. The purpose of the present paper is to provide the reader with a nontechnical description of the main ideas in [6].

4 Existence Theory for Suitable Solutions

Our goal in this section is to prove the following existence result.

Proposition 1 *For each $T > 0$ and each $f_{in} \in L^1(\mathbf{R}^3)$ such that $f_{in} \geq 0$ a.e. on $\mathbf{R}^3$ and*

$$\int_{\mathbf{R}^3} (1 + |v|^k + |\ln f_{in}(v)|) f_{in}(v) dv < +\infty \quad \text{for some } k > 3 ,$$

there exists $\mathcal{N} \subset [0, T]$ of Lebesgue measure 0, and an $(\mathcal{N}, q, C'_E)$-suitable solution f on $[0, T]$ with initial data f_{in} and

$$C'_E \equiv C'_E[T, q, f_{in}] > 0 , \qquad q := \frac{2k}{k+3} .$$

Two remarks are in order. First, there is no limitation on the length T of the time interval on which the suitable solution is defined, except that the larger T, the smaller the constant C'_E. Since $C'_E > 0$ is the strength of the parabolic regularizing effect in the Landau equation, one should avoid letting $T \to +\infty$ if this implies that $C'_E \to 0$. The second remark is about the set $\mathcal{N}$ of Lebesgue measure 0. This set $\mathcal{N}$ is not to be confused with the singular set $\mathbf{S}[f, (0, +\infty)]$, and may very well be of Hausdorff dimension $> \frac{1}{2}$ without ultimately affecting the Hausdorff dimension of the singular set $\mathbf{S}[f, (0, +\infty)]$.

4.1 Formal H Theorem

In this section, we propose a formal discussion of the Boltzmann H Theorem for the Landau equation, and of its truncated variant which is at the core of the notion of suitable solution. By formal, we mean that we proceed as if the solution f was smooth (although we are trying to prove much less), everywhere positive, rapidly decaying in v and such that $\nabla_v \ln f(t,v)$ has at most polynomial growth as $|v| \to +\infty$.

Under these assumptions, one has

$$\frac{d}{dt}\int_{\mathbf{R}^3} f(t,v)\ln f(t,v)dv$$
$$= -\int_{\mathbf{R}^6} \frac{f(t,v)f(t,w)}{16\pi|v-w|}\left|\Pi(v-w)\left(\frac{\nabla_v f(t,v)}{f(t,v)} - \frac{\nabla_w f(t,w)}{f(t,w)}\right)\right|^2 dvdw\,.$$

Next, we study the truncated variant of the identity above. For each $\kappa \geq 1$, one easily checks that

$$\frac{d}{dt}H_+(f(t,\cdot)|\kappa)$$
$$+\int_{\mathbf{R}^6} \frac{f(t,v)f(t,w)}{16\pi|v-w|}\left|\Pi(v-w)\left(\frac{\mathbf{1}_{f(t,v)>\kappa}\nabla_v f(t,v)}{f(t,v)} - \frac{\mathbf{1}_{f(t,w)>\kappa}\nabla_w f(t,w)}{f(t,w)}\right)\right|^2 dvdw$$
$$= -\int_{\mathbf{R}^6} f(t,v)f(t,w)a(v-w):\nabla_v(\ln\tfrac{f(t,v)}{\kappa})_+\otimes\nabla_w(\ln\tfrac{f(t,w)}{\kappa})_- dvdw\,.$$

A careful inspection of the term on the right hand side shows that

$$-\int_{\mathbf{R}^6} f(t,v)f(t,w)a(v-w):\nabla_v(\ln\tfrac{f(t,v)}{\kappa})_+\otimes\nabla_w(\ln\tfrac{f(t,w)}{\kappa})_- dvdw$$
$$= \int_{\mathbf{R}^6} a(v-w):\nabla_v f(t,v)\mathbf{1}_{f(t,v)\geq\kappa}\otimes\nabla_w f(t,w)\mathbf{1}_{f(t,w)<\kappa}\,dvdw$$
$$= \int_{\mathbf{R}^6} \mathrm{div}_v(\mathrm{div}_w\, a(v-w))(f(t,v)-\kappa)_+(\kappa-(f(t,w)-\kappa)_-)dvdw$$
$$\leq \kappa\int_{\mathbf{R}^3}(f(t,v)-\kappa)_+dv\,,$$

since one can check, by an elementary computation, that

$$\mathrm{div}_v(\mathrm{div}_w\, a(v-w)) = \delta_0(v-w) \geq 0 \qquad \text{in } \mathscr{D}'(\mathbf{R}^6)\,.$$

Eventually, one finds that

$$\frac{d}{dt}H_+(f(t,\cdot)|\kappa) + \int_{\mathbf{R}^6} \frac{f(t,v)f(t,w)}{16\pi|v-w|}\left|\Pi(v-w)\left(\frac{\mathbf{1}_{f(t,v)>\kappa}\nabla_v f(t,v)}{f(t,v)} - \frac{\mathbf{1}_{f(t,w)>\kappa}\nabla_w f(t,w)}{f(t,w)}\right)\right|^2 dvdw$$

$$\leq \kappa \int_{\mathbf{R}^3} (f(t,v)-\kappa)_+ dv\,.$$

The right hand side of this inequality is precisely the depleted nonlinear term which appears in the definition of the notion of suitable solution of the Landau equation.

4.2 The Desvillettes Theorem

In [5], Desvillettes explained how the nonlocal entropy production integral for the Landau equation can be replaced with a weighted variant of the Fisher information of f. This is an absolutely remarkable result, for several reasons, the first one being that it very clearly explains how Villani's notion of H-solution to the Landau equation is related to the usual notion of weak solution. Another truly fascinating consequence of this result is that it suggests the existence of some "dictionary" between the Navier–Stokes and the Landau equations, as far as the regularity of solutions is concerned. We shall return to this question in the final section of the present paper.

Theorem 2 ([5]) *For each $f \in L^1_2(\mathbf{R}^3)$ such that $f \geq 0$ a.e. and $f \ln f \in L^1(\mathbf{R}^3)$, one has*

$$\int_{\mathbf{R}^3} \frac{|\nabla\sqrt{f(v)}|^2 dv}{(1+|v|^2)^{3/2}} \leq C_D + C_D \int_{\mathbf{R}^6} \frac{|\Pi(v-w)(\nabla_v-\nabla_w)\sqrt{f(v)f(w)}|^2}{|v-w|} dvdw\,,$$

with

$$C_D \equiv C_D\left[\int_{\mathbf{R}^3} (1, v, |v|^2, |\ln f(v)|) f(v) dv\right] > 0\,.$$

Observe that this is a functional inequality, and not a property special to solutions of the Landau equation. The constant C_D is essentially explicit—at least, Desvillettes' proof of Theorem 2 provides an explicit estimate of C_D.

An interesting consequence of this result is the following observation on the propagation of moments for H-solutions of the Landau equation.

Theorem 3 ([5]) *Let $f_{in} \in L^1_k(\mathbf{R}^3))$ with $k > 2$ satisfy $f_{in} \geq 0$ a.e. on $\mathbf{R}^3$, and assume that $f_{in}|\ln f_{in}| \in L^1(\mathbf{R}^3)$. Then, any H-solution f of the Landau equation such that $f\big|_{t=0} = f_{in}$ satisfies*

$$f \in L^\infty(0,T; L^1_k(\mathbf{R}^3)) \qquad \text{for each } T > 0\,.$$

4.3 Sketch of the Proof of Proposition 1

This proof uses exactly the same approximating sequence as in [24]. In other words, while we do not know whether *all* H-solutions of the Landau equation are suitable solutions, our proof of Proposition 1 shows that the H-solutions constructed by Villani are indeed suitable solutions.

Replace a with its truncated variant: for each integer $n \geq 1$, set

$$a_n(z) := \tfrac{1}{8\pi} \min\left(\frac{1}{|z|}, n\right) \Pi(z)\,, \quad \text{satisfying } \operatorname{div}(\operatorname{div} a_n) \leq 0\,,$$

as in the construction of H-solutions in [24].

Next, use the first Desvillettes theorem (Theorem 2) to bound

$$\begin{aligned} &\tfrac{1}{C_D''} \int_{\mathbf{R}^3} \tfrac{|\nabla_v \sqrt{f(t,v)}|^2}{(1+|v|)^3} \mathbf{1}_{f(t,v)>\kappa} dv \\ &\leq \int_{\mathbf{R}^6} \tfrac{f(t,v)f(t,w)}{16\pi|v-w|} \left| \Pi(v-w) \left(\tfrac{\mathbf{1}_{f(t,v)>\kappa} \nabla_v f(t,v)}{f(t,v)} - \tfrac{\mathbf{1}_{f(t,w)>\kappa} \nabla_w f(t,w)}{f(t,w)} \right) \right|^2 dvdw \\ &\qquad + \int_{\mathbf{R}^3} (f(t,w) - \kappa)_+ dw\,. \end{aligned}$$

Using the Desvillettes propagation theorem (Theorem 3) with $p' = \frac{2}{q}$ (recall that $q = \frac{2k}{k+3} \in (1,2)$ since $k > 3$), one finds that

$$\begin{aligned} &\left\| \mathbf{1}_{f(t,v)>\kappa} \nabla_v f(t,v)^{1/q} \right\|^q_{L^q(\mathbf{R}^3)} \\ &\leq (\tfrac{2}{q})^q \| f(t,\cdot) \|^p_{L^p_{3p/2p'}(\mathbf{R}^3)} \left(\int_{\mathbf{R}^3} \tfrac{|\nabla_v \sqrt{f(t,v)}|^2 \mathbf{1}_{f(t,v)\geq\kappa}}{(1+|v|^2)^{3/2}} dv \right)^{1/p'}. \end{aligned}$$

The remaining part in the existence proof follows essentially [24].

5 The 1st De Giorgi Type Lemma

In [4], De Giorgi provided the missing piece in the resolution of Hilbert's 19th problem (on the analyticity of extremals in the calculus of variations). De Giorgi's striking result is a Hölder regularity estimate on weak solutions of elliptic equations in conservative form, with *bounded but discontinuous* diffusion coefficients. Because of the discontinuity of the diffusion coefficients, such an elliptic equation cannot be made close to Laplace's equation (with a constant coefficient Laplacian) by zooming in in the vicinity of one point where one seeks to prove that the weak solution is Hölder continuous. For instance, one can think of a diffusion equation on the plane in conservative form with scalar diffusion coefficient with a jump discontinuity across a

line. Zooming in at each point on the line of discontinuity will not eliminate the jump discontinuity in the diffusion coefficient, and therefore will not make the diffusion operator close to the Laplacian for the Euclidean metric. This simple observation explains why the De Giorgi regularity estimate is of a totally different nature than all the results obtained on PDEs with variable coefficients by the method of "frozen coefficients".

One particular feature in the De Giorgi method is a clever combination of a zooming transformation in the variables involved in the PDE of interest, and of nested truncations in the set of values of the weak solutions of the PDE of interest (which is also known as the Stampacchia truncation method). The latter feature is conveniently formulated in the truncated relative entropy inequality in the definition (Definition 1) of the notion of suitable solution of the Landau equation: see [8] for an application of the De Giorgi method to a reaction diffusion system, using a notion of entropy similar to the truncated relative entropy considered here. That the De Giorgi method applies to a parabolic system as in [8] is quite remarkable: in general, the De Giorgi method cannot be used on systems. However, the system considered in [8] enjoys a special structure including an entropy inequality similar to the Boltzmann H theorem, and some of the ideas and results presented below are reminiscent of the analysis in [8]. More recently, the De Giorgi method, originally written for elliptic equations, and easily extended to the case of parabolic equations, has been used in the more complicated case of kinetic models (see [7, 12] and the references therein).

Proposition 2 *Let f be a $(\mathscr{N}, q, C'_E)$–suitable solution to the Landau equation for $t \in [0,1]$ with $C'_E > 0$ and $q \in (\frac{6}{5}, 2)$. Then there exists $\eta_0 \equiv \eta_0[q, C'_E] > 0$ such that*

$$\int_{1/8}^1 H_+(f(t,\cdot)|\tfrac{1}{2})dt < \eta_0 \implies f(t,v) \le 2 \quad \text{a.e. on } [\tfrac{1}{2}, 1] \times \mathbf{R}^3 .$$

Proof Set

$$\begin{cases} t^k := \frac{1}{2} - \frac{1}{4} \cdot 2^{-k} , & \kappa_k := (1 + (2^{1/q} - 1)(1 - 2^{-k}))^q , \\ f_k^+(t,v) := \mu((f(t,v)^{1/q} - \kappa_k^{1/q})_+) , & \text{with } \mu(r) := \min(r, r^2) . \end{cases}$$

One easily checks that there exists $c_h > 0$ and, for each $\iota > 0$, there exists $C_\iota > 0$ such that

$$c_h \mu((r-1)_+) \le h_+(r) \le C_\iota (r-1)_+^\iota , \qquad r \ge 0 .$$

Consider the quantity

$$A_k := \operatorname*{ess\,sup}_{t^k \le t \le 1} \tfrac{c_h}{2} \int_{\mathbf{R}^3} f_k^+(t,v)^q dv + \tfrac{1}{4} C'_E \int_{t^k}^1 \left(\int_{\mathbf{R}^3} |\nabla_v f_k^+(t,v)|^q dv \right)^{2/q} dt .$$

Observe first that

$$f_{k+1}^+ > 0 \implies f_k^+ > \mu((2^{1/q}-1)\cdot 2^{-k-1}),$$

$$\text{so that} \quad A_{k+1} \le C_{q,\iota} 4^{(k+3)q(1+\iota)} \int_{t^k}^1 \int_{\mathbf{R}^3} f_k^+(\theta, v)^{q(1+\iota)} dv d\theta .$$

At this point, we apply the De Giorgi nonlinearization technique. Using the Hölder inequality and the Sobolev embedding with $\iota = \frac{2}{3}$, one arrives after some manipulations at the inequality

$$A_{k+1} \le M \Lambda^k A_k^\beta , \quad \beta := \tfrac{8}{3} - \tfrac{2}{q} > 1 \text{ and } \Lambda := 2 \cdot 4^{\frac{5q}{3}}$$

with $M \equiv M[q, C'_E] > 0$. Now, an easy induction argument shows that

$$A_0 < M^{-\frac{1}{\beta-1}} \Lambda^{-\frac{1}{(\beta-1)^2}} \implies A_k \to 0 \text{ as } k \to \infty .$$

With Fatou's lemma, the fact that $A_k \to 0$ as $k \to \infty$ implies that $f(t, v) \le 2$ a.e. on $[\frac{1}{2}, 1] \times \mathbf{R}^3$. It remains to prove that A_0 can be made arbitrarily small, which is done by using the truncated entropy.

6 The Improved De Giorgi Lemma

Next one seeks to apply Proposition 2 to a scaled suitable solution of the Landau equation. While zooming and scaling arguments are of considerable importance in classical PDE theory, such arguments do not easily apply to kinetic models. In general, moments of the distribution function such as the mass and kinetic energy densities, together with the Boltzmann H function are of considerable importance in the mathematical analysis of such models, and usually the group of scaling transformations leaving a kinetic model equation invariant is not rich enough to preserve simultaneously the mass, kinetic energy and entropy densities. This is precisely what happens in the case of the Landau equation. However, what truly matters is to keep the truncated relative entropy inequality in Definition 1 invariant, and this is a much weaker demand on the scaling transformations to be used.

Proposition 3 *Let f be a $(\mathscr{N}, q, C'_E)$-suitable solution of the Landau equation on $[0, 1]$ with $q \in (\frac{4}{3}, 2)$. There exists $\eta_1 \equiv \eta_1[q, C'_E] > 0$ and $\delta_1 \in (0, 1)$ such that*

$$\overline{\lim_{\epsilon \to 0^+}} \, \epsilon^{\gamma-3} \int_{1-\epsilon^\gamma}^1 \left\| \mathbf{1}_{f(T,\cdot) > \epsilon^{-\gamma}} \nabla_V f(T, \cdot)^{\frac{1}{q}} \right\|_{L^q(\mathbf{R}^3)}^2 dT < \eta_1$$
$$\implies f \in L^\infty((1-\delta_1, 1) \times \mathbf{R}^3)$$

with $\gamma := \frac{5q-6}{2q-2}$.

Proof The Landau equation is invariant under the following 2-parameter group of scaling transformations

$$f_{\lambda,\epsilon}(t,v) := \lambda f(\lambda t, \epsilon v)\,.$$

Let f be a $(\mathscr{N}, q, C'_E)$-suitable solution on $[0,1]$, with $\lambda = \epsilon^\gamma$: thus

$$H_+(f_{\lambda,\epsilon}(t,\cdot)|\epsilon^\gamma\kappa) = \epsilon^{\gamma-3}H_+(f(\epsilon^\gamma t,\cdot)|\epsilon^\gamma\kappa)$$

$$\int_{t_1}^{t_2}\int_{\mathbf{R}^3}(f_{\lambda,\epsilon}(t,v)-\epsilon^\gamma\kappa)_+dvdt = \frac{1}{\epsilon^3}\int_{\epsilon^\gamma t_1}^{\epsilon^\gamma t_2}\int_{\mathbf{R}^3}(f(T,V)-\kappa)_+dVdT\,,$$

while $\gamma := \frac{5q-6}{2q-2}$ implies that

$$\int_{t_1}^{t_2}\left(\int_{\mathbf{R}^3}|\mathbf{1}_{f_{\lambda,\epsilon}\geq\epsilon^\gamma\kappa}\nabla_v f_{\lambda,\epsilon}^{\frac{1}{q}}(t,v)|^q dv\right)^{2/q}dt$$

$$= \epsilon^{\gamma-3}\int_{\epsilon^\gamma t_1}^{\epsilon^\gamma t_2}\left(\int_{\mathbf{R}^3}|\mathbf{1}_{f\geq\kappa}\nabla_v f^{\frac{1}{q}}(T,V)|^q dV\right)^{2/q}dT\,.$$

Set

$$f_n(t,v) := \epsilon_n^\gamma f(1+\epsilon_n^\gamma(t-1),\epsilon_n v) \quad \text{with } \epsilon_n := 2^{-n}\,,$$

$$F_n(t,v) := \mu((f_n(t,v)^{1/q}-1)_+)\,, \quad \int_{\mathbf{R}^3}F_n(t,v)dv \leq \epsilon_n^{\gamma-3}\,.$$

Observe that f_n is a $(\mathscr{N}_n, q, C'_E)$-suitable solution of the Landau equation on $[0,1]$ with

$$\mathscr{N}_n := \{t \geq 0 \text{ s.t. } 1+\epsilon_n^\gamma(t-1) \in \mathscr{N}\}\,.$$

One key point (perhaps the most important point) in the argument is that the constant C'_E is unchanged by the scaling defined above.

Pick a positive integer N large enough so that

$$n \geq N \implies \int_0^1\left(\int_{\mathbf{R}^3}|\nabla_v F_n(t,v)|^q dv\right)^{2/q}dt$$

$$\leq 4\epsilon_n^{\gamma-3}\int_{1-\epsilon_n^\gamma}^1\left(\int_{\mathbf{R}^3}|\mathbf{1}_{f\geq\epsilon_n^{-\gamma}}\nabla_V f(T,V)^{1/q}|^q dV\right)^{2/q}dT < 8\eta_1\,.$$

Next we use an iteration argument vaguely reminiscent (although different in spirit, as we shall explain below) of the one used in the previous section. Using the Hölder and the Sobolev inequalities as in the proof of Proposition 2, isolating the term $\|\nabla_v F_{n+1}\|_{L^2_t L^q_v} = O(\eta_1)$, shows that the quantity

$$X_m := \operatorname*{ess\,sup}_{\frac{1}{2}<t<1}\int_{\mathbf{R}^3}F_{N+m}(t,v)^q dv$$

satisfies

$$X_{m+1} < \rho(\max(1, X_m)^\alpha + \max(1, X_{m-1})^\alpha)\,, \quad X_0, X_1 \le M\,,$$
$$\text{with } \alpha := q/3\,, \qquad \rho := D(q)\eta_1^{q/2}\,, \qquad M := 2^{(N+3)(3-\gamma)}\,.$$

Choose $\eta_1 > 0$ small enough so that $\rho < \frac{1}{4}$. Then, an easy induction argument shows that

$$\max(X_{2m}, X_{2m+1}) \le \max\left(2\rho, (2\rho)^{\frac{1-\alpha^m}{1-\alpha}} M^{\alpha^m}\right)$$

Since $q \in (\frac{6}{5}, 2)$, one has $\alpha \in (0, 2/3)$, and in particular $0 < \alpha < 1$. Therefore

$$\lim_{m\to\infty} \max\left(2\rho, (2\rho)^{\frac{1-\alpha^m}{1-\alpha}} M^{\alpha^m}\right) = \max\left(2\rho, (2\rho)^{\frac{1}{1-\alpha}}\right) = 2\rho$$

since $0 \le 2\rho < 1$ and $\frac{1}{1-\alpha} > 1$. Hence there exists an integer $m_0 \ge 1$ such that

$$X_{m_0} < 3D(q)\eta_1^{\frac{q}{2}} \ll 1$$

reducing $\eta_1 > 0$ further as needed. By undoing the scaling transformation used here and returning to the original variables, we easily check that this implies that f_{N+m_0+3} satisfies the assumption in Proposition 2. With this, the conclusion easily follows.

It is interesting to compare the treatments of the sequences X_m and A_k in this section and the previous one respectively. In the previous section, what matters is that $\beta > 1$. Provided that $A_0 > 0$ is small enough, the exponential increase of the exponent of A_0 in A_k offsets the linear increase of the exponent of Λ in A_k, even if $\Lambda > 0$ is very large. This is typical of the De Giorgi method, and it is indeed one of the clever ideas in this method to arrive at a nonlinear estimate for a linear problem.

In the present section on the contrary, the exponent α satisfies $0 < \alpha < 1$, and even if X_m satisfies an inequality of the same type as the one satisfied by A_k, the argument is totally different. Here, what matters is that the constant $\rho > 0$ can be made arbitrarily small by an appropriate choice of $\eta_1 > 0$. In other words, although X_m and A_k satisfy the same type of recursive inequalities, the arguments for obtaining the required bounds on these sequences are completely different.

7 Proof of the Partial Regularity Theorem

By Proposition 1, the initial data f_{in} launches a $(\mathcal{N}, q, C'_E)$ suitable solution with a constant $C'_E[T, f_{in}, q]$ for each $q \in (1, 2)$.

If $\tau \in \mathbf{S}[f, [1, 2]]$, apply Proposition 3 to the translated solution

$$f_\tau \equiv f_\tau(t, v) := f(t + \tau - 1, v)\,.$$

For each $q \in (\frac{4}{3}, 2)$, there exists $\epsilon(\tau) \in (0, \frac{1}{2})$ such that

$$\int_{\tau-\epsilon(\tau)^\gamma}^{\tau} \left(\int_{\mathbf{R}^3} |\nabla_v (f(t,v)^{1/q} - 1)_+|^q dv \right)^{2/q} dt \geq \tfrac{1}{2}\eta_1 \epsilon(\tau)^{3-\gamma} .$$

By Vitali's covering theorem (see for instance Sect. 1.6 in Chap. 1 of [21]) , there is a sequence $\tau_j \in \mathbf{S}[f, [1,2]]$ such that

$$\mathbf{S}[f, [1,2]] \subset \bigcup_{j\geq 1} (\tau_j - 5\epsilon(\tau_j)^\gamma, \tau_j + 5\epsilon(\tau_j)^\gamma)$$

with $(\tau_j - \epsilon(\tau_j)^\gamma, \tau_j + \epsilon(\tau_j)^\gamma)$ pairwise disjoint for $j \geq 1$.

Thus

$$\begin{aligned} \tfrac{1}{2}\eta_1 \sum_{j\geq 1} \epsilon(\tau_j)^{3-\gamma} &\leq \sum_{j\geq 1} \int_{\tau_j-\epsilon(\tau_j)^\gamma}^{\tau_j} \left(\int_{\mathbf{R}^3} |\nabla_v (f(t,v)^{1/q} - 1)_+|^q dv \right)^{2/q} dt \\ &\leq \int_0^2 \left(\int_{\mathbf{R}^3} |\nabla_v (f(t,v)^{1/q} - 1)_+|^q dv \right)^{2/q} dt < +\infty \end{aligned}$$

Since $\gamma = \frac{5q-6}{2q-2}$, one has $\frac{3-\gamma}{\gamma} = \frac{q}{5q-6}$, and the inequality above implies that

$$\mathscr{H}^{\frac{q}{5q-6}}(\mathbf{S}[f,1,2]) < \infty \quad \text{for each } q \in \left(\frac{4}{3}, 2\right) ,$$

where $\mathscr{H}^s$ designates the s-dimensional Hausdorff measure. Letting $k \to \infty$ (i.e. assuming that f_{in} has finite moments of all positive orders) implies that $q = \frac{2k}{k+3}$ (by Proposition 1) satisfies $q \to 2^-$, and therefore $\frac{q}{5q-6} \to (\frac{1}{2})^+$. The conclusion immediately follows from the very definition of the Hausdorff dimension.

8 Final Remarks and Open Problems

A fascinating outcome of the Desvillettes theorem is that it puts the regularity issue for the Landau equation in the same class as the regularity issue for the three-dimensional Navier–Stokes equations in terms of Lebesgue exponents, except for the $(1 + |v|)^{-3}$ weight in the Fisher information term. It is interesting to compare the following pieces of information coming from Leray's theory [15] in the case of the Navier–Stokes equations, and from the Villani and Desvillettes theory of H-solutions [5, 24] in the case of the Landau equation:

(a) in the case of the Navier–Stokes equations, the velocity field $u \equiv u(t,x) \in \mathbf{R}^3$ satisfies

$$u \in L^\infty(\mathbf{R}_+; L^2(\mathbf{R}^3; \mathbf{R}^3)) , \qquad \nabla_x u \in L^2(\mathbf{R}_+ \times \mathbf{R}^3; M_3(\mathbf{R})) ;$$

(c) in the case of the Landau equation, the distribution function $f \equiv f(t, v) \geq 0$ satisfies

$$\sqrt{f} \in L^\infty(\mathbf{R}_+; L^2(\mathbf{R}^3)) , \qquad \nabla_x \sqrt{f} \in L^2(\mathbf{R}_+; L^2_{-3}(\mathbf{R}^3; \mathbf{R}^3)) .$$

Perhaps more analogies between these two problems should be explored more systematically. For instance, according to Serrin's theorem [19] , if a Leray solution $u \equiv u(t, x)$ of the three-dimensional Navier–Stokes equations satisfies

$$u \in L^p_{loc}(\mathbf{R}^*_+; L^q_{loc}(\mathbf{R}^3)) \quad \text{with } \frac{2}{p} + \frac{3}{q} < 1 ,$$

then u is smooth. Is there a similar conditional regularity result for the Landau equation? specifically, if $f \equiv f(t, v)$ is a H-solution of the Landau equation with finite moments of all orders such that

$$\sqrt{f} \in L^p_{loc}(\mathbf{R}^*_+; L^q_{loc}(\mathbf{R}^3)) \quad \text{with } \frac{2}{p} + \frac{3}{q} < 1 ,$$

is f smooth? The limit case $p = \infty$ and $q = 3$ has been considered in [20]. (The same question could also be investigated for the "isotropic model Landau equation" introduced in the first section of this paper. The similarities and differences with the Navier–Stokes equations are perhaps more obvious on this model equation than on the original Landau equation.)

The analogy between the Landau equation and the Navier–Stokes equations suggests also that a partial regularity theorem in (t, v) "à la" Caffarelli-Kohn-Nirenberg [2] might be within reach. As a matter of fact, our approach to partial regularity through the De Giorgi method is inspired from Vasseur's approach to partial regularity in [23] (see also [8] for a problem closer to the one studied here).

There are however limitations in this analogy, due in particular to the negative weight in the Desvillettes lower bound for the entropy production in the Landau equation. For instance, the set of singular times of Leray solutions of the Navier–Stokes equations in three space dimensions is of $\mathscr{H}^{1/2}$-measure 0. Likewise, Caffarelli-Kohn-Nirenberg [2] prove that the set of singular (t, x) for a suitable solution of the Navier–Stokes equations in three space dimensions is of "parabolic, 1-dimensional Hausdorff measure" 0. Here, the word "parabolic" refers to the fact that the covering of the set of singular (t, x) involved in the definition of the measure uses space-time sets of the form

$$(t_j - \epsilon^2, t_j + \epsilon^2) \times B(x_j, \epsilon) , \qquad j \geq 1 .$$

By comparison, in the case of the Landau equation, we do not know whether $\mathscr{H}^{1/2}(\mathbf{S}[f, I])$ is equal to 0, or even finite, for each bounded time interval I and each suitable solution f.

References

1. L. Ambrosio, P. Tilli, *Topics on Analysis in Metric Spaces* (Oxford University Press, Oxford, 2004)
2. L. Caffarelli, R.V. Kohn, L. Nirenberg, Partial regularity of suitable weak solutions of the Navier-Stokes equations. Comm. Pure Appl. Math. **35**, 771–831 (1982)
3. T. Cazenave, A. Haraux, *An Introduction to Semilinear Evolution Equations* (Oxford University Press, Oxford, 1998)
4. E. De Giorgi, Sulla differenziabilità e l'analiticità delle estremali degli integrali multipli regolari. Mem. Accad. Sci. Torino Cl. Sci. Fis. Mat. Nat. **3**, 25–43 (1957)
5. L. Desvillettes, Entropy dissipation estimates for the Landau equation in the Coulomb case and applications. J. Funct. Anal. **269**, 1359–1403 (2015)
6. F. Golse, M.-P. Gualdani, C. Imbert, A. Vasseur, Partial regularity in time for the space homogeneous Landau equation with Coulomb potential. arXiv:1906.02841 [math.AP] to appear in Ann. Sci. Ec. Norm. Sup.
7. F. Golse, C. Imbert, C. Mouhot, A. Vasseur, Harnack inequality for kinetic Fokker-Planck equations with rough coefficients and application to the Landau equation. Ann. Sc. Norm. Super. Pisa Cl. Sci. **19**(5), 253–295 (2019)
8. T. Goudon, A. Vasseur, Regularity analysis for systems of reaction-diffusion equations. Ann. Sci. Ec. Norm. Sup. **43**, 117–142 (2010)
9. P.T. Gressman, J. Krieger, R.M. Strain, A non-local inequality and global existence. Adv. Math. **230**, 642–648 (2012)
10. M.P. Gualdani, N. Guillen, Estimates for radial solutions of the homogeneous Landau equation with Coulomb potential. Anal. PDE **9**, 1772–1809 (2016)
11. M.P. Gualdani, N. Guillen, On A_p weights and the Landau equation. Calc. Var. Part. Differ. Equ. **58**, no. 1, Art. 17, 55 (2019)
12. C. Imbert, L. Silvestre, The weak Harnack inequality for the Boltzmann equation without cut-off. J. Eur. Math. Soc. **22**, 507–592 (2020)
13. J. Krieger, R. Strain, Global solutions to a non-local diffusion equation with quadratic nonlinearity. Comm. P.D.E. **37**, 647–689 (2012)
14. L.D. Landau, Die kinetische Gleichung für den Fall Coulombscher Wechselwirkung. Phys. Z. Sowjet. **10**, 154–164 (1936)
15. J. Leray, Sur le mouvement d'un liquide visqueux emplissant l'espace. Acta Math. **63**, 193–248 (1934)
16. Fanghua Lin, A new proof of the Caffarelli-Kohn-Nirenberg theorem. Comm. Pure Appl. Math. **51**, 241–257 (1998)
17. E.M. Lifshitz, L.P. Pitaevskii, *Physical Kinetics* (Pergamon Press, Oxford, 1981)
18. V. Scheffer, The Navier-Stokes equations on a bounded domain. Commun. Math. Phys. **73**, 1–42 (1980)
19. J. Serrin, On the interior regularity of weak solutions of the Navier-Stokes equations. Arch. Rational Mech. Anal. **9**, 187–195 (1962)
20. L. Silvestre, Upper bounds for parabolic equations and the Landau equation. J. Differ. Equ. **262**, 3034–3055 (2017)
21. E. Stein, *Singular Integrals and Differentiability Properties of Functions* (Princeton University Press, Princeton, 1970)
22. M. Struwe, On partial regularity results for the Navier-Stokes equations. Comm. Pure Appl. Math. **41**, 437–458 (1988)
23. A. Vasseur, A new proof of partial regularity of solutions to Navier-Stokes equations. NoDEA Nonlin. Diff. Eq. Appl. **14**, 753–785 (2007)
24. C. Villani, On a new class of weak solutions to the spatially homogeneous Boltzmann and Landau equations. Arch. Rational Mech. Anal. **143**, 273–307 (1998)
25. C. Villani, A review of mathematical topics in collisional kinetic theory, in *Handbook of Mathematical Fluid Dynamics*, vol. I, eds. by S. Friedlander, D. Serre (North-Holland, Amsterdam, 2002), pp. 71–305

26. F. Weissler, Local existence and nonexistence for semilinear parabolic equations in L^p. Indiana Univ. Math. J. **29**, 79–102 (1980)

Recent Developments on the Well-Posedness Theory for Vlasov-Type Equations

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Abstract In these notes we summarise some recent developments on the existence and uniqueness theory for Vlasov-type equations, both on the torus and on the whole space.

Keywords Vlasov–Poisson · Plasma physics · Well-posedness

1 An Introduction to Vlasov-Type Equations in Plasma Physics

In this note, we discuss some recent results concerning a class of PDEs used in the modelling of plasma. Plasma is a state of matter abundant in the universe. It can be found in stars, the solar wind and the interstellar medium, and is therefore widely studied in astrophysics, as well as in many other contexts. For example, a major terrestrial application is in nuclear fusion research. For this reason, mathematical modelling of plasma is of interest, with different types of plasma models being suitable for different contexts.

A plasma consists of an ionised gas. It forms when an electrically neutral gas is subjected to high temperatures or a strong electromagnetic field, which causes the gas particles to dissociate into charged particles. These charged particles then interact through electromagnetic forces. The relatively long range nature of these interactions results in a collective behaviour distinct from that expected from a neutral gas.

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In this article, we will discuss the well-posedness of a certain class of PDE models for plasma. We will consider equations of Vlasov type, which describe particle systems with mean field interactions.

1.1 The Vlasov–Poisson System: The Electrons' View-Point

The ionisation process in the formation of a plasma produces two types of charged particle: positively charged ions and negatively charged electrons. It also generally contains neutral species, since not all of the particles of the original neutral gas will dissociate. However, typically the interactions with the neutral species are weak in comparison to the interactions of the charged species. For the purposes of these notes, we will neglect interactions with the neutral particles and concentrate on the modelling of the charged particles.

In fact, it is usual to make an assumption which decouples the dynamics of the two species. It is possible to do this because the mass of an electron is much smaller than the mass of an ion. The result is a separation between the timescales on which each species evolves: in short, the ions typically move much more slowly than the electrons. When modelling the electrons, it is thus common to assume that the ions are stationary over the time interval of observation.

The Vlasov–Poisson system is a well-known kinetic equation describing this situation. This equation was proposed by Jeans [20] as a model for galaxies. Its use in the plasma context dates back to the work of Vlasov [33]. The most commonly known version of the system models the electrons in the plasma. The electrons are described by a density function $f = f(t, x, v)$, which is the unknown in the following system of equations:

$$(VP) := \begin{cases} \partial_t f + v \cdot \nabla_x f + \frac{q_e}{m_e} E \cdot \nabla_v f = 0, \\ \nabla_x \times E = 0, \\ \epsilon_0 \operatorname{div}_x E = R_i + q_e \rho_f, \\ \rho_f(t, x) := \displaystyle\int_{\mathbb{R}^d} f(t, x, v)\, \mathrm{d}v, \\ f|_{t=0} = f_0 \geq 0. \end{cases} \tag{1}$$

Here q_e is the charge on each electron, m_e is the mass of an electron and ϵ_0 is the electric permittivity. $R_i : \mathbb{R}^d \to \mathbb{R}_+$ is the charge density contributed by the ions, which is independent of time since they are assumed to be stationary. The electrons experience a force $q_e E$, where E is the electric field induced by the plasma itself. This is found from the Gauss law

$$\nabla_x \times E = 0, \quad \epsilon_0 \operatorname{div}_x E = R_i + q_e \rho_f,$$

which arises as an electrostatic approximation of the full Maxwell equations.

The system (1) expresses the fact that each electron in the plasma feels the influence of the other particles in the plasma in an averaged sense, through the electric field E induced collectively by the whole plasma. This is a long-range interaction between particles. In particular, this equation does not account for collisions between particles of any species.

The Vlasov–Poisson system as written in Eq. (1) does not yet include a boundary condition. In this note we focus on two cases: either the periodic case where the spatial variable x lies in the d-dimensional flat torus $\mathbb{T}^d$ and the velocity variable v lies in the whole Euclidean space $\mathbb{R}^d$, or the whole space case where both x and v range over $\mathbb{R}^d$. We will use the notation $\mathscr{X}$ to denote the spatial domain, either $\mathbb{T}^d$ or $\mathbb{R}^d$ as appropriate, so that throughout this note we have $(x, v) \in \mathscr{X} \times \mathbb{R}^d$.

It is common to restrict in particular to the case where the background ion density R_i is spatially uniform. In the case of the torus, $\mathscr{X} = \mathbb{T}^d$, this results in the system

$$(VP) := \begin{cases} \partial_t f + v \cdot \nabla_x f + \frac{q_e}{m_e} E \cdot \nabla_v f = 0, \\ \nabla_x \times E = 0, \\ \epsilon_0 \operatorname{div}_x E = q_e \left(\rho_f - \int_{\mathbb{T}^d \times \mathbb{R}^d} f \, \mathrm{d}x \, \mathrm{d}v \right), \\ f|_{t=0} = f_0 \geq 0. \end{cases} \tag{2}$$

The ion charge density is chosen to be

$$R_i \equiv -q_e \int_{\mathbb{T}^d \times \mathbb{R}^d} f \, \mathrm{d}x \, \mathrm{d}v$$

so that the system is globally neutral. This is required from the point of view of the physics under consideration due to the conservation of charge, since the plasma forms from an electrically neutral gas. Note that any solution f of (2) satisfies a transport equation with a divergence free vector field, which implies that the mass of f is conserved by the evolution. Thus in fact

$$R_i \equiv -q_e \int_{\mathbb{T}^d \times \mathbb{R}^d} f_0 \, \mathrm{d}x \, \mathrm{d}v.$$

In mathematical treatments, it is common to see (2) written in the rescaled form

$$(VP) := \begin{cases} \partial_t f + v \cdot \nabla_x f + E \cdot \nabla_v f = 0, \\ \nabla_x \times E = 0, \\ \operatorname{div}_x E = \rho_f - 1, \\ f|_{t=0} = f_0 \geq 0, \ \int_{\mathbb{T}^d \times \mathbb{R}^d} f_0 \, \mathrm{d}x \, \mathrm{d}v = 1. \end{cases} \tag{3}$$

In the whole space case $\mathscr{X} = \mathbb{R}^d$, one often considers a vanishing background, in order to have a system with finite mass. This results in the system

$$\begin{cases} \partial_t f + v \cdot \nabla_x f + E \cdot \nabla_v f = 0, \\ \nabla_x \times E = 0, \\ \operatorname{div}_x E = \rho_f, \\ f|_{t=0} = f_0 \geq 0, \ \displaystyle\int_{\mathbb{R}^d \times \mathbb{R}^d} f_0 \, \mathrm{d}x \, \mathrm{d}v = 1. \end{cases} \tag{4}$$

1.2 The Vlasov–Poisson System with Massless Electrons: The Ions' View-Point

The previous section presented the Vlasov–Poisson system as a model for the electrons in a dilute, unmagnetised, collisionless plasma. A variant of the Vlasov–Poisson system may be used to model the ions in the plasma instead.

To derive an appropriate model, once again we make use of the large disparity between the masses of the two species. The resulting separation of timescales allows an approximation in which the two species are modelled separately. From the point of view of the ions, the electrons have a very small mass and so are very fast moving. Since the electrons are not stationary, a model of the form (3) is not appropriate.

Instead observe that, since the electrons move quickly relative to the ions, the frequency of electron-electron collisions is high in comparison to ion-ion or ion-electron collisions. Electron-electron collisions are expected to be relevant on the typical timescale of evolution of the ions, even while the frequencies of other kinds of collisions remain negligible. The expected effect of the electron-electron collisions is to drive the electron distribution towards its equilibrium configuration. In ion models it is therefore common in physics literature to assume that the electrons are close to thermal equilibrium.

In the limit of **massless electrons**, the ratio between the masses of the electrons and ions, m_e/m_i, tends to zero. Here m_e is the mass of an electron and m_i is the mass of an ion. In the limiting regime, it is assumed that the electrons instantaneously assume the equilibrium distribution. This approximation is often made in the physics literature, motivated by the fact that m_e/m_i is close to zero in applications.

