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Patrícia Gonçalves · Ana Jacinta Soares
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From Particle Systems to Partial Differential Equations

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Preface

This volume presents the proceedings of the fifth international conference on Particle Systems and Partial Differential Equations, "PS-PDEs V", which was held at the Centre of Mathematics of the University of Minho in Braga, Portugal, from November 28 to 30, 2016.

In the same spirit of the previous editions of PSPDE, this edition was intended to bring together prominent active researchers working in the fields of probability and partial differential equations, so that they could present their latest scientific findings in both areas, and to promote active discussions on some of their areas of expertise. Further, it was intended to introduce a vast and varied public, including young researchers, to the subject of interacting particle systems, its underlying motivation, and its relation to partial differential equations.

This volume includes eight contributed papers written by conference participants on essential and intriguing 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 meeting.

Lastly, we wish to gratefully acknowledge the financial support provided by Fundação para a Ciência e a Tecnologia through the FCT-FACC funds, to the Centre of Mathematics of the University of Minho, to the Centre for Mathematical Analysis, Geometry, and Dynamical Systems of the University of Lisbon, to the Centre of Mathematics, Fundamental Applications and Operations Research of the University of Lisbon, and to the Co-Lab initiative UT Austin-Portugal.

We really hope that you enjoy reading this book!

Braga, Portugal
June 2018

Patrícia Gonçalves
Ana Jacinta Soares

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Linear Boltzmann Equations: A Gradient Flow Formulation

Giada Basile

Abstract I present some results obtained together with D. Benedetto and L. Bertini on a gradient flow formulation of linear kinetic equations, in terms of an entropy dissipation inequality. The setting includes the current as a dynamical variable. As an application I discuss the diffusive limit of linear Boltzmann equations and show that the rescaled entropy inequality asymptotically provides the corresponding inequality for heat equation.

1 Introduction

Linear Boltzmann equations describe a wide class of transport phenomena. They depict the interaction of a population of independent particles or quasi-particles with a background medium. Classical examples are charge transport in a medium [22], neutron transport through matter [21], but also the evolution of a tagged particle in a Newtonian system in thermal equilibrium [28], and the propagation of lattice vibrations in insulating crystals [4]. Some of these equations have been derived from an underlying microscopic dynamics [4, 10, 17, 29]. On the other hand, several results on the asymptotic behavior of the one-particle distribution have been obtained. In particular, by considering non degenerate scattering rates, under a diffusive rescaling it has been proved that linear Boltzmann equations converge to a diffusion [3, 7, 16, 21].

Under reversibility assumption on the scattering operator, the general form of the linear Boltzmann equation is the following

$$(\partial_t + b(v)\cdot\nabla_x) f(t,x,v) = \int_{\mathscr{V}} \pi(\mathrm{d}v')\sigma(v,v')\big[f(t,x,v') - f(t,x,v)\big], \qquad (1)$$

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where $\pi(\mathrm{d}v)$ is a probability measure on the velocity space $\mathscr{V}$, b is the drift, $\sigma(v, v') = \sigma(v', v) \geq 0$ is the scattering kernel and f is the density of the one-particle distribution with respect to $\mathrm{d}x\,\pi(\mathrm{d}v)$. The velocity space $\mathscr{V}$ can be either $\mathbb{R}^d$, $\mathbb{S}^{d-1}$, $\mathbb{T}^d$ or a discrete state space.

From a probabilistic point of view, (1) is the Fokker–Planck equation of the process $(V(t), X(t))_{t\geq 0}$ where $V(\cdot)$ is an autonomous jump process with value in $\mathscr{V}$ defined by the generator

$$(\mathscr{L}g)(v) = \int_{\mathscr{V}} \pi(\mathrm{d}v')\sigma(v, v')\big[g(v') - g(v)\big], \tag{2}$$

and $X(\cdot)$ is an additive functional of V, namely $X(t) = \int_0^t b(V_s)ds$. The diffusive asymptotics corresponds to an invariance principle for $X(\cdot)$.

The homogeneous version of (1), corresponding to $b = 0$, is the Fokker–Planck equation associated to continuous time reversible Markov chains. Recently there have been a few attempts to formulate it as gradient flows [14, 23, 24], essentially in terms of so called energy variational inequalities. In a recent paper with D. Benedetto and L. Bertini [5], inspired by the general theory in [2, 12], we introduce a gradient flow approach based on an entropy dissipation inequality that can be applied naturally to the inhomogeneous case, i.e. in presence of a drift.

The gradient flow approach allows to express a differential equation as a variational inequality. Here is a simple example. Given a function $\Phi : \mathbb{R}^d \to \mathbb{R}$, smooth enough, consider the curve $x : [0, +\infty) \to \mathbb{R}^d$ such that

$$\frac{d}{dt}x(t) = -\nabla\Phi(x(t)), \qquad t \in [0, +\infty).$$

It is the curve which moves by choosing at each time the direction which makes the functional Φ decreasing as much as possible, i.e. the steepest descendant curve. This is the definition of "gradient flow". This curve produces the maximal dissipation rate. In fact, along every curve $w : [0, +\infty) \to \mathbb{R}^d$

$$-\frac{d}{dt}\Phi(w(t)) = -\nabla\Phi(w(t)) \cdot \dot{w}(t) \leq \frac{1}{2}|\dot{w}(t)|^2 + \frac{1}{2}|\nabla\Phi(w(t))|^2$$

and equality holds iff $\dot{w} = -\nabla\Phi(w)$. By integrating, the steepest descendant curve satisfies

$$\Phi(x(0)) - \Phi(x(t)) = \int_0^t ds\Big(\frac{1}{2}|\dot{x}(s)|^2 + \frac{1}{2}|\nabla\Phi(x(s))|^2\Big),$$

while for every curve the inequality $\leq$ holds. This observation leads to a variational characterization of the gradient flows as any curve $x(\cdot)$ (smooth enough) satisfying the inequality

$$\Phi(x(t)) + \int_0^t ds\Big(\frac{1}{2}|\dot{x}(s)|^2 + \frac{1}{2}|\nabla\Phi(x(s))|^2\Big) \leq \Phi(x(0)).$$

This approach works also in function spaces, with ordinary differential equations replaced by partial differential equations. In particular, a gradient flow structure has been recognized in equations of the form $\partial_t \rho - \nabla \cdot (\rho\, v) = 0$, with $v = \nabla \cdot (\rho \frac{\delta F}{\delta \rho})$ [19, 26].

In the same spirit we have formulated (1) as an entropy dissipation inequality. The basic observation is that the entropy is a Lyapunov functional for the evolution (1), and its rate of decrease is not affected by the transport term. An analogous approach can be found in [15], where a slightly different gradient flow formulation for the homogeneous (non linear) Boltzmann equation is introduced. In particular in [15] a notion of distance between probabilities is defined and the entropy dissipation inequality involves an entropy production term and the metric derivative with respect to this distance. In our approach the entropy production term is replaced by the Dirichlet form of the square root and the metric derivative by a kinematic term which involves also the current.

The functional giving rise to the entropy dissipation inequality is related to the large deviation asymptotics of Markov chains. More precisely, in the homogeneous case it corresponds to the large deviation rate function of the empirical measure of N independent jump processes defined by (2). We conjecture that this equivalence holds also in the non-homogeneous case, i.e. the functional defined in (14) is the large deviation rate function of the empirical measure of velocity and position of N independent particles evolving according to (1).

As an application, we have shown that the particle density, give by $\rho^\varepsilon(t, x) = \int \pi(\mathrm{d}v)\, f(\varepsilon^{-2}t, \varepsilon^{-1}x, v)$, converges weakly to the solution of the heat equation in the limit $\varepsilon \to 0$. This is proved by taking the limit $\varepsilon \to 0$ in the rescaled entropy dissipation inequality and deducing the corresponding inequality for the heat equation. In these notes I show the basic ideas of this approach overlooking the technical details.

2 A Gradient Flow Formulation of Heat Equation and Linear Boltzmann Equation

I discuss a gradient flow formulation of heat equation and linear Boltzmann equation in a setting that includes the current as a dynamical variable.

2.1 Heat Equation

Consider the heat equation on $\mathbb{T}^d$

$$\partial_t \rho = \nabla \cdot D \nabla \rho$$

where ρ is a probability density and the diffusion coefficient D is a positive symmetric $d \times d$ matrix. I introduce the currents as vector fields on $\mathbb{T}^d$, denoted by j. Given ρ, the associated current is $j^\rho := -D\nabla\rho$, then the heat equation reads

$$\begin{cases} \partial_t \rho + \nabla \cdot j = 0 \\ j = j^\rho. \end{cases} \tag{3}$$

The goal is to rewrite these equations as a variational inequality that expresses the decrease of the entropy.

Fix $T > 0$ and consider the set of paths $(\rho(t), j(t))$, $t \in [0, T]$ satisfying the continuity equation $\partial_t \rho + \nabla \cdot j = 0$. Observe that a suitable current can be found as soon as the path is absolutely continuous. On this set consider the action functional

$$I(\rho, j) = \frac{1}{2} \int_0^T \mathrm{d}t \int \mathrm{d}x \frac{1}{\rho(t)} \big[j(t) + D\nabla\rho(t) \big] \cdot D^{-1} \big[j(t) + D\nabla\rho(t) \big],$$

where $\cdot$ denotes the inner product in $\mathbb{R}^d$. This functional arises naturally by analyzing the large deviation asymptotics of N independent Brownians [11, 20] and its connection with the gradient flow formulation of the heat equation is discussed in [1]. To be precise, the rate function in [1, 11, 20] does not include the current as a dynamical variable but it can be extended to this case, see [8] for a similar functional in the context of stochastic lattice gases.

Observe that $I \geq 0$ and $I(\rho, j) = 0$ if and only if $j = j^\rho$. Hence the second equation in (3) is equivalent to $I(\rho, j) \leq 0$. By expanding the square one deduces

$$\int_0^T \mathrm{d}t \int \mathrm{d}x \left[\frac{1}{2} \frac{1}{\rho(t)} j(t) \cdot D^{-1} j(t) + \frac{1}{2} \frac{1}{\rho(t)} \nabla\rho(t) \cdot D\nabla\rho(t) + \frac{1}{\rho(t)} \nabla\rho(t) \cdot j(t) \right] \leq 0. \tag{4}$$

Since $(\nabla\rho)/\rho = \nabla \log \rho$, integrating by parts and using the continuity equation, the last term is the total derivative of the entropy $H(\rho(t))$ defined as usual as $H(\rho) = \int \mathrm{d}x \, \rho \log \rho$.

Observe that the second term is the integral of the *Fisher information* E, that can be defined as the Dirichlet form of square root, namely

$$E(\rho) = \frac{1}{2} \int \mathrm{d}x \frac{1}{\rho} \nabla\rho \cdot D\nabla\rho = 2 \int \mathrm{d}x \, \nabla\sqrt{\rho} \cdot D\nabla\sqrt{\rho}.$$

Finally, let the first term be the *kinematic term* R which is the functional on the set of paths $(\rho(t), j(t))$ defined by

$$R(\rho, j) = \frac{1}{2} \int_0^T \mathrm{d}t \int \mathrm{d}x \, \frac{1}{\rho(t)} j(t) \cdot D^{-1} j(t).$$

Then (4) reads as the following entropy dissipation inequality

$$H(\rho(T)) + \int_0^T \mathrm{d}t\, E(\rho(t)) + R(\rho, j) \le H(\rho(0)). \tag{5}$$

The precise formulation concerns a family of probabilities $\mu_t(\mathrm{d}x) = \rho(t,x)\mathrm{d}x$, $t \in [0,T]$ and vector valued measures $J(\mathrm{d}t, \mathrm{d}x) = j(t,x)\mathrm{d}t\mathrm{d}x$ (the currents). Given $T > 0$, let $C\big([0,T]; \mathscr{P}(\mathbb{T}^d)\big)$ be the set of continuous paths on $\mathscr{P}(\mathbb{T}^d)$ endowed with the topology of uniform convergence. Let also $\mathscr{M}\big([0,T] \times \mathbb{T}^d; \mathbb{R}^d\big)$ be the set of vector valued Radon measures on $[0,T] \times \mathbb{T}^d$ endowed with the weak* topology. Set $S := C\big([0,T]; \mathscr{P}(\mathbb{T}^d)\big) \times \mathscr{M}\big([0,T] \times \mathbb{T}^d; \mathbb{R}^d\big)$ endowed with the product topology.

Given a positive $d \times d$ matrix D, the Fisher information $E\colon \mathscr{P}(\mathbb{T}^d) \to [0, +\infty]$ can be defined by the variational formula

$$E(\mu) = 2 \sup_{\phi \in C^2(\mathbb{T}^d)} \Big\{ -\int \mathrm{d}\mu\, e^{-\phi} \nabla \cdot D \nabla e^{\phi} \Big\}, \tag{6}$$

which implies its lower semicontinuity and convexity. Also the kinematic term $R\colon S \to [0, \infty]$ admits the variational representation

$$R(\mu, J) = \sup_{w \in C([0,T] \times \mathbb{T}^d; \mathbb{R}^d)} \Big\{ J(w) - \frac{1}{2} \int_0^T \mathrm{d}t \int \mathrm{d}\mu_t\, w \cdot Dw \Big\}, \tag{7}$$

where $J(w) = \int_0^T \int \mathrm{d}J \cdot w$, which implies its lower semicontinuity and convexity. Then the entropy dissipation inequality (5) reads

$$\int_0^T \mathrm{d}t\, \mu_t(\partial_t \phi) + J(\nabla \phi) = 0, \qquad \phi \in C_c^1\big((0,T) \times \mathbb{T}^d\big) \tag{8}$$

$$H(\mu_T) + \int_0^T \mathrm{d}t\, E(\mu_t) + R(\mu, J) \le H(\nu), \tag{9}$$

where the first equation is the required continuity equation. Given $\nu \in \mathscr{P}(\mathbb{T}^d)$ with $H(\nu) < +\infty$, a path $(\mu, J) \in S$ is a solution of the heat equation with initial condition ν iff $\mu_0 = \nu$ and (8), (9) are satisfied ([5]).

The standard formulation of the heat equation as gradient flow of the entropy can be easily recovered from (9) by projecting on the density. Indeed, by the Benamou–Brenier lemma [6], one obtains that if (μ, J) is a solution to the (9) , then $\mu = (\mu_t)_{t \in [0,T]}$ satisfies

$$H(\mu_T) + \int_0^T \mathrm{d}t \left\{ E(\mu_t) + \frac{1}{2} \big|\dot{\mu}_t\big|^2 \right\} \le H(\nu) \tag{10}$$

where $\big|\dot{\mu}_t\big|$ is the metric derivative of $t \mapsto \mu_t$ with respect to the Wasserstein-2 distance.

2.2 Linear Boltzmann Equations

Let $\mathscr{V}$ be the velocity space. Consider a measure π on $\mathscr{V}$, a symmetric scattering kernel $\sigma : \mathscr{V} \times \mathscr{V} \to [0, +\infty)$ and a drift $b : \mathscr{V} \to \mathbb{R}^d$. Let $\mathscr{P}(\mathbb{T}^d \times \mathscr{V})$ be the set of probabilities on $\mathbb{T}^d \times \mathscr{V}$, endowed with the topology of the weak convergence. Given $P \in \mathscr{P}(\mathbb{T}^d \times \mathscr{V})$, the relative entropy $\mathscr{H}(P)$ of P with respect to the probability $\mathrm{d}x\,\pi(\mathrm{d}v)$ is $\mathscr{H}(P) = \iint \mathrm{d}x\pi(\mathrm{d}v)\, f \log f$ if $\mathrm{d}P = f\,\mathrm{d}x\,\pi(\mathrm{d}v)$ and $\mathscr{H}(P) = +\infty$ otherwise.

Fix $T > 0$. Given a path $(P_t)_{t\in[0,T]}$ on $\mathscr{P}(\mathbb{T}^d \times \mathscr{V})$ with $\mathrm{d}P_t = f(t, x, v)\,\mathrm{d}x\,\pi(\mathrm{d}v)$, set

$$\eta^f = \eta^f(t, x, v, v') := \sigma(f - f') = \sigma(v, v')\big[f(t, x, v) - f(t, x, v')\big], \tag{11}$$

where $f = f(t, x, v)$, $f' = f(t, x, v')$. The linear Boltzmann equation (1) can be rewritten as

$$\begin{cases} \big(\partial_t + b(v)\cdot\nabla_x\big) f(t, x, v) + \int \pi(dv')\,\eta(t, x, v, v') = 0, \\ \eta = \eta^f \end{cases} \tag{12}$$

where the first equation has to be satisfied weakly. We shall refer to it as the *balance* equation. The goal is again to express these equations as an entropy dissipation inequality. To this end, given $\varkappa > 0$ let $\Phi_\varkappa : \mathbb{R}_+ \times \mathbb{R}_+ \times \mathbb{R} \to [0, +\infty)$ be the convex function defined by

$$\Phi_\varkappa(p, q; \xi) := \sup_{\lambda\in\mathbb{R}} \Big\{\lambda\xi - \varkappa p\big(e^\lambda - 1\big) - \varkappa q\big(e^{-\lambda} - 1\big)\Big\}.$$

Given $p, q \in \mathbb{R}_+$ the map $\xi \mapsto \Phi_\varkappa(p, q; \xi)$ is positive (take $\lambda = 0$), and equal to zero iff $\xi = \varkappa(p - q)$. Explicitly $\Phi_\varkappa$ reads

$$\begin{aligned} \Phi_\varkappa(p, q; \xi) = \xi\Big[\operatorname{ash}\frac{\xi}{2\varkappa\sqrt{pq}} - \operatorname{ash}\frac{\varkappa(p - q)}{2\varkappa\sqrt{pq}}\Big] \\ - \Big[\sqrt{\xi^2 + 4\varkappa^2 pq} - \sqrt{\big[\varkappa(p - q)\big]^2 + 4\varkappa^2 pq}\Big] \end{aligned} \tag{13}$$

where the equality $\operatorname{ash}(z) = \log(z + \sqrt{1 + z^2})$ holds.

Fix a path $(f(t), \eta(t))$, $t \in [0, T]$ satisfying $\eta(t, x, v, v') = -\eta(t, x, v', v)$ and the balance equation in (12). The condition $\eta(t) = \eta^{f(t)}$, $t \in [0, T]$ is equivalent to

$$\mathscr{I}(f, \eta) := \int_0^T \mathrm{d}t \int \mathrm{d}x \iint \pi(\mathrm{d}v)\,\pi(\mathrm{d}v')\,\Phi_\sigma(f, f'; \eta) \le 0. \tag{14}$$

This functional is connected with the large deviations asymptotic of a Markov chain on $\mathscr{V}$ with transition rates $\sigma(v', v)\pi(\mathrm{d}v')$, see [9, 25].

Setting

$$\Phi_\varkappa(p,q;\xi) = \Phi_\varkappa(p,q;0) + \xi\frac{\partial}{\partial\xi}\Phi_\varkappa(p,q;0) + \Psi_\varkappa(p,q;\xi), \tag{15}$$

by explicit computations one obtains

$$\begin{aligned}
&\Phi_\varkappa(p,q;0) = \varkappa\big(\sqrt{p}-\sqrt{q}\big)^2\\
&\frac{\partial}{\partial\xi}\Phi_\varkappa(p,q;0) = \frac{1}{2}\log\frac{q}{p}\\
&\Psi_\varkappa(p,q;\xi) = \xi\,\mathrm{ash}\frac{\xi}{2\varkappa\sqrt{pq}} - \Big[\sqrt{\xi^2+4\varkappa^2pq} - 2\varkappa\sqrt{pq}\Big].
\end{aligned}$$

Observe that $\Psi_\varkappa$ has the variational representation

$$\Psi_\varkappa(p,q;\xi) = \sup_{\lambda\in\mathbb{R}}\Big\{\lambda\xi - 2\varkappa\sqrt{pq}\big[\mathrm{ch}\lambda - 1\big]\Big\}, \tag{16}$$

in particular, $\Psi_\varkappa \geq 0$ and the map $\xi \mapsto \Psi_\varkappa(p,q;\xi)$ is convex. Moreover, $\Psi_\varkappa(p,q;\xi) \sim \xi^2$ for ξ small and $\Psi_\varkappa(p,q;\xi) \sim |\xi|\log|\xi|$ for ξ large.

Observe now that for any path $(f(t),\eta(t)), t\in[0,T]$ satisfying the balance equation in (12)

$$\begin{aligned}
\frac{d}{dt}\mathscr{H}(f(t)) &= \int \mathrm{d}x \int \pi(\mathrm{d}v)\,\log f\big[-b(v)\cdot\nabla_x f - \int\pi(\mathrm{d}v)\,\eta(t,x,v,v')\big]\\
&= -\int \mathrm{d}x \iint \pi(\mathrm{d}v)\pi(\mathrm{d}v')\,\eta\log f
\end{aligned}$$

since the first term is a total derivative in x. Hence, by the antisymmetry of η,

$$\int \mathrm{d}x \iint \pi(\mathrm{d}v)\pi(\mathrm{d}v')\,\eta\frac{\partial}{\partial\xi}\Phi_\varkappa(f,f';0) = \frac{d}{dt}\mathscr{H}(f(t)).$$

for any $\varkappa>0$. Setting $\varkappa=\sigma$, inserting (15) and integrating in time we obtain that, for any $(f(t),\eta(t)), t\in[0,T]$ satisfying the balance equation, it holds

$$\begin{aligned}
&\mathscr{H}(f(T)) + \int_0^T \mathrm{d}t \int \mathrm{d}x \iint \pi(\mathrm{d}v)\pi(\mathrm{d}v')\big[\Phi_\sigma(f,f';0) + \Psi_\sigma(f,f';\eta)\big]\\
&\qquad = \mathscr{H}(f(0)) + \int_0^T \mathrm{d}t \int \mathrm{d}x \iint \pi(\mathrm{d}v)\pi(\mathrm{d}v')\,\Phi_\sigma(f,f';\eta).
\end{aligned} \tag{17}$$

Gathering the above computations, (14) can be rewritten as

$$\mathscr{H}(f(T)) + \int_0^T \mathrm{d}t\, \mathscr{E}(f(t)) + \mathscr{R}(f,\eta) \le \mathscr{H}(f(0)) \tag{18}$$

where

$$\mathscr{E}(f) = \int \mathrm{d}x \iint \pi(\mathrm{d}v)\pi(\mathrm{d}v')\,\sigma(v,v')\big[\sqrt{f'} - \sqrt{f}\big]^2 \tag{19}$$

and

$$\mathscr{R}(f,\eta) = \int_0^T \mathrm{d}t \int \mathrm{d}x \iint \pi(dv)\pi(dv')\,\Psi_\sigma(f, f'; \eta). \tag{20}$$

The inequality (18), formally analogous to (5), is the proposed gradient flow formulation of the linear Boltzmann equation (1).

The precise formulation concerns the measures $P(\mathrm{d}x\,\mathrm{d}v) = f(x,v)\,\mathrm{d}x\,\pi(\mathrm{d}v)$ and $\Theta(\mathrm{d}t, \mathrm{d}x, \mathrm{d}v, \mathrm{d}v') = \eta(t,x,v,v')\,\mathrm{d}t\,\mathrm{d}x\,\mathrm{d}v\,\mathrm{d}v'$.

Given $T > 0$, let $C\big([0,T]; \mathscr{P}(\mathbb{T}^d \times \mathscr{V})\big)$ be the set of continuous paths on $\mathscr{P}(\mathbb{T}^d \times \mathscr{V})$ endowed with the topology of uniform convergence. Denote by $\mathscr{M}_\mathrm{a}\big([0,T] \times \mathbb{T}^d \times \mathscr{V} \times \mathscr{V}\big)$ the set of finite Radon measures on $[0,T] \times \mathbb{T}^d \times \mathscr{V} \times \mathscr{V}$ anti-symmetric with respect to the exchange of the last two variables endowed with the weak* topology. Set $\mathscr{S} := C\big([0,T]; \mathscr{P}(\mathbb{T}^d \times \mathscr{V})\big) \times \mathscr{M}_\mathrm{a}\big([0,T] \times \mathbb{T}^d \times \mathscr{V} \times \mathscr{V}\big)$ endowed with the product topology. Let also $C_\mathrm{be}\big([0,T]; \mathscr{P}(\mathbb{T}^d \times \mathscr{V})\big)$ the set of paths $(P_t)_{t\in[0.T]}$ in $C\big([0,T]; \mathscr{P}(\mathbb{T}^d \times \mathscr{V})\big)$ such that $\sup_{t\in[0,T]} \mathscr{H}(P_t) < +\infty$ and let finally $\mathscr{S}_\mathrm{be} := C_\mathrm{be}\big([0,T]; \mathscr{P}(\mathbb{T}^d \times \mathscr{V})\big) \times \mathscr{M}_\mathrm{a}\big([0,T] \times \mathbb{T}^d \times \mathscr{V} \times \mathscr{V}\big)$.