1.2.1 The Maxwell–Boltzmann Law for Electrons

The equilibrium distribution can be identified by studying the equation for the evolution of electrons. Let the ion density $\rho[f_i]$ be fixed, and assume that all ions carry the same charge q_i. We have discussed that a possible model for the evolution of the electron density is the Vlasov–Poisson system (1). However, the Vlasov–Poisson system is a collisionless model. As discussed above, in the long time regime we consider we expect the effect of electron-electron collisions to be significant.

Collisions in a plasma are described by the Landau-Coulomb operator Q_L [21, Chap. 4], which is an integral operator defined as follows: for a given function $g =$

$g(v) : \mathbb{R}^d \to \mathbb{R}$,

$$Q_L(g) := \operatorname{div}_v \int_{\mathbb{R}^d} a(v - v_*) : [g(v_*)\nabla_v g(v) - g(v)\nabla_v g(v_*)]\, \mathrm{d}v_*.$$

The tensor a is defined by

$$a(z) = \frac{|z|^2 \mathbb{I} - z \otimes z}{|z|^3}.$$

We add this term to the Vlasov–Poisson system to model a plasma with collisions. This results in the following model for the electron density f_e:

$$\begin{cases} \partial_t f_e + v \cdot \nabla_x f_e + \dfrac{q_e}{m_e} E \cdot \nabla_v f_e = \dfrac{C_e}{m_e^2} Q_L(f_e), \\ \\ \nabla_x \times E = 0, \quad \epsilon_0 \operatorname{div}_x E = q_i \rho[f_i] + q_e \rho[f_e]. \end{cases} \tag{5}$$

Here C_e is a constant depending on physical quantities such as the electron charge q_e and number density n_e, but *not* on the electron mass m_e. For the derivation of the scaling C_e/m_e^2 in front of the Landau-Coulomb operator, see Bellan [4, Chap. 13, Eq. (13.46)].

Consider the rescaling

$$F_e(t, x, v) = m_e^{-\frac{d}{2}} f_e\left(t, x, \frac{v}{\sqrt{m_e}}\right).$$

Notice that this scaling preserves the macroscopic density: $\rho[F_e] = \rho[f_e]$. Then F_e satisfies

$$\begin{cases} \sqrt{m_e}\partial_t F_e + v \cdot \nabla_x F_e + q_e E \cdot \nabla_v F_e = C_e Q_L(F_e), \\ \\ \nabla \times E = 0, \quad \epsilon_0 \nabla \cdot E = q_i \rho[f_i] + q_e \rho[F_e]. \end{cases} \tag{6}$$

We assume that F_e converges to a stationary distribution $\bar{f}_e = \bar{f}_e(x, v)$ as m_e tends to zero, and focus on formally identifying $\bar{f}_e$.

To identify the possible forms of $\bar{f}_e$, we consider the entropy functional

$$H[f] := \int_{\mathscr{X} \times \mathbb{R}^d} f \log f \, \mathrm{d}x \, \mathrm{d}v.$$

For a solution F_e of Eq. (6),

$$\frac{\mathrm{d}}{\mathrm{d}t} H[F_e] = m_e^{-1/2} \int_{\mathscr{X} \times \mathbb{R}^d} (1 + \log F_e) \left[-\operatorname{div}_{x,v} ((v, E) F_e) + Q_L(F_e) \right] \mathrm{d}x \, \mathrm{d}v.$$

Integrating by parts formally, the transport term vanishes:

$$-\int_{\mathscr{X}\times\mathbb{R}^d}(1+\log F_e)\mathrm{div}_{x,v}\left((v,E)F_e\right)\mathrm{d}x\,\mathrm{d}v=\int_{\mathscr{X}\times\mathbb{R}^d}(v,E)\cdot\nabla_{x,v}F_e\,\mathrm{d}x\,\mathrm{d}v$$
$$=\int_{\mathscr{X}\times\mathbb{R}^d}\mathrm{div}_{x,v}\left((v,E)F_e\right)\mathrm{d}x\,\mathrm{d}v=0.$$

Thus

$$\frac{\mathrm{d}}{\mathrm{d}t}H[F_e]=m_e^{-1/2}\int_{\mathscr{X}\times\mathbb{R}^d}(1+\log F_e)\,Q_L(F_e)\,\mathrm{d}x\,\mathrm{d}v.$$

By substituting the definition of Q_L, one can calculate formally (see [10]) that

$$\frac{\mathrm{d}}{\mathrm{d}t}H[F_e]=-\frac{C}{\sqrt{m_e}}\int_{\mathscr{X}\times\mathbb{R}^d}\frac{1}{|v-v_*|}\cdot$$
$$\cdot\left|P_{(v-v_*)^\perp}\left[\nabla_v\sqrt{F_e(x,v)F_e(x,v_*)}-\nabla_{v_*}\sqrt{F_e(x,v)F_e(x,v_*)}\right]\right|^2\mathrm{d}v_*\,\mathrm{d}v\,\mathrm{d}x,\quad(7)$$

where $P_{(v-v_*)^\perp}$ denotes the operator giving the orthogonal projection onto the hyperplane perpendicular to $v-v_*$. For a stationary solution $\bar{f}_e$, we must have $\frac{\mathrm{d}}{\mathrm{d}t}H[\bar{f}_e]=0$, that is, the functional on the right hand side of (7) must vanish. If $\bar{f}_e\in L^1$, it follows (see for example [32, Lemma 3]) that $\bar{f}_e$ is a local Maxwellian of the form

$$\bar{f}_e(x,v)=\rho_e(x)\left(\pi\beta_e(x)\right)^{d/2}\exp\left[-\beta_e(x)|v-u_e(x)|^2\right].\quad(8)$$

The electron density ρ_e, mean velocity u_e and inverse temperature β_e can then be studied using an argument similar to the one given in the proof of [2, Theorem 1.1]. Substituting the form (8) into Eq. (5), we obtain the following identity for all x such that $\rho_e(x)\neq 0$ and all $v\in\mathbb{R}^d$:

$$-\nabla_x\beta_e\cdot(v-u_e)|v-u_e|^2-u_e\cdot\nabla_x\beta_e|v-u_e|^2+\beta_e(v-u_e)^\top\nabla_x u_e(v-u_e)$$
$$+(v-u_e)\cdot\left[\nabla_x\log\left(\rho_e\beta_e^{d/2}\right)-q_e\beta_e E+u_e\cdot\nabla_x u_e\right]+u_e\cdot\nabla_x\log\left(\rho_e\beta_e^{d/2}\right)=0.$$

For each fixed x, the left hand side is a polynomial in $v-u_e(x)$, whose coefficients must all be equal to zero. For example, by looking at the cubic term we see that $\nabla_x\beta_e=0$ and thus β_e must be a constant independent of x.

The quadratic term then gives

$$v^\top\nabla_x u_e v=0\qquad\text{for all } v\in\mathbb{R}^d,$$

which implies that $\nabla_x u_e$ is skew-symmetric. On a spatial domain for which a Korn inequality holds, this restricts the class of u_e that can occur. For example, in the case of the torus $\mathscr{X}=\mathbb{T}^d$, the fact that the symmetric part of $\nabla_x u_e$ vanishes implies that u_e is constant [11, Proposition 13].

Finally, from the linear term we obtain that

$$\nabla_x \log(\rho_e \beta_e^{d/2}) - q_e \beta_e E = 0.$$

Since $\nabla_x \times E = 0$, E is a gradient—that is, it can be written as $E = -\nabla U$ for some function U. Then

$$\nabla_x \log(\rho_e \beta_e^{d/2}) = -q_e \beta_e \nabla_x U.$$

From this we deduce that ρ_e should be of the form

$$\rho_e(x) = A \exp(-q_e \beta_e U),$$

for some constant $A > 0$. This is known as a **Maxwell–Boltzmann** law.

In the whole space case $\mathscr{X} = \mathbb{R}^d$, we include an additional spatial confinement of the electrons, by adding an additional potential Ψ to the electron dynamics. The equivalent of Eq. (6) is then

$$\begin{cases} \sqrt{m_e}\partial_t F_e + v \cdot \nabla_x F_e + (q_e E - \nabla \Psi) \cdot \nabla_v F_e = C_e Q_L(F_e), \\ \nabla \times E = 0, \quad \epsilon_0 \nabla \cdot E = q_i \rho[f_i] + q_e \rho[F_e]. \end{cases}$$

Repeating the previous argument, we can derive the following limiting distribution in the regime $m_e \to 0$:

$$\rho_e = A e^{-\beta_e(q_e U + \Psi)} = A g e^{-\beta_e q_e U},$$

where we let $g = e^{-\beta_e \Psi}$. We assume that the confining potential Ψ grows sufficiently quickly at infinity so that $g \in L^1 \cap L^\infty(\mathbb{R}^d \times \mathbb{R}^d)$.

Bardos, Golse, Nguyen and Sentis [2] studied the problem of rigorously identifying the Maxwell–Boltzmann law as the distribution of electrons in the massless limit. They consider coupled systems of the form

$$\begin{cases} \partial_t f_i + v \cdot \nabla_x f_i + \frac{q_i}{m_i} E \cdot \nabla_v f_i = 0, \\ \partial_t f_e + v \cdot \nabla_x f_e + \frac{q_e}{m_e} E \cdot \nabla_v f_e = C(m_e) Q(f_e), \\ \nabla_x \times E = 0, \quad \epsilon_0 \operatorname{div}_x E = q_i \rho[f_i] + q_e \rho[f_e]. \end{cases} \tag{9}$$

In the above, Q denotes a collision operator such as a BGK or Boltzmann operator. Under suitable hypotheses on the spatial domain and the collision rate $C(m_e)$, and assuming the existence of sufficiently regular solutions of the coupled system (9), they derive that, in the limit as m_e/m_i tends to zero, the electrons indeed take on a Maxwell–Boltzmann distribution. Moreover, solutions of the system (9) converge to a solution of a system of a similar form to Eq. (12) below, but where the electron temperature depends on time and is chosen to respect the conservation of energy. Other works on this topic include, for example, the work of Bouchut and Dolbeault [7] on the long time limit for the Vlasov–Poisson–Fokker–Planck system for one species—the massless electrons limit can be related to a long time limit since (6) can also be seen as a time rescaling. Herda [17] also considered the massless electron

limit in the case with an external magnetic field. In this case the limiting system is a fluid model for the electrons, coupled with a kinetic model for the ions.

1.2.2 The Vlasov–Poisson System in the Limit of Massless Electrons

From Eq. (5), we see that the electrostatic potential U induced by a distribution $\rho[f_i]$ of ions with a background of thermalised electrons should satisfy the following semilinear elliptic PDE:

$$-\epsilon_0 \Delta U = q_i \rho[f_i] + A q_e \, g \exp\left(-\frac{q_e U}{k_B T_e}\right), \tag{10}$$

where in the torus case $\mathscr{X} = \mathbb{T}^d$ we let $g \equiv 1$. The normalising constant A should be chosen so that the system is globally neutral, that is, the total charge is zero:

$$\int_{\mathscr{X}} q_i \rho[f_i] + A q_e \exp\left(-\frac{q_e U}{k_B T_e}\right) \mathrm{d}x = 0. \tag{11}$$

Indeed, on the torus $\mathscr{X} = \mathbb{T}^d$, the Poisson equation

$$\Delta U = h$$

can only be solved if h has total integral zero. Thus if (10) has a solution, global neutrality must hold automatically. Adjusting the choice of A corresponds to adding a constant to U. Thus without loss of generality we choose $A = 1$.

Then, the nonlinear equation (10) replaces the standard Poisson equation for the electrostatic potential in the Vlasov–Poisson system (1). After a suitable normalisation of physical constants, this leads to the following system for the ions:

$$(VPME) := \begin{cases} \partial_t f + v \cdot \nabla_x f + E \cdot \nabla_v f = 0, \\ E = -\nabla_x U, \\ \Delta U = e^U - \rho_f, \\ f|_{t=0} = f_0 \geq 0, \ \displaystyle\int_{\mathbb{T}^d \times \mathbb{R}^d} f_0 \, \mathrm{d}x \, \mathrm{d}v = 1. \end{cases} \tag{12}$$

This is known as the Vlasov–Poisson system **with massless electrons**, or **VPME** system.

In the whole space case $\mathscr{X} = \mathbb{R}^d$, we consider two versions of the VPME system, depending on the choice of the constant A. In one case, we let $A = 1$. With a suitable choice of dimensionless variables, this results in the following system:

$$\begin{cases} \partial_t f + v \cdot \nabla_x f + E \cdot \nabla_v f = 0, \\ E = -\nabla_x U, \\ \Delta U = g e^U - \rho_f, \\ f|_{t=0} = f_0 \geq 0, \int_{\mathbb{R}^d \times \mathbb{R}^d} f_0 \, \mathrm{d}x \, \mathrm{d}v = 1. \end{cases} \tag{13}$$

This system is structurally similar to the torus case (12) considered above. Note however that in this model the system is not necessarily globally neutral. In order to enforce global neutrality, we can instead choose A to be a normalising constant

$$A = \frac{1}{\int_{\mathbb{R}^d} g e^U \, \mathrm{d}x}.$$

Thus we obtain the following system:

$$\begin{cases} \partial_t f + v \cdot \nabla_x f + E \cdot \nabla_v f = 0, \\ E = -\nabla_x U, \\ \Delta U = \frac{g e^U}{\int_{\mathbb{R}^d} g e^U \, \mathrm{d}x} - \rho_f, \\ f|_{t=0} = f_0 \geq 0, \int_{\mathbb{R}^d \times \mathbb{R}^d} f_0 \, \mathrm{d}x \, \mathrm{d}v = 1. \end{cases} \tag{14}$$

The VPME system has been used in the physics literature in, for instance, numerical studies of the formation of ion-acoustic shocks [24, 29] and the development of phase-space vortices behind such shocks [5], as well as in studies of the expansion of plasma into vacuum [25]. A physically oriented introduction to the model (12) may be found in [14].

In [13], we consider the problem of proving well-posedness for the VPME system (12) under reasonable conditions on the initial datum f_0. The well-posedness of the systems (13) and (14) is considered in a forthcoming paper.

2 Well-Posedness for Vlasov Equations with Smooth Interactions

The Vlasov–Poisson system is an example of a more general class of nonlinear scalar transport equations known as **Vlasov equations**. A Vlasov equation takes the following form:

$$\begin{cases} \partial_t f + v \cdot \nabla_x f + F[f] \cdot \nabla_v f = 0, \\ F[f](t,x) = -\nabla_x W * \rho_f, \\ \rho_f(t,x) = \int_{\mathbb{R}^d} f(t,x,v) \, \mathrm{d}v, \\ f(0,x,v) = f_0(x,v) \geq 0. \end{cases} \tag{15}$$

The system (15) is a mean field model for a system of interacting particles with binary interactions described by a pair potential $W : \mathscr{X} \to \mathbb{R}$. The electron Vlasov–Poisson systems (3), (4) can be seen to be of the form (15) by choosing W to be the Green's function of the Laplacian on $\mathscr{X}$. By this we mean that G is a function satisfying the relation

$$-\Delta G = \delta_0 - 1 \quad \text{for } \mathscr{X} = \mathbb{T}^d, \quad \text{or} \quad -\Delta G = \delta_0 \quad \text{for } \mathscr{X} = \mathbb{R}^d. \tag{16}$$

The function $U = G * (\rho_f - 1)$ is a solution of the Poisson equation, respectively

$$-\Delta U = \rho_f - 1 \quad \text{on } \mathbb{T}^d \quad \text{or} \quad -\Delta U = \rho_f \quad \text{on } \mathbb{R}^d.$$

Thus the Vlasov–Poisson systems (3), (4) are of the form (15).

The available well-posedness theory for the system (15) depends on the choice of the interaction potential W, and in particular on the regularity of the force $-\nabla W$. For example, if ∇W is a Lipschitz function, then the system (15) is well-posed in the class $C\left([0,\infty); \mathscr{M}_+(\mathscr{X} \times \mathbb{R}^d)\right)$—the space of continuous paths taking values in the space $\mathscr{M}_+(\mathscr{X} \times \mathbb{R}^d)$ of finite measures on $\mathscr{X} \times \mathbb{R}^d$ equipped with the topology of weak convergence of measures. This case was considered for example by Braun and Hepp [8] and by Dobrushin [12].

A path $f \in C\left([0,\infty); \mathscr{M}_+(\mathscr{X} \times \mathbb{R}^d)\right)$ is a weak solution of the Vlasov equation (15) if, for all test functions $\phi \in C_c^1\left([0,\infty) \times \mathscr{X} \times \mathbb{R}^d\right)$,

$$\int_0^\infty \int_{\mathscr{X}\times\mathbb{R}^d} \left[\partial_t \phi + v \cdot \nabla_x \phi - \left(\nabla_x W *_x \rho_f\right) \cdot \nabla_v \phi\right] f(t, \mathrm{d}x, \mathrm{d}v)\, \mathrm{d}t + \int_{\mathscr{X}\times\mathbb{R}^d} \phi(0, x, v)\, f_0(\mathrm{d}x, \mathrm{d}v) = 0. \tag{17}$$

Under the assumption that ∇W is a Lipschitz function, it is known that weak solutions of the Vlasov equation (15) exist [8, 12] and are unique [12].

Theorem 1 *Assume that $\nabla W : \mathscr{X} \to \mathbb{R}^d$ is a Lipschitz function. Let f_0 be a finite non-negative measure with finite first moment:*

$$\int_{\mathbb{T}^d\times\mathbb{R}^d} (1 + |x| + |v|)\, f_0(\mathrm{d}x\, \mathrm{d}v) < +\infty.$$

Then there exists a unique weak solution $f \in C\left([0,+\infty); \mathscr{M}_+(\mathscr{X} \times \mathbb{R}^d)\right)$ of the Vlasov equation (15).

3 Well-Posedness for the Vlasov–Poisson System

In the case of the Vlasov–Poisson system for electrons (3), the interaction potential W is chosen to be the function G defined by the relation (16). The resulting force $K = -\nabla G$ is known as the Coulomb kernel. However, K is not a Lipschitz function and so the Vlasov–Poisson system does not satisfy the assumptions of Theorem 1. For example, in the whole space case, $\mathscr{X} = \mathbb{R}^d$, G takes the form

$$G_{\mathbb{R}^d}(x) = \begin{cases} -\frac{1}{2\pi} \log |x|, & d = 2, \\ \frac{1}{4\pi |x|}, & d = 3, \end{cases} \tag{18}$$

The Coulomb kernel $K_{\mathbb{R}^d} = -\nabla G_{\mathbb{R}^d}$ takes the form

$$K(x) = \begin{cases} \frac{x}{2\pi |x|^2}, & d = 2, \\ \frac{x}{4\pi |x|^3}, & d = 3, \end{cases} \tag{19}$$

and thus has a singluarity at $x = 0$.

On the torus $\mathscr{X} = \mathbb{T}^d$, it can be shown that $G_{\mathbb{T}^d}$ is smooth away from the origin: $G_{\mathbb{T}^d} \in C^\infty(\mathbb{T}^d \setminus \{0\})$. Near the singularity it is of the form

$$G_{\mathbb{T}^d} = G_{\mathbb{R}^d} + G_1,$$

where G_1 is a C^∞ function. Thus $K_{\mathbb{T}^d}$ possesses a singularity similar to that of $K_{\mathbb{R}^d}$.

Consequently, Theorem 1 does not apply to the Vlasov–Poisson system. It is not known whether the Vlasov–Poisson system is well-posed in the class of measure solutions. However, global well-posedness has been shown for solution classes with greater regularity.

Arsen'ev [1] introduced a notion of weak solution for the Vlasov–Poisson system (3) in dimension $d = 3$ and proved the existence of such solutions, globally in time, for initial data f_0 belonging to the space $L^1 \cap L^\infty(\mathbb{R}^6)$. The boundedness condition $f_0 \in L^\infty(\mathbb{R}^6)$ was later relaxed to $f_0 \in L^p(\mathbb{R}^6)$, for p sufficiently large, by Horst and Hunze [19].

In the case of classical C^1 solutions, in the two-dimensional case $d = 2$ Ukai and Okabe [31] proved global existence for initial data $f_0 \in C^1(\mathbb{R}^4)$ decaying sufficiently fast at infinity. This result was extended under similar assumptions to the case $d = 3$ by Pfaffelmoser [27]. Schaeffer gave a streamlined proof of the same result in [30], focusing however on the case of compactly supported initial data for clarity. Horst [18] extended these results to include non-compactly supported initial data with sufficiently fast decay at infinity, obtaining improved bounds on the time growth of the velocity of the particles. The methods of proof for these results are based on an analysis of the characteristic trajectories associated to system (3). This approach was adapted to the torus by Batt and Rein [3], who proved the existence of global-in-time

classical solutions for (3) posed on $\mathbb{T}^3 \times \mathbb{R}^3$, for initial data $f_0 \in C^1(\mathbb{T}^3 \times \mathbb{R}^3)$ with sufficiently fast decay at infinity.

An alternative approach to the construction of global-in-time solutions in dimension $d = 3$ was provided by Lions and Perthame [22]. Their method is based on proving the propagation of moments. They showed global existence of solutions, provided that the initial datum $f_0 \in L^1 \cap L^\infty(\mathbb{R}^d \times \mathbb{R}^d)$ has moments in velocity of sufficiently high order. However, their strategy is for the whole space case $x \in \mathbb{R}^d$, and differs from the strategies currently available for the torus.

Pallard [26] then extended the range of moments that could be propagated in the whole space case and showed propagation of moments on the torus $\mathbb{T}^3$, using a method based on an analysis of trajectories (more similar to [3, 27, 30]). Chen and Chen [9] adapted these techniques to further extend the range of moments that could be propagated for the torus case.

Lions and Perthame [22] proved a uniqueness criterion for their solutions under the additional technical condition that, for all $R, T > 0$,

$$\sup\left\{|\nabla f_0(y + vt, w)| : |y - x| \le R, |w - v| \le R\right\} \in L^\infty\left((0, T) \times \mathbb{R}^3_x; L^1 \cap L^2(\mathbb{R}^3_v)\right)\Big\}.$$

Robert [28] then proved uniqueness for solutions that are compactly supported in phase space for all time. Subsequently, Loeper [23] proved a uniqueness result which requires only boundedness of the mass density ρ_f, and therefore includes the compactly supported case. Loeper's result is based on proving a stability estimate on solutions of the VPME system (12) with bounded density, with respect to their initial data f_0—in particular, a quantitative estimate in terms of the second order Wasserstein distance W_2. In a similar vein, in the one dimensional case Hauray [16] proved a weak-strong uniqueness principle, showing that if a bounded density solution exists, then this solution is unique among measure-valued solutions. This result is also based on a Wasserstein stability result.

4 Well-Posedness Theory for the Vlasov–Poisson System with Massless Electrons

The VPME system for ions is in general less well understood than the Vlasov–Poisson system for electrons, due to the additional nonlinearity in the elliptic equation for the electrostatic potential. In the case of the well-posedness theory, weak solutions for the VPME system were constructed in dimension $d = 3$ in the whole space by Bouchut [6], globally in time. In one dimension, global-in-time weak solutions were constructed by Han-Kwan and Iacobelli [15] for measure data with a first moment. A weak-strong uniqueness principle was also proved for solutions satisfying $\rho_f \in L^\infty_{\text{loc}}([0, +\infty); L^\infty(\mathbb{T}))$: namely, if a solution with this regularity exists, then it is unique among measure solutions. However, a well-posedness theory for strong solutions in higher dimensions remained open.

In the article [13], global well-posedness is proved for the VPME system on the torus in dimension $d = 2$ and $d = 3$. The main result is stated in the following theorem.

Theorem 2 (Global well-posedness: $\mathbb{T}^d$) *Let $d = 2, 3$. Let the initial datum $f_0 \in L^1 \cap L^\infty(\mathbb{T}^d \times \mathbb{R}^d)$ be a probability density satisfying*

$$f_0(x, v) \leq \frac{C_0}{1 + |v|^{k_0}} \quad \text{for some } k_0 > d,$$

$$\int_{\mathbb{T}^d \times \mathbb{R}^d} |v|^{m_0} f_0(x, v)\, \mathrm{d}x\, \mathrm{d}v < +\infty \quad \text{for some } m_0 > d(d-1).$$

Then there exists a global-in-time weak solution $f \in C([0, \infty); \mathscr{P}(\mathbb{T}^d \times \mathbb{R}^d))$ of the VPME system (12) with initial data f_0. This is the unique solution of (12) with initial datum f_0 such that

$$\rho_f \in L^\infty_{loc}([0, +\infty); L^\infty(\mathbb{T}^d)).$$

In addition, if f_0 has compact support, then at each time t, $f(t)$ has compact support.

This theorem asks for no regularity on f_0, only that $f_0 \in L^1 \cap L^\infty(\mathbb{T}^d \times \mathbb{R}^d)$. The resulting solutions are therefore not C^1 classical solutions in general. It is thus useful to introduce a concept of *strong* solutions: the class of bounded distributional solutions f of (12) whose density ρ_f is uniformly bounded: $\rho_f \in L^\infty_{\mathrm{loc}}([0, +\infty); L^\infty(\mathscr{X}))$. Strong solutions have several convenient properties: in particular, their characteristic ODE system is well-posed and the resulting flow can be used to represent the solutions. A consequence of this is that if the initial datum f_0 is additionally assumed to be C^1, then the resulting strong solution is in fact a C^1 classical solution. Therefore we may also deduce global well-posedness for classical solutions of the VPME system.

In a forthcoming paper, we also consider the problem posed on the whole space; we are able to prove the following global well-posedness result for the whole space systems (13)and (14).

Theorem 3 (Global well-posedness: $\mathbb{R}^3$) *Let $f_0 \in L^1 \cap L^\infty(\mathbb{R}^3 \times \mathbb{R}^3)$ be a probability density satisfy*

$$f_0(x, v) \leq \frac{C}{(1 + |v|)^r} \quad \text{for some } r > 3,$$

$$\int_{\mathbb{R}^3 \times \mathbb{R}^3} |v|^{m_0} f_0(x, v)\, dx\, dv < +\infty \quad \text{for some } m_0 > 6.$$

Assume that $g \in L^1 \cap L^\infty(\mathbb{R}^3)$, with $g \geq 0$ satisfying $\int_{\mathbb{R}^3} g = 1$. Then there exists a unique solution $f \in L^\infty([0, T]; L^1 \cap L^\infty(\mathbb{R}^3 \times \mathbb{R}^3))$ of (13) (resp. (14)) with initial datum f_0 such that $\rho_f \in L^\infty([0, T]; L^\infty(\mathbb{R}^3))$.

Remark 1 In particular, these results provide well-posedness for the VPME system under the same conditions as were previously known for the Vlasov–Poisson system.

4.1 Strategy for $\mathbb{T}^d$

4.1.1 Analysis of the Electric Field

The first step of the proof is to obtain estimates on the regularity of the electric field E. We begin with a decomposition of the electric field, as was used in [15] for the one dimensional setting. The electric field E can be seen as a sum of the electric field appearing in the electron model (3), plus a more regular nonlinear term. For this, we use the notation $E = \bar{E} + \widehat{E}$, where

$$\bar{E} = -\nabla \bar{U}, \qquad \widehat{E} = -\nabla \widehat{U},$$

and $\bar{U}$ and $\widehat{U}$ solve respectively

$$\Delta \bar{U} = 1 - \rho_f, \qquad \Delta \widehat{U} = e^{\bar{U}+\widehat{U}} - 1. \tag{20}$$

We expect $\widehat{E}$ to be more regular than $\bar{E}$. The key point is to prove this rigorously, taking into account the nonlinearity in the equation satisfied by $\widehat{U}$. In particular we need to quantify the gain of regularity carefully.

To analyse $\widehat{E}$, we use techniques from the calculus of variations which allow us to deal with the nonlinearity in the equation for $\widehat{U}$. We then wish to quantify the gain of regularity in terms of its dependence on ρ_f. The key lemma is the following regularity estimate.

Lemma 1 *Let $d = 2, 3$. Assume that $\rho_f \in L^{\frac{d+2}{d}}$. There exist unique $\bar{U}, \widehat{U} \in W^{1,2}(\mathbb{T}^d)$ such that*

$$\Delta \bar{U} = 1 - \rho_f, \qquad \Delta \widehat{U} = e^{\bar{U}+\widehat{U}} - 1.$$

Moreover, there exists $\alpha > 0$ such that $\widehat{U} \in C^{2,\alpha}(\mathbb{T}^d)$, with the quantitative estimate

$$\|\widehat{U}\|_{C^{2,\alpha}(\mathbb{T}^d)} \leq C_{\alpha,d} \exp\exp\left(C_{\alpha,d}\left(1 + \|\rho_f\|_{L^{\frac{d+2}{d}}(\mathbb{T}^d)}\right)\right), \qquad \alpha \in \begin{cases} (0,1) \text{ if } d = 2 \\ (0, \frac{1}{5}] \text{ if } d = 3. \end{cases}$$

The choice of $(d+2)/d$ as the integrability exponent is relevant because this is a quantity that we expect to be bounded uniformly in time, as a consequence of the conservation of the following energy functional associated to the VPME system:

$$\mathscr{E}[f] := \frac{1}{2}\int_{\mathbb{T}^d \times \mathbb{R}^d} |v|^2 f \, \mathrm{d}x \, \mathrm{d}v + \frac{1}{2}\int_{\mathbb{T}^d} |\nabla U|^2 \, \mathrm{d}x + \int_{\mathbb{T}^d} U e^U \, \mathrm{d}x. \tag{21}$$

Lemma 2 *Let $f \geq 0$ satisfy, for some constant $C_0 > 0$,*

$$\|f\|_{L^\infty(\mathbb{T}^d \times \mathbb{R}^d)} \leq C_0, \qquad \mathscr{E}[f] \leq C_0,$$

where $\mathscr{E}$ is the energy functional defined in (21). Then the mass density

$$\rho_f(x) := \int_{\mathbb{R}^d} f(x, v)\, \mathrm{d}v \tag{22}$$

lies in $L^{(d+2)/d}(\mathbb{T}^d)$ with

$$\|\rho_f\|_{L^{\frac{d+2}{d}}(\mathbb{T}^d)} \leq C_1. \tag{23}$$

for some constant $C_1 > 0$ depending on C_0 and d only.

Using these estimates on the electric field, the proof of well-posedness is carried out in two main steps. First we prove the uniqueness of solutions for VPME under the condition that the mass density ρ_f is bounded in $L^\infty(\mathbb{T}^d)$. Then, we show the global existence of solutions with bounded density, given the assumptions of Theorem 2.

4.1.2 Uniqueness

The first part of the proof of well-posedness is to prove the uniqueness of strong solutions, i.e. uniqueness under the condition that

$$\rho_f \in L^\infty_{\mathrm{loc}}\left([0, +\infty); L^\infty(\mathbb{T}^d)\right).$$

For the electron Vlasov–Poisson system (3), Loeper [23] proved uniqueness of solutions under this condition. In the VPME setting, we make use of Loeper's strategy to handle the electric field $\bar{E}$. However, to deal with $\widehat{E}$ further nontrivial estimates are necessary. We prove the following estimate, which quantifies the stability of $\widehat{E}$ with respect to the charge density ρ_f.

Lemma 3 *For each $i = 1, 2$, let $\bar{U}_i$ and $\widehat{U}_i$ be respectively solutions of*

$$\Delta \bar{U}_i = h_i - 1, \qquad \Delta \widehat{U}_i = e^{\bar{U}_i + \widehat{U}_i} - 1.$$

where $h_i \in L^\infty \cap L^{(d+2)/d}(\mathbb{T}^d)$. Then there exists a constant $C_d > 0$ such that

$$\begin{aligned} &\|\nabla \widehat{U}_1 - \nabla \widehat{U}_2\|^2_{L^2(\mathbb{T}^d)} \\ &\quad \leq \exp\exp\left[C_d\left(1 + \max_i \|h_i\|_{L^{(d+2)/d}(\mathbb{T}^d)}\right)\right] \max_i \|h_i\|_{L^\infty(\mathbb{T}^d)}\, W_2^2(h_1, h_2). \end{aligned} \tag{24}$$

Using these estimates, we are able to prove the following stability estimate for solutions of the VPME system (12) relative to the initial datum, quantified in the

second order Wasserstein distance W_2. Uniqueness of strong solutions then follows immediately.

Proposition 1 (Stability for solutions with bounded density) *For $i = 1, 2$, let f_i be solutions of (12) satisfying for some constant M and all $t \in [0, T]$,*

$$\rho[f_i(t)] \leq M. \tag{25}$$

Then there exists a constant C, depending on M, such that, for all $t \in [0, T]$,

$$W_2\left(f_1(t),\, f_2(t)\right)^2 \leq \begin{cases} 16de \exp\left[\log \frac{W_2(f_1(0),\, f_2(0))^2}{16de} e^{-Ct}\right] & \text{if } t \leq t_0 \\ \max\left\{W_2\left(f_1(0),\, f_2(0)\right)^2, d\right\} e^{C(1+\log 16)(t-t_0)} & \text{if } t > t_0. \end{cases}$$

where the time t_0 is defined by

$$\begin{aligned} t_0 &= t_0\big(W_2\left(f_1(0),\, f_2(0)\right)\big) \\ &= \inf\left\{t \geq 0 : 16de \exp\left[\log \frac{W_2\left(f_1(0),\, f_2(0)\right)^2}{16de} e^{-Ct}\right] > d\right\}. \end{aligned}$$

4.1.3 Existence of Solutions

The proof of existence is based on controlling the moments of solutions. We first show an a priori estimate, proving that the VPME propagates velocity moments of sufficiently high order. This approach was previously used to prove global existence for the electron Vlasov–Poisson system, going back to the work of Lions and Perthame [22] for the problem posed on $\mathbb{R}^3$. Pallard [26] proved propagation of moments on the torus and extended the range of moments that could be propagated in the whole space, while Chen and Chen [9] further extended the range of moments available for the torus case. By extending these methods to the VPME case, we show global-in-time existence of solutions for the VPME system, for any initial datum $f_0 \in L^1 \cap L^\infty(\mathbb{T}^d \times \mathbb{R}^d)$ that has a finite velocity moment of order $m_0 > d$. Note that Theorem 2 requires moments of higher order than this, for the reason that stronger assumptions are required to show uniqueness.

The proposition below shows the propagation of moments for classical solutions of the VPME system. In the proof, the estimates from Lemma 1 on the nonlinear part of the potential $\widehat{U}$ are crucial.

Proposition 2 *Let the dimension $d = 2$ or $d = 3$. Let $0 \leq f_0 \in L^1 \cap L^\infty(\mathbb{T}^d \times \mathbb{R}^d)$ have a finite energy and finite velocity moment of order $m_0 > d$:*

$$\mathscr{E}[f] \leq C_0 < +\infty, \qquad \int_{\mathbb{T}^d \times \mathbb{R}^d} |v|^{m_0} f_0(x, v)\, \mathrm{d}x\, \mathrm{d}v = M_0 < +\infty.$$

Let f be a C^1 compactly supported solution of the VPME system (12). Then, for all $T > 0$,

$$\sup_{[0,T]} \int_{\mathbb{T}^d \times \mathbb{R}^d} |v|^{m_0} f(t,x,v)\,\mathrm{d}x\,\mathrm{d}v \leq C(T, C_0, M_0, m_0, \|f_0\|_\infty).$$

Using this estimate, we then prove the global existence of solutions for the VPME system under these assumptions.We first consider a regularized version of the VPME system:

$$\begin{cases} \partial_t f + v \cdot \nabla_x f - \chi_r *_x \nabla_x U \cdot \nabla_v f = 0, \\ \Delta U = e^U - \chi_r *_x \rho_f, \\ f|_{t=0} = f_0, \ \displaystyle\int_{\mathbb{T}^d \times \mathbb{R}^d} f_0\,\mathrm{d}x\,\mathrm{d}v = 1. \end{cases} \tag{26}$$

Here χ_r is a mollifier defined for $r > 0$ by

$$\chi_r(x) := r^{-d} \chi\left(\frac{x}{r}\right), \qquad \chi \in C_c^\infty(\mathbb{T}^d; [0, +\infty)),$$

where χ is a fixed smooth, radially symmetric function with compact support.

The regularized system (26) is globally well-posed. This can be proved using standard methods, for example by adapting the approach of Dobrushin [12]. The proof of Proposition 2 then provides moment estimates for the solutions of (26) that are uniform in the regularization parameter. We can then extract a limit point and show that it is a global solution of the VPME system. With this method of construction, no regularity is required on the initial datum f_0. Moreover, the conservation of the energy $\mathscr{E}[f]$ defined in (21) also follows—in comparison, the energy of the weak solutions constructed by Bouchut [6] is non-increasing but not necessarily conserved. We obtain the following existence result.

Theorem 4 *Let $d = 2, 3$. Consider an initial datum $f_0 \in L^1 \cap L^\infty(\mathbb{T}^d \times \mathbb{R}^d)$ satisfying*

$$\int_{\mathbb{T}^d \times \mathbb{R}^d} |v|^{m_0} f_0(x,v)\,\mathrm{d}x\,\mathrm{d}v < +\infty, \quad \textit{for some } m_0 > d.$$

Then there exists a global-in-time weak solution $f \in C([0,\infty); \mathscr{P}(\mathbb{T}^d \times \mathbb{R}^d))$ of the VPME system (12) with initial data f_0, such that for all $T > 0$,

$$\sup_{t \in [0,T]} \int_{\mathbb{T}^d \times \mathbb{R}^d} |v|^{m_0} f(t,x,v)\,\mathrm{d}x\,\mathrm{d}v < +\infty.$$

The proof of Theorem 2 is then completed by showing that, under the specified decay and moment assumption on f_0, the solution provided by Theorem 4 has bounded density. Proposition 1 then applies, proving the uniqueness of this solution.

4.2 Strategy for $\mathbb{R}^3$

In the whole space case, the overall strategy is similar to the torus case: we first analyse the electrostatic potential using the decomposition $U = \bar{U} + \widehat{U}$, where

$$-\Delta \bar{U} = \rho_f, \qquad \lim_{|x|\to 0} \bar{U}(x) = 0,$$

and the remainder $\widehat{U}$ satisfies either

$$\Delta \widehat{U} = g e^{\bar{U}+\widehat{U}} \quad \text{or} \quad \Delta \widehat{U} = \frac{g e^{\bar{U}+\widehat{U}}}{\int_{\mathbb{R}^3} g e^{\bar{U}+\widehat{U}} \, \mathrm{d}x}.$$

Once again, by using techniques from the calculus of variations we can show that the nonlinear remainder $\widehat{U}$ is more regular than $\bar{U}$. However, one first difference with the torus case is that we have to account for the behaviour of the potential at infinity.

A more significant difference occurs for the fixed charge model. Due to the normalisation of the electron charge, the nonlinearity takes a different form compared to the torus case. To deal with this, we use a different functional in the calculus of variations approach to the analysis of $\widehat{U}$.

For the uniqueness of strong solutions, once again we prove a stability estimate in W_2 using stability estimates for the electric field with respect to the charge density ρ_f. For $\bar{E}$ we use estimates devised by Loeper [23]. For $\widehat{E}$ we again need a version of Lemma 3, modified in the fixed charge case to handle the different nonlinearity.

To prove existence, we again use the propagation of moments. However the proof of the propagation of moments in the whole space is very different with respect to the propagation of moments on the torus, and we rely on the approach of Lions and Perthame [22], making use of the regularity estimates on $\widehat{U}$.