If $P \in \mathscr{P}(\mathbb{T}^d \times \mathscr{V})$ has finite entropy, the Dirichlet form of the square root $\mathscr{E}$ can be defined by the variational formula

$$\mathscr{E}(P) := \sup_{\phi \in C_\mathrm{b}(\mathbb{T}^d \times \mathscr{V})} \iint P(\mathrm{d}x, \mathrm{d}v)\pi(\mathrm{d}v')\,\sigma(v,v')\Big[1 - e^{\phi(x,v') - \phi(x,v)}\Big]. \tag{21}$$

The representation (21) corresponds to the Donsker–Varadhan large deviation for the empirical measure of the continuous time Markov chain on $\mathscr{V}$ with transition rates $\sigma(v',v)\pi(\mathrm{d}v')$ [13]. Indeed, $\mathscr{E}(P) = \sup_\phi\{-P(e^{-\phi}\mathscr{L}e^{\phi})\}$, with $\mathscr{L}$ defined in (2).

A variational representation for the kinematic term $\mathscr{R}$ is easily obtained by combining (16) with the simple observation that for positive p, q one has $-2\sqrt{pq} = \sup_{a>0}\big\{-ap - a^{-1}q\big\}$. Then $\mathscr{R}\colon \mathscr{S}_\mathrm{be} \to [0, +\infty]$ is the functional defined by

$$\begin{aligned}\mathscr{R}(P,\Theta) := \sup_{\zeta,\alpha} \Bigg\{ \Theta(\zeta) - \int_0^T \mathrm{d}t \iiint P_t(\mathrm{d}x, \mathrm{d}v)\pi(\mathrm{d}v')\,\sigma(v,v') \\ \times \big[\mathrm{ch}\zeta(t,x,v,v') - 1\big]\big[\alpha(t,x,v,v') + \alpha(t,x,v',v)^{-1}\big] \Bigg\},\end{aligned} \tag{22}$$

where the supremum is carried out over all continuous functions $\zeta\colon [0,T] \times \mathbb{T}^d \times \mathscr{V} \times \mathscr{V} \to \mathbb{R}$ with compact support and antisymmetric with respect to the exchange

of the last two variables and all bounded continuous functions $\alpha\colon [0,T]\times\mathbb{T}^d\times\mathscr{V}\times\mathscr{V}\to(0,+\infty)$ uniformly bounded away from zero.

Let $Q\in\mathscr{P}(\mathbb{T}^d\times\mathscr{V})$ with $\mathscr{H}(Q)<+\infty$. The entropy dissipation inequality formulation for $(P,\Theta)\in\mathscr{S}_{\mathrm{be}}$ solution to the linear Boltzmann equation, with initial condition $P_0=Q$, reads

$$\int_0^T \mathrm{d}t\, P_t(\partial_t\phi+b\cdot\nabla_x\phi)=\frac{1}{2}\int\Theta(\mathrm{d}t,\mathrm{d}x,\mathrm{d}v,\mathrm{d}v')\big[\phi(t,x,v)-\phi(t,x,v')\big], \quad (23)$$

$$\mathscr{H}(P_T)+\int_0^T \mathrm{d}t\,\mathscr{E}(P_t)+\mathscr{R}(P,\Theta)\le\mathscr{H}(Q). \quad (24)$$

for all continuous functions $\phi\colon(0,T)\times\mathbb{T}^d\times\mathscr{V}$ with compact support and continuously differentiable with respect to the first two variables.

3 Diffusive Scaling

Convergence of linear Boltzmann equation to a diffusion is a classical topic [7, 16, 21]. From a probabilistic point of view, it corresponds to the central limit theorem for additive functional of Markov chains. Here this convergence is achieved by performing limiting variational inequalities, according to a general scheme formalized in [27].

To carry out the analysis of the diffusive limit of linear Boltzmann equations a few extra conditions, implying in particular homogenization of the velocity, are needed. Let $\lambda\colon\mathscr{V}\to[0,+\infty)$ be the scattering rate defined by $\lambda(v)=\int\pi(\mathrm{d}v')\sigma(v',v)$, let $\tilde\pi$ be the probability on $\mathscr{V}$ defined by

$$\tilde\pi(\mathrm{d}v):=\frac{\lambda(v)}{\pi(\lambda)}\pi(\mathrm{d}v). \quad (25)$$

Assumption 1 The following conditions hold.

1. The drift $b:\mathscr{V}\to\mathbb{R}^d$ is centered with respect to the measure π, namely $\pi(b)=0$.
2. The scattering rate λ satisfies $\pi[\lambda=0]=0$.
3. $|b|^2/\lambda$ has all exponential moments, i.e. $\pi[\exp\{\gamma|b|^2/\lambda\}]<+\infty$ for any $\gamma>0$.
4. There exists a constant $C_0>0$ such that for any $g\in L^2(\tilde\pi)$ one has

$$\int\mathrm{d}\tilde\pi\big[g-\tilde\pi(g)\big]^2\le C_0\iint\tilde\pi(\mathrm{d}v)\tilde\pi(\mathrm{d}v')\frac{\sigma(v,v')}{\lambda(v)\lambda(v')}\big[g(v)-g(v')\big]^2. \quad (26)$$

Item 4 corresponds to the assumption that the continuous time Markov chain with transition rates $\frac{\sigma(v,v')}{\lambda(v)\lambda(v')}\tilde\pi(\mathrm{d}v')$ has a spectral gap. The generator of this Markov chain is $(K-\mathrm{Id})$, where K is given by

$$\big(Kg\big)(v) = \pi(\lambda) \int \tilde{\pi}(\mathrm{d}v') \frac{\sigma(v, v')}{\lambda(v)\lambda(v')} g(v'). \tag{27}$$

Observe that $-\mathscr{L} = \mathbb{I} - K$, where $\mathscr{L}$ is the generator of the original Markov chain as defined in (2). Assumption 1 implies that there exists $\xi \in L^2(\tilde{\pi}; \mathbb{R}^d)$ such that $-\mathscr{L}\xi = b$. Indeed, item 1 implies that b/λ is centered with respect to $\tilde{\pi}$, item 2 implies that $b/\lambda \in L^2(\tilde{\pi}; \mathbb{R}^d)$, and finally item 3 implies that $\xi := (\mathbb{I} - K)^{-1}(b/\lambda) \in L^2(\tilde{\pi}; \mathbb{R}^d)$.

Another technical condition is required in order to carry out a truncation on ξ which is used in the proof of the main theorem.

Assumption 2 At least one of the following alternatives holds

1. $(-\mathscr{L})^{-1}b$ is bounded, or
2. there exists $C < \infty$ such that $\big\|\big(\mathbb{I} - K\big)^{-1} f\big\|_\infty \le C\|f\|_\infty$, for any f such that $\tilde{\pi}(f) = 0$.

Let $\varepsilon > 0$ be the scaling parameter and denote by $(f^\varepsilon, \eta^\varepsilon)$ the rescaled solution of the linear Boltzmann equation. Accordingly with the gradient flow formulation, it satisfies

$$\partial_t f^\varepsilon(t, x, v) + \frac{1}{\varepsilon} b(v) \cdot \nabla_x f^\varepsilon(t, x, v) + \frac{1}{\varepsilon^2} \int \pi(\mathrm{d}v') \eta^\varepsilon(t, x, v, v') = 0 \tag{28}$$

$$\mathscr{H}(f^\varepsilon(T)) + \frac{1}{\varepsilon^2} \int_0^T \mathrm{d}t\, \mathscr{E}(f^\varepsilon(t)) + \frac{1}{\varepsilon^2} \mathscr{R}(f^\varepsilon, \eta^\varepsilon) \le \mathscr{H}(f_0^\varepsilon). \tag{29}$$

Set

$$\begin{aligned} \rho^\varepsilon(t, x) &= \int \pi(\mathrm{d}v) f^\varepsilon(t, x, v) \\ j^\varepsilon(t, x) &= \frac{1}{\varepsilon} \int \pi(\mathrm{d}v) f^\varepsilon(t, x, v) b(v). \end{aligned} \tag{30}$$

Since $\eta^\epsilon(t, x, v, v')$ is antisymmetric with respect to the exchange of v and v', by integrating (28) with respect to $\pi(dv)$ the following continuity equation holds

$$\partial_t \rho^\epsilon + \nabla \cdot j^\epsilon = 0. \tag{31}$$

Theorem 1 *Assume that $\rho_0^\varepsilon \to \rho_0$ in $\mathscr{P}(\mathbb{T}^d)$ and $\lim_{\varepsilon \to 0} \mathscr{H}(f_0^\varepsilon) = H(\rho_0)$. Then the sequence $(\rho^\varepsilon, j^\varepsilon)$ converges in $C([0, T]; \mathscr{P}(\mathbb{T}^d)) \times \mathscr{M}([0, T] \times \mathbb{T}^d; \mathbb{R}^d)$ to the solution to the heat equation, with initial datum ρ_0 and diffusion coefficient*

$$D = \pi\big(b \otimes (-\mathscr{L})^{-1} b\big). \tag{32}$$

Note that, by Assumption 1, b/λ and $\xi = (-\mathscr{L})^{-1}b$ are in $L^2(\tilde{\pi}; \mathbb{R}^d)$, hence the diffusion coefficient $D = \pi(\lambda)\, \tilde{\pi}\big((b/\lambda) \otimes \xi\big)$ is finite.

The proof of the theorem is achieved using a compactness result ([5], Lemma 3.5) and passing to the limit in inequality (29). By the hypothesis of the theorem,

$\mathscr{H}(f_0^\varepsilon) \to H(\rho_0)$, then we prove that the inferior limit of the left hand side of (29) majorizes the left hand side of (9). This is the content of Lemma 1. Observe that the Dirichlet form and the kinematic term exchange roles in the limit. This is actually a little bit surprising. As a partial explanation, one observes that for heat equation the Fisher information and the metric slope are the same object.

Lemma 1 *Assume that* $(\rho^\varepsilon, j^\varepsilon) \to (\rho, j)$. *Then*

$$\varliminf_{\varepsilon\to 0} \mathscr{H}(f^\varepsilon(t)) \geq H(\rho(t)),$$

$$\varliminf_{\varepsilon\to 0} \frac{1}{\varepsilon^2} \int_0^T \mathrm{d}t\, \mathscr{E}(f^\varepsilon(t)) \geq R(\rho, j), \tag{33}$$

for each $t \in [0, T]$, *and*

$$\varliminf_{\varepsilon\to 0} \frac{1}{\varepsilon^2} \mathscr{R}(f^\varepsilon, \eta^\varepsilon) \geq \int_0^T dt\, E(\rho(t)). \tag{34}$$

Sketch of the proof of Lemma 1. The first inequality is a direct consequence of the convexity and lower semicontinuity of the relative entropy. In order to prove the second inequality, consider the case where $(-\mathscr{L})^{-1}b$ is bounded. Fix $w \in C\big([0, T] \times \mathbb{T}^d;\, \mathbb{R}^d\big)$, then in the variational representation for $\mathscr{E}$ choose the test function $\log\big(1 + \varepsilon w(t, x) \cdot (-\mathscr{L})^{-1}b(v)\big)$, with ε small enough. By Taylor expansion

$$\varliminf_{\varepsilon\to 0} \frac{1}{\varepsilon^2} \int_0^T \mathrm{d}t\, \mathscr{E}(f^\varepsilon(t)) \geq \varliminf_{\varepsilon\to 0} \frac{1}{\varepsilon} \int_0^T \mathrm{d}t \int \mathrm{d}x \int \mathrm{d}\pi f^\varepsilon\, w \cdot b$$
$$- \varlimsup_{\varepsilon\to 0} \int_0^T \mathrm{d}t \int \mathrm{d}x \int \mathrm{d}\pi f^\varepsilon\, w \cdot (-\mathscr{L})^{-1} b\, w \cdot b.$$

Recalling (30) and the variational representation (7), it suffices to show

$$\varlimsup_{\varepsilon\to 0} \int_0^T \mathrm{d}t \int \mathrm{d}x \int \mathrm{d}\pi f^\varepsilon\, w \cdot b\, w \cdot (-\mathscr{L})^{-1} b \leq \frac{1}{2} \int_0^T \mathrm{d}t \int \mathrm{d}x \rho\, w \cdot Dw.$$

This is done with an homogenization procedure which uses Assumption 1. The third inequality can be proved in a similar way.

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Navier–Stokes Hydrodynamic Limit of BGK Kinetic Equations for an Inert Mixture of Polyatomic Gases

Marzia Bisi and Giampiero Spiga

Abstract We perform an hydrodynamic limit of BGK equations for an inert mixture of polyatomic gases, with molecular structure modelled by a set of discrete internal energy levels. An asymptotic Chapman–Enskog procedure provides consistent hydrodynamic equations at Navier–Stokes level for species number densities, global momentum and total (kinetic plus internal) energy. We explicitly compute diffusion velocities (with Fick matrix and Soret coefficients), pressure tensor (with the dynamical pressure typical of polyatomic gases), and heat flux (with Dufour effect).

Keywords Polyatomic gases · BGK models · Hydrodynamic equations Transport coefficients

1 Introduction

Most of the complex non-equilibrium problems of gas dynamics in important fields of application involve mixtures of polyatomic gases, possibly even reactive, and an accurate fluid–dynamic description originating consistently from kinetic theory would be highly desirable [12, 14]. In kinetic approaches, the non-translational degrees of freedom are accounted for by a suitable internal energy variable in a sort of semi-classical scheme, and such a variable may be either continuously ranging on the real line [10, 13], or discrete, in correspondence to an internal structure of energy levels [15]. Physical or mathematical requirements could make preferable one option or the other. Typically the continuous approach is more manageable, the discrete one is more realistic in a semiclassical frame. New important features are brought up by a polyatomic gas with respect to the classical monatomic kinetic the-

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ory, and, among them, the occurrence of the so-called dynamical pressure, or, in other words, of different non-equilibrium temperatures [2, 20]. These effects have been recently investigated at the Boltzmann level, for both continuous and discrete descriptions [9].

On the other hand, since the analytical investigation at the level of the Boltzmann equation is very heavy to manage, approximate simpler (but reliable) kinetic models are useful for applications, and in this respect relaxation models of BGK type seem to play the most important role. For the simplest conceivable reactive flows we may quote for instance the algorithms discussed in [7, 16, 18, 19], and the numerical implementations [1, 6, 17]. BGK collision models for a single polyatomic gas have been recently proposed and discussed in [4, 5], and even an ellipsoidal statistical version has been introduced [11]. The much more complicated problem of a mixture of polyatomic gases has been only recently addressed [3, 8], and remains, to a large extent, quite open.

In all of the literature quoted above one of the most important questions to be answered is the derivation of fluid–dynamic equations governing the evolution of the main macroscopic fields, which are power moments of the distribution functions, and correspond to physically observable quantities. Exact balance equations follow from kinetic theory by taking moments of the kinetic equations, but their closure requires constitutive equations for the additional moments and collision contributions which come up in the procedure, and which have to be expressed in terms of the main fields by means of suitable transport coefficients. This goal is usually achieved in the hydrodynamic limit of dominant collisions (small Knudsen number) by resorting to an asymptotic expansion with respect to such small parameter and performing the relevant asymptotic Chapman–Enskog analysis [12].

This is what the present paper is about, concerning the non-reactive case of an inert mixture and the Navier–Stokes hydrodynamic level (first order asymptotic corrections). Removing those restrictions is planned as future work. Specifically, we recall and briefly discuss in Sect. 2 the main features of the adopted BGK model for polyatomic mixtures [3], and perform then the consistent asymptotic procedure in the next three Sections. Manipulations are not easy at all, however they allow for explicit analytical results in terms of a set of collision parameters to be appropriately chosen, whereas the Boltzmann approach would remain at a formal level, implying the inversion of complicated integral operators. After deducing in Sect. 3 hydrodynamic variables and equilibria (Euler level), we proceed in Sect. 4 to the evaluation of the first order corrections to the distribution functions, and perform in Sect. 5 the closure of the macroscopic conservation laws by determining constitutive relations and relevant transport coefficients for diffusion velocities, dynamical pressure, viscous stress, and heat flux, yielding finally the sought Navier–Stokes fluid dynamic equations. All transport coefficients (Fick matrix, Soret factors, bulk viscosity, shear viscosity and thermal conductivity) are cast in explicit form in terms of the parameters and the relaxation times of the model.

2 BGK Model

We consider a mixture of Q gases G^i, $i = 1, \ldots, Q$, each one having N discrete energy levels. Each polyatomic constituent may be thus modelled as a mixture of N monatomic gases, with a proper distribution function for each of them. In this way, one has to manage QN different components, which for convenience are labeled according to a single index and ordered in such a way that the i-th gas may be regarded as the equivalence class of the indices s which are congruent to i modulo Q. Distribution functions will be denoted by $f^s(\mathbf{v})$, $s = 1, \ldots, QN$, and main macroscopic fields of the mixture may be recovered as suitable moments of this set of distributions. Specifically, the number density of the gas G^i is $N^i = \sum_{s \equiv i} n^s$, with

$$n^s = \int f^s(\mathbf{v})\, d\mathbf{v}\,,$$

while mass density is $\rho^i = m^i N^i$, with m^i denoting the particle mass of gas G^i (thus relevant also to all components $s \equiv i$); consequently, total number and mass densities of the mixture are provided by

$$n = \sum_{i=1}^{Q} N^i = \sum_{i=1}^{Q} \sum_{s \equiv i} n^s\,, \qquad \rho = \sum_{i=1}^{Q} m^i N^i\,.$$

Analogously, macroscopic velocity $\mathbf{u}$ of the mixture is defined as

$$\mathbf{u} = \frac{1}{n} \sum_{i=1}^{Q} \sum_{s \equiv i} n^s \mathbf{u}^s = \frac{1}{n} \sum_{i=1}^{Q} \sum_{s \equiv i} \int \mathbf{v} f^s(\mathbf{v})\, d\mathbf{v}\,,$$

while pressure tensor $\mathbf{P}$ and thermal heat flux $\mathbf{q}$ read as

$$\mathbf{P} = \sum_{i=1}^{Q} m^i \sum_{s \equiv i} \int (\mathbf{v} - \mathbf{u}) \otimes (\mathbf{v} - \mathbf{u}) f^s(\mathbf{v})\, d\mathbf{v}\,,$$

$$\mathbf{q} = \frac{1}{2} \sum_{i=1}^{Q} m^i \sum_{s \equiv i} \int (\mathbf{v} - \mathbf{u})\, |\mathbf{v} - \mathbf{u}|^2 f^s(\mathbf{v})\, d\mathbf{v}\,.$$

Kinetic temperature is related to the trace of pressure tensor as $T = \frac{1}{3nK} \operatorname{tr}(\mathbf{P})$ (where K is the Boltzmann constant), and internal energy of the mixture is given by $\sum_{i=1}^{Q} \sum_{s \equiv i} E^s n^s$, where E^s denotes the internal energy of molecules of s-th component.

As concerns the QN kinetic equations, in [3] a BGK approximation of the original Boltzmann model [15] has been proposed, reading as

$$\frac{\partial f^s}{\partial t} + \mathbf{v} \cdot \nabla_{\mathbf{x}} f^s = \nu^s \left(\mathscr{M}^s - f^s \right)$$

where $\forall i = 1, \ldots, Q$, $\forall s \equiv i$, collision operator is constituted by a $\mathbf{v}$–independent collision frequency ν^s multiplying the difference between an auxiliary distribution of Maxwellian type and the actual distribution function $f^s(\mathbf{v})$. The Maxwellian attractors are assumed to be accommodated at common fictitious velocity $\tilde{\mathbf{u}}$ and temperature $\tilde{T}$,

$$\mathscr{M}^s = \tilde{n}^s \left(\frac{m^i}{2\pi K \tilde{T}} \right)^{3/2} \exp\left(- \frac{m^i}{2K\tilde{T}} |\mathbf{v} - \tilde{\mathbf{u}}|^2 \right), \tag{1}$$

with the additional equilibrium assumption on fictitious number densities

$$\tilde{n}^s = \frac{\tilde{N}^i}{Z^i(\tilde{T})} \, \mathrm{e}^{-\frac{E^s - E^i}{K\tilde{T}}}, \qquad Z^i(\tilde{T}) = \sum_{s \equiv i} \mathrm{e}^{-\frac{E^s - E^i}{K\tilde{T}}}. \tag{2}$$

Here Z^i represents the partition function of the gas G^i, and constraints (2) relating auxiliary densities and temperature correspond to suppose that Maxwellians $\mathscr{M}^s$ are collision equilibria of the Boltzmann model for a mixture with discrete internal energies that we want to approximate [15]. As proven in [3], conservations of number densities N^i, of global mass velocity $\mathbf{u}$ and of total energy allow to cast auxiliary parameters in terms of the actual macroscopic fields as

$$\tilde{N}^i = \sum_{s \equiv i} \nu^s n^s \Big/ \left(\sum_{s \equiv i} \frac{\nu^s}{Z^i(\tilde{T})} \, \mathrm{e}^{-\frac{E^s - E^i}{K\tilde{T}}} \right), \tag{3}$$

$$\tilde{\mathbf{u}} = \sum_{i=1}^{Q} m^i \sum_{s \equiv i} \nu^s n^s \mathbf{u}^s \Big/ \left(\sum_{i=1}^{Q} m^i \sum_{s \equiv i} \nu^s n^s \right), \tag{4}$$

while $\tilde{T}$ is provided as the (unique) solution of a transcendental equation of the form $F(\tilde{T}) = \Lambda$, where

$$F(\tilde{T}) = \left(\sum_{i=1}^{Q} \sum_{r \equiv i} \nu^r n^r \right) \left[\frac{3}{2} K\tilde{T} + \frac{\sum_{s \equiv i} \nu^s E^s \, \mathrm{e}^{-\frac{E^s - E^i}{K\tilde{T}}}}{\sum_{p \equiv i} \nu^p \, \mathrm{e}^{-\frac{E^p - E^i}{K\tilde{T}}}} \right], \tag{5}$$

and Λ, whose cumbersome expression is not shown for brevity since it is not needed here, is explicit in terms of actual macroscopic fields.

This model of course reproduces, by its construction, the Maxwellian collision equilibria of the Boltzmann description, and the correct conservation laws of species

number densities, global momentum and energy. Moreover, fulfillment of the H–theorem has been proven [3] with the same logarithmic Lyapunov H–functional used for the Boltzmann equations for mixtures.

3 Hydrodynamic Limit: Conserved Quantities and Leading Order Accuracy

We consider a collision dominated regime and we rescale the BGK equations as

$$\frac{\partial f^s}{\partial t} + \mathbf{v} \cdot \nabla_{\mathbf{x}} f^s = \frac{1}{\varepsilon}\, \nu^s \big(\mathscr{M}^s - f^s \big), \qquad s = 1, \ldots, QN, \tag{6}$$

where ε stands for the Knudsen number. We expand distributions and macroscopic (actual and auxiliary) fields in powers of ε, as

$$f^s = f^{s(0)} + \varepsilon f^{s(1)},$$

and consequently

$$n^s = n^{s(0)} + \varepsilon\, n^{s(1)}, \qquad \mathbf{u}^s = \mathbf{u}^{s(0)} + \varepsilon\, \mathbf{u}^{s(1)}, \qquad T^s = T^{s(0)} + \varepsilon\, T^{s(1)},$$
$$\mathbf{P}^s = \mathbf{P}^{s(0)} + \varepsilon\, \mathbf{P}^{s(1)}, \qquad \mathbf{q}^s = \mathbf{q}^{s(0)} + \varepsilon\, \mathbf{q}^{s(1)}$$

for the main fluid–dynamic fields of single components, and

$$\tilde{n}^s = \tilde{n}^{s(0)} + \varepsilon\, \tilde{n}^{s(1)}, \qquad \tilde{\mathbf{u}} = \tilde{\mathbf{u}}^{(0)} + \varepsilon\, \tilde{\mathbf{u}}^{(1)}, \qquad \tilde{T} = \tilde{T}^{(0)} + \varepsilon\, \tilde{T}^{(1)}$$

for the auxiliary parameters appearing in the Maxwellian attractors $\mathscr{M}^s$.