References

1. A. Arsenev, Existence in the large of a weak solution to the Vlasov system of equations. Zh. Vychisl. Mat. i Mat. Fiz. **15**, 136–147 (1975)
2. C. Bardos, F. Golse, T.T. Nguyen, R. Sentis, The Maxwell-Boltzmann approximation for ion kinetic modeling. Phys. D **376**(377), 94–107 (2018)
3. J. Batt, G. Rein, Global classical solutions of the periodic Vlasov-Poisson system in three dimensions. C. R. Acad. Sci. Paris Sér. I Math. **313**, no. 6, 411–416 (1991)
4. P.M. Bellan, *Fundamentals of Plasma Physics* (Cambridge University Press, Cambridge, 2008)
5. G. Bonhomme, T. Pierre, G. Leclert, J. Trulsen, Ion phase space vortices in ion beam-plasma systems and their relation with the ion acoustic instability: numerical and experimental results. Plasma Phys. Control. Fusion **33**(5), 507–520 (1991)
6. F. Bouchut, Global weak solution of the Vlasov-Poisson system for small electrons mass. Comm. Part. Differ. Equ. **16**(8–9), 1337–1365 (1991)

7. F. Bouchut, J. Dolbeault, On long time asymptotics of the Vlasov-Fokker-Planck equation and of the Vlasov-Poisson-Fokker-Planck system with Coulombic and Newtonian potentials. Differ. Integr. Equ. **8**(3), 487–514 (1995)
8. W. Braun, K. Hepp, The Vlasov dynamics and its fluctuations in the $1/N$ limit of interacting classical particles. Comm. Math. Phys. **56**(2), 101–113 (1977)
9. Z. Chen, J. Chen, Moments propagation for weak solutions of the Vlasov-Poisson system in the three-dimensional torus. J. Math. Anal. Appl. **42**(1), 728–737 (2019)
10. L. Desvillettes, C. Villani, On the spatially homogeneous Landau equation for hard potentials part ii : h-theorem and applications. Commun. Part. Differ. Equ. **25**(1–2), 261–298 (2000)
11. L. Desvillettes, C. Villani, On the trend to global equilibrium for spatially inhomogeneous kinetic systems: the Boltzmann equation. Invent. Math. **159**, 245–316 (2005)
12. R.L. Dobrushin, Vlasov equations. Funktsional. Anal. i Prilozhen. **13**(2), 48–58 (1979)
13. M. Griffin-Pickering, M. Iacobelli, Global well-posedness in 3-dimensions for the Vlasov–Poisson system with massless electrons. arXiv:1810.06928
14. A.V. Gurevich, L.P. Pitaevsky, Non-linear dynamics of a rarefied ionized gas. Prog. Aerosp. Sci. **16**(3), 227–272 (1975)
15. D. Han-Kwan, M. Iacobelli, The quasineutral limit of the Vlasov-Poisson equation in Wasserstein metric. Commun. Math. Sci. **15**(2), 481–509 (2017)
16. M. Hauray, Mean field limit for the one dimensional Vlasov-Poisson equation. Séminaire Laurent Schwartz—Équations aux dérivées partielles et applications. Année 2012–2013, Exp. No. XXI, Sémin. Équ. Dériv. Partielles. École Polytech., Palaiseau (2014)
17. M. Herda, On massless electron limit for a multispecies kinetic system with external magnetic field. J. Differ. Equ. **260**(11), 7861–7891 (2016)
18. E. Horst, On the asymptotic growth of the solutions of the Vlasov-Poisson system. Math. Methods Appl. Sci. **16**(2), 75–86 (1993)
19. E. Horst, R. Hunze, Weak solutions of the initial value problem for the unmodified non- linear Vlasov equation. Math. Methods Appl. Sci. **6**(2), 262–279 (1984)
20. J.H. Jeans, On the theory of star-streaming and the structure of the universe. Mon. Not. R. Astron. Soc. **76**, 70–84 (1915)
21. E.M. Lifshitz, L.P. Pitaevskii, *Physical Kinetics*, vol. 10, Course of Theoretical Physics (Pergamon Press, Oxford, 1981)
22. P.L. Lions, B. Perthame, Propagation of moments and regularity for the 3-dimensional Vlasov-Poisson system. Invent. Math. **105**(2), 415–430 (1991)
23. G. Loeper, Uniqueness of the solution to the Vlasov-Poisson system with bounded density. J. Math. Pures Appl. **86**(9), no. 1, 68–79 (2006)
24. R.J. Mason, Computer simulation of ion-acoustic shocks. The diaphragm problem. Phys. Fluids **14**, no. 9, 1943–1958 (1971)
25. Y.V. Medvedev, Ion front in an expanding collisionless plasma. Plasma Phys. Control. Fusion **53**, no. 12, 125007 (2011)
26. C. Pallard, Moment propagation for weak solutions to the Vlasov-Poisson system. Comm. Part. Differ. Equ. **37**(7), 1273–1285 (2012)
27. K. Pfaffelmoser, Global classical solutions of the Vlasov-Poisson system in three dimensions for general initial data. J. Differ. Equ. **95**(2), 281–303 (1992)
28. R. Robert, Unicité de la solution faible à support compact de l'équation de Vlasov–Poisson. C. R. Acad. Sci. Paris Sér. I Math. **324**, no. 8, 873–877 (1997)
29. P. Sakanaka, C. Chu, T. Marshall, Formation of ion-acoustic collisionless shocks. Phys. Fluids **14**, no. 611, (1971)
30. J. Schaeffer, Global existence of smooth solutions to the Vlasov-Poisson system in three dimensions. Comm. Part. Differ. Equ. **16**(8–9), 1313–1335 (1991)
31. S. Ukai, T. Okabe, On classical solutions in the large in time of two-dimensional Vlasov's equation. Osaka J. Math. **15**(2), 245–261 (1978)
32. C. Villani, On the Cauchy problem for Landau equation: sequential stability, global existence. Adv. Differ. Equ. **1**(5), 793–816 (1996)
33. A.A. Vlasov, On the vibration properties of the electron gas. Zh. Eksper. Teor. Fiz. **8**, no. 3, 291 (1938)

Charge-Current Correlation Identities for Stochastic Interacting Particle Systems

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Abstract We adapt a recent proof of generic quantum-mechanical charge-current correlation identities with local conservation laws to stochastic interacting particle systems. Unlike in earlier proofs no translation invariance is required. We clarify the validity of an Onsager-type current symmetry that generally appears in hyperbolic systems of conservation laws that arise as hydrodynamic limits of stochastic interacting particle systems.

Keywords Stochastic interacting particle systems · Local conservation laws · Charge-current correlations · Current symmetry · Hydrodynamic limit

1 Introduction

The large-scale behaviour of d-dimensional translation invariant stochastic interacting particle systems with n local conservation laws is, in the presence of macroscopic stationary currents, on Euler scale generically described by hyperbolic systems of conservation laws [1]. The coarse-grained locally conserved quantities $q^\alpha(\mathbf{x}, t)$, $\alpha \in \{1, \ldots, n\}$ (that we shall call charges and arrange as a vector $\mathbf{q} \in \mathbb{R}^n$) and their associated currents $j_i^\alpha(\mathbf{x}, t)$ in space direction $i \in \{1, \ldots, d\}$ (arranged as vectors $\mathbf{j}_i \in \mathbb{R}^n$) evolve according to the system of partial differential equations

$$\frac{\partial}{\partial t}\mathbf{q} + \sum_{i=1}^{d} \frac{\partial}{\partial x_i}\mathbf{j}_i(\mathbf{q}) = 0, \quad \mathbf{q}, \mathbf{j}_i \in \mathbb{R}^n, \quad (\mathbf{x}, t) \in \mathbb{R}^d \times \mathbb{R} \tag{1}$$

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with a smooth family of currents j_i^α that depend on $(\mathbf{x}, t)$ only implicitly via the n charges $q^1(x,t), \ldots, q^n(x,t)$. The specific form of the current functions arises from the stationary current-charge relation of the particle system. The current Jacobian $J(\mathbf{q}) := D\mathbf{j}(\mathbf{q})$ has real eigenvalues $v^\alpha(\mathbf{q})$ at each point $\mathbf{q}$, see [2] with a focus on one dimension and references therein for the general case.

We do not discuss the conditions under which (1) is valid for a given particle system, but point out that hyperbolicity is a fundamental property that any Eulerian hydrodynamic limit of a physically meaningful particle system with macroscopic stationary currents *must* satisfy since, if (1) is valid, the eigenvalues v^α are the velocities of the fluctuation fields of the conserved charges [3] and as such take real values. In terms of the compressibility matrix $K(\mathbf{q})$—whose matrix elements are the stationary covariances of the space-integrated fluctuation fields—hyperbolicity is guaranteed by the current symmetry

$$JK = (JK)^T \tag{2}$$

since by the chain rule this implies that J expressed as a function of generalized fugacities of a grandcanonical ensemble is a real-symmetric matrix and hence has real eigenvalues.

This current symmetry—which is somewhat reminiscent of the Onsager relations—is significant not only on macroscopic level. It also guarantees that the thermodynamic entropy is a globally convex Lax entropy of the system (1) [4]. This fact plays an important role in extending Yau's relative entropy method [5] to prove rigorously the hydrodynamic limit (1) for particle systems with more than one conservation law up to times when no shocks are present.[1]

The current symmetry (2) has been known for a long time in different guises, see e.g. [8, 9]. However, its first rigorous proof dates back only to 2003 [4] and is specific to a family of particle systems whose invariant measure is a product measure. However, the product form of the invariant measure should not play a role for the current symmetry, as neither heuristic nor rigorous derivations of hydrodynamic limits require this property [10]. Indeed, subsequently a different proof [11] for rather general particle systems demonstrates that the assumptions on the invariant measure can be much weakened. Only mild assumptions, in particular, translation invariance, a grandcanonical form of the invariant measure with some conditions on differentiability, and a spatial decay of certain correlations involving the conserved charges and their associated currents, are sufficient to guarantee the current symmetry (2).

Further progress was made very recently, when it was shown in a quantum mechanical setting that the current symmetry (2) actually arises from an underlying general identity for space and time dependent correlations between local charges and currents

[1] Solutions of (1) generically develop shocks after a finite time that depends on the initial data [6, 7].

[12, 13], assuming implicitly a grandcanonical form of the stationary density matrix again with some conditions on differentiability and, explicitly, translation invariance and some assumptions on the decay stationary charge-current correlations.

The reliance on microscopic translation invariance in all arguments and rigorous proofs might appear natural as also in the macroscopic setting of the PDE (1) translation invariance is assumed. However, requiring translation invariance on *microscopic* scale is unsatisfactory as real macroscopic physical systems—for which one expects the current symmetry to be valid and for which one would like to derive it from the microscopic dynamics—are not microscopically translation invariant since any physical particle system has a boundary with some spatial structure on microscopic scale. This conceptual problem was finally resolved in [14] where it was proved, again in the quantum setting, that modified charge-current equalities—from which the current symmetry also follows under well-defined assumptions—are valid for systems that are *not* microscopically translation invariant.

It is the purpose of this article to adapt the results of [14] to the classical Markovian setting of stochastic interacting particle systems with more than one local conservation law [15, 16] and to discuss the significance of the decay of correlations and the differentiability conditions. In Sect. 2 we describe the setting and state the main results which are proved in Sect. 3. In Sect. 4 we conclude with the discussion of correlations and differentiability in the presence of shocks.

The main result from the perspective of large scale dynamics is Theorem 3 in Sect. 2. The more fundamental charge-current correlation identity from which Theorem 3 follows under further assumptions is established in Theorem 1. Additional details on the underlying assumptions can be found in [14] where a more extended discussion in the quantum setting is provided.

2 Classical Setting and Results

To begin with, we note that we work in one dimension on the discrete finite torus $\mathbb{T}_L := \mathbb{Z}/L\mathbb{Z}$ with $L \geq 2$ sites, counted from 0 to $L-1$ modulo L. The lattice sites are denoted by small letters $k, l, \ldots$. It will transpire that the extension of the results and the proofs to the d-dimensional torus $\mathbb{T}_L^d$ is obvious, as the one-dimensional argument can be applied to each space direction separately.

2.1 Notation and General Properties of the Interacting Particle System

We consider a stochastic interacting particle system with the state on site $k \in \mathbb{T}_L$ denoted by $\eta_k \in \mathbb{S}$ where $\mathbb{S}$ is a countable set. A full configuration of the system is denoted by $\eta := (\eta_0, \ldots, \eta_{L-1}) \in \mathbb{S}^L$. The lattice translation operator $T : \mathbb{S}^L \to \mathbb{S}^L$

acting on a configuration η is defined by the forward shift $\eta_k \mapsto \eta_{k+1}$. The lattice translation operator acting on functions $f : \mathbb{S}^L \to \mathbb{R}$ is defined by

$$\mathscr{T} f(\eta) := f(T\eta). \tag{3}$$

The Markovian stochastic dynamics is defined by a generator $\mathscr{L}$ (see e.g. [15]) with an invariant measure that we denote by π_L. We stress that we *not* assume translation invariance $\mathscr{T}\mathscr{L} = \mathscr{L}\mathscr{T}$ of the generator.

Specifically, we assume that the process has n locally conserved quantities $q_k^\alpha : \mathbb{S}^L \to \mathbb{R}$, $\alpha \in \{1, \ldots, n\}$, indexed by k that satisfy the discrete continuity equation

$$\mathscr{L} q_k^\alpha = j_{k-1}^\alpha - j_k^\alpha, \quad k \in \{0, \ldots, L-1\} \tag{4}$$

with the instantaneous currents j_k^α and the definition $j_{-1}^\alpha := j_{L-1}^\alpha$. As mentioned above, we refer to the quantities q_k^α as charges. As a consequence of the continuity Eq. (4) the global charges

$$Q^\alpha := \sum_{k=0}^{L-1} q_k^\alpha \tag{5}$$

are conserved. Since we do not assume translation invariance of the generator one has in general $j_{k-1}^\alpha \neq \mathscr{T} j_k^\alpha$.

The generator of the time-reversed process (w.r.t. the invariant measure π_L) is denoted by $\tilde{\mathscr{L}}$. The time-reversed currents are defined by the discrete continuity equation

$$\tilde{\mathscr{L}} q_k^\alpha = \tilde{j}_{k-1}^\alpha - \tilde{j}_k^\alpha \tag{6}$$

that is induced by the conservation law (4) [17].

We point out that the continuity equation does not uniquely define the instantaneous currents as without changing (4) one can add a function $f^\alpha : \mathbb{S}^L \to \mathbb{R}$ that does not depend on k. In more than one dimension there is even more freedom to add functions. E.g. in the discrete two-dimensional continuity equation with current components $j_{k,l}^{\alpha,i}$ for space direction $i \in \{1, 2\}$ also the modified current components $\tilde{j}_{k,l}^{\alpha,1} := j_{k,l}^{\alpha,1} + g_{k,l+1} - g_{k,l}$, $\tilde{j}_{k,l}^{\alpha,2} := j_{k,l}^{\alpha,2} - (g_{k+1,l} - g_{k,l})$ with an arbitrary measurable function $g_{k,l} : \mathbb{S}^{L^2} \to \mathbb{R}$ satisfy the same two-dimensional continuity equation. However, this ambiguity in the definition of the instantaneous current which is due to gauge invariance is not relevant to our discussion which can be straightforwardly generalized to the d-dimensional discrete torus in any dimension $d > 1$.

2.2 Some Important Expectation Values and General Properties of the Invariant Measure

Expectations of a measurable function $f : \mathbb{S}^L \to \mathbb{R}$ w.r.t. π_L are denoted by $\langle f \rangle_L$ and covariances are marked by an additional superscript c, i.e., $\langle f_1 f_2 \rangle_L^c := \langle f_1 f_2 \rangle_L - \langle f_1 \rangle_L \langle f_2 \rangle_L$. Due to stationarity, one-time expectations do not depend on time t. We define the stationary charge densities

$$q_L^\alpha(k) := \langle q_k^\alpha \rangle_L. \tag{7}$$

Notice that the stationary currents

$$j_L^\alpha := \langle j_k^\alpha \rangle_L \tag{8}$$

do not depend on k and one has

$$\tilde{j}_L^\alpha := \langle \tilde{j}_k^\alpha \rangle_L = -j_L^\alpha. \tag{9}$$

Here the subscript L denotes the dependence on the system size L.

Two-time expectations depend only on the time difference. Specifically, we consider the time-dependent correlation functions

$$S_L^{\alpha\beta}(k,l,t) := \langle q_k^\alpha(t) q_l^\beta(0) \rangle_L^c, \tag{10}$$

$$C_L^{\alpha\beta}(k,l,t) := \langle j_k^\alpha(t) q_l^\beta(0) \rangle_L^c, \tag{11}$$

$$\tilde{C}_L^{\alpha\beta}(k,l,t) := -\langle q_k^\alpha(t) \tilde{j}_l^\beta(0) \rangle_L^c. \tag{12}$$

By identifying all lattice sites modulo L, the correlation functions can be defined for all $k, l \in \mathbb{Z}$ with periodicity L for both space arguments k, l.[2] We note that when the distance $r_{k,l} := |(k-l) \mod L|$ between the sites k, l is much larger than the distance $r_{\max}(t) := (t \max_\alpha \{|v^\alpha|\} \mod L)$ travelled by the fastest fluctuation field and if charges and currents are local, then one expects by the classical analog of the quantum mechanical Lieb-Robinson bound [18] the correlation functions (10)–(12) to take their stationary values [19]. Otherwise, these correlations are, in general, highly nontrivial and encode the dynamical universality class of the fluctuation fields [20].

We do not assume reversibility of the process w.r.t. π_L nor uniqueness of π_L. The only assumptions on π_L that we shall make use of are the content of the following definition.

[2](a) Notice the negative sign and the appearance of the time-reversed current in the definition of $\tilde{C}_L^{\alpha\beta}(k,l,t)$, in contrast to the quantum case [14]. (b) For the distance $r = l - k$ between two sites the periodicity implies that distance $r = L - 1$ is the same as distance $r = -1$.

Definition 1 Let $\mathscr{L}$ be the generator of stochastic interacting particle system defined on $\mathbb{T}_L$ that has n local conservation laws. An invariant measure of the process is called *good* if the expectations (7)–(12) all exist for any fixed L and have well-defined thermodynamic limits $L \to \infty$.

To discuss some special cases we also introduce the notion of overlap between functions.

Definition 2 Two functions $f : \mathbb{S}^L \to \mathbb{R}$ and $g : \mathbb{S}^L \to \mathbb{R}$ are said to overlap if the intersection of the sets of occupation numbers η_k on which they depend non-trivially is not empty. Otherwise the two functions are called non-overlapping.

If a function $f(\cdot)$ has no overlap with either the instantaneous current j_l^α or with the reversed instantaneous current $\tilde{j}_l^\alpha$ then one has $\langle f j_l^\alpha \rangle_L = -\langle f \tilde{j}_l^\alpha \rangle_L$. An example of approximately non-overlapping functions are the charges and currents appearing in (7)–(12) if the Lieb-Robinson condition $r_{kl} \gg r^*(t)$ is met. On the other hand, these functions may be overlapping at all times for nonlocal charges in integrable systems [21] or in stochastic dynamics conditioned on large currents [22]. This is relevant to the present discussion in so far as overlap may prevent the decay of stationary correlations between these quantities that will play a role below.

2.3 Results

In Theorem 1 we present the fundamental charge-current identity in its local form. It requires only very few and mild assumptions on the stochastic dynamics and underlies all further results. In particular, it is valid also for finite lattices. In Theorem 2 some consequences of this fundamental identity are explored in the thermodynamic limit, with some mild assumptions on the decay of stationary charge-current correlations. Finally, Theorem 3 (along with Remark 5) establishes the validity of the current symmetry (2) for a generic class of grandcanonical invariant measures.

Definition 3 The quantities

$$A_L^{\alpha\beta}(k,t) := \frac{1}{L}\sum_{l=0}^{L-1} C_L^{\alpha\beta}(k,l,t), \quad \tilde{A}_L^{\alpha\beta}(l,t) := \frac{1}{L}\sum_{k=0}^{L-1} \tilde{C}_L^{\alpha\beta}(k,l,t) \tag{13}$$

are called the global charge-current correlations and

$$B_L^{\alpha\beta}(r,t) := \frac{1}{L}\sum_{k=0}^{L-1} C_L^{\alpha\beta}(k,k+r,t), \quad \tilde{B}_L^{\alpha\beta}(r,t) := \frac{1}{L}\sum_{k=0}^{L-1} \tilde{C}_L^{\alpha\beta}(k,k+r,t) \tag{14}$$

are called the space-averaged charge-current correlations.

These are the main quantities of interest.[3] Notice that for a translation invariant process with an invariant measure π_L that is also translation invariant one has

$$B_L^{\alpha\beta}(r,t) = \langle\, j_{-r}^{\alpha}(t) q_0^{\beta}(0) \,\rangle_L^c, \quad \tilde{B}_L^{\alpha\beta}(r,t) = -\langle\, q_{-r}^{\alpha}(t) \tilde{j}_0^{\beta}(0) \,\rangle_L^c. \tag{15}$$

Proposition 1 (Global charge-current correlation equality) *Let $\mathscr{L}$ be the generator of a stochastic interacting particle system with n local conservation laws and a good invariant measure π_L. For every $\alpha, \beta \in \{1, \dots, n\}$ the charge-current correlations (11), (12) satisfy the fundamental charge-current equality*

$$C_L^{\alpha\beta}(k-1,l,t) - C_L^{\alpha\beta}(k,l,t) + \tilde{C}_L^{\alpha\beta}(k,l-1,t) - \tilde{C}_L^{\alpha\beta}(k,l,t) = 0 \tag{16}$$

and the global charge-current correlations (13) are constants

$$A_L^{\alpha\beta}(k,t) = a_L^{\alpha\beta}, \quad \tilde{A}_L^{\alpha\beta}(l,t) = \tilde{a}_L^{\alpha\beta} \tag{17}$$

independent of space and time.

Remark 1 In a good canonical invariant measure where the conserved charges Q^{α} (5) have fixed (i.e. nonfluctuating) values one has $a_L^{\alpha\beta} = \tilde{a}_L^{\alpha\beta} = 0$ for any system size L.

Theorem 1 (Local charge-current correlation equality) *Let $\mathscr{L}$ be the generator of a stochastic interacting particle system with n local conservation laws and a good invariant measure π_L. Then for all $r \in \mathbb{T}_L$, $t \geq 0$, $\alpha, \beta \in \{1, \dots, n\}$ the space-averaged charge-current correlations (14) satisfy the charge-current equality*

$$B_L^{\alpha\beta}(r+1,t) - \tilde{B}_L^{\alpha\beta}(r,t) = d_L^{\alpha\beta} \tag{18}$$

with the constant $d_L^{\alpha\beta} := a_L^{\alpha\beta} - \tilde{a}_L^{\alpha\beta}$ given by the constants in Proposition 1.

Remark 2 In a good invariant canonical measure one has $d_L^{\alpha\beta} = 0$ and therefore the correlation equality $B_L^{\alpha\beta}(r+1,t) = \tilde{B}_L^{\alpha\beta}(r,t)$ for all $r \in \mathbb{T}_L$, $t \geq 0$ and for any L.

Remark 3 For an invariant product measure and for charges and currents that do not overlap for some distance $|r| > |r_0|$ one has $B_L^{\alpha\beta}(r+1,0) = \tilde{B}_L^{\alpha\beta}(r,0) = 0$ for $|r| > |r_0|$. This implies $d_L^{\alpha\beta} = 0$ and thus also $B_L^{\alpha\beta}(r+1,t) = \tilde{B}_L^{\alpha\beta}(r,t)$ for all $r \in \mathbb{T}_L$, $t \geq 0$ and L large enough to allow for non-overlap.

Next we elaborate on the consequences of decay of correlations.

Theorem 2 (Charge-current correlation equality with decay of correlations) *Let $\mathscr{L}$ be the generator of a stochastic interacting particle system with n local conservation laws and a good invariant measure π_L. If condition*

[3] We have redefined $A_L^{\alpha\beta}(k,t)$ by a factor of L compared to [14]. This makes formulas that appear in the proofs neater.

$$\mathbf{C}: \lim_{r\to\infty} B_\infty^{\alpha\beta}(r,t) = \lim_{r\to\infty} \tilde{B}_\infty^{\alpha\beta}(r,t) = 0 \tag{19}$$

on the decay of correlations in the thermodynamic limit $L \to \infty$ holds, then for every $\alpha, \beta \in \{1, \ldots, n\}$, $r \in \mathbb{Z}$, $t \geq 0$ the space-averaged charge-current correlations (14) satisfy the charge-current equality

$$B_\infty^{\alpha\beta}(r+1,t) = \tilde{B}_\infty^{\alpha\beta}(r,t). \tag{20}$$

Remark 4 We recall that no translation invariance is assumed. For a translation invariant process with π_L also translation invariant, Theorem 1 asserts that

$$\langle\, j_r^\alpha(t) q_0^\beta(0)\,\rangle_L^c + \langle\, q_{r+1}^\alpha(t) \tilde{j}_0^\beta(0)\,\rangle_L^c = d_L^{\alpha\beta} \quad \forall r \in \mathbb{T}_L, t \geq 0 \tag{21}$$

which for $d_L^{\alpha\beta} = 0$ (due to a canonical measure or decay of correlations as in Theorem 2) yields the classical lattice analog

$$\langle\, j_r^\alpha(t) q_0^\beta(0)\,\rangle_\infty^c = -\langle\, q_{r+1}^\alpha(t) \tilde{j}_0^\beta(0)\,\rangle_\infty^c \tag{22}$$

of the quantum continuum correlation equality of [13]. Taking the sum over r leads to the global correlation equality of [12] reproduced in Eq. (1) of [14].

Theorem 3 (Current symmetry) *Let $\mathscr{L}$ be the generator of a stochastic interacting particle system with n local conservation laws and a good invariant measure π_L with the further properties that for $\phi \in \mathbb{R}^n$ the large deviation function*

$$Z_L(\phi) := \langle\, e^{\sum_{\alpha=1}^n \phi^\alpha Q^\alpha}\,\rangle_L \tag{23}$$

is finite and twice differentiable inside a non-empty domain $X \subset \mathbb{R}^n$ around the origin of $\mathbb{R}^n$ and retains the modified invariant measure

$$\pi_{\phi,L} := \pi_L \frac{\exp\left(\sum_{\alpha=1}^n \phi^\alpha Q^\alpha\right)}{Z_L(\phi)} \tag{24}$$

good inside X. If the condition

$$\mathbf{C}': \lim_{L\to\infty} L[B_L^{\alpha\beta}(\lfloor L/2\rfloor + 1, 0) - \tilde{B}_L^{\alpha\beta}(\lfloor L/2\rfloor, 0)] = 0 \tag{25}$$

on the decay of correlations holds for some index pair α, β with expectation taken w.r.t. $\pi_{\phi,L}$, then, with the short-hand notation $\partial_\alpha := \partial/(\partial\phi^\alpha)$ and $j^\alpha = \lim_{L\to\infty} j_L^\alpha$, one has the current symmetry

$$\partial_\alpha j^\beta = \partial_\beta j^\alpha, \phi \in X \tag{26}$$

for the stationary currents in the thermodynamic limit.

Remark 5 The differentiability property of the large deviation function yields the current symmetry in the form (2).

3 Proofs

The proofs of the results use mostly the same ideas as in the quantum case [14]. One exception is the appearance of the time-reversed current. Throughout this section we assume $\mathscr{L}$ to be the generator of a particle system for which the discrete continuity Eq. (5) are valid and which has a good invariant measure.

3.1 *Proposition 1*

Proof The summation yields

$$A_L^{\alpha\beta}(k,t) = \langle\, j_k^\alpha(t) Q^\beta \,\rangle_L^c, \quad \tilde{A}_L^{\alpha\beta}(l,t) = -\langle\, Q^\alpha(t) \tilde{j}_l^\beta(0) \,\rangle_L^c. \tag{27}$$

Since global charges Q^α are conserved, the sums are independent of time. The conservation law also implies for the equal-time joint expectation taken in the invariant measure that $0 = \langle\, \mathscr{L}\left(q_k^\alpha Q^\beta\right) \rangle_L = \langle\, (j_{k-1}^\alpha - j_k^\alpha) Q^\beta \,\rangle_L$. This is true for any pair α, β and thus independence of the space coordinate of $\langle\, j_k^\alpha Q^\beta \,\rangle_L$ (and similarly of $\langle\, Q^\alpha \tilde{j}_l^\beta \,\rangle_L$) follows. Because of the space- independence of the currents (8), (9) this applies also to the covariances. □

3.2 *Theorems 1 and 2*

Theorem 2 is a consequence of Theorem 1 since under condition **C** one obtains $d_\infty^{\alpha\beta} = 0$. Hence we focus on Theorem 1.

Proof To prove the fundamental charge-current equality (16) we note that the time-derivative of the stationary charge-charge correlation function (10) can be taken in two different ways as

$$\frac{\mathrm{d}}{\mathrm{d}t} S_L^{\alpha\beta}(k,l;t) = \langle\, (\mathscr{L} q_k^\alpha(t)) q_l^\beta(0) \,\rangle = \langle\, q_k^\alpha(t) (\tilde{\mathscr{L}} q_l^\beta(0)) \,\rangle. \tag{28}$$

Using the discrete continuity Eqs. (4), (6) yields (16).

Next we define the two auxiliary functions

$$G_L^{\alpha\beta}(k,l,t) := \sum_{k'=1}^{k} \left[\tilde{C}_L^{\alpha\beta}(k',0,t) - \tilde{C}_L^{\alpha\beta}(k',l,t) \right] \tag{29}$$

$$g_L^{\alpha\beta}(r,t) := \frac{1}{L} \sum_{k=0}^{L-1} G_L^{\alpha\beta}(k,k+r,t) \tag{30}$$

which allow us to eliminate the requirement of local translation invariance in the existing proofs of Theorem 1. The periodicity of the correlation functions in the space arguments k and l implies $G_L^{\alpha\beta}(k,0,t) = G_L^{\alpha\beta}(0,l,t) = 0$ and the periodicity properties

$$G_L^{\alpha\beta}(k+mL,l+nL,t) = G_L^{\alpha\beta}(k,l,t), \quad g_L^{\alpha\beta}(r+mL,t) = g_L^{\alpha\beta}(r,t). \tag{31}$$

From the periodicity and (16) one gets

$$C_L^{\alpha\beta}(k,l,t) = C_L^{\alpha\beta}(0,l,t) + G_L^{\alpha\beta}(k,l,t) - G_L^{\alpha\beta}(k,l-1,t) \tag{32}$$

$$\tilde{C}_L^{\alpha\beta}(k,l,t) = \tilde{C}_L^{\alpha\beta}(k,0,t) + G_L^{\alpha\beta}(k-1,l,t) - G_L^{\alpha\beta}(k,l,t). \tag{33}$$

The next step is to set $l = k + r$ in (32) and sum over k and similar for (33). Using Theorem (1) this yields

$$B_L^{\alpha\beta}(r,t) = a_L^{\alpha\beta} + g_L^{\alpha\beta}(r,t) - g_L^{\alpha\beta}(r-1,t) \tag{34}$$

$$\tilde{B}_L^{\alpha\beta}(r-1,t) = \tilde{a}_L^{\alpha\beta} + g_L^{\alpha\beta}(r,t) - g_L^{\alpha\beta}(r-1,t). \tag{35}$$

Substracting the second from the first equality yields (18). □

Remark 6 The space-averaged charge-charge correlation function

$$s_L^{\alpha\beta}(r,t) := \frac{1}{L} \sum_{k} S_L^{\alpha\beta}(k,k+r,t) \tag{36}$$

satisfies [14]

$$\frac{\mathrm{d}}{\mathrm{d}t} s_L^{\alpha\beta}(r,t) = g_L^{\alpha\beta}(r+1,t) + g_L^{\alpha\beta}(r-1,t) - 2\, g_L^{\alpha\beta}(r,t) \tag{37}$$

where the r.h.s. has the form of a discrete Laplacian.

3.3 *Theorem 3*

Proof Because of the conservation law (5) the measure $\pi_{L,\phi}$ is an invariant measure and by hypothesis it is good inside the domain X. By construction, one has

$$\partial_\beta \frac{1}{Z_L} = -\frac{1}{Z_L} \langle\, Q^\beta \,\rangle_L \tag{38}$$

and therefore

$$\partial_\beta \langle\, j_k^\alpha \,\rangle_L = \langle\, j_k^\alpha Q^\beta \,\rangle_L^c. \tag{39}$$

Taking into account Proposition 1 thus yields

$$\partial_\beta \langle\, j^\alpha \,\rangle_L = L a_L^{\alpha\beta}. \tag{40}$$

Similarly, considering $\tilde{\jmath}_k^\alpha$ and taking the derivative w.r.t. ϕ^β yields with Proposition 1 and the change of sign in the second equality in (9),

$$\partial_\beta \langle\, \tilde{\jmath}^\alpha \,\rangle_L = L \tilde{a}_L^{\alpha\beta}. \tag{41}$$

From Theorem 1 one concludes that $\partial_\beta \langle\, j^\alpha \,\rangle_L - \partial_\beta \langle\, \tilde{\jmath}^\alpha \,\rangle_L = L[B_L^{\alpha\beta}(r+1,t) - \tilde{B}_L^{\alpha\beta}(r,t)]$. Condition $\mathbf{C}'$ on the decay of correlations then yields (26) by choosing $r = \lfloor L/2 \rfloor$ and taking the thermodynamic limit.

4 Comments on Phase Separation and the Decay of Correlations

Even in one space dimension, particle systems with more than one local conservation law exhibit very rich stationary behaviour [16], including a nonequilibrium analog of phase separation [23–25], albeit in certain cases with a random walking domain wall [26–29] rather than an immobile one. Such a domain wall is the microscopic realization (on lattice scale) of macroscopic shocks. Invariant measures with fluctuating microscopic shock position are an example where the differentiability condition in Theorem 4 may not be fullfilled.

This can be demonstrated explicitly for the discrete-time sublattice totally asymmetric simple exclusion process (dsTASEP) whose invariant measure is obtained in explicit form and studied in detail in [30, 31]. This process is a single-species exclusion process with a slow bond where particles jump with probability p, as opposed to deterministic hopping across all other bonds. With the critical density $\rho_c = p/2$ the current-density relation is given by

$$j(\rho) = \begin{cases} 2\rho & 0 \le \rho < \rho_c \\ p & \rho_c \le \rho \le 1/2 \end{cases} \tag{42}$$

The density regime with $\rho > 1/2$ follows from particle-hole symmetry. One sees that $j(\rho)$ is not differentiable at $\rho = \rho_c$ and in the grandcanocical ensemble with chemical potential $\phi(\rho) = \ln[2\rho/(1-2\rho)]$ the derivative $\mathrm{d}\phi/\mathrm{d}\rho$ is infinite at $\phi_c = \ln[p/(1-p)]$ as can be shown [31] using the matrix product approach of [32]

that expresses the invariant measure of the process in terms of scalar products in $\mathbb{R}^2$. The fact that the invariant measure is a convex combination with measures with a fluctuating microscopic shock position follows directly from the canonical approach of [30], but is actually a generic feature of matrix product measures with two-dimensional representations [33, 34].

Despite the failure of the differentiability condition of Theorem 3, the decay of correlations holds. Nevertheless, a macroscopically translation invariant description in terms of a conservation law of the form (1) cannot be expected to hold for arbitrary values of the blockage parameter p. This is in agreement with the rigorously established hydrodynamic limit for the usual (continuous-time) TASEP with a single defect [35–37]. An interesting open problem is the question whether condition $\mathbf{C}'$ is valid for *any* physical system where the charges q_k^α and associated instantaneous currents j_k^α are cylinder functions that depend only on a finite number of occupation variables in a finite distance around k.

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References

1. C. Kipnis, C. Landim, *Scaling Limits of Interacting Particle Systems* (Springer, Berlin, 1999)
2. A. Bressan, Hyperbolic systems of conservation laws in one space dimension, in *Proceedings of the ICM*, Beijing 2002, vol. 1 (2002), pp. 59–178. arXiv:math/0212392, Cited 3 Mar 2020
3. V. Popkov, G.M. Schütz, Shocks and excitation dynamics in a driven diffusive two-channel system. J. Stat. Phys. **112**, 523–540 (2003)
4. B. Tóth, B. Valkó, Onsager relations and Eulerian hydrodynamic limit for systems with several conservation laws. J. Stat. Phys. **112**, 497–521 (2003)
5. H.T. Yau, Relative entropy and hydrodynamics of Ginzburg–Landau models. Lett. Math. Phys. **22**, 63–80 (1991)
6. P.D. Lax, *Hyperbolic Systems of Conservation Laws and the Mathematical Theory of Shock Waves* (Society for Industrial and Applied Mathematics, Philadelphia, 1973)
7. D. Serre, *Systems of Conservation Laws* (Cambridge University Press, Cambridge, 1999)
8. D. Forster, *Hydrodynamic Fluctuations, Broken Symmetry, and Correlation Functions* (W. A. Benjamin Inc., Reading, MA, 1975)
9. H. Spohn, *Large Scale Dynamics of Interacting Particles* (Springer, Berlin, 1991)
10. C. Bahadoran, H. Guiol, K. Ravishankar, E. Saada, Euler hydrodynamics of one-dimensional attractive particle systems. Ann. Prob. **34**, 1339–1369 (2006)
11. R. Grisi, G.M. Schütz, Current symmetries for particle systems with several conservation laws. J. Stat. Phys. **145**, 1499–1512 (2011)
12. O.A. Castro-Alvaredo, B. Doyon, T. Yoshimura, Emergent hydrodynamics in integrable quantum systems out of equilibrium. Phys. Rev. X **6**, 041065 (2016)
13. J. De Nardis, D. Bernard, B. Doyon, Diffusion in generalized hydrodynamics and quasiparticle scattering. SciPost Phys. **6**, 049 (2019)
14. D. Karevski, G.M. Schütz, Charge-current correlation equalities for quantum systems far from equilibrium. SciPost Phys. **6**, 068 (2019)
15. T.M. Liggett, *Stochastic Interacting Systems: Contact Voter and Exclusion Processes* (Springer, Berlin, 1999)

16. G.M. Schütz, Critical phenomena and universal dynamics in one-dimensional driven diffusive systems with two species of particles. J. Phys. A: Math. Gen. **36**, R339–R379 (2003)
17. G.M. Schütz, Fluctuations in Stochastic Interacting Particle Systems, in *Stochastic Dynamics Out of Equilibrium. IHPStochDyn 2017*, eds. by G. Giacomin, S. Olla, E. Saada, H. Spohn, G. Stoltz. Springer Proceedings in Mathematics & Statistics, vol 282 (Springer, Cham, 2019)
18. E. Lieb, D. Robinson, The finite group velocity of quantum spin systems. Commun. Math. Phys. **28**, 251–257 (1972)
19. H. Spohn, Fluctuating hydrodynamics approach to equilibrium time correlations for anharmonic chains, in *Thermal Transport in Low Dimensions. From Statistical Physics to Nanoscale Heat Transfer*, ed. by S. Lepri. Lecture Notes in Physics, vo. 921 (Springer, Switzerland, 2016), pp. 107–158
20. V. Popkov, A. Schadschneider, J. Schmidt, G.M. Schütz, Fibonacci family of dynamical universality classes. Proc. Natl. Acad. Sci. (USA) **112**, 12645–12650 (2015)
21. A. Kundu, A. Dhar, Equilibrium dynamical correlations in the Toda chain and other integrable models. Phys. Rev. E **94**, 062130 (2016)
22. D. Karevski, G.M. Schütz, Conformal invariance in driven diffusive systems at high currents. Phys. Rev. Lett. **118**, 030601 (2017)
23. S. Ramaswamy, M. Barma, D. Das, A. Basu, Phase diagram of a two-species lattice model with a linear instability. Phase Trans. **75**, 363–375 (2002)
24. Y. Kafri, E. Levine, D. Mukamel, G.M. Schütz, R.D. Willmann, Phase-separation transition in one-dimensional driven models. Phys. Rev. E **68**, 035101(R) (2003)
25. S. Chakraborty, S. Pal, S. Chatterjee, M. Barma, Large compact clusters and fast dynamics in coupled nonequilibrium systems. Phys. Rev. E **93**, 050102(R) (2016)
26. P.A. Ferrari, L.R.G. Fontes, Shock fluctuations in the asymmetric simple exclusion process. Prob. Theory Relat. Fields **99**, 305–319 (1994)
27. M. Dudziński, G.M. Schütz, Relaxation spectrum of the asymmetric exclusion process with open boundaries. J. Phys. A: Math. Gen. **33**, 8351–8364 (2000)
28. V. Belitsky, G.M. Schütz, Diffusion and scattering of shocks in the partially asymmetric simple exclusion process. Electron. J. Prob. **7**, paper 11, 1–21 (2002)
29. J. de Gier, F.H.L. Essler, Exact spectral gaps of the asymmetric exclusion process with open boundaries. J. Stat. Mech. **P12011** (2006)
30. G. Schütz, Generalized Bethe ansatz solution of a one-dimensional asymmetric exclusion process on a ring with blockage. J. Stat. Phys. **71**, 471–505 (1993)
31. G.M. Schütz, On the phase transition in the deterministic sublattice TASEP with stochastic defect (2020). http://iopscience.iop.org/10.1088/1751-8121/abb042
32. H. Hinrichsen, S. Sandow, Deterministic exclusion process with a stochastic defect: matrix-product ground states. J. Phys. A: Math. Gen. **30**, 2745–2756 (1997)
33. K. Mallick, S. Sandow, Finite-dimensional representations of the quadratic algebra: Applications to the exclusion process. J. Phys. A: Math. Gen. **30**, 4513–4526 (1997)
34. F.H. Jafarpour, S.R. Masharian, Matrix product steady states as superposition of product shock measures in 1D driven systems. J. Stat. Mech. **P10013** (2007)
35. T. Seppäläinen, Hydrodynamic profiles for the totally asymmetric exclusion process with a slow bond. J. Stat. Phys. **102**, 69–96 (2001)
36. C. Bahadoran, Blockage hydrodynamics of one-dimensional driven conservative systems. Ann. Prob. **32**, 805–854 (2004)
37. P. Neijjar, Transition to Shocks in TASEP and Decoupling of Last Passage Times. Latin Am. J. Prob. Math. Stat. **15**, 1311–1334 (2018)

From the Hartree to the Vlasov Dynamics: Conditional Strong Convergence

Chiara Saffirio

Abstract We review the recent results [45, 46] concerning the semiclassical limit from the Hartree dynamics to the Vlasov equation with singular potentials and extend them to the case of more general radial interactions. We prove that, at positive temperature, the Hartree dynamics converges in trace norm to the Vlasov one, for a particular class of initial states.