We impose, as typical in the Chapman–Enskog procedure, that hydrodynamic variables corresponding to the collision invariants of the leading order kinetic operator (of BGK–relaxation type, in this paper) remain unexpanded. In the present polyatomic frame, macroscopic fields preserved by scattering are number densities N^i of each gas $i = 1, \ldots, Q$ (and therefore even n and ρ), global momentum $\rho\mathbf{u}$, and total energy $n\mathscr{E} = \frac{3}{2}\, nKT + \sum_{i=1}^{Q} \sum_{s \equiv i} E^s n^s$. Consequently

$$N^i = \sum_{s \equiv i} n^{s(0)}, \qquad \mathbf{u} = \mathbf{u}^{(0)},$$

and analogously for total energy

$$\frac{3}{2}\, nKT + \sum_{i=1}^{Q} \sum_{s \equiv i} E^s n^s = \frac{3}{2}\, nKT^{(0)} + \sum_{i=1}^{Q} \sum_{s \equiv i} E^s n^{s(0)}.$$

These requirements prescribe also that corresponding first order corrections must vanish, providing thus the constraints

$$\sum_{s\equiv i} n^{s(1)} = 0 \qquad i = 1, \dots, Q, \qquad \mathbf{u}^{(1)} = \mathbf{0}\,, \\ T^{(1)} = -\frac{2}{3}\frac{1}{nK}\sum_{i=1}^{Q}\sum_{s\equiv i} E^s n^{s(1)}. \tag{7}$$

Leading order terms of rescaled equations (6) provide immediately $f^{s(0)} = \mathscr{M}^{s(0)}$, hence actual and auxiliary parameters coincide:

$$n^{s(0)} = \tilde{n}^{s(0)}, \qquad \mathbf{u}^{s(0)} = \tilde{\mathbf{u}}^{(0)}, \qquad T^{s(0)} = \tilde{T}^{(0)} \qquad \forall s\,. \tag{8}$$

Last equalities mean that leading order velocities of all components take a common value, thus $\mathbf{u}^{s(0)} = \mathbf{u}\ \forall s$, and the same holds for temperatures, $T^{s(0)} = T^{(0)}$, where only the leading term of mixture temperature appears, in agreement with the fact that it is not an hydrodynamic variable. Moreover, the first of (8) implies that

$$N^i = \sum_{s\equiv i} n^{s(0)} = \sum_{s\equiv i} \tilde{n}^{s(0)} = \tilde{N}^{i(0)},$$

thus leading order number densities fulfill the laws (2), that for auxiliary parameters have been assumed from the beginning in the construction of the BGK operator. In conclusion, leading order distributions are nothing but collision equilibria

$$f^{s(0)} = n^{s(0)} \left(\frac{m^i}{2\pi K T^{(0)}}\right)^{3/2} \exp\left(-\frac{m^i}{2KT^{(0)}}|\mathbf{v}-\mathbf{u}|^2\right), \tag{9}$$

with

$$n^{s(0)} = \frac{N^i}{Z^i(T^{(0)})}\, \mathrm{e}^{-\frac{E^s - E^i}{KT^{(0)}}}. \tag{10}$$

The total energy (sum of kinetic and internal energies) at this collision equilibrium state is given by

$$n\mathscr{E} = n\mathscr{E}_{\mathsf{eq}} = \frac{3}{2}nKT^{(0)} + \sum_{i=1}^{Q}\sum_{s\equiv i} E^s n^{s(0)} = \frac{3}{2}nKT^{(0)} + \sum_{i=1}^{Q} N^i \bar{E}^i(T^{(0)}) \tag{11}$$

where

$$\bar{E}^i(T^{(0)}) = \frac{1}{Z^i(T^{(0)})}\sum_{s\equiv i} E^s \mathrm{e}^{-\frac{E^s - E^i}{KT^{(0)}}} \tag{12}$$

is a weighted average of the energy levels of gas G^i. Notice that Eq. (11) may be considered as a transcendental equation for $T^{(0)}$ for given $\mathscr{E}$, and as such it is just a particular case of (5), corresponding to the option of all equal ν^s. It is then uniquely solvable, and establishes a one-to-one relationship between $T^{(0)}$ and $\mathscr{E}$, which is a conserved quantity, so that $T^{(0)}$ is itself equivalent to an hydrodynamic variable. Therefore the $Q+4$ parameters defining equilibria (9) are cast in terms of the $Q+4$ conserved quantities, and we may choose as fluid dynamic fields in the sequel the variables N^i, $\mathbf{u}$, $T^{(0)}$.

Furthermore, the specific heat at constant volume of an inert mixture of polyatomic gases, defined as

$$c_v^*(T^{(0)}) = \frac{1}{K}\frac{\partial \mathscr{E}_{\mathsf{eq}}}{\partial T^{(0)}}$$

turns out to be, in the present BGK kinetic model,

$$c_v^*(T^{(0)}) = \frac{3}{2} + \frac{1}{n}\sum_{i=1}^{Q} N^i\,\sigma_i^*(T^{(0)})$$

where

$$\sigma_i^*(T^{(0)}) = \frac{1}{K}\frac{\partial \bar{E}^i(T^{(0)})}{\partial T^{(0)}} = \frac{1}{Z^i(T^{(0)})}\sum_{s\equiv i}\left[\frac{E^s - \bar{E}^i(T^{(0)})}{KT^{(0)}}\right]^2 \mathrm{e}^{-\frac{E^s-\bar{E}^i}{KT^{(0)}}}$$

is the expected correction due to the polyatomic structure of gases, analogous to the one found in [4] for a single polyatomic gas, that of course would vanish in case of monatomic mixture (only one energy level for each gas), reproducing the classical value $c_v^* = 3/2$.

4 First Order Distributions $f^{s(1)}$

From the rescaled BGK model (6) we deduce that the first order correction to the distribution functions is given by

$$f^{s(1)} = \mathscr{M}^{s(1)} - \frac{1}{\nu^{s(0)}}\left(\frac{\partial_0 f^{s(0)}}{\partial t} + \mathbf{v}\cdot\nabla_{\mathbf{x}} f^{s(0)}\right), \tag{13}$$

with appearance of the well known zero order time derivative [12]. Notice that, since collision frequencies ν^s may depend on macroscopic fields, they have been expanded as well. The final result will be quite similar to the corresponding one obtained in [4, 5] for a single gas, but we will repeat here all the fundamental steps in order to point out analogies and differences, and some new contributions typical of mixtures only. The term $\mathscr{M}^{s(1)}$ means the first order correction, with respect to the parameter ε, of

the Maxwellian attractor (1), provided by $\mathscr{M}^{s(1)} = \frac{\partial}{\partial\varepsilon}\mathscr{M}^{s}\Big|_{\varepsilon=0}$. It can be checked that for each $s \equiv i$, with $i = 1, \dots, Q$, we have

$$\begin{aligned}\mathscr{M}^{s(1)} = f^{s(0)} \left\{ \frac{\tilde{N}^{i(1)}}{N^i} + \frac{m^i}{KT^{(0)}}\, \tilde{\mathbf{u}}^{(1)} \cdot (\mathbf{v}-\mathbf{u}) \right. \\ \left. + \frac{\tilde{T}^{(1)}}{T^{(0)}} \left[\frac{1}{KT^{(0)}} \left(\frac{1}{2}\, m^i |\mathbf{v}-\mathbf{u}|^2 + E^s - \bar{E}^i(T^{(0)}) \right) - \frac{3}{2} \right] \right\}.\end{aligned} \tag{14}$$

For each index s, the attractor $\mathscr{M}^{s(1)}$ depends only on the total number density of the gas $i \equiv s$ which the component s belongs to, and not on the global number density of the mixture. Moreover, we remark also the appearance of the corrections of the auxiliary parameters $\tilde{N}^{i(1)}$, $\tilde{\mathbf{u}}^{(1)}$, $\tilde{T}^{(1)}$, which in the sequel need to be made explicit in terms of the hydrodynamic fields.

As concerns the streaming part in the relation (13), the derivatives of $f^{s(0)}$ may be expressed in terms of corresponding derivatives of N^i, $\mathbf{u}$, $T^{(0)}$, and the formal zero-order time derivatives have then to be eliminated, as usual in the Chapman–Enskog procedure, by the leading order Euler equations. We find

$$\begin{aligned}\frac{\partial_0 f^{s(0)}}{\partial t} + \mathbf{v}\cdot\nabla_{\mathbf{x}} f^{s(0)} = f^{s(0)} \left\{ \frac{1}{N^i} \left[\frac{\partial_0 N^i}{\partial t} + \mathbf{v}\cdot\nabla_{\mathbf{x}} N^i \right] \right. \\ + \frac{m^i}{KT^{(0)}} (\mathbf{v}-\mathbf{u}) \cdot \left[\frac{\partial_0 \mathbf{u}}{\partial t} + \mathbf{v}\cdot\nabla_{\mathbf{x}}\mathbf{u} \right] + \frac{1}{KT^{(0)}} \left[\frac{\partial_0 (KT^{(0)})}{\partial t} + \mathbf{v}\cdot\nabla_{\mathbf{x}} (KT^{(0)}) \right] \\ \left. \times \left[\frac{1}{KT^{(0)}} \left(\frac{1}{2}\, m^i |\mathbf{v}-\mathbf{u}|^2 + E^s - \bar{E}^i(T^{(0)}) \right) - \frac{3}{2} \right] \right\}.\end{aligned}$$

Euler equations provide immediately

$$\frac{\partial_0 N^i}{\partial t} = -\nabla_{\mathbf{x}} \cdot (N^i \mathbf{u})\,, \qquad \frac{\partial_0 \mathbf{u}}{\partial t} = -\mathbf{u}\cdot\nabla_{\mathbf{x}}\mathbf{u} - \frac{1}{\rho}\nabla_{\mathbf{x}} \big(nKT^{(0)} \big)\,,$$

while energy equation reads as

$$\begin{aligned}\frac{\partial_0}{\partial t} \left(\frac{1}{2}\,\rho |\mathbf{u}|^2 + \frac{3}{2}\, nKT^{(0)} + \sum_{i=1}^{Q} \sum_{s\equiv i} E^s n^{s(0)} \right) \\ = -\nabla_{\mathbf{x}} \cdot \left[\left(\frac{1}{2}\,\rho |\mathbf{u}|^2 + \frac{5}{2}\, nKT^{(0)} + \sum_{i=1}^{Q} \sum_{s\equiv i} E^s n^{s(0)} \right) \mathbf{u} \right],\end{aligned}$$

and yields

$$\begin{aligned}\frac{3}{2}\,n\,\frac{\partial_0(KT^{(0)})}{\partial t}+\sum_{i=1}^{Q}\sum_{s\equiv i}E^s\left(\frac{\partial_0 n^{s(0)}}{\partial t}+\nabla_{\mathbf{x}}\cdot(n^{s(0)}\mathbf{u})\right)\\ =-nKT^{(0)}\nabla_{\mathbf{x}}\cdot\mathbf{u}-\frac{3}{2}\,n\,\mathbf{u}\cdot\nabla_{\mathbf{x}}(KT^{(0)})\,.\end{aligned}\tag{15}$$

From the expression (10) for $n^{s(0)}$, with some computations it can be checked that

$$\begin{aligned}\frac{\partial_0 n^{s(0)}}{\partial t}+\nabla_{\mathbf{x}}\cdot(n^{s(0)}\mathbf{u})=\frac{N^i}{Z^i(T^{(0)})}\,\frac{1}{(KT^{(0)})^2}\,\mathrm{e}^{-\frac{E^s-E^i}{KT^{(0)}}}\\ \times\left(E^s-\bar{E}^i(T^{(0)})\right)\left[\frac{\partial_0(KT^{(0)})}{\partial t}+\mathbf{u}\cdot\nabla_{\mathbf{x}}(KT^{(0)})\right].\end{aligned}$$