Keywords Hartree equation · Vlasov equation · Semiclassical limit · Mean-field limit · Mixed states

1 Introduction

The Hartree dynamics. We consider the nonlinear Hartree-Fock equation

$$i\,\hbar\,\partial_t\,\omega_{N,t} = [\,\mathscr{H}_{\mathrm{HF}}\,,\,\omega_{N,t}\,]\,, \tag{1}$$

where $\omega_{N,t}$ is a one-particle fermionic operator, i.e. a nonnegative trace class operator over $L^2(\mathbb{R}^3)$ such that $\mathrm{tr}\;\omega_{N,t} = N$, $0 \leq \omega_{N,t} \leq 1$ and $N = \hbar^{-3}$. In (1) $[\mathscr{A}, \mathscr{B}]$ denotes the commutator between the operator $\mathscr{A}$ and the operator $\mathscr{B}$, $\mathscr{H}_{\mathrm{HF}}$ is the Hamilton operator given by

$$\mathscr{H}_{\mathrm{HF}} = -\hbar^2\Delta + (V * \rho_t) - \mathscr{X}_t\,, \tag{2}$$

where Δ is the Laplace operator, $V : \mathbb{R}^3 \to \mathbb{R}$ is a two-body interaction potential, $\rho_t : \mathbb{R}^3 \to \mathbb{R}$ is the density of fermions in the position space at time t, i.e. for $x \in \mathbb{R}^3$ $\rho_t(x) = N^{-1}\omega_{N,t}(x;x)$, and $\mathscr{X}_t$ is the exchange operator defined through its kernel $\mathscr{X}_t(x;y) = N^{-1}V(x-y)\omega_{N,t}(x;y)$, where we have used the notation $\mathscr{A}(\cdot;\cdot)$ to

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denote the kernel of the operator $\mathscr{A}$. We notice that the Hartree-Fock equation (1) propagates in time the fermionic structure of the operator ω_N. Namely if ω_N is a fermionic operator its evolution at time t according to the Hartree-Fock equation $\omega_{N,t}$ is also a fermionic operator, i.e. it satisfies the properties tr $\omega_{N,t} = N$ and $0 \leq \omega_{N,t} \leq 1$.

It has been shown in [5–7, 9, 11, 16, 20, 39, 41, 43, 44] that the Hartree-Fock equation is the mean-field approximation of the N-body fermionic Schrödinger dynamics for a class of quasi-free states exhibiting a semiclassical structure (see [12] for further readings). In particular, as first observed in [16], the mean-field scaling for a system of interacting fermions is naturally coupled with a semiclassical scaling through a rescaling of time, since the Planck constant $\hbar$ is proportional to $N^{-\frac{1}{3}}$, where N is the number of fermions.

As pointed out in [11], the energy contribution associated with the exchange term can be shown to be subleading. Hence, from now on we will drop the exchange term and consider the fermionic Hartree equation

$$i\,\hbar\,\partial_t\,\omega_{N,t} = [\mathscr{H}_{\mathrm{H}}\,,\ \omega_{N,t}]\,, \tag{3}$$

where $\mathscr{H}_{\mathrm{H}}$ is the Hamilton operator $\mathscr{H}_{\mathrm{HF}}$ defined in (2) with exchange term $\mathscr{X}_t = 0$.

The Vlasov equation. The Hartree equation (3) is N dependent because of the relation $\hbar = N^{-\frac{1}{3}}$ and the choice tr $\omega_{N,t} = N$. As we perform the limit $N \to \infty$, we are simultaneously performing the semiclassical limit $\hbar \to 0$. As first established by Narnhofer and Sewell in [37], the dynamics of N interacting fermions converges in the mean-field and semiclassical regime to a solution to the Vlasov equation

$$\partial_t \widetilde{W}_t + v \cdot \nabla_x \widetilde{W}_t + (\nabla V * \widetilde{\rho}_t) \cdot \nabla_v \widetilde{W}_t = 0\,, \tag{4}$$

where, for each $t \in \mathbb{R}_+$, $\widetilde{W}_t : \mathbb{R}^3 \times \mathbb{R}^3 \to \mathbb{R}$ is a probability density on the phase space representing the probability that a particle at time t is in position $x \in \mathbb{R}^3$ with velocity $v \in \mathbb{R}^3$. The function $\widetilde{\rho}_t : \mathbb{R}^3 \to \mathbb{R}$ is the spatial density of particles defined for each t as $\widetilde{\rho}_t(x) = \int_{\mathbb{R}^3} \widetilde{W}_t(x, v)\,dv$ and $V : \mathbb{R}^3 \to \mathbb{R}$ is a two-body interaction potential.

The Cauchy problem associated with Eq. (4) has been largely investigated. In [15] Dobrushin proved wellposedness in the case of potentials satisfying $V \in \mathscr{C}^2_c(\mathbb{R}^3)$. When the interaction is Coulomb or gravitational, existence of classical solutions under regularity assumptions on the initial datum has been established in [28] and [38] respectively in one and two dimensions. The three dimensional case has been addressed in [4] for small initial data and in a more general setting by Pfaffelmoser in [42] and by Lions and Perthame in [35].

The goal of this paper is to review recent results on the strong convergence of the Hartree equation (3) towards the Vlasov equation (4) when the interaction potential is singular.

Weyl and Wigner transforms. To study the semiclassical limit of Eq. (3), we observe that the solution of the Hartree equation (3) is an operator on $L^2(\mathbb{R}^3)$, whereas the solution to the Vlasov equation (4) is a function on the phase space $\mathbb{R}^3 \times \mathbb{R}^3$.

To compare them, we need to set the problem either on the space of operators on $L^2(\mathbb{R}^3)$ or on the space of functions on $\mathbb{R}^3 \times \mathbb{R}^3$. To this end, we introduce the notion of Wigner transform. We define the Wigner transform of the one-particle operator $\omega_{N,t}$ with kernel $\omega_{N,t}(\cdot\,;\,\cdot)$ as

$$W_{N,t}(x,v) = \left(\frac{\hbar}{2\pi}\right)^3 \int_{\mathbb{R}^3} \omega_{N,t}\left(x + \frac{\hbar y}{2}; x - \frac{\hbar y}{2}\right) e^{-iv\cdot y} dy\,. \tag{5}$$

Thus, for each $t > 0$, $W_{N,t} : \mathbb{R}^3 \times \mathbb{R}^3 \to \mathbb{R}$ and it is normalized, indeed

$$\int_{\mathbb{R}^3\times\mathbb{R}^3} W_{N,t}(x,v)dxdv = \hbar^3 \mathrm{tr}\,\omega_{N,t} = \hbar^3\, N = 1\,,$$

where in the last identity we used the relation $\hbar = N^{-1/3}$. Despite $W_{N,t}$ is normalized, in general it is not a probability density as it is not nonnegative.

The inverse transformation is called Weyl quantization. Given a function $W_{N,t}$ on the phase space, we define the Weyl quantization of $W_{N,t}$ by

$$\omega_{N,t}(x;\,y) = N \int W_{N,t}\left(\frac{x+y}{2}, v\right) e^{iv\cdot(x-y)/\hbar} dv\,, \tag{6}$$

where $\omega_{N,t}(x;\,y)$ is the kernel associated with the one-particle operator $\omega_{N,t}$. Therefore, the Weyl quantization transforms a function on the phase space into the kernel of a one-particle operator. Moreover, the quantity $\int_{\mathbb{R}^3} W_{N,t}(x,v)dv$ describes the density of fermions in position space at point $x \in \mathbb{R}^3$ and $\int_{\mathbb{R}^3} W_{N,t}(x,v)dx$ represents the density of particles with velocity $v \in \mathbb{R}^3$.

Initial states. We are interested in solutions to Eq. (3) which are evolutions of initial states describing equilibrium states of trapped systems. In the mean-field regime such equilibrium states are expected to be approximately quasi-free. In this paper we are interested in the evolution of quasi-free states at positive temperature, usually referred to as mixed states. More precisely, Shale-Stinespring condition (see Theorem 9.5 in [32]) guarantees that every one-particle operator ω_N such that $\mathrm{tr}\,\omega_N = N$ and $0 \le \omega_N \le 1$ is the one-particle reduced density of a quasi-free state with N fermions. When looking at the semiclassical limit, the advantage of considering mixed quasi-free states is that the associated Wigner transform is a regular function on the phase space. This is in general not the case when looking at zero temperature states (the so called pure states). See [10] for further reading on this matter.

State of art. The problem of obtaining the Vlasov equation as a classical limit of a dynamics of interacting quantum particles has been largely investigated. The first result in this direction is due to Narnhofer and Sewell. In [37] the authors consider a system of N fermions interacting through a two-body analytic potential $V \in \mathscr{C}^\omega(\mathbb{R}^3)$ and they obtain the Vlasov equation directly from the dynamics given by the N-fermion Schrödinger equation. In [47] the assumption on the interaction potential has been relaxed to $V \in \mathscr{C}^2(\mathbb{R}^3)$. The case of N bosons given by WKB

states in the mean-field regime combined with a semiclassical limit has been analysed in [26].

The semiclassical limit from the Hartree dynamics towards the Vlasov equation has been proven in weak topology for regular and singular interactions (here included the Coulomb potential) in [18, 34, 36]. This analysis has been extended to the Hartree-Fock equation in [21].

The above cited references establish weak convergence towards the solution to the Vlasov equation, but do not provide any control on the rate of convergence. The problem of obtaining explicit bounds on the convergence rate has been first addressed in [3] where the convergence from the Hartree equation to the Vlasov dynamics has been established in strong topology for regular interactions and later extended in [1, 2, 10, 41] and in [45, 46] for inverse power law potentials (included Coulomb interaction).

We also mention that a new approach has been initiated in [22, 23], where a notion of pseudo-distance reminiscent of the Monge-Kantorovich distance for classical probability measures has been introduced. Explicit bounds on the rate of convergence in the topology induced by such quantum analogous of the Monge-Kantorovich distance have been obtained for smooth (Cf. [23]) and singular potentials, including the Coulomb interaction (Cf. [29, 30]).

More recently, in the context of regular interactions, the joint mean-field and semiclassical limit for the dynamics of N fermions has been studied also in [14] by means of BBGKY type of hierarchy for the k-particle Husimi measure.

Main result. In this paper we are concerned with the strong convergence of the Hartree dynamics towards the Vlasov equation with interactions satisfying the following assumptions:

(a) let $V : \mathbb{R}^3 \to \mathbb{R}$ be a radially symmetric potential that is three times differentiable away from $x = 0$ and denote

$$V^{(m)}(|x|) := \frac{d^m}{d|x|^m} V(x) ;$$

(b) for $0 \leq m \leq 3$, assume

$$\lim_{|x|\to\infty} |x|^m V^{(m)}(|x|) = 0 ;$$

(c) for $\delta \in (0, 3/2]$, fix $k \in \mathbb{R}_+$ and assume

$$\int_0^k |r^2 V^{(3)}(r) - r V^{(2)}(r)| r^{\frac{9}{2}-\delta} dr < \infty .$$

We can think for instance to inverse power law interaction potentials, but more general interactions satisfying the above assumptions are included in the analysis performed in this paper. More precisely, assumptions (a) and (b) are needed to use a generalised version of Fefferman - De la Llave representation formula (see [27]), that is a key

tool in the proof of the main result of this paper. Assumption (c) is technical and has the advantage of making the presentation shorter and easier to read.

For some $a > 0$ and $k \in \mathbb{N}$, we introduce the weighed Sobolev spaces H^k_a, defined as the space of all square integrable functions f on the phase space $\mathbb{R}^3 \times \mathbb{R}^3$ such that the following norm is finite

$$\|f\|_{H^k_a} := \left(\sum_{|\beta| \leq k} \int (1 + x^2 + v^2)^a \, |\nabla^\beta f(x, v)|^2 \, dx \, dv \right)^{\frac{1}{2}}$$

where β is a multi-index and ∇^β can act on both x and v variables.

We are now ready to state our result.

Theorem 1 *Let V be a two-body potential satisfying assumptions* (a), (b) *and* (c) *above and $\hbar = N^{-\frac{1}{3}}$. Let ω_N be a sequence of fermionic operators, i.e. tr $\omega_N = N$ and $0 \leq \omega_N \leq 1$, and denote by $\omega_{N,t}$ the solution to the Hartree equation* (3) *with initial data ω_N. Let W_N be the Wigner transform of the operator ω_N and assume*[1] *that there exists a unique smooth solution $\widetilde{W}_{N,t}$ of the Vlasov equation* (4) *with initial data W_N such that $\nabla^2 \rho_t \in L^\infty(\mathbb{R}^3)$ for all $t \in [0, T]$ and $\|W_N\|_{H^6_4}$ is bounded uniformly in N.*

Assume moreover that there exists a time $T > 0$ and a constant $C > 0$ such that

$$\sup_{t \in [0,T]} \sum_{i=1}^{3} \left[\|\rho_{|[x_i, \widetilde{\omega}_{N,t}]|}\|_1 + \|\rho_{|[x_i, \widetilde{\omega}_{N,t}]|}\|_\infty \right] \leq C \, N \, \hbar \tag{7}$$

where

$$\rho_{|[x_i, \widetilde{\omega}_{N,t}]|}(x) := |[x_i \, , \, \widetilde{\omega}_{N,t}]|(x; x) \, . \tag{8}$$

Then there exist constants C_k, $k = 0, \ldots, 4$, depending only on T and on the H^{2+k}_4 norm of the Wigner transform of the initial data W_N such that

$$tr \, \left| \omega_{N,t} - \widetilde{\omega}_{N,t} \right| \leq C_0 \, N \, \hbar \left[1 + C_1 \hbar + C_2 \hbar^2 + C_3 \hbar^3 + C_4 \hbar^4 \right] . \tag{9}$$

Remark 1 We recall that tr $\omega_{N,t} = N$, hence the bound (9) is non-trivial, showing that the Vlasov equation is a good semiclassical approximation for the fermionic dynamics given by the Hartree equation with singular interaction potential V.

Remark 2 We observe that the exchange term in (1) is subleading in the limit of N large, i.e. as $\hbar \to 0$. For this reason the bound (9) is expected to remain correct if we consider the Hartree-Fock equation (1) instead of the Hartree equation (3).

[1] Such a solution indeed exists if the initial data are sufficiently regular. For the precise assumptions, see Remark 3 below.

Remark 3 In the statement of Theorem 1, we assumed a smooth solution to Eq. (4) to exist and to be unique. This is indeed the case whenever the following assumptions on the initial datum W_N are satisfied (Cf. [45, 46].):

(i) $W_N \in L^1 \cap L^\infty(\mathbb{R}^3 \times \mathbb{R}^3)$ and $\mathscr{M}_m(W_N) < \infty$ for all $m < m_0$, with $m_0 > 6$.
(ii) For all $R,\ T > 0$,

$$\begin{aligned} \operatorname*{ess\,sup}_{y,\,w} \{|\nabla^k W_N|(y + vt, w) \ : |y - x| \le R,\ |w - v| \le R\} \\ \in\ L^\infty((0, T) \times \mathbb{R}^3_x; L^1(\mathbb{R}^3_v) \cap L^2(\mathbb{R}^3_v)) \end{aligned} \tag{10}$$

for $k = 0, 1, \ldots, 5$.
(iii) There exists $C > 0$ independent of N such that $\|W_N\|_{H^6_4} \le C$.

Remark 4 Hypothesis (7) is a stringent assumption. At the moment we are not able to prove the bound (7) for the solution of the Vlasov equation. Nevertheless, there is a special situation in which the assumption is satisfied, that is for regular steady solutions of the Vlasov equation (4) when V is the gravitational potential. See [46] for extended explanations and examples.

Remark 5 In Theorem 1 we consider fermionic operators, i.e. operators ω_N such that $0 \le \omega_N \le 1$. However, the exact same proof holds in the bosonic case.

Strategy of the proof. The idea of the proof is to obtain a Grönwall type inequality to compare the solution $\omega_{N,t}$ of the Hartree equation (3) with a solution $\widetilde{\omega}_{N,t}$ to the Weyl transformed Vlasov equation, i.e. at the operator level and not as functions on the phase space. The operators $\omega_{N,t}$ and $\widetilde{\omega}_{N,t}$ are fermionic operators, i.e. they satisfy $0 \le \omega_{N,t} \le 1$ and $0 \le \widetilde{\omega}_{N,t} \le 1$, with the normalisation $\operatorname{tr} \omega_{N,t} = \operatorname{tr} \widetilde{\omega}_{N,t} = N$.

In the Grönwall type inequality we look for there are two terms appearing: the first one is the dominant term that will allow us to close the inequality; the second one is an subleding term and it will determine the rate of convergence of $\omega_{N,t}$ towards $\widetilde{\omega}_{N,t}$, as $\hbar = N^{-1/3} \to 0$. In the dominant term, the Laplace operator related to the kinetic part of the Hartree Hamiltonian (2) appears. To deal with it, we make use of a unitary transformation that acts as a change the reference frame, canceling the kinetic factor. Moreover, we deal with the singularity of the potential V by using a generalised version of the Fefferman and De la Llave representation formula. For general radially symmetric and fast decreasing potentials such a formula was provided in [27] (see Proposition 2). This is the key tool in the proof of Theorem 1, as it allows isolating the singularity of the potential V at zero and close the Grönwall inequality. To this end, we need to control the trace norm of the commutator between the Weyl transformed solution $\widetilde{\omega}_{N,t}$ of the Vlasov equation and the multiplication operator by a Gaussian $\chi_{(r,z)}(x) = \exp(-|x - z|^2/r^2)$ (see Lemma 2). This is the point at which the quantities (7)–(8) appear and the main reason why we have to restrict to initial data satisfying the bound (7) at time $t > 0$. To bound the error term, and therefore determine the convergence rate, we use again the generalized Fefferman - De la Llave representation formula for rapidly decreasing, radially symmetric interactions.

The paper is organised as follows: in Sect. 2 we present some auxiliary results, such as the precise statement of the generalized Fefferman - De la Llave representation formula and the key estimate on the commutator tr $|[\chi_{(r,z)}, \widetilde{\omega}_{N,t}]|$; in Sect. 3 we give the main steps to prove Theorem 1, focusing on the parts of the proof that differ from the Coulomb interaction case treated in [46].

2 Preliminary Estimates

Lemma 1 *Let $\omega_{N,t}$ be a solution to the Hartree equation (3) with initial datum ω_N. Denote by W_N the Wigner transform of ω_N and let $\widetilde{W}_{N,t}$ be the solution of the Vlasov equation (4) with initial data W_N. Denote by $\widetilde{\omega}_{N,t}$ the Weyl transform of $\widetilde{W}_{N,t}$. Then*

$$tr\,|\omega_{N,t} - \widetilde{\omega}_{N,t}| \leq \frac{1}{\hbar}\int_0^t tr\,\left|\left[V * (\rho_s - \widetilde{\rho}_s), \widetilde{\omega}_{N,s}\right]\right| ds + \frac{1}{\hbar}\int_0^t tr\,|B_s|\,ds \tag{11}$$

where, for every $s \in [0,t]$, B_s is the operator with kernel

$$B_s(x;y) = \left[(V * \widetilde{\rho}_s)(x) - (V * \widetilde{\rho}_s)(y) - \nabla (V * \widetilde{\rho}_s)\left(\frac{x+y}{2}\right) \cdot (x-y)\right] \widetilde{\omega}_{N,t}(x;y)\,. \tag{12}$$

Proof Applying the Weyl quantization to the Vlasov equation (4), we obtain the following equation for the operator $\widetilde{\omega}_{N,t}$:

$$i\,\hbar\,\partial_t\,\widetilde{\omega}_{N,t} = [-\hbar^2\,\Delta, \widetilde{\omega}_{N,t}] + \mathscr{A}_t \tag{13}$$

where $\mathscr{A}_t$ is the operator with integral kernel

$$\mathscr{A}_t(x;y) = \nabla (V * \widetilde{\rho}_t)\left(\frac{x+y}{2}\right) \cdot (x-y)\,\widetilde{\omega}_{N,t}(x;y)\,.$$

We introduce $\mathscr{U}(t;s)$, the two-parameter group of unitary transformations generated by the Hartree Hamiltonian $\mathscr{H}_{\mathrm{H}}(t) := -\hbar^2\Delta + V * \rho_t$

$$\begin{cases} i\,\hbar\,\partial_s\,\mathscr{U}(t;s) = \mathscr{H}_{\mathrm{H}}(t)\,\mathscr{U}(t;s) \\ \mathscr{U}(s;s) = 1 \end{cases}$$

so that $\omega_{N,t} = \mathscr{U}(t;0)\,\omega_N\,\mathscr{U}^*(t;0)$. The role of $\mathscr{U}(t;s)$ is to cancel the kinetic part of the Hamiltonian $\mathscr{H}_{\mathrm{H}}(t)$ by conjugating the difference between $\omega_{N,t}$ and $\widetilde{\omega}_{N,t}$ with $\mathscr{U}(t;s)$ and performing the time derivative. This leads to

$$
\begin{aligned}
i\,\hbar\,\partial_s\left(\mathscr{U}^*(t;s)\,(\omega_{N,s}-\widetilde{\omega}_{N,s})\,\mathscr{U}(t;s)\right)&\\
&=\mathscr{U}^*(t;s)\,[\mathscr{H}_{\mathrm{H}}(s),\omega_{N,s}-\widetilde{\omega}_{N,s}]\,\mathscr{U}(t;s)\\
&+\mathscr{U}^*(t;s)\,([\mathscr{H}_{\mathrm{H}}(s),\omega_{N,s}]-[-\hbar^2\Delta,\widetilde{\omega}_{N,s}]-\mathscr{A}_s)\,\mathscr{U}(t;s)\\
&=\mathscr{U}^*(t;s)\,\left(\left[V*\rho_s,\widetilde{\omega}_{N,t}\right]-\mathscr{A}_s\right)\,\mathscr{U}(t;s)\\
&=\mathscr{U}^*(t;s)\,\left(\left[V*(\rho_s-\widetilde{\rho}_s),\widetilde{\omega}_{N,s}\right]+\mathscr{B}_s\right)\,\mathscr{U}(t;s)
\end{aligned}
$$

where $\mathscr{B}_s$ is the operator with integral kernel (12). Recalling that $\widetilde{\omega}_{N,0}=\omega_N$, Duhamel's formula yields

$$
\begin{aligned}
\mathscr{U}^*(t;s)\,(\omega_{N,s}-\widetilde{\omega}_{N,s})\,\mathscr{U}(t;s)=\frac{1}{i\,\hbar}\int_0^t\mathscr{U}^*(t;s)\,\left[V*(\rho_s-\widetilde{\rho}_s),\widetilde{\omega}_{N,s}\right]\,\mathscr{U}(t;s)\,ds&\\
+\frac{1}{i\,\hbar}\int_0^t\mathscr{U}^*(t;s)\,\mathscr{B}_s\,\mathscr{U}(t;s)\,ds.&
\end{aligned}
\tag{14}
$$

The bound (11) follows by taking the trace norm in the above expression and using that $\mathscr{U}(t;s)$ is a family of unitary operators.

Proposition 1 *Under the same assumptions of Lemma 1 and Theorem 1, there exists a constant $C>0$ such that*

$$
tr\,\left|\left[V*(\rho_s-\widetilde{\rho}_s)\,,\,\widetilde{\omega}_{N,s}\right]\right|\leq C\,\hbar\,tr\,|\omega_{N,s}-\widetilde{\omega}_{N,s}|. \tag{15}
$$

The proof of Proposition 1 relies on the generalization proved in [27] of the Fefferman - De la Llave representation formula established in [17] for the Coulomb potential.

Proposition 2 (Theorem 1 in [27]) *For $n\geq 2$, let $V:\mathbb{R}^n\to\mathbb{R}$ be a radial function that is $[n/2]+2$ times differentiable away from $x=0$, where $[a]$ denotes the integer part of a. For $m\in\mathbb{N}_0$ denote $V^{(m)}(|x|)=d^m/d|x|^m\,V(x)$. Assume that $\lim_{|x|\to\infty}|x|^m V^{(m)}(|x|)=0$ for all $0\leq m\leq[n/2]+1$. Then*

$$
V(x)=\int_0^\infty\int_{\mathbb{R}^n}g(r)\,\mathbf{1}_{\{|x-z|\leq r\}}\mathbf{1}_{\{|z|\leq r\}}\,dz\,dr \tag{16}
$$

where

$$
\begin{aligned}
g(r)=\frac{(-1)^{[\frac{n}{2}]}}{\Gamma\left(\frac{n-1}{2}\right)}\frac{2}{(\pi\,r^2)^{\frac{(n-1)}{2}}}\left(\int_r^\infty ds\;V^{([\frac{n}{2}]+2)}(s)\left(\frac{d}{ds}\right)^{n-1-[\frac{n}{2}]}s(s^2-r^2)^{\frac{1}{2}(n-3)}\right.&\\
\left.+\,\mathbf{1}_{\{n=2k+1,\,k\in\mathbb{N}\}}V^{([\frac{n}{2}]+2)}(r)\,r(2r)^{\frac{1}{2}(n-3)}\Gamma\left(\frac{n-1}{2}\right)\right)&
\end{aligned}
\tag{17}
$$

where $\Gamma(\cdot)$ denotes the Gamma function.

Remark 6 We observe that the Coulomb potential $V(x) = \dfrac{1}{|x|}$ satisfies the assumptions in Proposition 2. In that case $g(r)$ has a simple expression and the Fefferman - De la Llave representation formula writes

$$\frac{1}{|x-y|} = \frac{1}{\pi}\int_0^\infty \int_{\mathbb{R}^n} \frac{1}{r^5}\, \mathbf{1}_{\{|x-z|\le r\}}\, \mathbf{1}_{\{|y-z|\le r\}}\, dz\, dr$$

Remark 7 We can easily replace the characteristic function $\mathbf{1}_{\{|x-z|\le r\}}$ by a smooth function varying on the same scale at the price of having a different constant in front of the expression. In what follows, we choose to use the Gaussian

$$\chi_{(r\,,\,z)}(x) := \exp\left(-\frac{|x-z|^2}{r^2}\right). \tag{18}$$

Hence, with the notations introduced in Proposition 2, the generalised Fefferman - De la Llave representation formula reads

$$V(x) = \frac{4}{\pi}\int_0^\infty \int_{\mathbb{R}^n} g(r)\, \chi_{(r,z)}(x)\, \chi_{(r,z)}(0)\, dz\, dr \tag{19}$$

Moreover, integrating out the z variable, we get

$$V(x) = \frac{4}{\pi}\int_0^\infty r^3\, g(r)\, \chi_{(\sqrt{2}r,x)}(0)\, dr \tag{20}$$

For later use, we recall here the definition of the Hardy-Littlewood maximal function:

Definition 1 For $z \in \mathbb{R}^3$ and B ball in $\mathbb{R}^3$ centred at zero, the Hardy-Littlewood maximal function of a function f is defined as

$$f^*(z) = \sup_{B\,:\,z\in B} \frac{1}{|B|}\int_B f(x)\, dx$$

We can now state the following Lemma, which gives a bound in trace norm on the commutator of $\widetilde{\omega}_{N,t}$ and the multiplication operator $\chi_{(r,z)}$.

Lemma 2 (Lemma 3.1 in [43]) *Let $\chi_{(r\,,\,z)}(x)$ be as in (18) and assume $\left[x_i, \widetilde{\omega}_{N,t}\right]$ to be trace class for all $t \in [0; T]$ and $i = 1, 2, 3$. Then, for all $\delta \in (0, 1/2)$, there exists a positive constant C such that the bound*

$$tr\,|[\chi_{(r,z)}\,,\,\widetilde{\omega}_{N,t}]| \le C\, r^{\frac{3}{2}-3\delta} \sum_{i=1}^{3} \|\rho_{|[x_i\,,\,\widetilde{\omega}_{N,t}]|}\|_{L^1}^{\frac{1}{6}+\delta} \left(\rho^*_{|[x_i\,,\,\widetilde{\omega}_{N,t}]|}(z)\right)^{\frac{5}{6}-\delta} \tag{21}$$

holds pointwise, where $\rho_{|[x_i\,,\,\widetilde{\omega}_{N,t}]|}$ is defined in (8) and $\rho^*_{|[x_i\,,\,\widetilde{\omega}_{N,t}]|}$ denotes the Hardy-Littlewood maximal function of $\rho_{|[x_i\,,\,\widetilde{\omega}_{N,t}]|}$ introduced in Definition 1.

Proof We consider the integral kernel of the commutator $[\chi_{(r,z)}, \widetilde{\omega}_{N,t}]$ and write it as

$$\begin{aligned}(x;\,y) &= \big(\chi_{(r\,,\,z)}(x) - \chi_{(r\,,\,z)}(y)\big)\,\widetilde{\omega}_{N,t}(x;\,y)\\ &= \int_0^1 ds\ \frac{d}{ds} e^{-\frac{(x-z)^2}{r^2}s}\widetilde{\omega}_{N,t}(x;\,y)e^{-\frac{(x-z)^2}{r^2}(1-s)}\\ &= -\int_0^1 ds\ e^{-s\frac{(x-z)^2}{r^2}}\left[\frac{(x-z)^2}{r^2}, \widetilde{\omega}_{N,t}\right](x;\,y)\,e^{-(1-s)\frac{(y-z)^2}{r^2}}\,.\end{aligned}$$

We can therefore write the commutator as

$$\begin{aligned}&[\chi_{(r\,,\,z)}, \widetilde{\omega}_{N,t}]\\ &= -\sum_{i=1}^3 \int_0^1 ds\ \chi_{(r/\sqrt{s}\,,\,z)}(x)\left(\frac{(x-z)_i}{r^2}\left[x_i, \widetilde{\omega}_{N,t}\right] + \left[x_i, \widetilde{\omega}_{N,t}\right]\frac{(x-z)_i}{r^2}\right)\chi_{(r/\sqrt{1-s}\,,\,z)}(x)\\ &= \sum_{i=1}^3 \mathfrak{A}_i^{(1)} + \mathfrak{A}_i^{(2)}\,.\end{aligned} \tag{22}$$

where, with an abuse of notation, we denote by $\chi_{(.,.)}(x)$ both the function of x and the corresponding multiplication operator.

We focus on the first term of the r.h.s. of (22) and fix $i = 1$. The other components of the first term, and the three components of the second term can then be treated similarly. By the spectral decomposition of the commutator $\left[x_1, \widetilde{\omega}_{N,t}\right]$ we have

$$[x_1, \widetilde{\omega}_{N,t}] = i\sum_j \lambda_j |\varphi_j\rangle\langle\varphi_j|$$

for a sequence of eigenvalues $\lambda_j \in \mathbf{R}$ and an orthonormal system φ_j in $L^2(\mathbf{R}^3)$ (we introduced $i = \sqrt{-1}$ on the r.h.s., because the commutator is anti self-adjoint). We find

$$\begin{aligned}\mathfrak{A}_1^{(1)} &= -\int_0^1 ds\ \chi_{(r/\sqrt{s},z)}(x)\frac{(x-z)_1}{r^2}\left[x_1, \widetilde{\omega}_{N,t}\right]\chi_{(r/\sqrt{1-s},z)}(x)\\ &= -\frac{i}{r}\sum_j \lambda_j \int_0^1 \frac{ds}{\sqrt{s}}\left|\chi_{(r/\sqrt{s}\,,\,z)}(x)\frac{(x-z)_1}{r/\sqrt{s}}\varphi_j\right\rangle\left\langle\chi_{(r/\sqrt{1-s}\,,\,z)}(x)\varphi_j\right|.\end{aligned}$$

Using that tr $||\psi_1\rangle\langle\psi_2|| = \|\psi_1\|\,\|\psi_2\|$ we obtain

$$\begin{aligned}\mathrm{tr}\,|\mathfrak{A}_1^{(1)}| &\leq \frac{1}{r}\sum_j |\lambda_j| \int_0^1 \frac{ds}{\sqrt{s}} \left\| \chi_{(r/\sqrt{s},z)}(x)\frac{|x-z|}{r/\sqrt{s}}\varphi_j \right\| \left\| \chi_{(r/\sqrt{1-s},z)}(x)\varphi_j \right\| \\ &\leq \frac{1}{r}\int_0^1 \frac{ds}{\sqrt{s}} \left(\sum_j |\lambda_j| \left\| \chi_{(r/\sqrt{s},z)}(x)\frac{|x-z|}{r/\sqrt{s}}\varphi_j \right\|^2 \right)^{1/2} \\ &\qquad \times \left(\sum_j |\lambda_j| \left\| \chi_{(r/\sqrt{1-s},z)}(x)\varphi_j \right\|^2 \right)^{1/2} . \end{aligned} \tag{23}$$

We compute

$$\begin{aligned}\sum_j |\lambda_j| \left\| \chi_{(r/\sqrt{1-s},z)}(x)\varphi_j \right\|^2 &= \int dx\, e^{-2(1-s)(x-z)^2/r^2} \rho_{|[x,\widetilde{\omega}_{N,t}]|}(x) \\ &\leq C\frac{r^3}{(1-s)^{3/2}}\, \rho^*_{|[x,\widetilde{\omega}_{N,t}]|}(z) \end{aligned} \tag{24}$$

where $\rho^*_{|[x_i,\widetilde{\omega}_{N,t}]|}$ is the Hardy-Littlewood maximal function associated with $\rho_{|[x_i,\widetilde{\omega}_{N,t}]|}$. To prove (24), we write

$$\begin{aligned} e^{-2(1-s)(x-z)^2/r^2} &= \int_0^1 \chi(t \leq e^{-2(1-s)(x-z)^2/r^2})dt \\ &= \int_0^1 \chi\left(|x-z| \leq \sqrt{\frac{r^2\log(1/t)}{2(1-s)}} \right) dt \end{aligned}$$

and, using Fubini, we find

$$\begin{aligned} &\int dx\, e^{-2(1-s)(x-z)^2/r^2} \rho_{|[x,\widetilde{\omega}_{N,t}]|}(x) \\ &\quad = \int_0^1 dt \int dx\, \chi\left(|x-z| \leq \sqrt{\frac{r^2\log(1/t)}{2(1-s)}} \right) \rho_{|[x,\widetilde{\omega}_{N,t}]|}(x) \\ &\quad \leq C\frac{r^3}{(1-s)^{3/2}}\, \rho^*_{|[x,\widetilde{\omega}_{N,t}]|}(z) \int_0^1 (\log(1/t))^{3/2} \\ &\quad \leq C\frac{r^3}{(1-s)^{3/2}}\, \rho^*_{|[x,\widetilde{\omega}_{N,t}]|}(z) \end{aligned}$$

which shows (24). Similarly to (24), we also find

$$\sum_j |\lambda_j| \left\| \chi_{(r/\sqrt{s},z)}(x)\frac{|x-z|}{r/\sqrt{s}}\varphi_j \right\|^2 \leq C\frac{r^3}{s^{3/2}}\rho^*_{|[x_1,\widetilde{\omega}_{N,t}]|}(z)\,.$$

Combining this bound with the simpler estimate

$$\sum_j |\lambda_j| \left\| \chi_{(r/\sqrt{s},z)}(x) \frac{|x-z|}{r/\sqrt{s}} \varphi_j \right\|^2 \leq C \sum_j |\lambda_j| = \|\rho_{|[x_1,\widetilde{\omega}_{N,t}]|}\|_1$$

we obtain

$$\sum_j |\lambda_j| \left\| \chi_{(r/\sqrt{s},z)}(x) \frac{|x-z|}{r/\sqrt{s}} \varphi_j \right\|^2 \leq C \frac{r^{3\gamma} \, \|\rho_{|[x_1,\widetilde{\omega}_{N,t}]|}\|_1^{1-\gamma}}{s^{3\gamma/2}} \left(\rho^*_{|[x_1,\widetilde{\omega}_{N,t}]|}(z)\right)^{\gamma}$$

for any $0 \leq \gamma \leq 1$. Inserting the last bound and (24) on the r.h.s. of (23) we conclude

$$\begin{aligned} \operatorname{tr} |\mathfrak{A}_1^{(1)}| \leq C r^{(1+3\gamma)/2} \|\rho_{|[x_1,\widetilde{\omega}_{N,t}]|}\|_1^{(1-\gamma)/2} \left(\rho^*_{|[x_1,\widetilde{\omega}_{N,t}]|}(z)\right)^{(1+\gamma)/2} \\ \times \int_0^1 ds \frac{1}{s^{1/2+3\gamma/4}(1-s)^{3/4}} \, . \end{aligned}$$

Hence, for all $\delta > 0$ we find (putting $\gamma = 2/3 - 2\delta$)

$$\operatorname{tr} |\mathfrak{A}_1^{(1)}| \leq C r^{3/2-3\delta} \|\rho_{|[x_1,\widetilde{\omega}_{N,t}]|}\|_1^{1/6+\delta} \left(\rho^*_{|[x_1,\widetilde{\omega}_{N,t}]|}(z)\right)^{5/6-\delta}$$

which concludes the proof.

Proof (*Proof of Proposition* 1) We write explicitly the convolution appearing on the l.h.s. of (15) and get the following expression for the commutator

$$[V * (\rho_s - \widetilde{\rho}_s) \, , \, \widetilde{\omega}_{N,s}] = \int (\rho_s(z) - \widetilde{\rho}_s(z)) \, [V(\cdot - z) \, , \, \widetilde{\omega}_{N,s}] \, dz \, .$$

By (19) and (18), we can rewrite the potential V as

$$V(x-z) = \frac{4}{\pi} \int_0^\infty r^3 \, g(r) \, \chi_{(\sqrt{2}r,z)}(x) \, dr \, .$$

Plugging (2) into (27) and taking the trace norm of (27), we obtain the bound

$$\begin{aligned} &\operatorname{tr} |[V*(\rho_s - \widetilde{\rho}_s) \, , \, \widetilde{\omega}_{N,s}]| \\ &\qquad \leq C \int |\rho_s(z) - \widetilde{\rho}_s(z)| \int_0^\infty r^3 \, |g(r)| \operatorname{tr} |[\chi_{(\sqrt{2}r,z)} \, , \, \widetilde{\omega}_{N,s}]| \, dr \, dz. \end{aligned}$$

We choose $k > 0$ and split the integral in the r variable into two parts: the set $r \in [0,k)$ and the set $r \in [k,\infty)$.

For $r \in [0,k)$, we use Lemma 2 and get

$$\begin{aligned}
&\int_0^k r^3\,|g(r)|\,\mathrm{tr}\,|[\chi_{(\sqrt{2}r,z)}\,,\,\widetilde{\omega}_{N,s}]|\,dr \\
&\qquad\le \int_0^k r^{\frac{9}{2}-3\delta}|g(r)|\sum_{i=1}^3 \|\rho_{|[x_i,\widetilde{\omega}_{N,s}]|}\|_{L^1}^{\frac{1}{6}+\delta}\left(\rho^*_{|[x_i,\widetilde{\omega}_{N,s}]|}(z)\right)^{\frac{5}{6}-\delta}\,dr \\
&\qquad\le \int_0^k r^{\frac{9}{2}-3\delta}|g(r)|\sum_{i=1}^3 \|\rho_{|[x_i,\widetilde{\omega}_{N,s}]|}\|_{L^1}^{\frac{1}{6}+\delta}\|\rho^*_{|[x_i,\widetilde{\omega}_{N,s}]|}\|_{L^\infty}^{\frac{5}{6}-\delta}\,dr \\
&\qquad\le C\sum_{i=1}^3 \|\rho_{|[x_i,\widetilde{\omega}_{N,s}]|}\|_{L^1}^{\frac{1}{6}+\delta}\|\rho_{|[x_i,\widetilde{\omega}_{N,s}]|}\|_{L^\infty}^{\frac{5}{6}-\delta}
\end{aligned}$$

where in the last inequality we used that $\|\rho^*_{|[x_i,\widetilde{\omega}_{N,s}]|}\|_{L^\infty} \le \|\rho_{|[x_i,\widetilde{\omega}_{N,s}]|}\|_{L^\infty}$ and that the integral in r converges by assumption c) on the potential V.

As for $r \in [k,\infty)$, following the same lines of the proof of Lemma 2 and choosing the parameter $\gamma = 0$, we simply bound the trace norm of the commutator $[\chi_{(\sqrt{2}r,z)}, \widetilde{\omega}_{N,s}]$ as

$$\mathrm{tr}\,|[\chi_{(\sqrt{2}r,z)}, \widetilde{\omega}_{N,s}]| \le C\|\rho_{|[x_i,\widetilde{\omega}_{N,s}]|}\|_{L^1}\,.$$

Then we are left with the integral in r. Using assumption b) on the potential V, we conclude that

$$\int_k^\infty r^3\,|g(r)|\,dr = C\int_k^\infty \left|\,r\,V^{(2)}(r) - r^2\,V^{(3)}(r)\,\right|\,dr < +\infty\,.$$

Hence

$$\begin{aligned}
&\mathrm{tr}\,|[V*(\rho_s-\widetilde{\rho}_s)\,,\,\widetilde{\omega}_{N,s}]| \\
&\qquad\le C\int |\rho_s(z)-\widetilde{\rho}_s(z)|\sum_{i=1}^3\left(\|\rho_{|[x_i,\widetilde{\omega}_{N,s}]|}\|_{L^1}^{\frac{1}{6}+\delta}\|\rho_{|[x_i,\widetilde{\omega}_{N,s}]|}\|_{L^\infty}^{\frac{5}{6}-\delta} + \|\rho_{|[x_i,\widetilde{\omega}_{N,s}]|}\|_{L^1}\right).
\end{aligned}$$

Moreover, using the dual definition of L^1 norm, we get

$$\begin{aligned}
\int |\rho_s(z)-\widetilde{\rho}_s(z)|\,dz &= \sup_{\substack{\mathscr{O}\in L^\infty\\ \|\mathscr{O}\|_\infty\le 1}}\left|\int \mathscr{O}(z)\,(\rho_s(z)-\widetilde{\rho}_s(z))\,dz\right| \\
&\le \frac{1}{N}\sup_{\substack{\mathscr{O}\in\mathfrak{B}\\ \|\mathscr{O}\|\le 1}}\left|\mathrm{tr}\,\mathscr{O}\,(\omega_{N,s}-\widetilde{\omega}_{N,s})\right| \\
&= \frac{1}{N}\,\mathrm{tr}\,|\omega_{N,s}-\widetilde{\omega}_{N,s}|
\end{aligned}$$

where $\mathfrak{B}$ denotes the set of bounded operators and $\|\cdot\|$ the operator norm. This concludes the proof.

Proposition 3 *Let $\mathscr{B}_t$ be the operator associated with the (12). Then, there exists a constant $C > 0$ depending on $\|\widetilde{W}_{N,t}\|_{H^2_4}$, $\|\nabla^2\widetilde{\rho}_t\|$ such that*

$$tr\,|\mathscr{B}_t| \leq C\,N\,\hbar^2\left(1+\sum_{k=1}^{4}\hbar^k\|\widetilde{W}_{N,t}\|_{H^{k+2}_4}\right). \tag{25}$$

The proof can be found in [44] and it is based on the following procedure: we write the identity operator as

$$\mathbf{1} = (1-\hbar^2\Delta)^{-1}(1+x^2)^{-1}(1+x^2)(1-\hbar^2\Delta).$$

By Cauchy-Schwarz inequality we have

$$\mathrm{tr}\,|\mathscr{B}_t| \leq \|(1-\hbar^2\Delta)^{-1}(1+x^2)^{-1}\|_{\mathrm{HS}}\,\|(1+x^2)(1-\hbar^2\Delta)\mathscr{B}_t\|_{\mathrm{HS}}. \tag{26}$$

We notice that for some $C > 0$ the following bound holds

$$\|(1-\hbar^2\Delta)^{-1}(1+x^2)^{-1}\|_{\mathrm{HS}} \leq C\sqrt{N}$$

where we have used the explicit form of the kernel of the operator $(1-\hbar^2\Delta)^{-1}$ and the fact that $\hbar^3 = N$.

We denote by U_s the convolution of the interaction with the spatial density at time s

$$U_s := V * \widetilde{\rho}_s. \tag{27}$$

We introduce the notation

$$\widetilde{\mathscr{B}} := (1-\hbar^2\Delta)\mathscr{B}_s$$

and observe that the kernel of $\widetilde{\mathscr{B}}$ reads

$$\widetilde{\mathscr{B}}(x;x') := \sum_{j=1}^{7}\widetilde{\mathscr{B}}_j(x;x') \tag{28}$$

where

$$\widetilde{\mathscr{B}}_1(x;x') = N\left[U_t(x)-U_t(x')-\nabla U_t\left(\frac{x+x'}{2}\right)\cdot(x-x')\right]\int\widetilde{W}_{N,t}\left(\frac{x+x'}{2},v\right)e^{iv\cdot\frac{(x-x')}{\hbar}}dv$$

$$\widetilde{\mathscr{B}}_2(x;x')$$

$$= -N\hbar^2\left[\Delta U_t(x)-\frac{1}{4}\Delta\nabla U_t\left(\frac{x+x'}{2}\right)\cdot(x-x')-\frac{1}{2}\Delta U_t\left(\frac{x+x'}{2}\right)\right]\int\widetilde{W}_{N,t}\left(\frac{x+x'}{2},v\right)e^{iv\cdot\frac{(x-x')}{\varepsilon}}dv$$

$$\widetilde{\mathscr{B}}_3(x;x')$$

$$= -\frac{N\hbar^2}{4}\left[U_t(x)-U_t(x')-\nabla U_t\left(\frac{x+x'}{2}\right)\cdot(x-x')\right]\int(\Delta_1\widetilde{W}_{N,t})\left(\frac{x+x'}{2},v\right)e^{iv\cdot\frac{(x-x')}{\hbar}}dv$$

$$\widetilde{\mathscr{B}}_4(x;x') = N\left[U_t(x) - U_t(x') - \nabla U_t\left(\frac{x+x'}{2}\right)\cdot(x-x')\right]\int \widetilde{W}_{N,t}\left(\frac{x+x'}{2},v\right)v^2 e^{i\,v\cdot\frac{(x-x')}{\hbar}}dv$$

$$\widetilde{\mathscr{B}}_5\,(x;x')$$

$$= -\frac{N\hbar^2}{2}\left[\nabla U_t(x) - \frac{1}{2}\nabla^2 U_t\left(\frac{x+x'}{2}\right)(x-x') - \nabla U_t\left(\frac{x+x'}{2}\right)\right]\int (\nabla_1 \widetilde{W}_{N,t})\left(\frac{x+x'}{2},v\right)e^{i\,v\cdot\frac{(x-x')}{\hbar}}dv$$

$$\widetilde{\mathscr{B}}_6(x;x')$$

$$= -N\hbar\left[\nabla U_t(x) - \frac{1}{2}\nabla^2 U_t\left(\frac{x+x'}{2}\right)(x-x') - \nabla U_t\left(\frac{x+x'}{2}\right)\right]\int \widetilde{W}_{N,t}\left(\frac{x+x'}{2},v\right)v e^{i\,v\cdot\frac{(x-x')}{\hbar}}dv$$

$$\widetilde{\mathscr{B}}_7(x;x') = -N\hbar\left[U_t(x) - U_t(x') - \nabla U_t\left(\frac{x+x'}{2}\right)\cdot(x-x')\right]\int (v\cdot\nabla_1 \widetilde{W}_{N,t})\left(\frac{x+x'}{2},v\right)e^{i\,v\cdot\frac{(x-x')}{\hbar}}dv$$

where we used the notation ∇_1 and Δ_1 to indicate derivatives with respect to the first variable.

In order to gain extra powers of $\hbar$, we write

$$\begin{aligned}
&U_t(x) - U_t(x') - \nabla U_t\left(\frac{x+x'}{2}\right)\cdot(x-x') \\
&= \int_0^1 d\lambda\left[\nabla U_t\left(\lambda x + (1-\lambda)x'\right) - \nabla U_t\left(\frac{(x+x')}{2}\right)\right]\cdot(x-x') \\
&= \sum_{i,j=1}^{3}\int_0^1 d\lambda\left(\lambda - \frac{1}{2}\right)\int_0^1 d\mu\;\partial_i\partial_j U_t\left(h(\lambda,\mu,x,x')\right)(x-x')_i(x-x')_j\,,
\end{aligned}$$

where $h(\lambda,\mu,x,x') := \mu(\lambda x + (1-\lambda)x') + (1-\mu)\dfrac{(x+x')}{2}$.

We notice that U_t defined in (27) has a convolution structure. Therefore derivatives of U_t are equivalent to derivatives of the spatial density $\widetilde{\rho}_t$. Hence, Fefferman - De la Llave representation formula (19) leads to

$$\begin{aligned}
&U_s(x) - U_s(x') - \nabla U_s\left(\frac{x+x'}{2}\right)\cdot(x-x') \\
&\quad= \sum_{i,j=1}^{3}\int_0^1 d\lambda\left(\lambda - \frac{1}{2}\right)\int_0^1 d\mu \\
&\qquad\int_0^\infty r^3 g(r)\int dy\;\chi_{(r,y)}\left(h(\lambda,\mu,x,x')\right)\partial_i\partial_j\widetilde{\rho}_s(y)\,(x-x')_i(x-x')_j\,.
\end{aligned} \tag{29}$$

Plugging (29) into the definition of $\widetilde{\mathscr{B}}_1$ and using twice the identity

$$(x-x')\int \widetilde{W}_{N,t}\left(\frac{x+x'}{2},v\right)e^{iv\cdot\frac{x-x'}{\hbar}}dv = -i\hbar\int \nabla_v \widetilde{W}_{N,t}\left(\frac{x+x'}{2},v\right)dv \tag{30}$$

and Young's inequality, we get

$$
\begin{aligned}
&|\widetilde{\mathscr{B}}_1(x;x')| \\
&\leq C\,N\,\hbar^2 \sum_{i,j=1}^{3} \int_0^1 d\lambda \left|\lambda - \frac{1}{2}\right| \int_0^1 d\mu \left| \int_0^\infty r^3 g(r) \right. \\
&\left. \int dy\, \chi_{(r,y)}(h(\lambda,\mu,x,x'))\partial^2_{i,j}\widetilde{\rho}_s(y) \int dv\, \partial^2_{v_i,v_j} \widetilde{W}_{N,s}\left(\frac{x+x'}{2}, v\right) e^{iv\cdot\frac{(x-x')}{\hbar}} \right|.
\end{aligned}
$$

Therefore, the Hilbert-Schmidt norm of the operator $(1+x^2)\widetilde{\mathscr{B}}_1$, where $(1+x^2)$ is the multiplication operator, can be estimated as follows:

$$
\begin{aligned}
&\|(1+x^2)\widetilde{\mathscr{B}}_1\|^2_{\mathrm{HS}} \\
&\quad = N\hbar^4 \int dq \int dp' \left[1+q^2+\hbar^2 p^2\right]^2 \left| \sum_{i,j=1}^{3} \int_0^1 d\lambda \left(\lambda - \frac{1}{2}\right) \int_0^1 d\mu \int_0^\infty r^3 g(r) \right. \\
&\quad \left. \int dy\, \chi_{(r,y)}(q+\hbar\mu(\lambda-1/2)p)\partial^2_{v_i,v_j}\widetilde{\rho}_s(y) \int dv\, \partial^2_{v_i,v_j} \widetilde{W}_{N,s}\,(q,v)\, e^{iv\cdot p} \right|^2
\end{aligned}
$$

where we performed the change of variables

$$
q = \frac{x+x'}{2}, \qquad p = \frac{x-x'}{\hbar} \tag{31}
$$

with Jacobian $J = 8\,\hbar^3 = 8\,N^{-1}$.

We fix $k > 0$ and divide the integral into the two sets $\mathcal{A}_< := \{r \in \mathbb{R}_+ \mid r \leq k\}$ and $\mathcal{A}_> := \{r \in \mathbb{R}_+ \mid r > k\}$, so that

$$
\begin{aligned}
&\|(1+x^2)\widetilde{\mathscr{B}}_1\|^2_{\mathrm{HS}} \\
&\leq CN\hbar^4 \int dq \int dp [1+q^2+\hbar^2 p^2]^2 \sum_{i,j=1}^{3} \int_0^1 d\lambda \left|\lambda - \frac{1}{2}\right| \int_0^1 d\mu \\
&\quad \left| \int_{\mathcal{A}_<} r^3 g(r) \int dy\, \chi_{(r,y)}(q+\hbar\mu(\lambda-1/2)p)\partial^2_{v_i,v_j}\widetilde{\rho}_s(y) \int dv\, \partial^2_{v_i,v_j} \widetilde{W}_{N,s}\,(q,v)\, e^{iv\cdot p} \right|^2 \\
&+ CN\hbar^4 \int dq \int dp [1+q^2+\hbar^2 p^2]^2 \sum_{i,j=1}^{3} \int_0^1 d\lambda \left|\lambda - \frac{1}{2}\right| \int_0^1 d\mu \\
&\quad \left| \int_{\mathcal{A}_>} r^3 g(r) \int dy\, \chi_{(r,y)}(q+\hbar\mu(\lambda-1/2)p)\partial^2_{v_i,v_j}\widetilde{\rho}_s(y) \int dv\, \partial^2_{v_i,v_j} \widetilde{W}_{N,s}\,(q,v)\, e^{iv\cdot p} \right|^2 .
\end{aligned} \tag{32}
$$

Denote by $\mathfrak{A}_<$ and $\mathfrak{A}_>$ the first and the second term of the sum on the r.h.s. of (32) respectively. For $\mathfrak{A}_<$ we use Young inequality and Hölder inequality with conjugated exponents $\theta = 1$ and $\theta' = \infty$, then we perform the integral in the y variable to extract r^3 which cancels the singularity at zero in the expression for $g(r)$ (Cf. (17)) together with assumption c) on V, thus leading to the bound

$$\mathfrak{A}_< \leq CN\hbar^4 \int dq \int dv (1+q^2)^2 |\nabla_v^2 \widetilde{W}_{N,s}(q,v)|^2 + CN\hbar^8 \int dq \int dv \, |\nabla_v^4 \widetilde{W}_{N,s}(q,v)|^2 \tag{33}$$

where C depends on $\|\nabla^2 \widetilde{\rho}_s\|_{L^\infty}$.

For $\mathfrak{A}_>$, we integrate by parts twice in the y variable and recall that $e^{-|z-y|^2/r^2}(1 + |z-y|^2/r^2)$ is bounded uniformly in $z \in \mathbb{R}^3$. Since $\widetilde{\rho}_s \in L^1(\mathbb{R}^3)$ we get the bound

$$\mathfrak{A}_> \leq CN\hbar^4 \int dq \int dv (1+q^2)^2 |\nabla_v^2 \widetilde{W}_{N,s}(q,v)|^2 + CN\hbar^8 \int dq \int dv \, |\nabla_v^4 \widetilde{W}_{N,s}(q,v)|^2 \tag{34}$$

where C depends on $\|\widetilde{\rho}_s\|_{L^1}$ and we have used the expression (17) for $g(r)$ and assumption b) for V.

Whence, the estimates (33) and (34) lead to

$$\|(1+x^2)\widetilde{\mathscr{B}}_1\|_{\mathrm{HS}} \leq C\sqrt{N}\hbar^2 \|\widetilde{W}_{N,s}\|_{H^2_2} + C\sqrt{N}\hbar^4 \|\widetilde{W}_{N,s}\|_{H^4} \tag{35}$$

where $C = C(\|\widetilde{\rho}_s\|_{L^1}, \|\nabla^2 \widetilde{\rho}_s\|_{L^\infty})$.

The Hilbert-Schmidt norms $\|(1+x^2)\widetilde{\mathscr{B}}_3\|_{\mathrm{HS}}$, $\|(1+x^2)\widetilde{\mathscr{B}}_4\|_{\mathrm{HS}}$ and $\|(1+x^2)\widetilde{\mathscr{B}}_7\|_{\mathrm{HS}}$ can be handled analogously, thus obtaining

$$\|(1+x^2)\widetilde{\mathscr{B}}_3\|_{\mathrm{HS}} \leq C\sqrt{N}\hbar^4 \|\widetilde{W}_{N,s}\|_{H^4_4} + C\sqrt{N}\hbar^6 \|\widetilde{W}_{N,s}\|_{H^6_4} \tag{36}$$

$$\|(1+x^2)\widetilde{\mathscr{B}}_4\|_{\mathrm{HS}} \leq C\sqrt{N}\hbar^2 \|\widetilde{W}_{N,s}\|_{H^2_4} + C\sqrt{N}\hbar^4 \|\widetilde{W}_{N,s}\|_{H^4_4} \tag{37}$$

$$\|(1+x^2)\widetilde{\mathscr{B}}_7\|_{\mathrm{HS}} \leq C\sqrt{N}\hbar^3 \|\widetilde{W}_{N,s}\|_{H^2_3} + C\sqrt{N}\hbar^5 \|\widetilde{W}_{N,s}\|_{H^5_2} \tag{38}$$

To bound the $\widetilde{\mathscr{B}}_i$ terms, $i = 2, 5, 6$, in which higher order derivatives of U appear, we proceed as for $\widetilde{\mathscr{B}}_1$ and obtain the following bounds:

$$\|(1+x^2)\widetilde{\mathscr{B}}_2\|_{\mathrm{HS}} \leq C\sqrt{N}\hbar^4 \|\widetilde{W}_{N,s}\|_{H^2_2} + C\sqrt{N}\hbar^6 \|\widetilde{W}_{N,s}\|_{H^4} \tag{39}$$

$$\|(1+x^2)\widetilde{\mathscr{B}}_5\|_{\mathrm{HS}} \leq C\sqrt{N}\hbar^4 \|\widetilde{W}_{N,s}\|_{H^4_2} + C\sqrt{N}\hbar^6 \|\widetilde{W}_{N,s}\|_{H^6} \tag{40}$$

$$\|(1+x^2)\widetilde{\mathscr{B}}_6\|_{\mathrm{HS}} \leq C\sqrt{N}\hbar^3 \|\widetilde{W}_{N,s}\|_{H^2_2} + C\sqrt{N}\hbar^5 \|\widetilde{W}_{N,s}\|_{H^4} \tag{41}$$

where $C = C(\|\widetilde{\rho}_s\|_{L^1}, \|\nabla^2 \widetilde{\rho}_s\|_{L^\infty})$. We refer to [46] for a detailed proof.

Gathering together all the terms, we get

$$\begin{aligned} &\|(1+x^2)\widetilde{\mathscr{B}}\|_{\mathrm{HS}} \\ &\leq C\sqrt{N}\left[\hbar^2 \|\widetilde{W}_{N,s}\|_{H^2_4} + \hbar^3 \|\widetilde{W}_{N,s}\|_{H^3_4} + \hbar^4 \|\widetilde{W}_{N,s}\|_{H^4_4} + \hbar^5 \|\widetilde{W}_{N,s}\|_{H^5_4} + \hbar^6 \|\widetilde{W}_{N,s}\|_{H^6_4}\right]. \end{aligned} \tag{42}$$

3 Proof of Theorem 1

From Lemma 1 we have

$$\mathrm{tr}\,|\omega_{N,t}-\widetilde{\omega}_{N,t}| \leq \frac{1}{\hbar}\int_0^t \mathrm{tr}\,|[V*(\rho_s-\widetilde{\rho}_s),\widetilde{\omega}_{N,s}]|\,ds+\frac{1}{\hbar}\int_0^t \mathrm{tr}\,|B_s|\,ds\,. \tag{43}$$

From Propositions 1 and 3, we get the following estimate on the terms on the r.h.s. of Eq. (43):

$$\mathrm{tr}\,|\omega_{N,t}-\widetilde{\omega}_{N,t}| \leq C\int_0^t \mathrm{tr}\,|\omega_{N,s}-\widetilde{\omega}_{N,s}|\,ds+CN\hbar\int_0^t\left(1+\sum_{k=1}^4\|\widetilde{W}_{N,s}\|_{H_4^{k+2}}\right)ds\,. \tag{44}$$

We further observe that the quantity $\|\widetilde{W}_{N,s}\|_{H_4^{k+2}}$ is bounded uniformly in N if $\|W_N\|_{H_4^{k+2}} \leq C$ for $k=1,\dots,4$. These regularity estimates can be obtained by simply adapting the proof of Lions and Perthame (cf. [35]). The details can be found in [45].

Whence, by Grönwall lemma we have

$$\mathrm{tr}\,|\omega_{N,t}-\widetilde{\omega}_{N,t}| \leq CN\hbar\left(1+\sum_{k=1}^4\|W_N\|_{H_4^{k+2}}\right),$$

where $C=C(t,\|\widetilde{\rho}\|_{L^1},\|\nabla^2\widetilde{\rho}_s\|_{L^\infty})$. The boundedness of $\|\nabla^2\widetilde{\rho}_s\|_{L^\infty}$ follows from an adaptation of [35] (cf. [45] for the details of the proof).

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References

1. L. Amour, M. Khodja, J. Nourrigat, The semiclassical limit of the time dependent Hartree-Fock equation: the Weyl symbol of the solution. Anal. PDE **6**(7), 1649–1674 (2013)
2. L. Amour, M. Khodja, J. Nourrigat, The classical limit of the Heisenberg and time dependent Hartree-Fock equations: the Wick symbol of the solution. Math. Res. Lett. **20**(1), 119–139 (2013)
3. A. Athanassoulis, T. Paul, F. Pezzotti, M. Pulvirenti, Strong semiclassical approximation of Wigner functions for the Hartree dynamics. Rend. Lincei Mat. Appl. **22**, 525–552 (2011)
4. C. Bardos, P. Degond, Global existence for the Vlasov-Poisson equation in 3 space variables with small initial data. Ann. Inst. H. Poincaré Anal. Non Linéaire **2**, 101–118 (1985)
5. V. Bach, S. Breteaux, S. Petrat, P. Pickl, T. Tzaneteas, Kinetic energy estimates for the accuracy of the time-dependent Hartree-Fock approximation with Coulomb interaction. J. Math. Pures Appl. **105**(1), 1–30 (2016)
6. C. Bardos, F. Golse, A.D. Gottlieb, N.J. Mauser, Mean field dynamics of fermions and the time-dependent Hartree-Fock equation. J. Math. Pures Appl. **82**(6), 665–683 (2003)

7. C. Bardos, F. Golse, A.D. Gottlieb, N.J. Mauser, Accuracy of the time-dependent Hartree-Fock approximation for uncorrelated initial states. J. Stat. Phys. **115**, 1037–1055 (2004)
8. C. Bardos, B. Ducomet, F. Golse, A. Gottlieb, N. Mauser, The TDHF approximation for Hamiltonians with m-particle interaction potentials. Commun. Math. Sci. suppl. 1, 1–9 (2007)
9. N. Benedikter, V. Jaksic, M. Porta, C. Saffirio, B. Schlein, Mean-field evolution of fermionic mixed states. Commun. Pure Appl. Math. **69**, 2250–2303 (2016)
10. N. Benedikter, M. Porta, C. Saffirio, B. Schlein, From the Hartree-Fock dynamics to the Vlasov equation. Arch. Ration. Mech. Anal. **221**(1), 273–334 (2016)
11. N. Benedikter, M. Porta, B. Schlein, Mean-field evolution of fermionic systems. Commun. Math. Phys. **331**, 1087–1131 (2014)
12. N. Benedikter, M. Porta, B. Schlein, Effective evolution equations from quantum mechanics. Springer Briefs in Mathematical Physics, vol. 7 (2016)
13. N. Benedikter, M. Porta, B. Schlein, Mean-field dynamics of fermions with relativistic dispersion. J. Math. Phys. **55**(2) (2014)
14. L. Chen, J. Lee, M. Liew, Combined mean-field and semiclassical limits of large fermionic systems (2019). ArXiv:1910.09892v2
15. R.L. Dobrushin, Vlasov equations. Funct. Anal. Appl. **13**(2), 115–123 (1979)
16. A. Elgart, L. Erdős, B. Schlein, H.-T. Yau, Nonlinear Hartree equation as the mean field limit of weakly coupled fermions. J. Math. Pures Appl. (9) **83**(10), 1241–1273 (2004)
17. C.L. Fefferman, R. de la Llave, Relativistic stability of matter-I. Rev. Mat. Iberoam. **2**(2), 119–213 (1986)
18. A. Figalli, M. Ligabò, T. Paul, Semiclassical limit for mixed states with singular and rough potentials. Indiana Univ. Math. J. **61**(1), 193–222 (2012)
19. S. Fournais, M. Lewin, J.P. Solovej, The semi-classical limit of large fermionic systems. Calc. Var. Partial Differ. Equ. **57–105**, 1–42 (2018)
20. J. Fröhlich, A. Knowles, A microscopic derivation of the time-dependent Hartree-Fock equation with Coulomb two-body interaction. J. Stat. Phys. **145**(1), 23–50 (2011)
21. I. Gasser, R. Illner, P.A. Markowich, C. Schmeiser, Semiclassical, $t \to \infty$ asymptotics and dispersive effects for HF systems. Math. Modell. Numer. Anal. **32**, 699–713 (1998)
22. F. Golse, C. Mouhot, T. Paul, On the mean field and classical limits of quantum mechanics. Commun. Math. Phys. **343**, 165–205 (2016)
23. F. Golse, T. Paul, The Schrödinger equation in the mean-field and semiclassical regime. Arch. Rational Mech. Anal. **223**, 57–94 (2017)
24. F. Golse, T. Paul, Empirical measures and quantum mechanics: applications to the mean-field limit. Commun. Math. Phys. (2019). https://doi.org/10.1007/s00220-019-03357-z
25. F. Golse, T. Paul, M. Pulvirenti, On the derivation of the Hartree equation in the mean field limit: uniformity in the Planck constant. To appear in J. Funct. Anal. arXiv:1606.06436
26. S. Graffi, A. Martinez, M. Pulvirenti, Mean-field approximation of quantum systems and classical limit. Math. Models Methods Appl. Sci. **13**(1), 59–73 (2003)
27. C. Hainzl, R. Seiringer, General decomposition of radial functions on ^{n} and applications to $\mathbb{R}N$-body quantum systems. Lett. Math. Phys. **61**(1), 75–84 (2002)
28. S.V. Iordanskii, The Cauchy problem for the kinetic equation of plasma. Trudy Mat. Inst. Steklov **60**, 181–194 (1961)
29. L. Laflèche, Propagation of moments and semiclassical limit from Hartree to Vlasov equation. J. Stat. Phys. **177**(1), 20–60 (2019)
30. L. Laflèche, Global semiclassical limit from Hartree to Vlasov equation for concentrated initial data (2019). ArXiv:1902.08520
31. M. Lewin, P.S. Madsen, A. Triay, Semi-classical limit of large fermionic systems at positive temperature (2019). ArXiv:1902.00310
32. E.H. Lieb, Thomas-Fermi and related theories of atoms and molecules. Rev. Mod. Phys. **53**(4), 603–641 (1981)
33. E.H. Lieb, B. Simon, The Thomas-Fermi theory of atoms, molecules and solids. Adv. Math. **23**, 22–116 (1977)
34. P.-L. Lions, T. Paul, Sur les mesures de Wigner. Rev. Mat. Iberoamericana **9**, 553–618 (1993)

35. P.-L. Lions, B. Perthame, Propagation of moments and regularity for the 3-dimensional Vlasov-Poisson system. Invent. Math. **105**, 415–430 (1991)
36. P.A. Markowich, N.J. Mauser, The classical limit of a self-consistent quantum Vlasov equation. Math. Models Methods Appl. Sci. **3**(1), 109–124 (1993)
37. H. Narnhofer, G.L. Sewell, Vlasov hydrodynamics of a quantum mechanical model. Commun. Math. Phys. **79**(1), 9–24 (1981)
38. S. Okabe, T. Ukai, On classical solutions in the large in time of the two-dimensional Vlasov equation. Osaka J. Math. **15**, 245–261 (1978)
39. S. Petrat, Hartree corrections in a mean-field limit for fermions with Coulomb interaction. J. Phys. A **50**(24), 244004 (2017)
40. S. Petrat, P. Pickl, A new method and a new scaling for deriving fermionic mean-field dynamics.Math. Phys. Anal. Geom. **19**, 3 (2016)
41. F. Pezzotti, M. Pulvirenti, Mean-field limit and semiclassical expansion of a quantum particle system. Ann. H. Poincaré **10**(1), 145–187 (2009)
42. K. Pfaffelmoser, Global existence of the Vlasov-Poisson system in three dimensions for general initial data. J. Differ. Equ. **95**, 281–303 (1992)
43. M. Porta, S. Rademacher, C. Saffirio, B. Schlein, Mean field evolution of fermions with Coulomb interaction. J. Stat. Phys. **166**, 1345–1364 (2017)
44. C. Saffirio, Mean-field evolution of fermions with singular interaction. Springer Proc. Math. Stat. **270**, 81–99 (2018)
45. C. Saffirio, Semiclassical limit to the Vlasov equation with inverse power law potentials. Commun. Math. Phys. https://doi.org/10.1007/s00220-019-03397-5
46. C. Saffirio, From the Hartree equation to the Vlasov-Poisson system: strong convergence for a class of mixed states. ArXiv:1903.06013
47. H. Spohn, On the Vlasov hierarchy. Math. Methods Appl. Sci. **3**(4), 445–455 (1981)

From the Boltzmann Description for Mixtures to the Maxwell–Stefan Diffusion Equations

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Abstract This article reviews some recent results on the diffusion limit of the Boltzmann system for gaseous mixtures to the Maxwell–Stefan diffusion equations.

Keywords Boltzmann system · Maxwell–Stefan equations · Cross-diffusion

1 Introduction

The Maxwell-Stefan system [25, 29] has been derived in the 19th century for describing the diffusion behaviour of multicolored gaseous mixtures. These equations are very popular in the context of chemical engineering [30] and have been extensively studied in the 20th century from the numerical point of view [17, 18]. Starting from [10, 12], a renewed interest in the Maxwell–Stefan equations arose in the mathematical community and several colleagues have worked for better understanding the mathematical properties of these equations.

The goal of this article is to review the recent literature devoted to a specific topic: the Maxwell–Stefan limit of kinetic equations for gaseous mixtures.

The starting point, in the case of non-reacting mixtures, is the standard extension of the Boltzmann equation [5], derived by Ludwig Boltzmann in 1872. However, many other variants of this model exist: we quote, for example, [26, 28], which provide two very popular examples of kinetic equations for gaseous mixtures. In the reactive case, the situation is similar. Several models have been proposed (for example, [21]), but the Maxwell-Stefan asymptotics has been mainly studied starting from the models proposed and studied in [16] and in [24].

The structure of the article is the following. We first introduce the Maxwell–Stefan equations and two of the main kinetic models for non-reactive and reactive mixtures. Then, we consider the diffusive limit of the non-reactive system to the

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Maxwell–Stefan equations at the formal level. The scaling has been introduced in [13], and subsequently developed in [11, 23]. After describing these formal results, we summarize the result by Bondesan and Briant [8], which provides a rigorous description of the limiting procedure. The next chapter is devoted to the reactive case, and is essentially based on the recent articles [2–4]. We conclude this review by quoting the most recent literature on some strictly related subjects.

2 The Maxwell–Stefan Equations

The classical Maxwell–Stefan system describes the diffusive behaviour of an ideal gaseous mixture, composed by $\mathscr{I} \in \mathbb{N}^*$ species. Let $\Omega \subset \mathbb{R}^3$ be a bounded domain with regular boundary. The unknowns of the problem are the $\mathscr{I}$ densities $c_i : \mathbb{R}^+ \times \Omega \to \mathbb{R}$ and the $\mathscr{I}$ fluxes $J_i : \mathbb{R}^+ \times \Omega \to \mathbb{R}^3$, which obey to the following cross-diffusion relationships:

$$\begin{cases} \partial_t c_i + \nabla_x \cdot J_i = 0, & (t,x) \in \mathbb{R}^+ \times \Omega \\ \nabla_x c_i = -\displaystyle\sum_{j \neq i} k_{ij}(c_j J_i - c_i J_j). \end{cases} \tag{1}$$

Here we use a notation which is more adapted from the mathematical point of view with respect to the traditional notation used in the applications: $k_{ij} = 1/Đ_{ij}$, where the constants $Đ_{ij}$ are suitable symmetric binary diffusion coefficients (i.e. $Đ_{ij} = Đ_{ji}$ for all $i, j = 1, \ldots, \mathscr{I}$) .

Because of the symmetry of the whole set of binary diffusion coefficients, it is immediate to see that the flux-gradient relationships in (1) are linearly dependent. For this reason, an additional constitutive equation has to be added to (1) in order to have a closed set of equations. The usual assumption – which guarantees the diffusive behaviour of the mixture – is the *equimolar diffusion condition*

$$\sum_{i=1}^{\mathscr{I}} J_i = 0. \tag{2}$$

Usually, the system of PDEs (1) is supplemented with appropriate initial and boundary conditions. When dealing with isolated systems, it is standard to suppose that the solution of (1)–(2) satisfies homogeneous Neumann boundary conditions:

$$c_i(0,x) = c_i^{\text{in}}(x) \in L^\infty(\Omega), \qquad J_i(t,x) \cdot n_x|_{(t,x)\in(0,\infty)\times\partial\Omega} = 0 \tag{3}$$

for all $i = 1, \ldots, \mathscr{I}$, where $n_x \in \mathbb{S}^2$ is the outward normal unit vector to the domain Ω starting from a given point $x \in \partial\Omega$. The Maxwell–Stefan system (1)–(2) is often written in terms of molar fraction. In this case, it is supposed that $c_i^{\text{in}} \geq 0$ and that

$$\sum_{i=1}^{\mathscr{I}} c_i^{\text{in}}(x) = 1.$$

This normalization property is conserved by the time evolution of the system. It means that

$$\sum_{i=1}^{\mathscr{I}} c_i(t,x) = 1 \text{ for a.e. } (t,x) \in \mathbb{R}^+ \times \Omega. \tag{4}$$

3 The Boltzmann System for Monatomic Inert Gaseous Mixtures

The Boltzmann system for a mixture of ideal monatomic non-reacting gases $\mathscr{A}_i$, $i = 1, \ldots, \mathscr{I}$ with $\mathscr{I} \geq 2$, subject to elastic mechanical collisions, describes the time evolution of the species by means of $\mathscr{I}$ distribution functions f_i, defined on the phase space of the system. The particles of each species are identical and can be modelled as point masses. Their main physical quantities are therefore the mass $m_i \in \mathbb{R}^+$ and the velocity $v \in \mathbb{R}^3$. The standard assumption on the density function is of L^1-type, i.e. $f_i(t,\cdot,\cdot) \in L^1_{\text{loc}}(\mathbb{R}^3_x; L^1(\mathbb{R}^3))$, for all $t \in \mathbb{R}^+$. This requirement guarantees that the system has finite mass. In what follows, we assume that the system is isolated, so that no external force acts on the particles. Moreover, we suppose that only elastic binary collisions are allowed. Therefore, momentum and kinetic energy are conserved during the interaction process. Under the previous hypotheses, the time evolution of the distribution functions f_i is governed by the Cauchy problem

$$\partial_t f_i + v \cdot \nabla_x f_i = \sum_{j=1}^{\mathscr{I}} Q_{ij}(f_i, f_j) \qquad \text{for } (t,x,v) \in (0,\infty) \times \mathbb{R}^3 \times \mathbb{R}^3 \tag{5}$$

$$f_i(0,x,v) = f_i^{\text{in}}(x,v) \qquad \text{for } (x,v) \in \mathbb{R}^3 \times \mathbb{R}^3 \tag{6}$$

for each $i = 1, \ldots, \mathscr{I}$, where $Q_{ij}(\cdot,\cdot)$ denotes the bilinear integral operator describing the collisions of molecules of species $\mathscr{A}_i$ with molecules of species $\mathscr{A}_j$.

A given particle follows a rectilinear trajectory, until it collides with another particle. When two particles belonging to the species $\mathscr{A}_i$ and $\mathscr{A}_j$, with masses m_i, m_j, and pre-collisional velocities v', v'_* collide, they exchange kinetic energy and momentum. A microscopic collision is a local in space and instantaneous in time phenomenon. It modifies the velocities of the particles, which become v and v_*, under the constraint of conserving the total kinetic energy and the total momentum:

$$m_i v' + m_j v'_* = m_i v + m_j v_*, \qquad \frac{1}{2} m_i |v'|^2 + \frac{1}{2} m_j |v'_*|^2 = \frac{1}{2} m_i |v|^2 + \frac{1}{2} m_j |v_*|^2. \tag{7}$$

The previous equations can be easily inverted:

$$v' = \frac{1}{m_i + m_j}(m_i v + m_j v_* + m_j |v - v_*| \sigma), \quad v'_* = \frac{1}{m_i + m_j}(m_i v + m_j v_* - m_i |v - v_*| \sigma), \tag{8}$$

where $\sigma \in \mathbb{S}^2$ is a unit vector which allows to keep into account the two degrees of freedom arising in inverting (7).

If f_i and f_j are two nonnegative functions, the operator describing the collisions between molecules of species $\mathscr{A}_i$ and molecules of species $\mathscr{A}_j$ is defined by

$$Q_{ij}(f_i, f_j)(v) := \iint\limits_{\mathbb{R}^3 \times \mathbb{S}^2} B_{ij}(v, v_*, \sigma)\Big[f_i(v') f_j(v'_*) - f_i(v) f_j(v_*)\Big] \mathrm{d}\sigma \, \mathrm{d}v_*. \tag{9}$$

The expressions of v' and v'_*, are given by (8).

The quantities B_{ij} $(i, j = 1, \ldots, \mathscr{I})$ are usually called *cross sections*. They satisfy the Galilean invariance and the *microreversibility assumptions*

$$B_{ij}(v, v_*, \sigma) = B_{ji}(v_*, v, \sigma) = B_{ij}(v', v'_*, \sigma).$$

Because of the Galilean invariance, it is possible to prove that the collision kernels B_{ij} only depend on the modulus of the relative velocity and on the cosine of the deviation angle:

$$B_{ij}(v, v_*, \sigma) = B_{ij}\,(|v - v_*|, \cos\theta) \quad \text{with} \quad \cos\theta = \frac{v - v_*}{|v - v_*|} \cdot \sigma.$$

The choice of the collision kernels B_{ij} has a deep influence on the properties of the Boltzmann equation. In the classical elastic case,

$$B_{ij}(\sigma, v - v_*) = K_{ij}\,|v - v_*|, \qquad K_{ij} > 0, \tag{10}$$

for a gas of three-dimensional hard spheres. This type of cross section is called *hard-sphere cross section*. When the binary forces between particles are proportional to the inverse of the s-th power of the relative distance (for example, $s = 2$ corresponds to the gravitational force or to the Coulomb force and $s = 7$ corresponds to the Van der Waals interaction, see [31] for more details), B_{ij} can be factorized:

$$B_{ij}(\sigma, v - v_*) = \Phi_{ij}(|v - v_*|) b_{ij}(\cos\theta).$$

In particular, in three space dimensions,

$$\Phi_{ij}(|v - v_*|) = |v - v_*|^\gamma, \quad \gamma = (s - 5)/(s - 1),$$

and all the b_{ij} are locally smooth functions with a non integrable singularity when $\theta \to 0$:

$$b_{ij}(\cos\theta) \sin\theta \sim K_{ij} \theta^{-(1+\eta)}, \quad \eta = 2/(s - 1).$$

The quantities Φ_{ij} are known in the literature as the *kinetic collision kernels*, and the terms b_{ij} are the *angular collision kernels*. The family of collision kernels whose kinetic term has the form $\Phi_{ij}(|v - v_*|) = |v - v_*|^\gamma$ is usually classified in the literature in three sub-classes: hard potentials, when $\gamma > 0$, soft potentials, when $\gamma < 0$, and Maxwellian potentials when $\gamma = 0$.

For simplifying the mathematical treatment of the angular cross section, Grad introduced an *angular cut-off assumption*, by supposing that angular collision kernel is integrable with respect to the angular variable [19, 20].

The link between the macroscopic description and the kinetic formulation is given by the moments of the distribution functions $f_i(t, x, v)$. In particular, the number densities c_i, mass densities ρ_i, mean velocities u_i and kinetic temperatures T_i of each species are respectively given by

$$c_i(t, x) = \int_{\mathbb{R}^3} f_i(t, x, v)\, \mathrm{d}v, \tag{11}$$

$$\rho_i(t, x) = m_i n_i(t, x), \tag{12}$$

$$u_i(t, x) = \frac{1}{c_i(t, x)} \int_{\mathbb{R}^3} v f_i(t, x, v) \mathrm{d}v, \tag{13}$$

$$T_i(t, x) = \frac{1}{3k_B c_i(t, x)} \int_{\mathbb{R}^3} m_i |v - u_i(t, x)|^2 f_i(t, x, v) \mathrm{d}v, \tag{14}$$

where $k_B = 1.380649 \times 10^{-23}$ m^2 kg s^{-2} K^{-1} is the Boltzmann constant.

It is important to underline that the Boltzmann constant has an exact value. It is indeed one of the seven *defining constants* in the 2019 redefinition of SI base units. In particular, the value of the Boltzmann constant k_B allows to define the unit of temperature T (the kelvin), in terms of the SI unit of energy (the joule), because it is the proportionality constant between the thermodynamic temperature and the average thermal energy of a gas. Unfortunately, the numerical value of the Boltzmann constant has not been, in the mathematical community, the focus of attention and often, for simplifying the computations, many articles and books simply suppose that $k_B = 1$. In the author's opinion, however, this attitude should change because of the central meaning of the Boltzmann constant as defining constant of the SI base units, and therefore k_B should explicitly appear in all the computations. This approach would allow moreover an easier transfer of the mathematical studies in kinetic theory to other scientific communities.