Since, bearing in mind the definition of the average energy (12), we have

$$\sum_{s\equiv i}E^s\mathrm{e}^{-\frac{E^s-E^i}{KT^{(0)}}}\left(E^s-\bar{E}^i(T^{(0)})\right)=\sum_{s\equiv i}\left(E^s-\bar{E}^i(T^{(0)})\right)^2\mathrm{e}^{-\frac{E^s-E^i}{KT^{(0)}}},$$

the energy equation (15) simply yields

$$\frac{\partial_0(KT^{(0)})}{\partial t}=-\mathbf{u}\cdot\nabla_{\mathbf{x}}(KT^{(0)})-\frac{KT^{(0)}}{c_v^*(T^{(0)})}\nabla_{\mathbf{x}}\cdot\mathbf{u}\,,$$

formally identical to the case of a single polyatomic gas [4]. Taking all of these results into account we finally get

$$\begin{aligned}-\frac{1}{\nu^{s(0)}}\left(\frac{\partial_0 f^{s(0)}}{\partial t}+\mathbf{v}\cdot\nabla_{\mathbf{x}}f^{s(0)}\right)=-\frac{f^{s(0)}}{\nu^{s(0)}}\left\{(\mathbf{v}-\mathbf{u})\cdot\left[\frac{\nabla_{\mathbf{x}}N^i}{N^i}-\frac{m^i}{\rho}\,\nabla_{\mathbf{x}}n\right]\right.\\ \left.+\frac{m^i}{KT^{(0)}}(\mathbf{v}-\mathbf{u})\otimes(\mathbf{v}-\mathbf{u}):\nabla_{\mathbf{x}}\mathbf{u}\right.\\ -\frac{1}{c_v^*(T^{(0)})}\left[\frac{m^i}{2KT^{(0)}}|\mathbf{v}-\mathbf{u}|^2+\frac{E^s-\bar{E}^i(T^{(0)})}{KT^{(0)}}+\frac{1}{n}\sum_{i=1}^{Q}N^i\,\sigma_i^*(T^{(0)})\right]\nabla_{\mathbf{x}}\cdot\mathbf{u}\\ +\frac{1}{KT^{(0)}}\left[\frac{m^i}{2KT^{(0)}}|\mathbf{v}-\mathbf{u}|^2+\frac{E^s-\bar{E}^i(T^{(0)})}{KT^{(0)}}-\frac{3}{2}-\frac{m^i n}{\rho}\right](\mathbf{v}-\mathbf{u})\cdot\nabla_{\mathbf{x}}(KT^{(0)}),\end{aligned}\tag{16}$$

where i is the unique index $i=1,\ldots,Q$ such that $s\equiv i$. Notice that in case of single gas, the gradients of number densities, namely the content of the square brackets in the first line of (16), would disappear, and moreover, in the last line of (16), we would have $m^i n/\rho=1$. In the present frame, the dependence on number density gradients will allow to recover the Fick matrix (in the diffusion velocities) and the Dufour effect (in the thermal heat flux), typical of gas mixtures [12, 14]. The first order distribution $f^{s(1)}$ is finally provided by the sum of (14) and (16).

5 Asymptotic Closure and Navier–Stokes Equations

We aim now at finding a consistent Navier–Stokes closure (namely, at first order accuracy) of the macroscopic conservation equations for an inert mixture that, as well known [12], may be cast as

$$\begin{aligned}
&\frac{\partial N^i}{\partial t} + \nabla_{\mathbf{x}} \cdot (N^i\,\mathbf{u}) + \varepsilon\,\nabla_{\mathbf{x}} \cdot \left(\sum_{s \equiv i} n^{s(0)} \mathbf{u}^{s(1)} \right) = 0\,, \qquad i = 1, \ldots, Q,\\
&\frac{\partial}{\partial t}(\rho \mathbf{u}) + \nabla_{\mathbf{x}} \cdot (\rho\,\mathbf{u} \otimes \mathbf{u}) + \nabla_{\mathbf{x}} \big(nKT^{(0)} \big) + \varepsilon\,\nabla_{\mathbf{x}} \cdot \mathbf{P}^{(1)} = \mathbf{0}\,,\\
&\frac{\partial}{\partial t} \left(\frac{1}{2}\,\rho |\mathbf{u}|^2 + \frac{3}{2}\,nKT^{(0)} + \sum_{i=1}^{Q} N^i \bar{E}^i(T^{(0)}) \right)\\
&+ \nabla_{\mathbf{x}} \cdot \left[\left(\frac{1}{2}\,\rho |\mathbf{u}|^2 + \frac{5}{2}\,nKT^{(0)} + \sum_{i=1}^{Q} N^i \bar{E}^i(T^{(0)}) \right) \mathbf{u} \right]\\
&+ \varepsilon\,\nabla_{\mathbf{x}} \cdot \big(\mathbf{P}^{(1)} \cdot \mathbf{u} \big) + \varepsilon\,\nabla_{\mathbf{x}} \cdot \mathbf{q}^{(1)} + \varepsilon\,\nabla_{\mathbf{x}} \cdot \left(\sum_{i=1}^{Q} \sum_{s \equiv i} E^s\, n^{s(0)} \mathbf{u}^{s(1)} \right) = 0\,.
\end{aligned} \tag{17}$$

We need thus constitutive equations for pressure tensor $\mathbf{P}^{(1)}$, heat flux $\mathbf{q}^{(1)}$ and diffusion velocities $\mathbf{u}^{s(1)}$, affecting both number density equations and energy equation, where the quantity $\sum_{i=1}^{Q} \sum_{s \equiv i} E^s\, n^{s(0)} \mathbf{u}^{s(1)}$ represents an additional heat flux due to internal energy of the polyatomic gases. These macroscopic fields may be explicitly computed as suitable moments of first order distributions $f^{s(1)}$ (given by (14) + (16)). Notice that the closure procedure needs also the computation of corrections of auxiliary parameters $\tilde{N}^{i(1)}$, $\tilde{\mathbf{u}}^{(1)}$, $\tilde{T}^{(1)}$, which affect the distributions (14).

5.1 Computation of Number Densities

By direct integration of the distribution $f^{s(1)}$ it can be checked that

$$\begin{aligned}
n^{s(1)} = \int f^{s(1)}(\mathbf{v})\,d\mathbf{v} &= n^{s(0)}\,\frac{\tilde{N}^{i(1)}}{N^i} + n^{s(0)}\,\frac{E^s - \bar{E}^i(T^{(0)})}{KT^{(0)}}\,\frac{\tilde{T}^{(1)}}{T^{(0)}}\\
&+ \frac{1}{c_v^*(T^{(0)})}\,\frac{n^{s(0)}}{\nu^{s(0)}}\,\frac{E^s - \bar{E}^i(T^{(0)})}{KT^{(0)}}\,\nabla_{\mathbf{x}} \cdot \mathbf{u}\,.
\end{aligned} \tag{18}$$

Bearing in mind the first of constraints (7), $\sum_{s \equiv i} n^{s(1)} = 0$, $\forall i$, we get an explicit expression for each auxiliary number density $\tilde{N}^{i(1)}$:

$$\tilde{N}^{i(1)} = -\,\frac{1}{c_v^*(T^{(0)})} \sum_{s \equiv i} \frac{n^{s(0)}}{\nu^{s(0)}}\,\frac{E^s - \bar{E}^i(T^{(0)})}{KT^{(0)}}\,\nabla_{\mathbf{x}} \cdot \mathbf{u}\,. \tag{19}$$

When G^i is a monatomic gas (with only one energy level) this correction turns out to vanish, consistently with the fact that in such a case the auxiliary number density $\tilde{N}^i$ coincides with the actual density N^i [3], which is an (unexpanded) hydrodynamic variable.

Notice that the densities $n^{s(1)}$ do not appear explicitly in the system (17) to be closed; however they will be needed in the next steps, where also the still unknown $\tilde{T}^{(1)}$ will be specified.

5.2 Computation of Diffusion Velocities

Diffusion velocities of single components $s = 1, \ldots, QN$ are defined as

$$\mathbf{u}^{s(1)} = \frac{1}{n^{s(0)}} \int (\mathbf{v} - \mathbf{u}) f^{s(1)}(\mathbf{v})\, d\mathbf{v}\,,$$

thus from (14) + (16) we get

$$\begin{aligned} \mathbf{u}^{s(1)} = \tilde{\mathbf{u}}^{(1)} - \frac{1}{\nu^{s(0)}} KT^{(0)} \left[\frac{\nabla_{\mathbf{x}} N^i}{\rho^i} - \frac{\nabla_{\mathbf{x}} n}{\rho} \right] \\ - \frac{1}{\nu^{s(0)}} \left[\frac{1}{m^i} \frac{E^s - \bar{E}^i(T^{(0)})}{KT^{(0)}} + \frac{1}{m^i} - \frac{n}{\rho} \right] \nabla_{\mathbf{x}} (KT^{(0)}) \end{aligned} \tag{20}$$

where all other terms vanish by parity arguments. This result may also be cast as

$$\begin{aligned} \mathbf{u}^{s(1)} = \tilde{\mathbf{u}}^{(1)} - \frac{1}{\nu^{s(0)}\, m^i} \frac{E^s - \bar{E}^i(T^{(0)})}{KT^{(0)}} \nabla_{\mathbf{x}} (KT^{(0)}) \\ - \frac{1}{\nu^{s(0)}} \left[\frac{\nabla_{\mathbf{x}} (N^i KT^{(0)})}{\rho^i} - \frac{\nabla_{\mathbf{x}} (nKT^{(0)})}{\rho} \right], \end{aligned} \tag{21}$$

where we may note that the second line, containing gradients of species scalar pressures, would vanish in case of a single gas.

At this stage $\mathbf{u}^{s(1)}$ is not completely explicit, since it depends on the auxiliary field $\tilde{\mathbf{u}}^{(1)}$. By imposing now the second constraint of (7), namely

$$\mathbf{u}^{(1)} = \sum_{i=1}^{Q} m^i \sum_{s \equiv i} \left(n^{s(0)} \mathbf{u}^{s(1)} + n^{s(1)} \mathbf{u} \right) = \sum_{i=1}^{Q} m^i \sum_{s \equiv i} n^{s(0)} \mathbf{u}^{s(1)} = \mathbf{0}\,, \tag{22}$$

from (21) we get

$$\tilde{\mathbf{u}}^{(1)} = \frac{1}{\rho}\sum_{i=1}^{Q}\sum_{s\equiv i}\frac{n^{s(0)}}{\nu^{s(0)}}\,\frac{E^s-\bar{E}^i(T^{(0)})}{KT^{(0)}}\,\nabla_{\mathbf{x}}(KT^{(0)}) + \frac{1}{\rho}\sum_{i=1}^{Q}\sum_{s\equiv i}\frac{n^{s(0)}}{\nu^{s(0)}}\left[\frac{\nabla_{\mathbf{x}}(N^iKT^{(0)})}{N^i}-\frac{m^i}{\rho}\,\nabla_{\mathbf{x}}(nKT^{(0)})\right]. \tag{23}$$

By inserting (23) into (21), or equivalently into (20), the computation of diffusion velocities is completed. As concerns velocity corrections of single gases G^i, $i = 1,\dots,Q$, defined as

$$\mathbf{u}^{i(1)} = \frac{1}{N^i}\sum_{s\equiv i} n^{s(0)}\mathbf{u}^{s(1)},$$

we note that their constitutive equations may be cast in the form

$$\mathbf{u}^{i(1)} = \sum_{j=1}^{Q}\mathscr{F}^{ij}\,\nabla_{\mathbf{x}}N^j + \alpha^i\nabla_{\mathbf{x}}(KT^{(0)}) \tag{24}$$

where

$$\mathscr{F}^{ij} = \frac{KT^{(0)}}{\rho}\left(\frac{1}{N^j}\sum_{s\equiv j}\frac{n^{s(0)}}{\nu^{s(0)}}+\frac{1}{N^i}\sum_{s\equiv i}\frac{n^{s(0)}}{\nu^{s(0)}}\right) - \frac{\delta_{ij}KT^{(0)}}{N^i\rho^i}\sum_{s\equiv i}\frac{n^{s(0)}}{\nu^{s(0)}} - \frac{KT^{(0)}}{\rho^2}\sum_{h=1}^{Q}m^h\sum_{s\equiv h}\frac{n^{s(0)}}{\nu^{s(0)}} \tag{25}$$

(with δ_{ij} standing for the Kronecker delta), and

$$\alpha^i = -\frac{1}{\rho^i}\sum_{j=1}^{Q}\left(\delta_{ij}-\frac{\rho^i}{\rho}\right)\sum_{s\equiv j}\frac{n^{s(0)}}{\nu^{s(0)}}\left(\frac{E^s-\bar{E}^j(T^{(0)})}{KT^{(0)}}+1-\frac{m^jn}{\rho}\right). \tag{26}$$

Coefficients $\mathscr{F}^{ij}$ form the so-called Fick matrix, which relates diffusion velocities with gradients of number densities of single gases. It may be easily seen that such matrix is symmetric ($\mathscr{F}^{ij} = \mathscr{F}^{ji}$) and satisfies the relation

$$\sum_{j=1}^{Q}\rho^j\mathscr{F}^{ij} = 0\,, \qquad \forall\, i = 1,\dots,Q\,. \tag{27}$$

Moreover, all its diagonal terms are negative:

$$\mathscr{F}^{ii} = -\frac{KT^{(0)}}{N^i\rho^i}\left(1-\frac{\rho^i}{\rho}\right)^2\sum_{s\equiv i}\frac{n^{s(0)}}{\nu^{s(0)}} - \frac{KT^{(0)}}{\rho^2}\sum_{h\neq i}m^h\sum_{s\equiv h}\frac{n^{s(0)}}{\nu^{s(0)}} < 0\,.$$

Coefficients α^i given in (26) provide the Soret effect, namely the dependence of diffusion velocities $\mathbf{u}^{i(1)}$ on the gradient of kinetic temperature (see (24)). Again we obviously have

$$\sum_{i=1}^{Q} \rho^i \alpha^i = 0\,, \tag{28}$$

and properties (27) and (28) guarantee fulfillment of constraint (22). Result (24) also determines the first order corrections to the mass conservations (continuity equations) in (17), since

$$\sum_{s\equiv i} n^{s(0)} \mathbf{u}^{s(1)} = N^i \mathbf{u}^{i(1)} = N^i \sum_{j=1}^{Q} \mathscr{F}^{ij}\, \nabla_{\mathbf{x}} N^j + N^i \alpha^i \nabla_{\mathbf{x}} (KT^{(0)}).$$

In case of single polyatomic gas, coefficients $\mathscr{F}^{11}$ and α^1 are both vanishing (since $\rho^1 = \rho = mn$), reproducing the fact that mean velocity of the gas is an hydrodynamic (unexpanded) variable.