A central role in the study of kinetic equations and systems is played by local and global Maxwellians (i.e. Gaussians in the language of kinetic theory).

In three space dimensions, *Local Maxwellians* have the form

$$M(c_i^*, u_i^*, T_i^*) = c_i^*(t, x) \left(\frac{m_i}{2\pi k_B T_i^*(t, x)} \right)^{3/2} e^{-m_i \frac{|v - u_i^*(t,x)|^2}{2k_B T_i^*(t,x)}}, \tag{15}$$

for some space-time dependent functions c_i^*, u_i^* and T_i^* $(1 \leq i \leq \mathscr{I})$. *Global Maxwellians* have the same structure as local Maxwellians, but the quantities c_i^*, u_i^* and T_i^* are constant in space and time. It is clear that

$$c_i(t,x) = \int_{\mathbb{R}^3} M(c_i, u_i, T_i)\,\mathrm{d}v,$$

$$u_i(t,x) = \frac{1}{c_i(t,x)} \int_{\mathbb{R}^3} vM(c_i, u_i, T_i)\mathrm{d}v,$$

$$T_i(t,x) = \frac{1}{3k_B c_i(t,x)} \int_{\mathbb{R}^3} m_i|v - u_i(t,x)|^2 M(c_i, u_i, T_i)\mathrm{d}v,$$

in agreement with Eqs. (11)–(14).

It is possible to prove that, in the mono-species case, a local Maxwellian is a local equilibrium of the system for any choice of velocity and temperature. However, when the mixture is composed of more than one species, the local Maxwellian state is still an equilibrium for the whole system only when the velocities and the kinetic temperatures of the species composing the mixture are exactly the same.

4 The Boltzmann System for Polyatomic Reactive or Non-reactive Gas Mixtures

The model described in the previous section is designed for mixtures of monatomic gases. However, when the species which compose the mixture are of polyatomic type, it is not possible to neglect the additional – rotational and vibrational – degrees of freedom induced by the polyatomic structure of the molecules. In this case, not only the kinetic energy, but also the internal energy of the molecules must be taken into account in the energy balance. Moreover, when chemical reactions are allowed, the collisions may modify the species involved in the process: the species of the incoming particles may be different from the species of the outgoing particles. This behaviour needs to be carefully modelled both at the level of the binary encounters and at the level of the time evolution of the density functions.

In this section, we describe the kinetic system proposed in [16], based on the Borgnakke-Larsen procedure [9], which describes a mixture of polyatomic gases, either of reactive or non-reactive type. The model is defined on an enlarged phase-space: the independent variables of the unknowns f_i have the physical meanings of time ($t \in \mathbb{R}^+$), space ($x \in \mathbb{R}^3$), velocity ($v \in \mathbb{R}^3$) and internal energy ($I \in \mathbb{R}^+$).

Note that the internal energy is defined on $\mathbb{R}^+$. This choice allows to "forget" the complicate structure of the discrete energy levels predicted by quantum mechanics, once implemented a strategy for capturing the correct macroscopic behaviour of the mixture. This goal is achieved by introducing a set of suitable measures $\varphi_i(I)\mathrm{d}I$,

which allow to relate, in a simple and computable way, the Boltzmann level with the macroscopic parameters of the corresponding reactive fluid equations and guarantee that the model is consistent at the macroscopic level, with the energy law of virtually any type of polyatomic gas.

Among the various possible dynamics of a chemically reacting mixture, the authors of [16] have chosen to describe a mixture of four species A_1, A_2, A_3 and A_4, which may react in a reversible way through the formula

$$A_1 + A_2 \leftrightharpoons A_3 + A_4\,. \tag{16}$$

For each species A_i, with $i = 1, 2, 3, 4$, the authors introduce the corresponding distribution function $f_i = f_i(t, x, v, I)$, the molecular mass m_i, the chemical binding energy E_i and the weight $\varphi_i(I)$. During a chemical reaction of type (16), the conservation of mass requires that

$$m_1 + m_2 = m_3 + m_4 = M, \tag{17}$$

and the balance of binding energies, i.e.

$$E = E_3 + E_4 - E_1 - E_2, \tag{18}$$

means that the forward reaction $A_1 + A_2 \to A_3 + A_4$ is endothermic when $E > 0$ or exothermic if $E < 0$.

In this description, the moments of the distribution function $f_i(t, x, v, I)$ are defined in $L^1\left(\varphi_i(I)\mathrm{d}I\,\mathrm{d}v\right)$. In particular, the number density c_i, mass density ρ_i, mean velocity u_i and temperature T_i of each species are respectively given by

$$c_i(t,x) = \int_{\mathbb{R}^3}\int_0^{+\infty} f_i(t,x,v,I)\varphi_i(I)\,\mathrm{d}I\,\mathrm{d}v, \quad \rho_i(t,x) = m_i c_i(t,x),$$

$$u_i(t,x) = \frac{1}{c_i(t,x)}\int_{\mathbb{R}^3}\int_0^{+\infty} v\, f_i(t,x,v,I)\varphi_i(I)\,\mathrm{d}I\,\mathrm{d}v,$$

$$T_i(t,x) = \frac{1}{3k_B c_i(t,x)}\int_{\mathbb{R}^3}\int_0^{+\infty} m_i|v - u_i(t,x)|^2 f_i(t,x,v,I)\varphi_i(I)\,\mathrm{d}I\,\mathrm{d}v.$$

The possible collisions – of binary type – between the molecules of the mixtures are either elastic or reactive.

In the case of elastic encounters, the particles involved in the collision modify their velocities and internal energies, but the chemical composition of the particles is unchanged. If we denote the velocities and internal energies of the colliding particles before the collision by v_i, v_j and I_i, I_j respectively, and their corresponding post-collisional values by v_i', v_j' and I_i', I_j', the conservation laws of momentum and total energy for elastic collisions are given by

$$m_i v_i + m_j v_j = m_i v_i' + m_j v_j', \tag{19}$$

$$\frac{1}{2} m_i |v_i|^2 + I_i + \frac{1}{2} m_j |v_j|^2 + I_j = \frac{1}{2} m_i |v_i'|^2 + I_i' + \frac{1}{2} m_j |v_j'|^2 + I_j'. \tag{20}$$

In particular, $i \neq j$ for bi-species collisions and $i = j$ for mono-species collisions.

Reactive collisions occur among particles of species A_1, A_2 or A_3, A_4. In this case, the velocities and the internal energies are modified by the collision and, moreover, the reactants are transformed into the products of the reaction. By following the notation of [2], the rearrangement of mass and the redistribution of chemical binding energy are formalized as follows.

If A_i, A_j and A_k, A_l represent the reactants and products of the chemical reaction, with $(i, j, k, l) \in \{(1, 2, 3, 4), (2, 1, 4, 3)\}$ and $(i, j, k, l) \in \{(3, 4, 1, 2), (4, 3, 2, 1)\}$ for the forward and backward chemical reactions respectively, the conservation laws of momentum and total energy (kinetic energy, internal energies and chemical binding energy) for reactive collisions are given by

$$m_i v_i + m_j v_j = m_k v_k' + m_l v_l', \tag{21}$$

$$\frac{1}{2} m_i |v_i|^2 + I_i + E_i + \frac{1}{2} m_j |v_j|^2 + I_j + E_j = \frac{1}{2} m_k |v_k'|^2 + I_k' + E_k + \frac{1}{2} m_l |v_l'|^2 + I_l' + E_l. \tag{22}$$

Note that Eq. (22) can be written in an equivalent form as

$$\frac{1}{2} m_i |v_i|^2 + I_i + \frac{1}{2} m_j |v_j|^2 + I_j - \frac{E}{2} = \frac{1}{2} m_k |v_k'|^2 + I_k' + \frac{1}{2} m_l |v_l'|^2 + I_l' + \frac{E}{2}$$

where E has been defined in (18).

The post-collisional velocities can be expressed in terms of pre-collisional velocities and the corresponding expressions are derived from the conservation laws for reactive collisions (21), (22) and for non-reactive collisions (19), (20). They are deduced by applying the Borgnakke-Larsen procedure [9], which distributes the total energy of the colliding pair into kinetic and internal energies, when the collisions are non-reactive, or into kinetic, internal and chemical binding energies, when the collisions are reactive.

If we denote with $\mu_{ij} = m_i m_j / (m_i + m_j)$ the reduced mass of the colliding pair and introduce the two Borgnakke-Larsen parameters $R,\ r \in [0, 1]$, we have, in the case of non-reactive elastic collisions,

$$v_i' = \frac{m_i v_i + m_j v_j}{m_i + m_j} + \frac{m_j}{m_i + m_j} \sqrt{\frac{2R\mathscr{E}}{\mu_{ij}}}\, T_\omega \left[\frac{v_i - v_j}{|v_i - v_j|} \right]$$

$$v_j' = \frac{m_i v_i + m_j v_j}{m_i + m_j} - \frac{m_i}{m_i + m_j} \sqrt{\frac{2R\mathscr{E}}{\mu_{ij}}}\, T_\omega \left[\frac{v_i - v_j}{|v_i - v_j|} \right],$$

where $\mathscr{E} = (\mu_{ij}|v_i - v_j|^2/2 + I_i + I_j) = (\mu_{ij}|v_i' - v_j'|^2/2 + I_i' + I_j')$ is the energy in the center of mass reference frame, $\omega \in \mathbb{S}^2$ is a unit vector and $T_\omega[x] = x - 2(\omega \cdot x)\omega$ is the symmetry with respect to the plane $\{\omega\}^\perp$.

Suppose now that the collisions induce a forward chemical reaction and denote by $\mathscr{E}^*$ the total energy of the colliding pair. In this case, the conservation laws (21) and (22), give the post-collisional velocities, parameterized by a unit vector $\omega \in \mathbb{S}^2$:

$$v_3' = \frac{m_1 v_1 + m_2 v_2}{m_1 + m_2} + \frac{m_4}{m_3 + m_4}\sqrt{\frac{2}{\mu_{34}}}\left(R\mathscr{E}^* - \frac{E}{6}\right)^{1/2} T_\omega\left[\frac{v_1 - v_2}{|v_1 - v_2|}\right]$$

$$v_4' = \frac{m_1 v_1 + m_2 v_2}{m_1 + m_2} - \frac{m_3}{m_3 + m_4}\sqrt{\frac{2}{\mu_{34}}}\left(R\mathscr{E}^* - \frac{E}{6}\right)^{1/2} T_\omega\left[\frac{v_1 - v_2}{|v_1 - v_2|}\right].$$

The reactive post-collisional velocities for the backward reaction in terms of pre-collisional velocities are

$$v_1' = \frac{m_3 v_3 + m_4 v_4}{m_3 + m_4} + \frac{m_2}{m_1 + m_2}\sqrt{\frac{2}{\mu_{12}}}\left(R\mathscr{E}^* + \frac{E}{6}\right)^{1/2} T_\omega\left[\frac{v_3 - v_4}{|v_3 - v_4|}\right]$$

$$v_2' = \frac{m_3 v_3 + m_4 v_4}{m_3 + m_4} - \frac{m_1}{m_1 + m_2}\sqrt{\frac{2}{\mu_{12}}}\left(R\mathscr{E}^* + \frac{E}{6}\right)^{1/2} T_\omega\left[\frac{v_3 - v_4}{|v_3 - v_4|}\right].$$

The evolution of the distribution functions f_i, with $i = 1, \ldots, 4$, is governed by the system of kinetic equations

$$\frac{\partial f_i}{\partial t} + v \cdot \nabla_x f_i = \sum_{j=1}^{4} Q_{ij}^e(f_i, f_j) + Q_i^{react}, \qquad i = 1, \ldots, 4. \tag{23}$$

In the sum written above, when $i \neq j$, the notation Q_{ij}^e represents the bi-species elastic operator associated to collisions between one particle of constituent i and another one of constituent j. When $i = j$, the operator Q_{ii}^e is nothing but the standard mono-species elastic collisional operator. Moreover, Q_i^{react} represents the reactive collisional operator. The operators Q_{ij}^e and Q_i^{react} are defined as follows. For non-reactive interactions, the operators are

$$Q_{ij}^e(f_i, f_j) = \int_{\mathbb{R}^3}\int_0^{+\infty}\int_0^1\int_0^1\int_{\mathbb{S}^2}\Big[f_i(v_i', I_i')f_j(v_j', I_j') - f_i(v, I)f_j(v_j, I_j)\Big] \times B_{ij}(v, v_j, I, I_j, R, r, \omega)(1 - R)\left|v - v_j\right|^{-1}\varphi_i(I)^{-1}\,\mathrm{d}\omega\,\mathrm{d}r\,\mathrm{d}R\,\mathrm{d}I_j\,\mathrm{d}v_j,$$

where B_{ij} are suitable cross sections and v_i', v_j', I_i' and I_j' are given by

$$v_i' = \frac{m_i v + m_j v_j}{m_i + m_j} + \frac{m_j}{m_i + m_j}\sqrt{\frac{2R\mathscr{E}}{\mu_{ij}}}\, T_\omega\left[\frac{v - v_j}{|v - v_j|}\right],$$

$$v_j' = \frac{m_i v + m_j v_j}{m_i + m_j} - \frac{m_i}{m_i + m_j}\sqrt{\frac{2R\mathscr{E}}{\mu_{ij}}}\, T_\omega\left[\frac{v - v_j}{|v - v_j|}\right],$$

$$I_i' = \left(\frac{\mu_{ij}}{2}|v - v_j|^2 + I + I_j\right) r(1 - R),\ I_j' = \left(\frac{\mu_{ij}}{2}|v - v_j|^2 + I + I_j\right)(1 - r)(1 - R).$$

The reactive collisional operators are more involved. Let $B^{react} : \mathbb{R}^3 \times \mathbb{R}^3 \times \mathbb{R}^+ \times \mathbb{R}^+ \times [0,1]^2 \times \mathbb{S}^2 \to \mathbb{R}^+$ be a suitable cross-section.

In the case of the forward reaction, we define the total energy as

$$\mathscr{E}_1^* = \frac{1}{2}\mu_{12}|v - v_2|^2 + I + I_2 - \frac{E}{2}.$$

Then, the reactive post-collisional velocities and internal energies can be written in terms of the pre-collisional quantities in the following way:

$$v_3' = \frac{m_1 v + m_2 v_2}{m_1 + m_2} + \frac{m_4}{m_3 + m_4}\sqrt{\frac{2}{\mu_{34}}}\left(R\mathscr{E}_1^* - \frac{E}{6}\right)^{1/2} T_\omega\left[\frac{v - v_2}{|v - v_2|}\right],$$

$$v_4' = \frac{m_1 v + m_2 v_2}{m_1 + m_2} - \frac{m_3}{m_3 + m_4}\sqrt{\frac{2}{\mu_{34}}}\left(R\mathscr{E}_1^* - \frac{E}{6}\right)^{1/2} T_\omega\left[\frac{v - v_2}{|v - v_2|}\right],$$

$$I_3' = r(1 - R)\mathscr{E}_1^* - \frac{E}{6}, \qquad I_4' = (1 - r)(1 - R)\mathscr{E}_1^* - \frac{E}{6}.$$

Consider the set

$$F_1 = \Bigg\{(I, I_2, r, R, v, v_2) :\ \ I \geq \frac{E}{6},\ I_2 \geq \frac{E}{6},\ R\mathscr{E}_1^* \geq \frac{E}{6},$$
$$\frac{\mu_{12}}{2}|v - v_2|^2 \geq \frac{E}{6},\ (1-R)r\mathscr{E}_1^* \geq \frac{E}{6},\ (1-R)(1-r)\mathscr{E}_1^* \geq \frac{E}{6}.\Bigg\}.$$

Then, the collisional integral describing the forward chemical reaction is

$$Q_1^{react}(v, I) = \int_{\mathbb{R}^3}\int_0^{+\infty}\int_0^1\int_0^1\int_{\mathbb{S}^2}\left[\left(\frac{m_1 m_2}{m_3 m_4}\right)^3 f_3(v_3', I_3') f_4(v_4', I_4') - f_1(v, I) f_2(v_2, I_2)\right]$$
$$\times\, \mathbb{1}_{\xi \in F_1} B^{react}(v, v_2, I, I_2, R, r, \omega)\frac{(1 - R)}{(m_1 m_2)^2 |v - v_2|\, \varphi_1(I)}\, \mathrm{d}\omega\, \mathrm{d}r\, \mathrm{d}R\, \mathrm{d}I_2\, \mathrm{d}v_2.$$

The structure of Q_2^{react} is similar. We define the total energy

$$\mathscr{E}_2^* = \frac{1}{2}\mu_{12}|v - v_1|^2 + I + I_1 - \frac{E}{2},$$

the reactive post-collisional velocities and internal energies

$$v_3' = \frac{m_1 v_1 + m_2 v}{m_1 + m_2} + \frac{m_4}{m_3 + m_4}\sqrt{\frac{2}{\mu_{34}}}\left(R\mathscr{E}_2^* - \frac{E}{6}\right)^{1/2} T_\omega\left[\frac{v_1 - v}{|v_1 - v|}\right],$$

$$v_4' = \frac{m_1 v_1 + m_2 v}{m_1 + m_2} - \frac{m_3}{m_3 + m_4}\sqrt{\frac{2}{\mu_{34}}}\left(R\mathscr{E}_2^* - \frac{E}{6}\right)^{1/2} T_\omega\left[\frac{v_1 - v}{|v_1 - v|}\right],$$

$$I_3' = r(1-R)\mathscr{E}_2^* - \frac{E}{6}, \quad I_4' = (1-r)(1-R)\mathscr{E}_2^* - \frac{E}{6},$$

and the set

$$F_2 = \Big\{(I, I_1, r, R, v, v_1): \ I \geq \frac{E}{6}, \ I_1 \geq \frac{E}{6}, \ R\mathscr{E}_2^* \geq \frac{E}{6},$$
$$\frac{\mu_{12}}{2}|v - v_1|^2 \geq \frac{E}{6}, \ (1-R)r\mathscr{E}_2^* \geq \frac{E}{6}, \ (1-R)(1-r)\mathscr{E}_2^* \geq \frac{E}{6}\Big\}.$$

The collisional integral Q_2^{react} describing the forward chemical reaction is hence

$$Q_2^{react}(v, I) = \int_{\mathbb{R}^3}\int_0^{+\infty}\int_0^1\int_0^1\int_{\mathbb{S}^2}\left[\left(\frac{m_1 m_2}{m_3 m_4}\right)^3 f_3(v_3', I_3') f_4(v_4', I_4') - f_2(v, I) f_1(v_1, I_1)\right]$$
$$\times \mathbb{1}_{\xi \in F_2} B^{react}(v, v_1, I, I_1, R, r, \omega)\frac{(1-R)}{(m_1 m_2)^2 |v - v_1| \varphi_2(I)}\, \mathrm{d}\omega\, \mathrm{d}r\, \mathrm{d}R\, \mathrm{d}I_1\, \mathrm{d}v_1.$$

In the case of the backward reaction we treat two collisional terms. Denote

$$\mathscr{E}_3^* = \frac{1}{2}\mu_{34}|v - v_4|^2 + I + I_4 + \frac{E}{2}$$

the total energy. We can write the reactive post collisional velocities and internal energies as follows:

$$v_1' = \frac{m_3 v + m_4 v_4}{m_3 + m_4} + \frac{m_2}{m_1 + m_2}\sqrt{\frac{2}{\mu_{12}}}\left(R\mathscr{E}_3^* + \frac{E}{6}\right)^{1/2} T_\omega\left[\frac{v - v_4}{|v - v_4|}\right],$$

$$v_2' = \frac{m_3 v + m_4 v_4}{m_3 + m_4} - \frac{m_1}{m_1 + m_2}\sqrt{\frac{2}{\mu_{12}}}\left(R\mathscr{E}_3^* + \frac{E}{6}\right)^{1/2} T_\omega\left[\frac{v - v_4}{|v - v_4|}\right],$$

$$I_1' = r(1-R)\mathscr{E}_3^* + \frac{E}{6}, \quad I_2' = (1-r)(1-R)\mathscr{E}_3^* + \frac{E}{6}.$$

The admissible set F_3 is

$$F_3 = \Big\{(I_4, r, R, v_4): \quad I_4 \geq 0, \quad v_4 \in \mathbb{R}^3, \quad r, R \in [0,1]\Big\}.$$

The collisional integral Q_3^{react} describing the backward reaction is defined by

$$Q_3^{react}(v, I) = \int_{\mathbb{R}^3}\int_0^{+\infty}\int_0^1\int_0^1\int_{\mathbb{S}^2}\left[\left(\frac{m_3 m_4}{m_1 m_2}\right)^3 f_1(v_1', I_1') f_2(v_2', I_2') - f_3(v, I) f_4(v_4, I_4)\right]$$
$$\times \mathbb{1}_{\xi \in F_3} B^{react}(v, v_4, I, I_4, R, r, \omega) \frac{(1-R)}{(m_3 m_4)^2 |v - v_4| \varphi_3(I)} \, \mathrm{d}\omega \, \mathrm{d}r \, \mathrm{d}R \, \mathrm{d}I_4 \, \mathrm{d}v_4.$$

Finally, let

$$\mathscr{E}_4^* = \frac{1}{2}\mu_{34}|v - v_3|^2 + I + I_3 + \frac{E}{2}$$

be the total energy of the binary encounter. Then, we can write the reactive post-collisional velocities and internal energies in the following way:

$$v_1' = \frac{m_3 v_3 + m_4 v}{m_3 + m_4} + \frac{m_2}{m_1 + m_2}\sqrt{\frac{2}{\mu_{12}}}\left(R\mathscr{E}_4^* + \frac{E}{6}\right)^{1/2} T_\omega\left[\frac{v_3 - v}{|v_3 - v|}\right],$$

$$v_2' = \frac{m_3 v_3 + m_4 v}{m_3 + m_4} - \frac{m_1}{m_1 + m_2}\sqrt{\frac{2}{\mu_{12}}}\left(R\mathscr{E}_4^* + \frac{E}{6}\right)^{1/2} T_\omega\left[\frac{v_3 - v}{|v_3 - v|}\right].$$

$$I_1' = r(1-R)\mathscr{E}_4^* + \frac{E}{6}, \quad I_2' = (1-r)(1-R)\mathscr{E}_4^* + \frac{E}{6}.$$

The admissible set F_4 is

$$F_4 = \Big\{(I_3, r, R, v_3): \quad I_3 \geq 0, \quad v_3 \in \mathbb{R}^3, \quad r, R \in [0,1]\Big\},$$

and the reactive collisional integral Q_4^{react}, describing the backward reaction, is defined by

$$Q_4^{react}(v, I) = \int_{\mathbb{R}^3}\int_0^{+\infty}\int_0^1\int_0^1\int_{\mathbb{S}^2}\left[\left(\frac{m_3 m_4}{m_1 m_2}\right)^3 f_1(v_1', I_1') f_2(v_2', I_2') - f_4(v, I) f_3(v_3, I_3)\right]$$
$$\times \mathbb{1}_{\xi \in F_4} B^{react}(v, v_3, I, I_3, R, r, \omega) \frac{(1-R)}{(m_3 m_4)^2 |v - v_3| \varphi_4(I)} \, \mathrm{d}\omega \, \mathrm{d}r \, \mathrm{d}R \, \mathrm{d}I_3 \, \mathrm{d}v_3.$$

In [16], the equilibria for the kinetic system (23) have been studied in two steps, first by assuming that the mechanical equilibrium is reached, and then by considering the chemical equilibrium associated to the reactive collisional operator.

These equilibria are again called Maxwellians, because they play the same role as the Maxwellian functions of the classical Boltzmann equation. Let $c_i \geq 0$, $i = 1, \ldots, 4$, $u \in \mathbb{R}^3$ and $T > 0$. Then, the reactive Maxwellians of the model have the form

$$\mathscr{M}(c_i, u, T) = \frac{c_i(t,x)}{q_i(T(t,x))} \left(\frac{m_i}{2\pi k_B T(t,x)}\right)^{3/2} \exp\left(-\frac{m_i\,|v-u(t,x)|^2}{2k_B T(t,x)} - \frac{I}{k_B T(t,x)}\right)$$

where

$$q_i(T(t,x)) = \int_0^{+\infty} \varphi_i(I)\, \exp\left(-\frac{I}{k_B T(t,x)}\right) \mathrm{d}I \tag{24}$$

can be interpreted as a Laplace transform of φ_i for all i.

Note that this model may describe a non-reactive mixture of polyatomic gases, by simply neglecting the reactive collision kernels. In this case, it can be viewed as a generalization of [14], which studied non-reactive polyatomic gaseous mixtures.

5 The Maxwell–Stefan Diffusion Limit for Non-reactive Boltzmann Systems

In the previous section, we have described two kinetic models for reactive and non-reactive mixtures. The diffusive limit of these systems is based on the study of the asymptotic behaviour, as the mean free path tends to zero, of the rescaled kinetic system in the diffusive scaling, by supposing that the solutions are perturbations of the local Maxwellian state. It is indeed clear that, if the initial conditions are local Maxwellians, there are no reasons which guarantee that the Maxwellian structure is kept by the time evolution. However, it is possible to prove that the solutions of the system stay close to Maxwellian functions, with a reminder which is small as the mean free path tends to zero.

We first describe the formal asymptotics, then we consider the rigorous derivation of the diffusive system.

5.1 The Formal Asymptotics

In [13], Boudin, Grec, and Salvarani study the Boltzmann system described in Sect. 3, in a spatial domain Ω, in the case of Maxwellian molecules, i.e. by supposing that each cross section B_{ij} depends on v, v_* and σ only through the deviation angle $\theta \in [0, \pi]$ between $(v - v_*)$ and σ. This means that, for each (i, j), there exists a function $b_{ij} : [-1, 1] \to \mathbb{R}^+$ such that

$$B_{ij}(v, v_*, \sigma) = b_{ij}\left(\frac{v - v_*}{|v - v_*|} \cdot \sigma\right) = b_{ij}\left(\cos\theta\right).$$

In the article is moreover supposed that b_{ij} is even and that $b_{ij} \in L^1(-1, 1)$ (Grad's angular cutoff assumption).

After introducing the mean free path $\varepsilon > 0$, the authors wrote the kinetic system in the diffusive scaling. By denoting with $(f_i^\varepsilon)_{1 \le i \le \mathscr{I}}$ the corresponding unknowns in this regime, each distribution function f_i^ε solves

$$\varepsilon\, \partial_t f_i^\varepsilon + v \cdot \nabla_x f_i^\varepsilon = \frac{1}{\varepsilon} \sum_{j=1}^{\mathscr{I}} Q_{ij}(f_i^\varepsilon, f_j^\varepsilon), \quad \text{on } \mathbb{R}_*^+ \times \Omega \times \mathbb{R}^3. \tag{25}$$

The analysis has been carried out in the isothermal case, i.e. by supposing that the temperature T is constant with respect to the time variable and homogeneous with respect to the spatial variable. Once introduced the quantities

$$c_i^\varepsilon : \mathbb{R}^+ \times \Omega \to \mathbb{R}^+, \qquad u_i^\varepsilon : \mathbb{R}^+ \times \Omega \to \mathbb{R}^3, \qquad 1 \le i \le \mathscr{I},$$

the article assumes that the system evolution leaves the distribution functions, up to a correction of lower order, in the local Maxwellian state,

$$f_i^\varepsilon = c_i^\varepsilon(t, x)\left(\frac{m_i}{2\pi k_B T}\right)^{3/2} e^{-m_i|v - \varepsilon u_i^\varepsilon(t,x)|^2/2k_B T}(1 + \mathscr{O}(\varepsilon)), \ \ t > 0, \ (x, v) \in \Omega \times \mathbb{R}^3,$$

where the quantity $\varepsilon u_i^\varepsilon$ is the bulk velocity, of order ε, whose precise form may depend on the considered species of the mixture. By supposing that all the initial quantities

$$c_i^{\text{in}} : \Omega \to \mathbb{R}^+, \qquad u_i^{\text{in}} : \Omega \to \mathbb{R}^3, \qquad 1 \le i \le \mathscr{I},$$

do not depend on ε and that

$$\sum_{i=1}^{\mathscr{I}} c_i^{\text{in}} = 1 \quad \text{on } \Omega,$$

the authors prove that, in the limit $\varepsilon \to 0$, for $(t, x) \in \mathbb{R}^+ \times \Omega$, by supposing the existence of the limits

$$c_i(t, x) = \lim_{\varepsilon \to 0^+} c_i^\varepsilon(t, x), \qquad J_i(t, x) = \lim_{\varepsilon \to 0^+} c_i^\varepsilon(t, x) u_i^\varepsilon(t, x)$$

and that

$$c := \sum_{i=1}^{\mathscr{I}} c_i = \sum_{i=1}^{\mathscr{I}} c_i^{\text{in}} = 1 \quad \text{on } \Omega,$$

the pairs (c_i, J_i) formally satisfy the Maxwell–Stefan diffusion system (1) and give an explicit form of the binary diffusion coefficients:

$$k_{ij} = \frac{2\pi\ m_i m_j \|b_{ij}\|_{L^1}}{(m_i + m_j)k_B T}. \tag{26}$$

These binary diffusion coefficients are symmetric ($k_{ij} = k_{ji}$ for all $i, j = 1, \ldots, \mathscr{I}$) and depend on the cross-section (in this case, the cross-section of Maxwell molecules with Grad's angular cutoff).

The authors have not deduced, in the limiting procedure, the equimolar closure relationship (2). However, they have proved that, formally,

$$\nabla_x \cdot \left(\sum_{i=1}^{\mathscr{I}} J_i \right) = 0.$$

Other cross sections give different forms of the binary diffusion coefficients. In particular, Hutridurga and Salvarani [23] derived the expression of the binary diffusion coefficients under suitable assumptions on the collision kernels B_{ij}. They suppose that the collision kernels B_{ij} depend on the modulus of the relative velocity $|v - v_*|$ and on the cosine of the deviation angle θ, i.e.

$$B_{ij}(v, v_*, \sigma) = \Phi(|v - v_*|) b_{ij}(\cos\theta). \tag{27}$$

Moreover, they assume that the angular collision kernels b_{ij} belong to the class $L^1(-1, +1)$ and that they are even functions with respect to their argument. Furthermore, they suppose that the kinetic collision kernel $\Phi(|v - v_*|)$ is analytic in the following sense: there exists a family $\{a_n\}_{n\in\mathbb{N}^*} \subset \mathbb{R}$ such that Φ can be written as a uniformly converging even power series:

$$\Phi(|v - v_*|) = \sum_{n\in\mathbb{N}^*} a_n |v - v_*|^{2n}.$$

Under these hypotheses, the binary diffusion coefficients computed in [23] have the form

$$k_{ij} = \left\{ a_0 \frac{2\pi m_i m_j \|b_{ij}\|_{L^1}}{(m_i + m_j)k_B T} + a_1 10\pi \|b_{ij}\|_{L^1} + \right.$$

$$\sum_{n\geq 2} a_n \frac{2\pi \|b_{ij}\|_{L^1} (m_i m_j)}{(m_i + m_j)k_B T} \Bigg(\sum_{n_1+n_2+n_3=n} \frac{n!}{n_1! n_2! n_3!} \sum_{\substack{\alpha,\beta,\gamma,\delta,\rho,\eta\in 2\mathbb{N}^* \\ \alpha+\beta=2n_1 \\ \gamma+\delta=2n_2 \\ \rho+\eta=2n_3}} \frac{(2n_1)!}{\alpha!\beta!} \frac{(2n_2)!}{\gamma!\delta!} \frac{(2n_3)!}{\rho!\eta!}$$

$$\left. \times \mathscr{E}(\alpha, \beta, \gamma, \delta, \rho, \eta) \left(\frac{k_B T}{m_i} \right)^{(\alpha+\gamma+\rho)/2} \left(\frac{k_B T}{m_j} \right)^{(\beta+\delta+\eta)/2} \Bigg) \right\},$$

where

$$\mathscr{E}(\alpha,\beta,\gamma,\delta,\rho,\eta)=((\alpha-1)(\alpha-3)\cdots 1)((\beta-1)(\beta-3)\cdots 1)\,((\gamma-1)(\gamma-3)\cdots 1)$$
$$\times\,((\delta-1)(\delta-3)\cdots 1)\,((\rho-1)(\rho-3)\cdots 1)\,((\eta-1)(\eta-3)\cdots 1)\,.$$

The binary diffusion coefficients depend on the reduced mass of the species, on the temperature and on the cross sections of the kinetic model. Therefore, by tuning the coefficients a_n in the kinetic cross section (27), it is possible to obtain several forms of temperature dependency for the binary diffusion coefficients and compare them with the experiments. When $a_i = 0$ for all $i \geq 1$, the formula written above corresponds to the binary diffusion coefficients already deduced in Eq. (26).

A gas of hard spheres of fixed diameter is not included in the previous analysis. The study of this case has been carried out by Anwasia [1].

In [11], Boudin, Grec and Pavan provide another approach for going beyond Maxwellian molecules. They propose a semi-explicit link between the Maxwell–Stefan diffusion coefficients and the cross sections of the corresponding rescaled Boltzmann system for monatomic gaseous mixtures in the diffusive scaling, for general cross sections $B_{ij} = B_{ij}(v, v_*, \sigma)$ satisfying the Galilean invariance and the microreversibility assumptions, under Grad's angular cut-off hypothesis. They prove that

$$k_{ij} = \int\int\int B_{ij}(v,v_*,\sigma)\exp\left[-\frac{m_i}{2\pi k_B T}|v|^2-\frac{m_j}{2\pi k_B T}|v_*|^2\right]\left[m_i(v'-v)\right]^2 \mathrm{d}\sigma,\mathrm{d}v_*\mathrm{d}v$$

$$= \frac{m_i m_j}{6(k_B T)^2(m_i+m_j)}\left(\frac{m_i}{2\pi k_B T}\right)^{3/2}\left(\frac{m_j}{2\pi k_B T}\right)^{3/2}\int\int\int B_{ij}(v,v_*,\sigma)\times$$

$$\exp\left[-\frac{m_i}{2\pi k_B T}|v|^2-\frac{m_j}{2\pi k_B T}|v_*|^2\right]\left(v-v_*+|v'-v|\sigma\right)\cdot\left(m_i v-m_j v_*\right)\mathrm{d}\sigma,\mathrm{d}v_*\mathrm{d}v.$$

These two equivalent forms of the binary diffusion coefficients show their positivity as well as their symmetry.

We moreover quote [22], which derived, by using the same approach, a system of Maxwell–Stefan type when the temperature is not uniform in space nor constant in time. In the diffusive limit, the authors show that the kinetic temperature of each species of the mixture tends to the same temperature function $T = T(t, x)$, $(t, x) \in (0, \infty) \times \Omega$, $\Omega \subseteq \mathbb{R}^3$ as $\varepsilon \to 0$. The structure of the system they derived is:

$$\begin{cases} \partial_t c_i + \nabla_x \cdot J_i = 0 & \text{in } (0,\infty)\times\Omega, \quad i = 1,\ldots,\mathscr{I} \\ \nabla_x\,(c_i T) = -\displaystyle\sum_{j\neq i} k_{ij}^*\left(c_j J_i - c_i J_j\right) & \text{in } (0,\infty)\times\Omega, \quad i = 1,\ldots,\mathscr{I}, \end{cases} \tag{28}$$

The binary diffusion coefficients k_{ij}^*, as in the previously described articles, depend on the cross sections. In particular, if the hypotheses on the cross sections are the same as in [1, 11, 13] or [23] respectively, then the binary diffusion coefficients in (28) are of the form $k_{ij}^* = T(t,x)k_{ij}$, where k_{ij} are the binary diffusion coefficients described in [1, 11, 13] or [23].

5.2 The Rigorous Diffusive Asymptotics

The article by Bondesan and Briant [8] studies the Maxwell–Stefan asymptotics, in the 3-dimensional torus $\mathbb{T}^3$, of the system of coupled Boltzmann equations for mixtures (5)–(6), with collisional integrals of the form (8)–(9) and suitable cross sections (of cutoff Maxwellian type, or hard potentials, or hard spheres). The starting point is the Cauchy theory, proved by the same authors in [7], whose precise result is the following.

Theorem 1 *Let $s > 3$ be an integer, $\bar{u} : \mathbb{R}^+ \times \mathbb{T}^3 \to \mathbb{R}^3$ be in $L^\infty(\mathbb{R}^+; H^s(\mathbb{T}^3))$ with $\nabla_x \cdot \bar{u} = 0$, and consider $\bar{\mathbf{c}} > 0$. Suppose that there exist δ_{MS}, C_{MS}, C'_{MS}, $\lambda_{MS} > 0$ such that for all $\varepsilon \in (0,1]$ and for any initial datum $(\tilde{\mathbf{c}}^{\,\mathrm{in}}, \tilde{\mathbf{u}}^{\,\mathrm{in}}) \in H^s(\mathbb{T}^3) \times H^{s-1}(\mathbb{T}^3)$, for almost any $x \in \mathbb{T}^3$ and for any $1 \le i \le \mathscr{I}$, the following requirement are satisfied:*

(i) Mass compatibility: $\displaystyle\sum_{i=1}^{\mathscr{I}} \tilde{c}_i^{\,\mathrm{in}}(x) = 0 \quad \text{and} \quad \int_{\mathbb{T}^3} \tilde{c}_i^{\,\mathrm{in}}(x)\mathrm{d}x = 0,$

(ii) Mass positivity: $\bar{c}_i + \varepsilon \tilde{c}_i^{\,\mathrm{in}}(x) > 0,$

(iii) Moment compatibility: $\nabla_x \tilde{c}_i^{\,\mathrm{in}} = \displaystyle\sum_{j \neq i} k_{ij} c_i^{\,\mathrm{in}} c_j^{\,\mathrm{in}} \left(\tilde{u}_j^{\,\mathrm{in}} - \tilde{u}_i^{\,\mathrm{in}}\right),$

(iv) Smallness assumptions: $\left\|\tilde{\mathbf{c}}^{\,\mathrm{in}}\right\|_{H_x^s} \le \delta_{MS} \quad \text{and} \quad \|\bar{u}\|_{L_t^\infty H_x^s} \le \delta_{MS}.$

Then, there exists a unique weak solution

$$(\mathbf{c}, \mathbf{u}) = \left(\bar{\mathbf{c}} + \varepsilon \tilde{\mathbf{c}}, \bar{\mathbf{u}} + \varepsilon \tilde{\mathbf{u}}\right)$$

in $L^\infty\left(\mathbb{R}^+; H^s(\mathbb{T}^3)\right) \times L^\infty\left(\mathbb{R}^+; H^{s-1}(\mathbb{T}^3)\right)$ to the incompressible Maxwell–Stefan system

$$\partial_t c_i + \nabla_x \cdot (c_i u_i) = 0, \tag{29}$$

$$-\nabla_x c_i = \sum_{j=1}^{\mathscr{I}} k_{ij} c_i c_j (u_i - u_j), \tag{30}$$

$$\nabla_x \cdot \left(\sum_{i=1}^{\mathscr{I}} c_i u_i \right) = 0, \tag{31}$$

such that initially $(\tilde{\mathbf{c}}, \tilde{\mathbf{u}})\,|_{t=0} = \left(\tilde{\mathbf{c}}^{\,\mathrm{in}}, \tilde{\mathbf{u}}^{\,\mathrm{in}}\right)$ *a.e. on* $\mathbb{T}^3$. *In particular, if* $s > 4$ *and* $\bar{u} \in C^0\left(\mathbb{R}^+; H^s(\mathbb{T}^3)\right)$, *then the pair* $(\mathbf{c}, \mathbf{u})$ *also belongs to* $C^0\left(\mathbb{R}^+; H^{s-1}(\mathbb{T}^3)\right) \times C^0\left(\mathbb{R}^+; H^{s-2}(\mathbb{T}^3)\right)$. *Moreover,* $\mathbf{c}$ *is positive and the following relations hold a.e. on* $\mathbb{R}^+ \times \mathbb{T}^3$:

$$\langle \mathbf{c}, \tilde{\mathbf{u}} \rangle = \sum_{i=1}^{\mathscr{I}} c_i(t,x)\tilde{u}_i(t,x) = 0 \quad \textit{and} \quad \int_{\mathbb{T}^3} \tilde{c}_i(t,x)\mathrm{d}x = 0.$$

Finally, for almost any time $t \geq 0$

$$\|\tilde{\mathbf{c}}\|_{H^s_x\left(\bar{\mathbf{c}}^{-\frac{1}{2}}\right)} \leq e^{-t\lambda_{MS}} \left\|\tilde{\mathbf{c}}^{\,\mathrm{in}}\right\|_{H^s_x\left(\bar{\mathbf{c}}^{-\frac{1}{2}}\right)}, \quad \|\tilde{\mathbf{u}}\|_{H^{s-1}_x} \leq C_{MS} e^{-t\lambda_{MS}} \left\|\tilde{\mathbf{c}}^{\,\mathrm{in}}\right\|_{H^s_x\left(\bar{\mathbf{c}}^{-\frac{1}{2}}\right)},$$
$$\int_0^t e^{2(t-\tau)\lambda_{MS}} \|\tilde{\mathbf{u}}(\tau)\|^2_{H^s_x}\,\mathrm{d}\tau \leq C'_{MS} \left\|\tilde{\mathbf{c}}^{\,\mathrm{in}}\right\|^2_{H^s_x\left(\bar{\mathbf{c}}^{-\frac{1}{2}}\right)}.$$

The constants δ_{MS}, λ_{MS}, C_{MS} *and* C'_{MS} *are constructive and only depend on* s, *the number of species* $\mathscr{I}$, *the diffusion coefficients* $(k_{ij})_{1\leq i,j\leq \mathscr{I}}$ *and the constant vector* $\bar{\mathbf{c}}$. *In particular, they are independent of the parameter* ε.

This theorem guarantees the possibility of building a Cauchy theory around the macroscopic state $(\bar{\mathbf{c}}, \bar{\mathbf{u}})$, instead of considering the equilibrium $(\bar{\mathbf{c}}, \mathbf{0})$. It is hence possible to give a complete description of systems having an equilibrium state with a constant mass vector $\bar{\mathbf{c}}$. Actually, this theorem does not provide strong uniqueness for the solutions, because infinitely many solutions to the Maxwell–Stefan system can be constructed by considering different constant $\bar{\mathbf{c}}$ and $\bar{\mathbf{u}}$ satisfying the incompressible condition. However, as soon as it is possible to fix a macroscopic equilibrium $(\bar{\mathbf{c}}, \bar{\mathbf{u}})$, then strong uniqueness is recovered around this specific state.

The next step by Bondesan and Briant has been a Cauchy theory for the Boltzmann system (5) having the property of being uniform with respect to the Knudsen number ε. Their result allows to prove that, in the limit $\varepsilon \to 0$, the Maxwell–Stefan equation are rigorously derived. The authors work in the three-dimensional torus $\mathbb{T}^3$.

The assumptions on the cross sections B_{ij} at the kinetic level are the following:

(H1) All the B_{ij} satisfy a symmetry property with respect to the interchange of the indices i and j, i.e.:

$$B_{ij}(|v - v_*|, \cos\theta) = B_{ji}(|v - v_*|, \cos\theta), \quad \text{for all } v, v_* \in \mathbb{R}^3 \text{ and for all } \theta \in \mathbb{R}.$$

(H2) All cross sections B_{ij} can be decomposed as the product of a kinetic part $\Phi_{ij} \geq 0$ and of an angular part $b_{ij} \geq 0$:

$$B_{ij}(|v - v_*|, \cos\theta) = \Phi_{ij}(|v - v_*|)b_{ij}(\cos\theta), \text{ for all } v, v_* \in \mathbb{R}^3 \text{ and for all } \theta \in \mathbb{R}.$$

(H3) The kinetic part is derived from an hard or a Maxwellian ($\gamma = 0$) potential:

$$\Phi_{ij}(|v - v_*|) = C^{\Phi}_{ij}|v - v_*|^{\gamma}, \quad C^{\Phi}_{ij} > 0, \quad \gamma \in [0, 1], \quad \text{for all } v, v_* \in \mathbb{R}^3.$$

(H4) The angular part satisfies Grad's angular cutoff in strong form [19]: there exists a constant $C > 0$ such that

$$0 < b_{ij}(\cos\theta) \le C|\sin\theta||\cos\theta|, \qquad b'_{ij}(\cos\theta) \le C, \qquad \theta \in [0,\pi].$$

Moreover,

$$\inf_{\sigma_1,\sigma_2\in\mathbb{S}^2} \int_{\mathbb{S}^2} \min\{b_{ii}(\sigma_1\cdot\sigma_3), b_{ii}(\sigma_2\cdot\sigma_3)\}\mathrm{d}\sigma_3 > 0.$$

The precise statement of their theorem is the following [8]:

Theorem 2 *Let the collision kernels B_{ij} satisfy assumptions* (H1)–(H2)–(H3)–(H4)*, and let $\boldsymbol{\mu}$ be the unique global equilibrium of the mixture. Consider the local Maxwellian vector $\mathbf{M}^\varepsilon = (M_1^\varepsilon, \dots, M_I^\varepsilon)$, where*

$$M_1^\varepsilon = c_i(t,x)\left(\frac{m_i}{2\pi}\right)^{3/2}\exp\left(-\frac{m_i}{2}|v-\varepsilon u_i(t,x)|^2\right), \qquad i = 1,\dots,\mathscr{I}.$$

There exist $s_0 \in \mathbb{N}^*$, $\bar{\delta}_{MS} > 0$ and $\varepsilon_0 \in (0,1]$ such that the following statements hold for any integer $s \ge s_0$.

(i) There exist three sets of positive constants $\left(a_\alpha^{(s)}\right)_\alpha^s$, $\left(b_{\alpha,k}^{(s)}\right)_{\alpha,k}^s$ and $\left(d_{\alpha,\beta}^{(s)}\right)_{\alpha,\beta}^s$ such that, for all $\varepsilon \in (0,\varepsilon_0]$, the following norms are equivalent:

$$\|\cdot\|_{\mathscr{H}_\varepsilon^s} \sim \left(\|\cdot\|^2_{L^2_{x,v}\left(\boldsymbol{\mu}^{-\frac12}\right)} + \sum_{|\alpha|\le s}\left\|\partial_x^\alpha\cdot\right\|^2_{L^2_{x,v}\left(\boldsymbol{\mu}^{-\frac12}\right)} + \varepsilon^2\sum_{\substack{|\alpha|+|\beta|\le s\\ |\beta|\ge 1}}\left\|\partial_v^\beta\partial_x^\alpha\cdot\right\|^2_{L^2_{x,v}\left(\boldsymbol{\mu}^{-\frac12}\right)}\right)^{\frac12}.$$

(ii) Let $\boldsymbol{L}$ be the vector of linearized mono-species Boltzmann operators around the global Maxwellian equilibrium of the mixture $\boldsymbol{\mu}$,

$$\mathbf{T}^\varepsilon = \varepsilon^{-2}\boldsymbol{L} - \varepsilon^{-1}v\cdot\nabla_x$$

and $\pi_{\mathbf{T}^\varepsilon}$ be the orthogonal projection onto $\ker\mathbf{T}^\varepsilon$ in $L^2(\mathbb{R}^3,\boldsymbol{\mu}^{-\frac12})$.
There exists $\delta_B > 0$ such that, for all $\varepsilon \in (0,\varepsilon_0]$, for all $\delta_{MS} \in [0,\bar{\delta}_{MS}]$ and for any initial datum $\mathbf{f}^{\text{in}}$ in $H^s\left(\mathbb{T}^3\times\mathbb{R}^3,\boldsymbol{\mu}^{-\frac12}\right)$ with

$$\left\|\mathbf{f}^{\text{in}}\right\|_{\mathscr{H}_\varepsilon^s} \le \delta_B, \qquad \left\|\pi_{\mathbf{T}^\varepsilon}(\mathbf{f}^{\text{in}})\right\|_{L^2_{x,v}\left(\boldsymbol{\mu}^{-\frac12}\right)} \le C\delta_{MS},$$

for some positive constant $C > 0$ independent of the parameters ε and δ_{MS}, there exists a unique $\mathbf{f} \in C^0\left(\mathbb{R}^+; H^s\left(\mathbb{T}^3\times\mathbb{R}^3,\boldsymbol{\mu}^{-\frac12}\right)\right)$ such that $\mathbf{F}^\varepsilon = \mathbf{M}^\varepsilon + \varepsilon\mathbf{f}$ is the unique weak solution of the Boltzmann multi-species equation (25)*. Moreover,*

if $\mathbf{F}^{\varepsilon,\,\mathrm{in}} = \mathbf{M}^{\varepsilon,\,\mathrm{in}} + \varepsilon \mathbf{f}^{\,\mathrm{in}} \geq 0$, *then* $\mathbf{F}^{\varepsilon}(t, x, v) \geq 0$ *almost everywhere on* $\mathbb{R}^+ \times \mathbb{T}^3 \times \mathbb{R}^3$. *Finally, for any time* $t \geq 0$, $\mathbf{F}^{\varepsilon}$ *satisfies the stability property*

$$\|\mathbf{F}^{\varepsilon} - \mathbf{M}^{\varepsilon}\|_{\mathscr{H}^s_{\varepsilon}} \leq \varepsilon \delta_B, \quad \text{for all } \varepsilon \in (0, \varepsilon_0].$$

The constant δ_B *is explicit and only depend on the number of species* $\mathscr{I}$, *on the atomic masses* $(m_i)_{1 \leq i \leq \mathscr{I}}$, *and on the cross sections* $(B_{ij})_{1 \leq i,j \leq \mathscr{I}}$. *In particular, it is independent of the parameters* ε *and* δ_{MS}.

The strategy of proof consists in constructing perturbations of local Maxwellian states whose fluid quantities are perturbative solutions of the Maxwell–Stefan equations (29)–(31). Then, they plug the perturbation into the rescaled Boltzmann system (25). They obtain a system composed of four terms: the rescaled free transport operator, a linearized operator, a bilinear operator and a source term, which encodes the distance between the Maxwell–Stefan system and the fluid part of the perturbed Boltzmann equation.

However, the central spectral gap property cannot be directly recovered, because local Maxwellians are not local equilibria of the system, unless they share the same temperature and velocity (see Sect. 3). Nonetheless, the authors notice that the loss of the spectral gap has a lower order of magnitude. By introducing a modified Sobolev norm, they recover a coercivity property and close the energy estimates on the non-linear terms.

Uniqueness is proved in a perturbative regime only.

A possible research direction consists in extending the previous strategy to the rigorous derivation of the Maxwell–Stefan equations in the non-isothermal setting.

6 The Maxwell–Stefan Diffusion Limit for Reactive Kinetic Systems

When chemical reactions are allowed, temperature may vary in space and time. Moreover, the structure of the target system depends on the relative order of magnitude of the reactive collisional terms with respect to the non-reactive ones.

In what follows, we will describe the situation of a quaternary reacting mixture, which is the most common situation considered in the literature. The extension to other types of mixture is straightforward.

Starting from the SRS kinetic model [24] for a mixture of four ideal gases undergoing a reversible chemical reaction of bimolecular type, Anwasia, Gonçalves and Soares derive in [4] the corresponding Maxwell–Stefan asymptotics in the diffusive scaling, in the vanishing limit of the mean free path, when all the collisional integrals have the same order of magnitude. The authors first define the reactive cross sections for the direct and reverse chemical reactions in terms of their threshold relative velocities. Let $d_i > 0$ be the diameter of the particles of the i-th species ($i = 1, \ldots, 4$) and define, for any pair of species

$$\sigma_{ij}^2 = \frac{1}{4}(d_i + d_s)^2, \qquad i = 1, \ldots, 4, \qquad j = 1, \ldots, 4.$$

Then

$$\sigma_{12}'^2 = \begin{cases} \beta_{12}\sigma_{12}^2 & \langle \epsilon, v_1 - v_2 \rangle \geq \Xi_{12} \\ 0 & \langle \epsilon, v_1 - v_2 \rangle < \Xi_{12} \end{cases} \qquad \sigma_{34}'^2 = \begin{cases} \beta_{34}\sigma_{34}^2 & \langle \epsilon, v_3 - v_4 \rangle \geq \Xi_{34} \\ 0 & \langle \epsilon, v_3 - v_4 \rangle < \Xi_{34} \end{cases}$$

where the coefficients $\beta_{ij} \in [0, 1]$ represent the fraction of colliding pairs with enough kinetic energy to produce a chemical reaction.

By neglecting external forces, the SRS kinetic equations are given by

$$\frac{\partial f_i}{\partial t} + v_i \cdot \nabla_x f_i = J_i\,, \quad \text{in} \quad \mathbb{R}_+ \times \Omega \times \mathbb{R}^3,$$

with $J_i = J_i^E + J_i^R$, for $i = 1, 2, 3, 4$. For each species, J_i^E denotes the elastic collision operator and J_i^R the reactive collision operator. Their precise form is

$$\begin{aligned} J_i^E = {} & \sigma_{ii}^2 \int_{\mathbb{R}^3} \int_{\mathbb{S}_+^2} \left[{f_i}' f_{i_*}' - f_i f_{i_*} \right] \langle \epsilon, v_i - v_{i_*} \rangle \, d\epsilon \, dv_{i_*} \\ & + \sum_{\substack{s=1 \\ s \neq i}}^{4} \sigma_{is}^2 \int_{\mathbb{R}^3} \int_{\mathbb{S}_+^2} \left[{f_i}' f_s' - f_i f_s \right] \langle \epsilon, v_i - v_s \rangle \, d\epsilon \, dv_s \\ & - \beta_{ij} \sigma_{ij}^2 \int_{\mathbb{R}^3} \int_{\mathbb{S}_+^2} \left[{f_i}' {f_j}' - f_i f_j \right] \Theta \left(\langle \epsilon, v_i - v_j \rangle - \Xi_{ij} \right) \langle \epsilon, v_i - v_j \rangle \, d\epsilon \, dv_j, \end{aligned}$$

$$J_i^R = \beta_{ij} \sigma_{ij}^2 \int_{\mathbb{R}^3} \int_{\mathbb{S}_+^2} \left[\left(\frac{\mu_{ij}}{\mu_{kl}} \right)^2 f_k^\circ f_l^\circ - f_i f_j \right] \Theta \left(\langle \epsilon, v_i - v_j \rangle - \Xi_{ij} \right) \langle \epsilon, v_i - v_j \rangle \, d\epsilon \, dv_j,$$

where $f_i' = f(t, x, v_i')$, $f_{i*}' = f(t, x, v_{i*}')$, $f_s' = f(t, x, v_s')$, ${f_k}^\circ = f(t, x, v_k^\circ)$, ${f_l}^\circ = f(t, x, v_l^\circ)$, and Θ is the Heaviside step function.

Then Anwasia, Gonçalves and Soares prove that, in the limit, the concentrations c_i and the diffusive fluxes $\mathbf{J}_i$ satisfy an equation of Maxwell–Stefan type:

$$\begin{cases} \dfrac{\partial c_i}{\partial t} + \nabla_x \cdot \mathbf{J_i} = \sigma_{ij}^2 \left(\dfrac{2\pi \mu_{ij}}{k_B T} \right)^{\frac{1}{2}} \left[\left(\dfrac{\mu_{ij}}{\mu_{kl}} \right)^{\frac{1}{2}} c_k \, c_l \, \exp\left(\dfrac{E}{k_B T} \right) - c_i \, c_j \right] \\ \qquad\qquad \times \left[\dfrac{2 k_B T}{\mu_{ij}} \Gamma(2, z_i^*) - \left(\dfrac{\Xi_{ij}}{c_0} \right)^2 \Gamma(1, z_i^*) \right] \\ \nabla_x c_i = \dfrac{32}{3} \displaystyle\sum_{\substack{s=1 \\ s \neq i}}^{4} \sigma_{is}^2 \left(\dfrac{2\pi \mu_{ij}}{k_B T} \right)^{\frac{1}{2}} \left(c_i \mathbf{J}_s - c_s \mathbf{J}_i \right), \end{cases}$$

with

$$\mu_{ij} = \frac{m_i m_j}{m_i + m_j}, \qquad z_i^* = \frac{\mu_{ij}}{2k_B T}\left(\frac{\Xi_{ij}}{c_0}\right)^2,$$

where E is the reaction heat defined by the balance of chemical binding energies (18), Γ denotes the incomplete gamma function, c_0 denotes the characteristic speed of sound in the mixture at a reference temperature T_0, ζ_i is the activation energy for each of the species and $\Xi_{ij} = \sqrt{2\zeta_i/\mu_{ij}}$ is the threshold relative velocity.

It is worth noticing that no influence of the chemical reaction appears in the limiting Maxwell–Stefan equations written above.

In [3], the same authors modify the scaling, by supposing that both mechanical collisions and chemical reactions have comparable relaxation times, much smaller than the characteristic time of the flow. The reactive Maxwell–Stefan equations under this scaling have the form:

$$\nabla_x(c_i T) = -\sum_{\substack{s=1\\ s\neq i}}^{4}\left(\frac{c_s \mathbf{J}_s - c_i \mathbf{J}_s}{D_{is}}\right) + \frac{c_j \mathbf{J}_i - c_i \mathbf{J}_j}{D_{ij}} + \frac{c_l \mathbf{J}_k}{D_k} + \frac{c_k \mathbf{J}_l}{D_l} - \frac{c_j \mathbf{J}_i}{D_i} - \frac{c_i \mathbf{J}_j}{D_j},$$

where the indices (i, j, k, l) take the values $(1, 2, 3, 4)$, $(2, 1, 4, 3)$, $(3, 4, 1, 2)$ or $(4, 3, 2, 1)$, and the quantities D_{is}, D_{ij}, D_k, D_l, D_i are explicitly computed diffusion coefficients, based on the kinetic parameters of the model.

We conclude this section with the formal derivation of the Maxwell–Stefan asymptotics starting from the kinetic model for reactive gases by Desvillettes, Monaco and Salvarani [16] whose precise form is described in Sect. 4, under the standard diffusive scaling and when mechanical collisions are predominant with respect to reacting collisions.

The formal limit as $\varepsilon \to 0$, when the angular collision kernels of both the elastic bi-species and the reactive operators are odd functions of $\cos\theta$, has been studied by Anwasia, Bisi, Salvarani and Soares [2]. The resulting target equations have the structure of a system of balance equations coupled with the corresponding temperature-dependent flux-gradient relationships and with an equation describing the energy balance:

$$\frac{\partial c_i}{\partial t} + \nabla_{\boldsymbol{x}} \cdot J_i = -\lambda_i A \quad i = 1, 2, 3, 4$$

$$\nabla_{\boldsymbol{x}}\left(c_i k_B T\right) = -\sum_{\substack{j=1\\ j\neq i}}^{4} \frac{c_j \mathbf{J}_i - c_i \mathbf{J}_j}{D_{ij}} \quad i = 1, 2, 3, 4$$

$$\frac{\partial}{\partial t}\left[\sum_{i=1}^{4} c_i \left(\frac{3}{2}k_B T + \frac{q_i^*(T)}{q_i(T)}\right)\right] + \nabla_{\boldsymbol{x}} \cdot \left[\sum_{i=1}^{4}\left(\frac{5}{2}k_B T + \frac{q_i^*(T)}{q_i(T)}\right) J_i\right] = -EA,$$

where the production term A is given by

$$A = \left[\left(\frac{m_3 m_4}{m_1 m_2}\right)^{3/2} \frac{c_1 c_2}{q_1(T(t,\boldsymbol{x}))q_2(T(t,\boldsymbol{x}))} \exp\left(-\frac{E}{k_B T(t,\boldsymbol{x})}\right) \right.$$
$$\left. - \frac{c_3 c_4}{q_3(T(t,\boldsymbol{x}))q_4(T(t,\boldsymbol{x}))} \right] \frac{4}{\sqrt{\pi}(m_3 m_4)^2} \Gamma\left(\frac{\gamma+2}{2}\right) \left(\frac{2k_B T}{\mu_{34}}\right)^{(\gamma-1)/2}$$
$$\times \int_0^{+\infty} \int_0^{+\infty} \int_0^1 \int_0^1 \int_{\mathbb{S}^2} \exp\left(-\frac{I+I_4}{k_B T}\right) \Phi^{react}(I, I_4, R, r)$$
$$\times b^{react}(\cos\theta)\, \cos\theta\, (1-R)\, \mathrm{d}\sigma \mathrm{d}r \mathrm{d}R \mathrm{d}I_4 \mathrm{d}I,$$

and the diffusion coefficients D_{ij} are

$$\frac{1}{D_{ij}} = \frac{4}{3\sqrt{\pi}} \mu_{ij}^{(3-\gamma)/2} (2k_B T(t,\boldsymbol{x}))^{(\gamma-1)/2} \frac{1}{q_i(T(t,\boldsymbol{x}))q_j(T(t,\boldsymbol{x}))}$$
$$\times \Gamma\left(\frac{\gamma+4}{2}\right) \int_0^{+\infty} \int_0^{+\infty} \int_0^1 \int_0^1 \int_{\mathbb{S}^2} \exp\left(-\frac{I+I_j}{k_B T(t,\boldsymbol{x})}\right) \Phi_{ij}(I, I_j, R, r)$$
$$\times \cos\theta (1-R) b_{ij}(\cos\theta)\, \mathrm{d}\sigma \mathrm{d}r \mathrm{d}R \mathrm{d}I_j \mathrm{d}I\,.$$

In the previous formulas, Γ denotes the complete Gamma function and the quantities q_i are given by (24), whereas

$$q_i^*(T(t,x)) = \int_0^{+\infty} I\varphi_i(I)\, \exp\left(-\frac{I}{k_B T(t,x)}\right) \mathrm{d}I.$$

The structure of these equations takes into account the effects of the chemical reactions and their consequences with respect to the evolution of the temperature of the mixtures. We underline that they are compatible with the energy law of polyatomic gases and the law of mass action. Indeed, at the equilibrium, it is possible to deduce the law of mass action

$$\frac{c_1 c_2}{c_3 c_4} = \left(\frac{m_1 m_2}{m_3 m_4}\right)^{3/2} \frac{q_1(T(t,\boldsymbol{x}))q_2(T(t,\boldsymbol{x}))}{q_3(T(t,\boldsymbol{x}))q_4(T(t,\boldsymbol{x}))} \exp\left(\frac{E}{k_B T(t,\boldsymbol{x})}\right),$$

which depends on the choice of the functional forms of the weights φ_i. The choice of these weights can be adapted to the physical situation of the mixture.

7 Some Related Research Directions

Some other articles consider problems with a strong relationship with the subject of this note.

Bondesan, Boudin and Grec [6] derive a numerical method for the Euler equations describing a mixture, stable with respect to the relaxation parameter, whose limit is the Maxwell–Stefan system.

Briant and Grec have studied in [15] the asymptotics of the Boltzmann system (5)–(6) in a framework different from the one studied in [8]. They suppose that, at the leading order, the species velocities are identical and obtain a cross-diffusion system of Fick type, not equivalent to the Maxwell–Stefan systems because the two matrices linking fluxes and concentrations are not invertible.

A relationship between the Fick diffusion and Maxwell–Stefan diffusion has been investigated by Salvarani and Soares in [27]. They rigorously prove the relaxation of the Maxwell–Stefan system, together with the equimolar closure relationship (2), towards a system of uncoupled linear diffusion equations of Fickian type.

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References

1. B. Anwasia, The Maxwell-Stefan diffusion limit of a hard-sphere kinetic model for mixtures, *From Particle Systems to Partial Differential Equations* (Springer, 2021), pp. 15–36
2. B. Anwasia, M. Bisi, F. Salvarani, A.J. Soares, On the Maxwell-Stefan diffusion limit for a reactive mixture of polyatomic gases in non-isothermal setting. Kineti. Relat. Models **13**, 63 (2020)
3. B. Anwasia, P. Gonçalves, A.J. Soares, On the formal derivation of the reactive Maxwell-Stefan equations from the kinetic theory. EPL (Europhys. Lett.) **129**(4), 40005 (2020)
4. B. Anwasia, P. Gonçalves, A.J. Soares, From the simple reacting sphere kinetic model to the reaction-diffusion system of Maxwell-Stefan type. Commun. Math. Sci. **17**(2), 507–538 (2019)
5. L. Boltzmann, Weitere Studien über das Wärmegleichgewicht unter Gasmoläkulen. Sitzungsberichte der Akademie der Wissenschaften **66**, 275–370 (1872)
6. A. Bondesan, L. Boudin, B. Grec, A numerical scheme for a kinetic model for mixtures in the diffusive limit using the moment method. Numer. Methods Partial Differ. Equs. **35**(3), 1184–1205 (2019)
7. A. Bondesan, M. Briant, Perturbative Cauchy theory for a flux-incompressible Maxwell-Stefan system in a non-equimolar regime. arXiv:1910.03279
8. A. Bondesan, M. Briant, Stability of the Maxwell-Stefan system in the diffusion asymptotics of the Boltzmann multi-species equation. arXiv:1910.08357
9. C. Borgnakke, P.S. Larsen, Statistical collision model for Monte Carlo simulation of polyatomic gas mixture. J. Comput. Phys. **18**(4), 405–420 (1975)
10. D. Bothe, On the Maxwell-Stefan approach to multicomponent diffusion, in *Parabolic Problems*, *Volume 80 of Progress Nonlinear Differential Equations Application* (Birkhäuser/Springer Basel AG, Basel, 2011), pp. 81–93
11. L. Boudin, B. Grec, V. Pavan, The Maxwell-Stefan diffusion limit for a kinetic model of mixtures with general cross sections. Nonlinear Anal. **159**, 40–61 (2017)
12. L. Boudin, B. Grec, F. Salvarani, A mathematical and numerical analysis of the Maxwell-Stefan diffusion equations. Discret. Contin. Dyn. Syst. Ser. B **17**(5), 1427–1440 (2012)
13. L. Boudin, B. Grec, F. Salvarani, The Maxwell-Stefan diffusion limit for a kinetic model of mixtures. Acta Appl. Math. **136**, 79–90 (2015)
14. J.-F. Bourgat, L. Desvillettes, P. Le Tallec, B. Perthame, Microreversible collisions for polyatomic gases and Boltzmann's theorem. European J. Mech. B Fluids **13**(2), 237–254 (1994)

15. M. Briant, B. Grec, Rigorous derivation of the Fick cross-diffusion system from the multi-species Boltzmann equation in the diffusive scaling. arXiv:2003.07891
16. L. Desvillettes, R. Monaco, F. Salvarani, A kinetic model allowing to obtain the energy law of polytropic gases in the presence of chemical reactions. Eur. J. Mech. B Fluids **24**(2), 219–236 (2005)
17. A. Ern, V. Giovangigli, *Multicomponent Transport Algorithms*, vol. 24. Lecture Notes in Physics Monographs New Series M (Springer, Berlin, 1994)
18. V. Giovangigli, *Multicomponent Flow Modeling*. Modeling and Simulation in Science, Engineering and Technology (Birkhäuser Boston Inc., Boston, MA, 1999)
19. H. Grad, Principles of the kinetic theory of gases, in *Handbuch der Physik (herausgegeben von S. Flügge), Bd. 12, Thermodynamik der Gase* (Springer-Verlag, Berlin-Göttingen-Heidelberg, 1958), pp. 205–294
20. H. Grad, Asymptotic theory of the Boltzmann equation. II, in *Rarefied Gas Dynamics (Proceedings 3rd International Symposium, Palais de l'UNESCO, Paris, 1962), Vol. I*, pages 26–59. Academic Press, New York, 1963
21. M. Groppi, G. Spiga, Kinetic approach to chemical reactions and inelastic transitions in a rarefied gas. J. Math. Chem. **26**(1–3), 197–219 (1999)
22. H. Hutridurga, F. Salvarani, Maxwell-Stefan diffusion asymptotics for gas mixtures in non-isothermal setting. Nonlinear Anal. **159**, 285–297 (2017)
23. H. Hutridurga, F. Salvarani, On the Maxwell-Stefan diffusion limit for a mixture of monatomic gases. Math. Methods Appl. Sci. **40**(3), 803–813 (2017)
24. M.T. Marron, Simple collision theory of reactive hard spheres. J. Chem. Phys **52**(8), 4060–4061 (1970)
25. J.C. Maxwell, On the dynamical theory of gases. Philos. Trans. R. Soc. **157**, 49–88 (1866)
26. T.F. Morse, Kinetic model equations for a gas mixture. Phys. Fluids **7**, 908–918 (1964)
27. F. Salvarani, A.J. Soares, On the relaxation of the Maxwell-Stefan system to linear diffusion. Appl. Math. Lett. **85**, 15–21 (2018)
28. L. Sirovich, Kinetic modeling of gas mixtures. Phys. Fluids **5**(8), 908–918 (1962)
29. J. Stefan, Über das Gleichgewicht und die Bewegung insbesondere die Diffusion von Gasgemengen. Akad. Wiss. Wien **63**, 63–124 (1871)
30. R. Taylor, R. Krishna, *Multicomponent Mass Transfer*, vol. 2 (Wiley, New York, 1993)
31. C. Villani, A review of mathematical topics in collisional kinetic theory, in *Handbook of Mathematical Fluid Dynamics*, vol. I (North-Holland, Amsterdam, 2002), pp. 71–305

Alternative Quantum Formulations and Systems at the Classical-Quantum Border

R. Vilela Mendes

Abstract There are, at least, three completely equivalent formulations of quantum mechanics: the Hilbert space approach, the phase-space deformation approach and the tomographic one. The Hilbert space approach is the most widely used to describe dynamics at the microscopic level. However, with the recent emergence of "quantum technology" it became important to have appropriate models for systems with behavior at the classical-quantum border. For these systems, the deformation and tomographic approaches turn out to be more convenient than the Hilbert space one. This paper presents a short review of the alternative quantum formalisms as well as some applications, one of them discussed at the Nice conference.

Keywords Phase-space deformation · Quantum tomography · Quantum kinetics · Quantum complexity

1 Introduction

There are, at least, three completely equivalent formulations of quantum mechanics: the Hilbert space approach, the phase-space deformation approach and the tomographic one.[1] In the Hilbert space approach quantum states are mapped to rays in Hilbert space and physical measurable quantities are obtained from expectation values of the self-adjoint operators that represent observables. This is the most widely used formalism to describe dynamics at the microscopic level. However, with the recent developments in quantum technology it became important to have suitable models for systems with a behavior at the classical-quantum border. For these systems, it would be convenient to have a "smooth" transition between the phase space

[1] For other formulations of quantum mechanics see D. F. Styer et al. Am. J. Phys. 70 (2002) 288–297. Here however I have emphasized those that seem most useful to describe systems at the classical-quantum border.

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description of classical dynamics and the quantum phenomena. This is achieved by a phase space formulation of quantum mechanics, the quantum effects corresponding to a replacement of the classical commutative algebra of velocity and momenta by a non-commutative algebra. Likewise the non-commutative nature of quantum observables is circumvented in the tomographic approach by dealing with linear combinations of the noncommuting observables, the full scope of quantum dynamics being obtained by varying the coefficients in the linear combination. The Hilbert space approach being very familiar, this paper only presents a short review of the other two quantum formalisms as well as some applications. Finally it is pointed out that the alternative approaches corresponding to a replacement of the operators by functions (operator symbols) with a non-commutative algebra, it is, in principle, possible to develop many other equivalent formalisms for quantum mechanics. This is formalized in a quantizer-dequantizer framework.

2 Quantum Mechanics and Deformation Theory

The phase space of classical mechanics is a symplectic manifold $W = (T^*M, \omega)$ where T^*M is the cotangent bundle over the configuration space M and ω is a symplectic form. In local (Darboux) coordinates (p_i, q_i) the symplectic form is

$$\omega = \sum dp_i \wedge dq_i \tag{1}$$

The Poisson bracket gives a Lie algebra structure to the C^∞-functions on W, namely

$$\{f, g\} = \sum_i \frac{\partial f}{\partial q_i}\frac{\partial g}{\partial p_i} - \frac{\partial f}{\partial p_i}\frac{\partial g}{\partial q_i} \tag{2}$$

in local coordinates.

The transition to quantum mechanics is now regarded as a deformation of this Poisson algebra [1]. Let for example $T^*M = \boldsymbol{R}^{2n}$. Then,

$$\omega = \sum_{1 \le i,j \le n} \omega_{ij} dx^i \wedge dx^j = \sum_{1 \le i \le n} dx^i \wedge dx^{i+n} \tag{3}$$

Consider the following bidifferential operator

$$P^r(f, g) = \sum_{\substack{i_1 \cdots i_r \\ j_1 \cdots j_r}} \omega^{i_1 j_1} \cdots \omega^{i_r j_r}\, \partial_{i_1} \cdots \partial_{i_r}(f) \partial_{j_1} \cdots \partial_{j_r}(g) \tag{4}$$

$P^1(f, g)$ is the Poisson bracket. $P^3(f, g)$ is a non-trivial 2-cocycle and, barring obstructions, one expects the existence of non-trivial deformations of the Poisson

algebra. Existence of non-trivial deformations have indeed been proved in a very general context [2–5]. They always exist if W is finite-dimensional and for a flat Poisson manifold they are all equivalent to the Moyal [6] bracket

$$[f, g]_M = \frac{2}{\hbar} sin\left(\frac{\hbar}{2}P\right)(f, g) = \{f, g\} - \frac{\hbar^2}{4.3!}P^3(f, g) + \cdots \tag{5}$$

Moreover $[f, g]_M = \frac{1}{i\hbar}(f *_\hbar g - g *_\hbar f)$ where $f *_\hbar g$ is an associative star-product

$$f *_\hbar g = \exp\left(i\frac{\hbar}{2}P(f, g)\right) \tag{6}$$

Correspondence with quantum mechanics formulated in Hilbert space is obtained by the Weyl quantization prescription. Let $f(p, q)$ be a function in phase space and $\widetilde{f}$ its Fourier transform. Then, if to the function f we associate the Hilbert space operator

$$\boldsymbol{\Omega}(f) = \int \widetilde{f}(x_i, y_i) e^{-\frac{i}{\hbar}\sum x_i Q_i + y_i P_i}\, dx_i dy_i \tag{7}$$

where $Q_i \boldsymbol{\psi} = \boldsymbol{x}_i \boldsymbol{\psi}$ and $P_i = -i\hbar \frac{\partial}{\partial x_i}\boldsymbol{\psi}$, one finds

$$[\boldsymbol{\Omega}(f), \boldsymbol{\Omega}(g)] = i\hbar \boldsymbol{\Omega}([f, g]_M) \tag{8}$$

with, in the left-hand side, the usual commutator for Hilbert space operators and in right hand side the Moyal bracket. Therefore quantum mechanics may be described either by associating self-adjoint operators in Hilbert space to the observables or, equivalently, staying in the classical setting of phase-space functions but deforming their product to a $*_\hbar$- product and their Poisson brackets to Moyal brackets.

Time evolution of the observables is described by the Moyal equation

$$\frac{\partial}{\partial t} f = [f, H]_M = \frac{1}{i\hbar}(f *_\hbar H - H *_\hbar f) \tag{9}$$

Somewhat related to quantization by deformation is the geometric quantization theory. Geometric quantization [7] is a very nice and profound theory. Starting from a classical phase-space it aims to construct, in a consistent manner, a Hilbert space representing the corresponding quantum theory. The final product being a Hilbert space, a setting quite different from the classical phase-space, geometric quantization is probably not so useful to study systems at the classical-quantum border. I might be wrong.

Here is a brief sketch of the geometric quantization scheme: One starts from a manifold M with a symplectic structure ω and construct a Hermitean line bundle L with a connection of curvature $-i\omega$. L is the prequantization line bundle and the Hilbert space H_0 of square-integrable sections of L is the prequantum Hilbert space. Smooth functions on M are mapped to operators on H_0 taking Poisson brackets to

commutators. H_0 is in general too big a space. H_0 is then cut down by polarization, which picks out a subspace P_x of the complexified tangent space at $x \in M$. The quantum Hilbert space H is then defined to be the space of square-integrable sections of L that yield zero when we take their covariant derivative at any point x in the direction of any vector in P_x.

3 Quantum Mechanics in the Tomography Approach

The tomography approach may be used both for classical and quantum mechanics, which makes the classical-quantum transition quite easy. One therefore starts by describing the tomography formulation of classical statistical mechanics. States in classical statistical mechanics are described by a function $\rho\,(x,\ p)$, which is the probability distribution in phase space,

$$\rho\,(x,\ p) \geq 0\,, \qquad \int \rho\,(x,\ p)\ dp = P(x)\,, \qquad \int \rho\,(x,\ p)\ dx = \widetilde{P}(p)\,, \tag{10}$$

$P(x)$ and $\widetilde{P}(p)$ being the (marginal) probability distributions for position and momentum.

The density function $\rho\,(x,\ p)$ is normalized

$$\int \rho\,(x,\ p)\ dx\,dp = 1\,.$$

Consider now a parametrized observable, a linear function on the phase space of the system,

$$X\,(x,\ p) = \mu x + \nu p\,, \tag{11}$$

The variable $X\,(x,\ p)$ can be considered as the position of the system when measured in a rotated and rescaled reference frame in the classical phase space. All the position and momentum features of the system are obtained by varying the μ and ν parameters. The tomography map is defined as

$$M\,(X,\ \mu,\ \nu) = \frac{1}{2\,\pi} \int e^{-ik(X-\mu x-\nu p)}\ \rho\,(x,\ p)\ dx\,dp\,dk\,. \tag{12}$$

which is an homogeneous function,

$$M\,(\lambda X,\ \lambda\mu,\ \lambda\nu) = |\lambda|^{-1} M\,(X,\ \mu,\ \nu)\,, \tag{13}$$

and the Eq. (12) can be inverted,

$$\rho\,(x,\ p) = \frac{1}{4\,\pi^2}\int M\,(X,\ \mu,\ \nu)\,\exp\left[-i\,(\mu x + \nu p - X)\right]\,dX\,d\mu\,d\nu\,. \tag{14}$$

Therefore the classical system may be equivalently described by the phase space density $\rho\,(x,\ p)$ or by the tomography map. The tomography map cannot be an arbitrary function, it must be such that the corresponding $\rho\,(x,\ p)$ in (12) is a nonnegative function. As seen from (12) the classical tomography map is the Fourier transform of a characteristic function

$$M\,(X) = \frac{1}{2\,\pi}\int \langle e^{ikX}\rangle e^{-ikX}\,dk \tag{15}$$

which is a real nonnegative function. Furthermore

$$M\,(X) = \int \rho\,(x,\ p)\ \delta\,(X(x,\ p) - X)\ dx\,dp\,. \tag{16}$$

and

$$\int M\,(X)\ dX = \int \rho\,(x,\ p)\ dx\,dp = 1\,. \tag{17}$$

The evolution equation for the classical phase space density of a particle with mass $m = 1$ and potential $V(x)$,

$$\frac{\partial\rho\,(x,\ p,\ t)}{\partial t} + p\,\frac{\partial\rho\,(x,\ p,\ t)}{\partial x} - \frac{\partial V(x)}{\partial x}\,\frac{\partial\rho\,(x,\ p,\ t)}{\partial p} = 0 \tag{18}$$

can be rewritten in terms of the tomography map $M\,(X,\ \mu,\ \nu,\ t)$

$$\dot{M} - \mu\frac{\partial}{\partial\nu}M - \frac{\partial V}{\partial x}\,(\widetilde{q})\left[\nu\frac{\partial}{\partial X}M\right] = 0\,, \tag{19}$$

with the argument of the function $\partial V/\partial x$ being replaced by the operator

$$\widetilde{q} = -\left(\frac{\partial}{\partial X}\right)^{-1}\frac{\partial}{\partial\mu}\,. \tag{20}$$

For the mean value of position in classical statistical mechanics, one has

$$\langle x\rangle = \int \rho\,(x,\ p)\,x\,dx\,dp = i\int M\,(X,\ \mu,\ \nu)\,e^{iX}\,\delta'\,(\mu)\ \delta\,(\nu)\ dX\,d\mu\,d\nu\,. \tag{21}$$

In quantum mechanics one considers the observable ($\hbar = 1$)

$$\widehat{X} = \mu\hat{q} + \nu\hat{p}\,, \tag{22}$$

$\hat{q}$ and $\hat{p}$ being the quantum position and momentum. The quantum tomography map may be defined directly from the wave function or the density matrix. However it was originally defined [8–12] in terms of the Wigner function $W(q,\ p)$ as follows:

$$M\,(X,\ \mu,\ \nu) = \int \exp\left[-ik(X - \mu q - \nu p)\right] W(q,\ p)\,\frac{dk\,dq\,dp}{(2\pi)^2}\,. \tag{23}$$

One sees that the formula (23) is identical to (12) of the classical case. For a pure state, with wave function $\Psi\,(y)$, the quantum tomography map has the form [13]

$$M\,(X,\ \mu,\ \nu) = \frac{1}{2\,\pi\,|\nu|}\left|\int \Psi\,(y) \exp\left(\frac{i\,\mu y^2}{2\nu} - \frac{iyX}{\nu}\right) dy\right|^2. \tag{24}$$

From Eq. (24) one sees that the tomography map is the amplitude squared of a projection of the quantum state on the eigenvectors of the operator $\widehat{X}$ in (22).