It is interesting to note that, by resorting to (25) and (26), diffusion velocities may be cast as

$$\mathbf{u}^{i(1)} = \sum_{j=1}^{Q} \frac{\mathscr{F}^{ij}}{KT^{(0)}} \nabla_{\mathbf{x}} (N^j KT^{(0)}) + \frac{1}{\rho^i} \sum_{j=1}^{Q} \left(\frac{\rho^i}{\rho} - \delta_{ij} \right) \sum_{s\equiv j} \frac{n^{s(0)}}{\nu^{s(0)}} \frac{E^s - \bar{E}^j(T^{(0)})}{KT^{(0)}} \nabla_{\mathbf{x}} (KT^{(0)}), \tag{29}$$

where the first addend constitutes the Onsager relation, relating species velocities to species pressures via the symmetric matrix $\mathscr{F}^{ij}/KT^{(0)}$ (Onsager's reciprocity), whereas the second addend is a sort of thermal diffusion effect contributed by the internal structure of energy levels in each polyatomic species, which would disappear in the mono-atomic limit. Such an "excitation" contribution would disappear also if all relaxation parameters of the model were taken equal to each other within the same species, namely $\nu^{s(0)} = \nu^{i(0)}, \quad \forall s \equiv i$.

5.3 Computation of Dynamical Pressure and of Viscous Stress Tensor

It is well known that in a polyatomic gas the classical equilibrium scalar pressure is not the trace of the pressure tensor, but must be corrected by an additional term, usually referred to as "dynamical pressure". This macroscopic field is typical of the polyatomic structure of molecules, and it does not appear in monatomic gases [20]. For this reason, the simplest fluid–dynamic description of a polyatomic gas beyond the Euler level is the so-called "6–moment theory", in which the dynamical pressure Π represents the sixth field, additional with respect to classical variables n, $\mathbf{u}$, T of Euler equations [2, 9]. This feature is clearly related to the fact that kinetic

temperature is not a conserved quantity, and there is a correction with respect to the equilibrium value.

In the present frame, dynamical pressure of our inert mixture is provided by

$$\Pi = nKT^{(1)} = \frac{1}{3}\sum_{i=1}^{Q}\sum_{s\equiv i} m^i \int |\mathbf{v}-\mathbf{u}|^2 f^{s(1)}(\mathbf{v})\, d\mathbf{v}\,,$$

and by explicit computation we get

$$nKT^{(1)} = nK\tilde{T}^{(1)} - \frac{2}{3}\frac{KT^{(0)}}{c_v^*(T^{(0)})}\frac{1}{n}\sum_{j=1}^{Q} N^j\,\sigma_j^*(T^{(0)})\sum_{i=1}^{Q}\sum_{s\equiv i}\frac{n^{s(0)}}{\nu^{s(0)}}\,\nabla_{\mathbf{x}}\cdot\mathbf{u}\,. \tag{30}$$

More precisely, $nK\tilde{T}^{(1)}$ is the unique contribution arising from the Maxwellian attractors (14) (all other terms vanish, taking into account also that $\sum_{i=1}^{Q}\tilde{N}^{i(1)}=0$), while the addend involving the divergence of mean velocity comes from the streaming part (16). The third constraint in (7) together with the expressions (18) for $n^{s(1)}$ and (19) for $\tilde{N}^{i(1)}$ provide

$$\begin{aligned}\frac{3}{2}nKT^{(1)} &= -\sum_{i=1}^{Q}\sum_{s\equiv i}E^s n^{s(1)} = -\sum_{i=1}^{Q}\left\{\bar{E}^i(T^{(0)})\tilde{N}^{i(1)} + \sum_{s\equiv i}E^s n^{s(0)}\frac{E^s-\bar{E}^i(T^{(0)})}{KT^{(0)}}\frac{\tilde{T}^{(1)}}{T^{(0)}}\right.\\ &\qquad\left. + \frac{1}{c_v^*(T^{(0)})}\sum_{s\equiv i}E^s\,\frac{n^{s(0)}}{\nu^{s(0)}}\,\frac{E^s-\bar{E}^i(T^{(0)})}{KT^{(0)}}\,\nabla_{\mathbf{x}}\cdot\mathbf{u}\right\}\\ &= -\sum_{i=1}^{Q}N^i\,\sigma_i^*(T^{(0)})\,K\tilde{T}^{(1)} - \frac{1}{c_v^*(T^{(0)})}\sum_{i=1}^{Q}\sum_{s\equiv i}\frac{n^{s(0)}}{\nu^{s(0)}}\,\frac{\left[E^s-\bar{E}^i(T^{(0)})\right]^2}{KT^{(0)}}\,\nabla_{\mathbf{x}}\cdot\mathbf{u}\,.\end{aligned} \tag{31}$$

By comparing (30) with (31) we get a linear equation for $\tilde{T}^{(1)}$ leading to

$$\begin{aligned}nK\tilde{T}^{(1)} = \frac{KT^{(0)}}{\left[c_v^*(T^{(0)})\right]^2}&\left\{\frac{1}{n}\sum_{j=1}^{Q}N^j\,\sigma_j^*(T^{(0)})\sum_{i=1}^{Q}\sum_{s\equiv i}\frac{n^{s(0)}}{\nu^{s(0)}}\right.\\ &\left.-\sum_{i=1}^{Q}\sum_{s\equiv i}\frac{n^{s(0)}}{\nu^{s(0)}}\left[\frac{E^s-\bar{E}^i(T^{(0)})}{KT^{(0)}}\right]^2\right\}\nabla_{\mathbf{x}}\cdot\mathbf{u}\,,\end{aligned} \tag{32}$$

and consequently dynamical pressure may be cast in the expected form [20]

$$\Pi = -\,\varsigma\,\nabla_{\mathbf{x}}\cdot\mathbf{u}\,, \tag{33}$$

where coefficient ς is the bulk viscosity

$$\varsigma = \frac{2}{3}\,\frac{KT^{(0)}}{\left[c_v^*(T^{(0)})\right]^2}\left\{\left(\frac{1}{n}\sum_{j=1}^{Q} N^j\,\sigma_j^*(T^{(0)})\right)^2 \sum_{i=1}^{Q}\sum_{s\equiv i}\frac{n^{s(0)}}{\nu^{s(0)}} + \frac{3}{2}\sum_{i=1}^{Q}\sum_{s\equiv i}\frac{n^{s(0)}}{\nu^{s(0)}}\left[\frac{E^s - \bar{E}^i(T^{(0)})}{KT^{(0)}}\right]^2\right\} > 0\,, \tag{34}$$

which of course would vanish in case of monatomic gases (with each gas G^i having a fixed internal energy E^i, thus $\sigma_i^*(T^{(0)}) = 0$).

Analogously, viscous stress tensor, traceless deviatoric part of the pressure tensor correction $\mathbf{P}^{(1)}$, may be obtained by direct computation as

$$\begin{aligned} p_{hk}^{(1)} &= \sum_{i=1}^{Q}\sum_{s\equiv i} m^i \int\left[(v_h - u_h)(v_k - u_k) - \frac{1}{3}\,|\mathbf{v}-\mathbf{u}|^2\delta_{hk}\right] f^{s(1)}(\mathbf{v})\,d\mathbf{v} \\ &= \sum_{i=1}^{Q}\sum_{s\equiv i} m^i \int (v_h - u_h)(v_k - u_k)\, f^{s(1)}(\mathbf{v})\,d\mathbf{v} - \Pi\,\delta_{hk}\,. \end{aligned} \tag{35}$$

From (14) we have

$$\sum_{i=1}^{Q}\sum_{s\equiv i} m^i \int (v_h - u_h)(v_k - u_k)\,\mathscr{M}^{s(1)}(\mathbf{v})\,d\mathbf{v} = nK\tilde{T}^{(1)}\,\delta_{hk}\,,$$

while (16) provides

$$\begin{aligned} &-\sum_{i=1}^{Q}\sum_{s\equiv i}\frac{m^i}{\nu^{s(0)}}\int (v_h - u_h)(v_k - u_k)\left(\frac{\partial_0 f^{s(0)}}{\partial t} + \mathbf{v}\cdot\nabla_{\mathbf{x}} f^{s(0)}\right)d\mathbf{v} \\ &\quad = -\left(\sum_{i=1}^{Q}\sum_{s\equiv i}\frac{n^{s(0)}}{\nu^{s(0)}}\right) KT^{(0)}\left(\frac{\partial u_h}{\partial x_k} + \frac{\partial u_k}{\partial x_h} + \nabla_{\mathbf{x}}\cdot\mathbf{u}\,\delta_{hk}\right) \\ &+\frac{KT^{(0)}}{c_v^*(T^{(0)})}\left(\sum_{i=1}^{Q}\sum_{s\equiv i}\frac{n^{s(0)}}{\nu^{s(0)}}\right)\left(\frac{5}{2} + \frac{1}{n}\sum_{j=1}^{Q} N^j\,\sigma_j^*(T^{(0)})\right)\nabla_{\mathbf{x}}\cdot\mathbf{u}\,\delta_{hk}\,. \end{aligned}$$

Putting last two results together, and subtracting the dynamical pressure Π (given in (33)) to the diagonal terms, we get, as usual, that viscous stress is proportional to the strain rate tensor

$$p_{hk}^{(1)} = -\,\mu\left(\frac{\partial u_h}{\partial x_k} + \frac{\partial u_k}{\partial x_h} - \frac{2}{3}\,\nabla_{\mathbf{x}}\cdot\mathbf{u}\,\delta_{hk}\right) \tag{36}$$

by means of the shear viscosity coefficient

$$\mu = \left(\sum_{i=1}^{Q} \sum_{s \equiv i} \frac{n^{s(0)}}{\nu^{s(0)}} \right) KT^{(0)} > 0 \,. \tag{37}$$

5.4 Computation of Thermal Heat Flux

Finally, in order to complete closure at Navier–Stokes level we need a constitutive relation for thermal heat flux. An explicit computation provides

$$\begin{aligned} \mathbf{q}^{(1)} &= \frac{1}{2} \sum_{i=1}^{Q} \sum_{s \equiv i} m^i \int (\mathbf{v} - \mathbf{u}) |\mathbf{v} - \mathbf{u}|^2 f^{s(1)}(\mathbf{v}) \, d\mathbf{v} \\ &= \frac{5}{2} nKT^{(0)} \tilde{\mathbf{u}}^{(1)} - \frac{5}{2} (KT^{(0)})^2 \sum_{i=1}^{Q} \sum_{s \equiv i} \frac{n^{s(0)}}{\nu^{s(0)}} \left[\frac{\nabla_{\mathbf{x}} N^i}{\rho^i} - \frac{\nabla_{\mathbf{x}} n}{\rho} \right] \\ &- \frac{5}{2} KT^{(0)} \sum_{i=1}^{Q} \sum_{s \equiv i} \frac{n^{s(0)}}{\nu^{s(0)}} \left[\frac{1}{m^i} \frac{E^s - \bar{E}^i(T^{(0)})}{KT^{(0)}} + \frac{2}{m^i} - \frac{n}{\rho} \right] \nabla_{\mathbf{x}} (KT^{(0)}) \,, \end{aligned} \tag{38}$$

where the term involving $\tilde{\mathbf{u}}^{(1)}$ is due to (14), while all other contributions involving gradients of number densities and of temperature arise from (16). In the computation we have used the simple property

$$\int |\mathbf{v} - \mathbf{u}|^{2k} f^{s(0)}(\mathbf{v}) \, d\mathbf{v} = n^{s(0)} \left(\frac{2\, KT^{(0)}}{m^i} \right)^k \frac{2}{\sqrt{\pi}} \, \Gamma \left(k + \frac{3}{2} \right), \qquad k \in \mathbb{N} \,,$$

where Γ stands for the Euler Gamma function.