The formula (23) can be inverted and, as in the classical case, the Wigner function can be expressed in terms of the tomography map [8],

$$W(q,\ p) = \frac{1}{2\pi}\int M\,(X,\ \mu,\ \nu) \exp\left[-i\,(\mu q + \nu p - X)\right]\,d\mu\,d\nu\,dX\,. \tag{25}$$

As was shown in [10], for systems with the Hamiltonian

$$H = \frac{\hat{p}^2}{2} + V(\hat{q})\,, \tag{26}$$

the tomography map satisfies a quantum time-evolution equation

$$\begin{aligned}\dot{M} - \mu\,\frac{\partial}{\partial\nu}\,M - i\left[V\left(-\frac{1}{\partial/\partial X}\,\frac{\partial}{\partial\mu} - i\,\frac{\nu}{2}\,\frac{\partial}{\partial X}\right)\right.\\ \left. - V\left(-\frac{1}{\partial/\partial X}\,\frac{\partial}{\partial\mu} + i\,\frac{\nu}{2}\,\frac{\partial}{\partial X}\right)\right] M = 0\,,\end{aligned} \tag{27}$$

which is an alternative to the Schrödinger equation.

The evolution Eq. (27) can also be presented in the form

$$\dot{w} - \mu\,\frac{\partial w}{\partial\nu} - \frac{\partial V}{\partial x}\,(\widetilde{q})\,\nu\,\frac{\partial}{\partial X}\,w + 2\sum_{n=1}^{\infty}\frac{V^{2n+1}\,(\widetilde{q})}{(2n+1)!}\left(\frac{\nu}{2}\,\frac{\partial}{\partial X}\right)^{2n+1}(-1)^{n+1}w = 0\,, \tag{28}$$

where $\widetilde{q}$ is given by (20) and

$$V^{2n+1}\,(\widetilde{q}) \equiv \frac{d^{2n+1}V}{dq^{2n+1}}\,(\widetilde{q})\,.$$

This evolution equation is in fact Moyal equation (9) in the tomography representation.

The tomography approach has another interesting application in another classical, but non-commutative, context. In signal processing one deals with time and frequency which, as $\hat{q}$ and $\hat{p}$, are also non-commutative variables. Then, the tomography map, being a positive quantity with a probability interpretation, provides a robust and unambiguous tool for feature extraction in signal processing [13–18].

4 Applications

In this section one illustrates the use of the alternative quantum formulations in two situations where the classical-quantum border is quite apparent. The deformation approach is quite appropriate to obtain the quantum formulation, or quantum corrections, to the kinetic equations, because the natural setting of such equations is the phase space of positions and momenta. On the other hand, another notion that is very useful in classical mechanics is the notion of sensitive dependence to initial conditions or chaotic behavior. In classical mechanics this notion finds a rigorous formulation through the Lyapunov exponents of the dynamics. However, it is not obvious how to correctly carry the notion of Lyapunov exponent to quantum mechanics in the Hilbert space formulation. By first defining classical Lyapunov exponents in a tomographic formulation it becomes an easy matter to carry them to quantum mechanics and then, if needed, to carry the definition to Hilbert space. Of course this is possible because all the alternative formulations are equivalent. To use one or another is a question of computational and conceptual convenience. Another situation of current interest at the classical-quantum border is the cooling of levitated nanoparticles [19].

4.1 Kinetic Equations and Quantum Corrections

A kinetic equation deals with the evolution of a probability density $f(t, x, p)$ of particles in phase space. The typical form is

$$\frac{\partial}{\partial t} f + \frac{p}{m} \cdot \nabla_x f + F_{ext} \cdot \nabla_p f = S(f) \tag{29}$$

the left hand side being a drift term defining the characteristics along which the particles move between collisions and the right hand side a collision term. It is therefore an equation involving a probability distribution in the (x, p) phase space. In quantum mechanics $f(x, p)$ cannot be a classical probability distribution because x and p are non-commuting variables. However $f(x, p)$ may be interpreted as a functional of elements in an algebra with a deformed product and, as discussed before, this leads to the correct quantum results.

It is therefore tempting, to obtain the quantum corrections to Eq. (29), by simply replacing all products by deformed products. However, recalling that at the basis of the deformation interpretation of quantum mechanics is the deformation of a Poisson algebra, it is more appropriate to deform the kinetic equation when their (canonical or non-canonical) Hamiltonian structure is exhibited. This is the approach that will be followed.

4.1.1 The Poisson–Vlasov Equation

The Poisson–Vlasov equation describing a collisionless plasma with purely electrostatic interactions is

$$\frac{\partial f}{\partial t} + \frac{p}{m} \cdot \frac{\partial f}{\partial x} - e \frac{\partial \phi}{\partial x} \cdot \frac{\partial f}{\partial p} = 0 \tag{30}$$

with

$$\triangle \phi = -e \int dp f\,(x, p, t) \tag{31}$$

It is a non-canonical Hamiltonian system [20], with Hamiltonian,

$$H_{PV} = \frac{1}{2} \int \left| \frac{p}{2m} \right|^2 f\,(x, p, t)\, dxdp + e \int dx \phi\,(x) \int f\,(x, p, t)\, dp \tag{32}$$

the time evolution of arbitrary phase-space functions given by

$$\frac{dF}{dt} = [F, H_{PV}] \tag{33}$$

the Poisson structure $[\cdot, \cdot]$ being

$$[F, G] = \int f \left\{ \frac{\delta F}{\delta f}, \frac{\delta G}{\delta f} \right\} dxdp \tag{34}$$

where $\{\cdot, \cdot\}$ stands for the usual Poisson bracket for functions of x and p

$$\{A, B\} = \sum_i \left(\frac{\partial A}{\partial x_i} \frac{\partial B}{\partial p_i} - \frac{\partial A}{\partial p_i} \frac{\partial B}{\partial x_i} \right) \tag{35}$$

and the functional derivative $\frac{\delta F}{\delta f}$ being related to the Fréchet derivative by

$$\left(D_f F\right) \cdot f' = \int \frac{\delta F}{\delta f} f' dxdv \tag{36}$$

Taking into attention that

$$\frac{\delta f\,(y,\mu,t)}{\delta f\,(x,p,t)} = \delta^3\,(y-x)\,\delta^3\,(\mu-p)$$
$$\frac{\delta H_{PV}}{\delta f\,(x,p,t)} = \frac{1}{2m}\,|p|^2 + e\phi\,(x) \tag{37}$$

and using Eq. (34) one obtains the classical Poisson–Vlasov equation

$$\frac{df}{dt} = [f, H_{PV}] = -\frac{p}{m}\cdot\nabla_x f + e\nabla_x\phi\cdot\nabla_p f \tag{38}$$

For the quantum version all one has to do is to replace in Eq. (34) the Poisson bracket (35) by the Moyal bracket (5).

$$\frac{df}{dt} = \int d^3x d^3p f\,(x,p,t)\,\frac{2}{\hbar}\sin\left(\frac{\hbar}{2}P\right)\left(\frac{\delta f}{\delta f},\frac{\delta H_{PV}}{\delta f}\right) \tag{39}$$

P being the bidifferential operator in (4).

Of special interest is the leading quantum correction. The 6-dimensional ω matrix in the symplectic form (3) has $\omega_{i,i+3} = -\omega_{i+3,i} = 1$ with all the other elements being zero. Because $\frac{\delta H_{PV}}{\delta f(x,p,t)}$ is quadratic in p, all terms in $\omega_{i,i+3}\omega_{j,j+3}\omega_{k,k+3}$ vanish. Finally one obtains in leading $\hbar^2$ order,

$$\frac{df}{dt} = \left[f, H_{PV}\right]_M = -\frac{p}{m}\cdot\nabla_x f + e\nabla_x\phi\cdot\nabla_p f - e\frac{\hbar^2}{24}\sum_{i,j,k=1}^{3}\frac{\partial^3 f}{\partial p_i\partial p_j\partial p_k}\frac{\partial^3\phi}{\partial x_i\partial x_j\partial x_k} + O\left(\hbar^4\right) \tag{40}$$

4.1.2 The Maxwell–Vlasov Equation

The Maxwell–Vlasov equation,

$$\frac{\partial f}{\partial t} + v\cdot\nabla_x f + \frac{e}{m}\left(E + \frac{v\times B}{c}\right)\cdot\nabla_v f = 0 \tag{41}$$

describing a classical collisionless plasma in an electromagnetic field, is also a non-canonical Hamiltonian system. There are several variational formulations of the Maxwell–Vlasov system, the most complete one being probably the one by Marsden and Weinstein [21]. However, in their formulation, part of the dynamics is coded on the Poisson structure rather than on the Hamiltonian and to apply the deformation theory for the transition to quantum mechanics, one would also need to handle the deformation of the electromagnetic field dynamics, not just the replacement of the Poisson bracket involving position and momentum of the particles. Hence, because here one only wants to obtain the quantum corrections to the f dynamics, it is more convenient to use the Low [22] Hamiltonian,

$$H_{MV} = \int d^3x d^3p \left\{ \frac{1}{2m} \left(p - \frac{e}{c} A \right)^2 + e\phi\,(x) \right\} f\,(x,\, p,\, t) + \int d^3x \left(E^2 + B^2 \right) \tag{42}$$

where $E = -\nabla_x \phi - \frac{1}{c} \frac{\partial A}{\partial t}$, $B = \nabla \times A$ in terms of the independent variables $(\phi,\, A)$.

The Poisson structure is the same as in (34) for the f dynamics. With this Hamiltonian

$$\frac{\delta H_{MV}}{\delta f\,(x,\, p,\, t)} = \frac{1}{2m} \left(p^2 - \frac{e}{c} \left(p \cdot A + A \cdot p \right) + \frac{e^2}{c^2} A^2 \right) + e\phi\,(x) \tag{43}$$

Then, using (34) and (35) one obtains for the classical equation

$$\begin{aligned} \frac{\partial f}{\partial t} &= -\frac{1}{m} \left(p - \frac{e}{c} A \right) \cdot \nabla_x f + \left(\frac{e}{m} \nabla_x \phi - \frac{e}{mc} p \cdot \nabla_x A + \frac{e^2}{2mc^2} \nabla_x A^2 \right) \cdot \nabla_p f \\ &= -\frac{1}{m} \left(p - \frac{e}{c} A \right) \cdot \nabla_x f + \left(-eE - \frac{e}{c} v \times B - \frac{e}{c} \frac{dA}{dt} \right) \cdot \nabla_p f \end{aligned} \tag{44}$$

with

$$\begin{aligned} \frac{dA}{dt} &= \frac{\partial A}{\partial t} + v \cdot \nabla_x A \\ v &= \frac{1}{m} \left(p - \frac{e}{c} A \right) \end{aligned} \tag{45}$$

Equation (44) is the same as (41) written in the variables $(x,\, p)$ instead of $(x,\, v)$. The first set is the most convenient one because the Moyal bracket deformation acts on these variables. Then, the quantum Maxwell–Vlasov equation becomes[2]

$$\frac{\partial f}{\partial t} = \int d^3x d^3p f\,(x,\, p,\, t)\, \frac{2}{\hbar} \sin \left(\frac{\hbar}{2} P \right) \left(\frac{\delta f}{\delta f},\, \frac{\delta H_{MV}}{\delta f} \right) \tag{46}$$

and, computing the leading quantum corrections, one obtains

$$\begin{aligned} \frac{\partial f}{\partial t} ==& -\frac{1}{m} \left(p - \frac{e}{c} A \right) \cdot \nabla_x f + \left(-eE - \frac{e}{c} v \times B - \frac{e}{c} \frac{dA}{dt} \right) \cdot \nabla_p f \\ &- \frac{e\hbar^2}{24} \sum_{i,j,k=1}^{3} \frac{\partial^3 f}{\partial p_i \partial p_j \partial p_k} \frac{\partial^3}{\partial x_i \partial x_j \partial x_k} \left(\phi + \frac{e}{2mc^2} A^2 \right) \\ &+ \frac{e\hbar^2}{24mc} \sum_{i,j,k=1}^{3} \left(\frac{\partial^3 f}{\partial p_i \partial p_j \partial p_k} p \cdot \frac{\partial^3 A}{\partial x_i \partial x_j \partial x_k} - 3 \frac{\partial^3 f}{\partial x_i \partial p_j \partial p_k} \frac{\partial^2 A_k}{\partial x_j \partial x_k} \right) + O\left(\hbar^4 \right) \end{aligned} \tag{47}$$

[2]Notice that in the Hamiltonian, products should also be replaced by $*$-products. However $p * A + A * p = 2p \cdot A$.

4.2 A Quantum Lyapunov Exponent

Bounded classical systems that are chaotic, display exponential growth of initial perturbations and other interesting long-time asymptotics, like exponential decay of correlations. In contrast, quantum Hamiltonians of bounded systems with time-independent potentials, having discrete spectrum, their wave functions are almost periodic functions. For this reason the work on "quantum chaos" has shifted from consideration of long-time properties to the statistics of energy levels of quantum systems with a chaotic classical counterpart.

However, quantum systems with bounded configuration space but time-dependent interactions (for example particles in an accelerator subjected to electromagnetic kicks or the systems used in quantum control) may have continuous spectrum. Therefore the estimation and control, of the rate of growth of the perturbed matrix elements of observables, becomes an issue of both theoretical and practical concern.

In classical mechanics the most important asymptotic indicator of chaotic behavior is the Lyapunov exponent (an ergodic invariant). Therefore a natural first step to discuss rates of growth in quantum mechanics seems to be the construction of a quantum Lyapunov exponent.

The tomography approach, because of the similarity of its structure in the classical and the quantum cases, seems to be an appropriate setting to carry out this construction. As a precondition it is necessary to carry the definition of Lyapunov exponent, usually defined in terms of orbits and tangent maps, to a definition in terms of densities. This was carried out in [23]. Given an initial density $\rho\,(x,\ p,\ t=0) \equiv \rho\,(x,\ p)$ for a classical particle, let it have a general time evolution defined by a smooth kernel

$$\rho\,(x,\,p,\,t) = \int \mathscr{K}\left(x,\,p,\,x',\,p',\,t\right)\rho\left(x',\,p'\right)\,dx'\,dp'. \tag{48}$$

The evolution of the distribution $\rho\,(x,\,p,\,t)$, described by Eq. (48), is equivalent to the action of the Frobenius–Perron operator used in [23, 24]. Consider now a small perturbation in the initial condition

$$\widetilde{\rho}\,(x,\,p) = \rho\,(x,\,p) + \varepsilon\,(\mathbf{n}\boldsymbol{\nabla})\,\delta(q)\,\delta(p)\,, \tag{49}$$

where

$$\mathbf{n} = (n_1, n_2)\,, \qquad \mathbf{n}^2 = 1\,, \qquad \boldsymbol{\nabla} = \left(\frac{\partial}{\partial x}, \frac{\partial}{\partial p}\right),$$

and

$$(\mathbf{n}\boldsymbol{\nabla}) = n_1\frac{\partial}{\partial x} + n_2\frac{\partial}{\partial p}\,.$$

The perturbed initial density evolves like

$$\rho(x, p, t) = \int \mathscr{K}\left(x, p, x', p', t\right)\left[\rho\left(x', p'\right) + \varepsilon\left(\mathbf{n}\nabla'\right)\delta(x')\,\delta(p')\right] dx'\,dp', \tag{50}$$

where

$$\nabla' = \left(\frac{\partial}{\partial x'}, \frac{\partial}{\partial p'}\right).$$

Let us now compare the expectation values, for example, of the position of the perturbed and unperturbed initial densities at time t

$$\Delta x(t) = \int x\left[\widetilde{\rho}(x, p, t) - \rho(x, p, t)\right] dx\,dp\,, \tag{51}$$

which equals

$$\Delta x(t) = \varepsilon \int x\mathscr{K}\left(x, p, x', p', t\right)\left(\nabla'\mathbf{n}\right)\delta(x')\delta(p')\,dx'\,dp'. \tag{52}$$

In order to obtain the Lyapunov exponent one computes

$$\lambda = \lim_{t\to\infty} \frac{1}{t} \log\left|\frac{\Delta x(t)}{\Delta x(0)}\right|. \tag{53}$$

leading to

$$\lambda = \lim_{t\to\infty} \frac{1}{t}\left\{\log \mid \varepsilon \int x\mathscr{K}\left(x, p, x', p', t\right) \times \left(\nabla'\mathbf{n}\right)\delta(x')\delta(p')\,dx'\,dp' - \log \mid \Delta x(0) \mid\right\}. \tag{54}$$

To translate this procedure to the tomography framework of classical mechanics, the initial probability density is transformed to an initial tomography map

$$\rho(x, p) \to M(X, \mu, \nu, t = 0) \equiv M(X, \mu, \nu)\,. \tag{55}$$

The density $\delta(x - x_0)\,\delta(p - p_0)$ is mapped to the tomography map

$$M_\delta(X, \mu, \nu) = \delta(X - \mu q_0 - \nu p_0)\,, \tag{56}$$

and the perturbed term

$$\widetilde{\rho}(x, p) - \rho(x, p) = (\mathbf{n}\nabla)\,\delta(x - x_0)\;\delta(p - p_0) \tag{57}$$

is mapped to the tomographic perturbation

$$M_\eta(X, \mu, \nu) = (n_1\mu + n_2\nu)\,\delta'(X - \mu q_0 - \nu p_0)\,, \tag{58}$$

The unperturbed and perturbed initial tomography maps evolve with the classical propagator $\Pi_{\mathrm{cl}}\left(X,\ \mu,\ \nu,\ X',\ \mu',\ \nu',\ t_2,\ t_1\right)$ that connects the maps at times t_1 and $t_2\ (t_2 > t_1)$

$$M\left(X,\mu,\nu,t_2\right) = \int \Pi_{\mathrm{cl}}\left(X,\mu,\nu,X',\mu',\nu',t_2,t_1\right) M\left(X',\mu',\nu',t_1\right)\, dX'\, d\mu'\, d\nu'. \tag{59}$$

the propagator satisfying the equation

$$\begin{aligned}&\frac{\partial \Pi_{\mathrm{cl}}}{\partial t_2} - \mu\,\frac{\partial}{\partial \nu}\Pi_{\mathrm{cl}} - \frac{\partial V}{\partial x}\left(\widetilde{q}\right)\nu\,\frac{\partial}{\partial X}\Pi_{\mathrm{cl}}\\ &= \delta\left(t_2 - t_1\right)\delta\left(X - X'\right)\delta\left(\mu - \mu'\right)\delta\left(\nu - \nu'\right).\end{aligned}$$

hence,

$$\begin{aligned}M_\eta\left(X,\mu,\nu,t\right) = &\int \Pi_{\mathrm{cl}}\left(X,\mu,\nu,X',\mu',\nu',t\right)\\ &\times\left(n_1\mu' + n_2\nu'\right)\delta'\left(X' - \mu' q_0 - \nu' p_0\right)\, dX'\, d\mu'\, d\nu'.\end{aligned} \tag{60}$$

The position perturbations at time zero and time t are

$$\Delta x(0) = \varepsilon \int M_\eta\left(X,\mu,\nu\right) e^{iX}\delta'(\mu)\,\delta(\nu)\, dX\, d\mu\, d\nu$$

$$\Delta x(t) = \varepsilon \int M_\eta\left(X,\mu,\nu,t\right) e^{iX}\delta'(\mu)\,\delta(\nu)\, dX\, d\mu\, d\nu$$

and by replacement in (53) the classical Lyapunov exponent is expressed as a function of the tomography maps.

For the quantum Lyapunov exponent all one has to do is to obtain the quantum values of $\Delta x(0)$ and $\Delta x(t)$. This is obtained by replacing, in the Eqs. (59) and (60), the classical by the quantum propagator which satisfies the equation

$$\begin{aligned}&\frac{\partial \Pi}{\partial t_2} - \mu\,\frac{\partial \Pi}{\partial \nu} - \frac{\partial V}{\partial x}\left(\widetilde{q}\right)\nu\,\frac{\partial \Pi}{\partial X} + 2\sum_{n=1}^{\infty}\frac{V^{2n+1}\left(\widetilde{q}\right)}{(2n+1)!}\left(\frac{\nu}{2}\frac{\partial}{\partial X}\right)^{2n+1}(-1)^{n+1}\Pi\\ &= \delta\left(t_2 - t_1\right)\delta\left(X - X'\right)\delta\left(\mu - \mu'\right)\delta\left(\nu - \nu'\right),\end{aligned} \tag{61}$$

the quantum Lyapunov exponent being also obtained from (53).

After some algebra one arrives at the Lyapunov exponent expression in the quantum-mechanical case,

$$\begin{aligned}\lambda = \lim_{t\to\infty}\frac{1}{t}\log\Big|\int &dX\, d\mu'\, d\nu'\, X\left(n_1\mu' + n^2\nu'\right)\\ &\times\frac{\partial \Pi}{\partial X'}\left(X,1,0,X' \to \mu' q_0 + \nu' p_0,\mu',\nu',t\right)\Big|\ .\end{aligned} \tag{62}$$

A satisfactory construction was thus achieved [25] in the sense that the phase-space observables that are used are exactly the same in classical and quantum mechanics. The only difference between the classical and the quantum exponent lies in the time evolution dynamics.

It is of some interest to express this results in the Hilbert space framework of quantum mechanics [26]. The tomographic maps being related to traces of operators, it turns out that the quantum Lyapunov exponent measures the rate of growth of the trace of position and momentum observables starting from a singular initial density matrix. A positive Lyapunov exponent would correspond to exponential growth of these traces. However, the same quantities may serve to characterize other types of growth, leading to a generalized notion of quantum sensitive dependence.

There are examples where exponential rates of growth (as in classical chaos) are also found in quantum systems [25]. However, in many other cases, quantum mechanics seems to have a definite taming effect on classical chaos. Therefore, a generalized notion of quantum sensitive dependence, corresponding to rates of growth milder than exponential, might be of interest to classify different types of quantum complexity or to characterize the degree of accuracy achievable in quantum control.

As a first step rewrite the result for the quantum Lyapunov exponent along the phase-space vector $\nu = (\nu_1 \nu_2)$

$$\lambda_\nu = \lim_{t\to\infty} \frac{1}{t} \log \left\| \int d^n X\, d^n \mu\, d^n \nu e^{iX\bullet \mathbf{1}} \left(\begin{pmatrix} \nabla_\mu \\ \nabla_\nu \end{pmatrix} \delta^n(\mu)\delta^n(\nu) \right) M_t(X,\mu,\nu) \right\|$$

$$M_t(X,\mu,\nu) = \int \Pi\left(X,\ \mu,\ \nu,\ X',\ \mu',\ \nu',\ t,\ 0\right) M_0(X,\mu,\nu)\, dX'^n d\mu'^n d\nu'^n$$

$$M_0\left(X',\mu',\nu'\right) = \left((\nu_1 \circledast \mu' + \nu_2 \circledast \nu') \bullet \nabla_{X'}\right) \delta^n\left(X' - \mu' q_0 - \nu' p_0\right) \tag{63}$$

with $(a \circledast b)_i = a_i b_i$.

For a system with Hamiltonian

$$H = \frac{p^2}{2} + V(q)\,, \tag{64}$$

the evolution equation for the quantum propagator of the tomographic densities is

$$\begin{array}{l} \frac{\partial \Pi}{\partial t} - \mu \bullet \nabla_\nu \Pi - \nabla_x V(\widetilde{q}) \bullet (\nu \circledast \nabla_X \Pi) \\ + \frac{2}{\hbar} \sum_{n=1}^{\infty} (-1)^{n+1} \left(\frac{\hbar}{2}\right)^{2n+1} \frac{\nabla_{i_1 \cdots i_{2n+1}} V(\widetilde{q})}{(2n+1)!} (\nu \circledast \nabla_X)_{i_1} \cdots (\nu \circledast \nabla_X)_{i_{2n+1}} \Pi \\ = 0 \end{array} \tag{65}$$

with initial condition

$$\lim_{t\to t_0} \Pi\left(X,\mu,\nu,X',\mu',\nu',t,t_0\right) = \delta^n\left(X - X'\right) \delta^n\left(\mu - \mu'\right) \delta^n\left(\nu - \nu'\right) \tag{66}$$

reducing for $\hbar = 0$ to the classical evolution equation.

In the tomographic formulation, classical and quantum mechanics are both described by a set of positive probability distributions $M_t(X, \mu, \nu)$, the $\hbar$-deformation appearing only in the time-evolution. It is this fact that allows the notion of Lyapunov exponent to be carried over without ambiguity from classical to quantum mechanics. However, to relate the Lyapunov exponent to the behavior of operator matrix elements and the spectral properties of the Hamiltonian, it is more convenient to rewrite it as a functional of the density matrix $\rho\left(x, x^{'}\right)$. The first step is to consider the Fourier transform $G_t(\mu, \mu)$ of the tomographic density $M_t(X, \mu, \nu)$

$$G_t(\mu, \nu) \doteq G_t(1, \mu, \nu) = \int d^n X\, e^{iX\bullet\mathbf{1}} M_t(X, \mu, \nu) \tag{67}$$

and perform the integrals in (63) to obtain

$$\lambda\begin{pmatrix}\nu_1\\ \nu_2\end{pmatrix} = \lim_{t\to\infty}\frac{1}{t}\log\left\|\begin{array}{c}\nabla_\mu G_t(\mu, \nu)\mid_{\mu=\nu=0}\\ \nabla_\nu G_t(\mu, \nu)\mid_{\mu=\nu=0}\end{array}\right\| \tag{68}$$

Now, using the relation between the tomographic densities and the density matrix, namely

$$G_t(\mu, \nu) = \left(\frac{1}{2\pi}\right)^n \int d^n X\, d^n p d^n x d^n x^{'}\, e^{i\left(X\bullet\mathbf{1} - p\bullet\left(x-x^{'}\right)\right)}\rho_t\left(x, x^{'}\right) \tag{69}$$
$$\delta^n\left(X - \mu\circledast\left(\frac{x+x^{'}}{2}\right) + \nu\circledast p\right)$$

one easily obtains

$$\lambda\begin{pmatrix}\nu_1\\ \nu_2\end{pmatrix} = \lim_{t\to\infty}\frac{1}{t}\log\left\|\begin{array}{c}Tr\{\rho_t x\}\\ Tr\{\rho_t p\}\end{array}\right\| \tag{70}$$

the density matrix at time zero (corresponding to $M_0\left(X^{'}, \mu^{'}, \nu^{'}\right)$ in Eq. (63)) being

$$\rho_0\left(x, x^{'}\right) = -e^{ip_0\bullet\left(x-x^{'}\right)}\left\{(\nu_1\bullet\nabla)\,\delta^n\left(q_0 - \frac{x+x^{'}}{2}\right) + i\nu_2\bullet\left(x-x^{'}\right)\delta^n\left(q_0 - \frac{x+x^{'}}{2}\right)\right\} \tag{71}$$

Equation (70) means that the quantum Lyapunov exponent measures the exponential rate of growth of the expectation values of position and momentum, starting from the initial singular perturbation ρ_0. This is a rather appealing and intuitive form for the Lyapunov exponent.

Using the time-dependent operators in the Heisenberg picture

$$\begin{aligned}x_H(t) &= U^{\dagger}xU\\ p_H(t) &= U^{\dagger}pU\end{aligned} \tag{72}$$

one has an equivalent form for $\lambda_{\vec{v}}$

$$\lambda \begin{pmatrix} v_1 \\ v_2 \end{pmatrix} = \lim_{t\to\infty} \frac{1}{t} \log \left\| \begin{matrix} Tr' \{\rho_0 x_H(t)\} \\ Tr' \{\rho_0 p_H(t)\} \end{matrix} \right\| \tag{73}$$

where we have also defined

$$Tr' \{\rho_0 x_H(t)\} = Tr \{\rho_0 x_H(t)\} / Tr \{\rho_0 x_H(0)\}$$

Whenever $\rho_0 x_H(t)$ is a trace class operator, the term corresponding to $\mathrm{Tr}\{\rho_0 x_H(0)\}$ has no contribution in the $t \to \infty$ limit. On the other hand, by taking the appropriate cut-off and a limiting procedure, the above expression may also make mathematical sense even in some non-trace class cases.

5 Quantizers and Dequantizers: An Unified View of Alternative Quantum Formulations

Tomography maps may be framed not only as amplitudes of projections on a complete basis of eigenvectors of a family of operators, as in (24), but also as operator symbols [27]. That is, as a map of operators to a space of functions where the operators non-commutativity is replaced by a modification of the usual product to a star-product.

Let $\hat{A}$ be an operator in Hilbert space $\mathscr{H}$ and $\hat{U}(\mathbf{x})$, $\hat{D}(\mathbf{x})$ two families of operators called *dequantizers* and *quantizers*, respectively, such that

$$\mathrm{Tr}\left\{ \hat{U}(\mathbf{x}) \hat{D}(\mathbf{x}') \right\} = \delta(\mathbf{x} - \mathbf{x}') \tag{74}$$

The labels $\mathbf{x}$ (with components $x_1, x_2, \ldots x_n$) are coordinates in a linear space V where the functions (operator symbols) are defined. Some of the coordinates may take discrete values, then the delta function in (74) should be understood as a Kronecker delta. Provided the property (74) is satisfied, one defines the *symbol of the operator* $\hat{A}$ by the formula

$$f_A(\mathbf{x}) = \mathrm{Tr}\left\{ \hat{U}(\mathbf{x}) \hat{A} \right\}, \tag{75}$$

assuming the trace to exist. In view of (74), one has the reconstruction formula

$$\hat{A} = \int f_A(x) \hat{D}(\mathbf{x})\, d\mathbf{x} \tag{76}$$

The role of quantizers and dequantizers may be exchanged. Then

$$f_A^d(\mathbf{x}) = \mathrm{Tr}\left\{\hat{D}(\mathbf{x})\,\hat{A}\right\} \tag{77}$$

is called the dual symbol of $f_A(\mathbf{x})$ and the reconstruction formula is

$$\hat{A} = \int f_A^d(x)\hat{U}(\mathbf{x})\,d\mathbf{x} \tag{78}$$

Symbols of operators can be multiplied using the star-product kernel as follows

$$f_A(\mathbf{x}) \star f_B(\mathbf{x}) = \int f_A(\mathbf{y})\,f_B(\mathbf{z})\,K(\mathbf{y},\mathbf{z},\mathbf{x})\,d\mathbf{y}\,d\mathbf{z} \tag{79}$$

the kernel being

$$K(\mathbf{y},\mathbf{z},\mathbf{x}) = \mathrm{Tr}\left\{\hat{D}(\mathbf{y})\hat{D}(\mathbf{z})\hat{U}(\mathbf{x})\right\} \tag{80}$$

The star-product is associative,

$$(f_A(\mathbf{x}) \star f_B(\mathbf{x})) \star f_C(\mathbf{x}) = f_A(\mathbf{x}) \star (f_B(\mathbf{x}) \star f_C(\mathbf{x})) \tag{81}$$

this property corresponding to the associativity of the product of operators in Hilbert space.

With the dual symbols the trace of an operator may be written in integral form

$$\mathrm{Tr}\left\{\hat{A}\hat{B}\right\} = \int f_A^d(\mathbf{x})\,f_B(\mathbf{x})\,d\mathbf{x} = \int f_B^d(\mathbf{x})\,f_A(\mathbf{x})\,d\mathbf{x}. \tag{82}$$

For two different symbols $f_A(\mathbf{x})$ and $f_A(\mathbf{y})$ corresponding, respectively, to the pairs $(\hat{U}(\mathbf{x}),\hat{D}(\mathbf{x}))$ and $(\hat{U}_1(\mathbf{y}),\hat{D}_1(\mathbf{y}))$, one has the relation

$$f_A(\mathbf{x}) = \int f_A(\mathbf{y})K(\mathbf{x},\mathbf{y})\,d\mathbf{y}, \tag{83}$$

with intertwining kernel

$$K(\mathbf{x},\mathbf{y}) = \mathrm{Tr}\left\{\hat{D}_1(\mathbf{y})\hat{U}(\mathbf{x})\right\} \tag{84}$$

Let now a wave function be identified with the projection operator Π_ψ on the function $\psi\,(t)$, denoted by

$$\Pi_\psi = |\psi\rangle\,\langle\psi| \tag{85}$$

Then the tomography maps (tomograms), and also other transforms, are symbols of the projection operators for several choices of quantizers and dequantizers.

Some examples:

Denote position and momentum by q and p (for signal processing the corresponding set of non-commuting variable would be t and ω).

The *Wigner–Ville function*: is the symbol of $|\,\psi\rangle\langle\psi\,|$ corresponding to the dequantizer

$$\hat{U}(\mathbf{x}) = 2\hat{\mathscr{D}}(2\alpha)\hat{P}, \qquad \alpha = \frac{q+ip}{\sqrt{2}} \tag{86}$$

where $\hat{P}$ is the inversion operator

$$\hat{P}\psi(q) = \psi(-q) \tag{87}$$

and $\hat{\mathscr{D}}(\gamma)$ is a "displacement" operator

$$\hat{\mathscr{D}}(\gamma) = \exp\left[\frac{1}{\sqrt{2}}\gamma\left(q - \frac{\partial}{\partial q}\right) - \frac{1}{\sqrt{2}}\gamma^*\left(q + \frac{\partial}{\partial q}\right)\right] \tag{88}$$

The quantizer operator is

$$\hat{D}(\mathbf{x}) := \hat{D}(q, p) = \frac{1}{2\pi}\hat{U}(q, p), \tag{89}$$

The Wigner function is

$$W(q, p) = 2\mathrm{Tr}\left\{|\,\psi\rangle\langle\psi\,|\,\hat{D}(2\alpha)\hat{D}\right\} \tag{90}$$

or, in integral form

$$W(q, p) = 2\int \psi^*(q)\hat{\mathscr{D}}(2\alpha)\psi(-q)\,dq \tag{91}$$

The *symplectic tomogram* (position-momentum or time-frequency in signal processing) tomogram of $|\,\psi\rangle\langle\psi\,|$ corresponds to the dequantizer

$$\hat{U}(\mathbf{x}) := \hat{U}(X, \mu, \nu) = \delta\left(X\hat{1} - \mu\hat{q} - \nu\hat{p}\right), \tag{92}$$

Here the notation $\delta\left(X\hat{1} - \mu\hat{q} - \nu\hat{p}\right)$ stands for the projector on the eigenvector of $\mu\hat{q} + \nu\hat{p}$ corresponding to the eigenvalue X and

$$\hat{q}\psi(q) = q\psi(q), \qquad \hat{p}\psi(t) = -i\frac{\partial}{\partial q}\psi(q) \tag{93}$$

and $X, \mu, \nu \in R$. The quantizer of the symplectic tomogram is

$$\hat{D}(\mathbf{x}) := \hat{D}(X, \mu, \nu) = \frac{1}{2\pi} \exp\left[i\left(X\hat{1} - \mu\hat{q} - \nu\hat{p}\right)\right] \tag{94}$$

The *optical tomogram* is the same as above for the case

$$\mu = \cos\theta, \qquad \nu = \sin\theta. \tag{95}$$

Thus the optical tomogram is

$$\begin{aligned} M(X,\theta) &= \mathrm{Tr}\left\{|\,\psi\rangle\langle\psi\,|\,\delta\left(X\hat{1} - \mu\hat{q} - \nu\hat{p}\right)\right\} \\ &= \frac{1}{2\pi}\int \psi^*(q)e^{ikX}\exp\left[ik\left(X - q\cos\theta + i\,\frac{\partial}{\partial q}\sin\theta\right)\right]\psi(q)\,dq\,dk \\ &= \frac{1}{2\pi|\sin\theta|}\left|\int \psi(q)\exp\left[i\left(\frac{\cot\theta}{2}q^2 - \frac{Xq}{\sin\theta}\right)\right]dq\right|^2. \end{aligned} \tag{96}$$

One important feature of the formulation of tomograms as operator symbols is that one may work with deterministic functions $\psi\,(q)$ as easily as with probabilistic ones. In this latter case the projector in (85) would be replaced by

$$\Pi_p = \int p_\mu\,|\psi_\mu\rangle\langle\psi_\mu|\,d\mu \tag{97}$$

with $\int p_\mu d\mu = 1$, the tomogram being the symbol of this new operator.

This also provides a framework for an algebraic formulation of signal processing, perhaps more general than the one described in [28]. There, a signal model is a triple $(\mathscr{A}, \mathscr{M}, \Phi)$ $\mathscr{A}$ being an algebra of linear filters, $\mathscr{M}$ a $\mathscr{A}$-module and Φ a map from the vector space of signals to the module. With the operator symbol interpretation, both deterministic or random signals and linear or nonlinear transformations on signals are operators. By the application of the dequantizer (Eq. 75) they are mapped to functions, the filter operations becoming star-products.

References

1. F. Bayen, M. Flato, C. Fronsdal, C. Lichnerowicz, D. Sternheimer, Deformation theory and quantization. Ann. Phys (NY) **111**, 61–151 (1978)
2. J. Vey, Déformation du crochet de Poisson sur une variété symplectique. Comment. Math. Helv. **50**, 421–454 (1975)
3. M. De Wilde, P. Lecomte, Existence of star-products and of formal deformations of the Poisson Lie algebra of arbitrary symplectic manifolds. Lett. Math. Phys. **7**, 487–496 (1983)
4. O.M. Neroslavsky, A.T. Vlassov, Sur les deformations de l'algebre des fonctions d'une variété symplectique. C. R. Acad. Sci. Paris **292**(I), 71–73 (1981)
5. M. Cahen, S. Gutt, Regular star-representations of Lie algebras. Lett. Math. Phys. **6**, 395–404 (1982)

6. J. Moyal, Quantum mechanics as a statistical theory. Proc. Cambridge Phil. Soc. **45**, 99–124 (1949)
7. S. Bates, A. Weinstein, *Lectures on the Geometry of Quantization, Berkeley Mathematics Lecture Notes 8* (American Mathematical Society, Providence, 1997)
8. S. Mancini, V.I. Man'ko, P. Tombesi, Wigner function and probability distribution for shifted and squeezed quadratures. Quantum Semiclass. Opt. **7**, 615–623 (1995)
9. G.M. D'Ariano, S. Mancini, V.I. Man'ko, P. Tombesi, Reconstructing the density operator by using generalized field quadratures. Quantum Semiclass. Opt. **8**, 1017–1027 (1996)
10. S. Mancini, V.I. Man'ko, P. Tombesi, Symplectic tomography as classical approach to quantum systems. Phys. Lett. A **213**, 1–6 (1996)
11. S. Mancini, V.I. Man'ko, P. Tombesi, Classical-like description of quantum dynamics by means of symplectic tomography. Found. Phys. **27**, 801–824 (1997)
12. O. Man'ko, V.I. Man'ko, Quantum states in probability representation and tomography. J. Russ. Laser Res. **18**, 407–444 (1997)
13. V.I. Man'ko, R. Vilela Mendes, Noncommutative time–frequency tomography. Phys. Lett. A **263**, 53–61 (1999)
14. M.A. Man'ko, V.I. Man'ko, R. Vilela Mendes, Tomograms and other transforms: a unified view. J. Phys. A: Math. Gen. **34**, 8321–8332 (2001)
15. F. Clairet, F. Briolle, B. Ricaud, S. Heuraux, New signal processing technique for density profile reflectometry on Tore Supra. Rev. Sci. Instrum. **82**, 083502 (2011)
16. C. Aguirre, R. Vilela Mendes, Signal recognition and adapted filtering by non-commutative tomography. IET Signal Proc. 8, 67–75 (2014)
17. R. Vilela Mendes, H.C. Mendes, T. Araújo, Signals on graphs: Transforms and tomograms. Phys. A **450**, 1–17 (2016)
18. R. Vilela Mendes, Non-commutative tomography and signal processing. Phys. Scr. **90**, 07402 (2015)
19. R. Vilela Mendes, J. Leitão, V.I. Man'ko, The classical-quantum transition in the cooling of levitated nanoparticles, in preparation
20. P.J. Morrison, Hamiltonian and action principle formulations of plasma physics. Phys. Plasmas **12**, 058102 (2005)
21. J.E. Marsden, A. Weinstein, The Hamiltonian structure of the Maxwell-Vlasov equations. Phys. D **4**, 394–406 (1982)
22. F.E. Low, A Lagrangian formulation of the Boltzmann-Vlasov equation for plasmas. Proc. R. Soc. Lond. Ser. A **248**, 282–287 (1958)
23. R. Vilela Mendes, Sensitive dependence in quantum systems: some examples and results. Phys. Lett. A **171**, 253–258 (1992)
24. R. Vilela Mendes, R. Coutinho, On the computation of quantum characteristic exponents. Phys. Lett. A **239**, 239–245 (1998)
25. V.I. Man'ko, R. Vilela Mendes, Lyapunov exponent in quantum mechanics. A phase-space approach. Phys. D **145**, 330–348 (2000)
26. V.I. Man'ko, R. Vilela Mendes, Quantum sensitive dependence. Phys. Lett. A **300**, 353–360 (2002)
27. F. Briolle, V.I. Man'ko, B. Ricaud, R. Vilela Mendes, Noncommutative tomography: A tool for data analysis and signal processing. J. Russian Laser Res. **33**, 103–121 (2012)
28. M. Puschel, J.F. Moura, Algebraic signal processing theory: 1-D space. IEEE Trans. Signal Proc. **56**, 3586–3599 (2008)