The result (38) may be rewritten as

$$\begin{aligned} \mathbf{q}^{(1)} &= \frac{5}{2} nKT^{(0)} \tilde{\mathbf{u}}^{(1)} - \frac{5}{2} KT^{(0)} \sum_{i=1}^{Q} \sum_{s \equiv i} \frac{n^{s(0)}}{\nu^{s(0)}} \frac{1}{m^i} \frac{E^s - \bar{E}^i(T^{(0)})}{KT^{(0)}} \nabla_{\mathbf{x}} (KT^{(0)}) \\ &- \frac{5}{2} KT^{(0)} \sum_{i=1}^{Q} \sum_{s \equiv i} \frac{n^{s(0)}}{\nu^{s(0)}} \left[\frac{\nabla_{\mathbf{x}} (N^i KT^{(0)})}{\rho^i} - \frac{\nabla_{\mathbf{x}} (nKT^{(0)})}{\rho} + \frac{1}{m^i} \nabla_{\mathbf{x}} (KT^{(0)}) \right], \end{aligned} \tag{39}$$

hence, by a direct comparison with (21), we note that

$$\begin{aligned} \mathbf{q}^{(1)} &= -\lambda \, \nabla_{\mathbf{x}} T^{(0)} + \frac{5}{2} KT^{(0)} \sum_{i=1}^{Q} \sum_{s \equiv i} n^{s(0)} \mathbf{u}^{s(1)} \\ &= -\lambda \, \nabla_{\mathbf{x}} T^{(0)} + \frac{5}{2} KT^{(0)} \sum_{i=1}^{Q} N^i \, \mathbf{u}^{i(1)} \,, \end{aligned} \tag{40}$$

where the conduction coefficient λ reads as

$$\lambda = \frac{5}{2} K^2 T^{(0)} \sum_{i=1}^{Q} \sum_{s \equiv i} \frac{1}{m^i} \frac{n^{s(0)}}{\nu^{s(0)}} > 0 \,. \tag{41}$$

Formula (40) for thermal heat flux is in agreement with the expected result for a multi-component inert mixture [12, 14], at least for simple intermolecular potentials (for instance, of Maxwell–molecule type). Bearing in mind the expressions (24) and (29) for species velocities, we obviously have that the heat flux involves also gradients of number densities (Dufour effect, which of course would vanish in case of a single gas). In conclusion, in the Navier–Stokes equation for energy, the global heat flux, sum of the thermal one and of a contribution due to the internal energy levels, results in

$$\mathbf{q}^{(1)} + \sum_{i=1}^{Q} \sum_{s \equiv i} E^s n^{s(0)} \mathbf{u}^{s(1)} = -\lambda \nabla_{\mathbf{x}} T^{(0)} + \sum_{i=1}^{Q} \sum_{s \equiv i} \left(\frac{5}{2} K T^{(0)} + E^s \right) n^{s(0)} \mathbf{u}^{s(1)} \,.$$

It is clear that diffusion velocities $\mathbf{u}^{s(1)}$ bring in Fick matrix and Soret coefficients also in the expression of heat flux.

6 Conclusion and Perspectives

In this paper we have provided a consistent Navier–Stokes closure of macroscopic fluid dynamic equations for an inert mixture of polyatomic gases, by means of a Chapman–Enskog asymptotic analysis of a kinetic model of BGK type. All transport coefficients have been explicitly computed, recovering the Fick matrix and the Soret effect in the diffusion velocities (24), and the Dufour effect in the heat flux (40), as expected in any hydrodynamic description for gas mixtures. Moreover, for polyatomic particles an additional macroscopic field arises in the pressure tensor, the dynamical pressure (33), which represents the difference between the energy of internal motion evaluated at the current (non-equilibrium) state and the corresponding equilibrium scalar pressure; indeed, in the present polyatomic frame kinetic temperature is not a conserved variable, since in collisions among particles there is transfer from kinetic energy into internal energy, and vice versa.

The consistent mathematical procedure has allowed to cast all transport coefficients $\mathscr{F}^{ij}$, α^i, ς, μ, λ in terms of the fluid–dynamic fields N^i, $\mathbf{u}$, $\mathscr{E}$ (or its equivalent $T^{(0)}$), as well as of the internal molecular structures, namely the energy levels E^s (and their byproducts $\bar{E}^i$ and c_v^*). Of course also the free parameters of the model (inverse relaxation times) $\nu^{s(0)}$, which may depend on fields variables themselves, play an essential role. Such free parameters can be used for a best fit of transport coefficients with known or experimental values, for a better approach at kinetic level.

We would get for instance

$$\frac{\lambda}{\mu} = \frac{5}{2} K \sum_{i=1}^{Q} \frac{\beta^i}{m^i} \Big/ \sum_{i=1}^{Q} \beta^i, \qquad \beta^i = \sum_{s \equiv i} \frac{n^{s(0)}}{\nu^{s(0)}},$$

by which one can avoid the typical drawback of BGK equations for a single monatomic gas $\frac{\lambda}{\mu} = \frac{5}{2} \frac{K}{m} = c_p$, providing an incorrect Prandtl number.

In view of physical applications, it would be interesting to generalize these fluid–dynamic closure to mixtures of gases subject also to chemical reactions. This goal is expected to be really ambitious, because of the additional constraints implied by chemistry, especially the equilibrium mass action law, a transcendental equation relating equilibrium number densities with equilibrium kinetic temperature. Some preliminary steps in this direction have been made in [8], where a suitable closure of balance equations for number densities has been achieved for a reacting mixture of four gases with continuous internal energy (having thus a unique distribution function for each gas). However, the understanding of the effects of chemical energy into Navier–Stokes equations for polyatomic mixtures, with the computation of chemical contributions possibly appearing in the dynamical pressure and in the heat flux, is still an open problem.

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Quantization of Probability Densities: A Gradient Flow Approach

François Golse

Abstract This paper introduces a gradient flow in infinite dimension, whose long-time dynamics is expected to be an approximation of the quantization problem for probability densities, in the sense of Graf and Luschgy (Lecture Notes in Mathematics, vol 1730. Springer, Berlin, 2000). Quantization of probability distributions is a problem which one encounters in a great variety of contexts, such as signal processing, pattern or speech recognition, economics… The present work describes a dynamical approach of the optimal quantization problem in space dimensions one and two, involving (systems of) parabolic equations. This is an account of recent work in collaboration with Caglioti et al. (Math Models Methods Appl Sci 25:1845–1885, 2015 and arXiv:1607.01198 (math.AP), to appear in Ann. Inst. H. Poincaré, Anal. Non Lin. https://doi.org/10.1016/j.anihpc.2017.12.003).

Keywords Quantization of probability densities · Wasserstein distance Gradient flow · Parabolic equations

1 Introduction

The quantization problem for probability densities can be formulated as follows.

Problem: To find "best approximations" of a probability density ρ on $\mathbf{R}^d$ by convex combinations of Dirac masses.

Applications of quantization of probability densities are frequently encountered in various contexts, such as

- information theory, signal compressing,
- pattern or speech recognition,
- mathematical economics (optimal location of service centers),

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- stochastic processes (sampling design),
- numerical analysis (quadrature formulas, Monte-Carlo and quasi-Monte-Carlo methods)...

Example: the well-known Koksma inequality recalled below can be thought of in terms of quantization for the uniform distribution $\rho = \mathbf{1}_{[0,1]}$ in the unit interval.

For each finite $S \subset [0, 1)$ and $\phi \in BV(0, 1)$

$$\left| \frac{1}{\#S} \sum_{x \in S} \phi(x + 0) - \int_0^1 \phi(x) dx \right| \leq \mathrm{TV}(\phi) D^*(S) \,,$$

where $D^*(S)$ is the star-discrepancy of S defined by the equality

$$\#S \cdot D^*(S) := \sup_{0 \leq y < 1} |\#([0, y) \cap S) - y \cdot \#S| \geq \tfrac{1}{2} \,.$$

Koksma's inequality is sharp (set $\phi_n = \mathbf{1}_{[0,y_n)}$ for a maximizing y_n). Indeed, the inequality above can be recast as

$$\sup_{\mathrm{TV}(\phi) \leq 1} p_\phi \left(\frac{1}{\#S} \sum_{x \in S} \delta_x - \rho \right) \leq D^*(S) \,,$$

where p_ϕ is the seminorm defined on the set of bounded Borel measures μ on $[0, 1]$ such that $\mu(\{1\}) = 0$ by the formula

$$p_\phi(\mu) := \left| \int_0^1 \phi(x + 0) \mu(dx) \right|$$

for all $\phi \in \mathrm{BV}(0, 1)$. (See Theorem 5.1 in Sect. 2.5 of [1].)

There are generalizations of the Koksma inequality to higher dimensions, including the Koksma-Hlawka inequality for functions ϕ of finite Hardy-Krause variation (a nontrivial extension of the notion of functions with bounded variation to the case of a space dimension higher than one): see for instance Theorem 5.5 in Sect. 2.5 of [1].

Low discrepancy sequences are widely used in numerical integration—specifically, in the context of quasi-Monte-Carlo methods. See for instance [2, 3] for a presentation of these methods.

2 A Compendium of Quantization Theory

First we recall the notion of Monge-Kantorovich(-Vasershtein) distances. For each Borel $\mathscr{X} \subset \mathbf{R}^d$, let $\mathscr{P}(\mathscr{X})$ be the set of Borel probability measures on $\mathscr{X}$ and let

$$\mathscr{P}_r(\mathscr{X}) := \left\{ \mu \in \mathscr{P}(\mathscr{X}) \text{ s.t. } \int_{\mathscr{X}} |x|^r \mu(dx) < \infty \right\} .$$

For each $\mu, \nu \in \mathscr{P}(\mathscr{X})$, we denote by $\Pi(\mu, \nu)$ the set of $\pi \in \mathscr{P}(\mathscr{X} \times \mathscr{X})$ with first and second marginals μ and ν, i.e.

$$\iint_{\mathscr{X}\times\mathscr{X}} (\phi(x) + \psi(y))\pi(dxdy) = \int_{\mathscr{X}} \phi(x)\mu(dx) + \int_{\mathscr{X}} \psi(y)\nu(dy)$$

for all $\phi, \psi \in C_b(\mathscr{X})$. Such probability measures π are referred to as a *coupling* of μ and ν.

For each $\mu, \nu \in \mathscr{P}_r(\mathscr{X})$ with $r \geq 1$, the Monge-Kantorovich(-Vasershtein) distance of exponent r is given by the formula

$$\mathrm{dist}_{\mathrm{MK,r}}(\mu, \nu) := \left(\inf_{\pi \in \Pi(\mu,\nu)} \iint_{\mathscr{X}\times\mathscr{X}} |x - y|^r \pi(dxdy) \right)^{1/r} .$$

The Monge-Kantorovich distance is known to metrize the topology of weak convergence of probability measures on $\mathscr{P}_r(\mathscr{X})$, in the following sense: for each sequence $\mu_n \in \mathscr{P}_r(\mathscr{X})$ and each $\mu \in \mathscr{P}_r(\mathscr{X})$, then

$$\mathrm{dist}_{\mathrm{MK,r}}(\mu_n, \mu) \to 0 \text{ iff } \int_{\mathscr{X}} \phi(x)(1 + |x|^r)\mu_n(dx) \to \int_{\mathscr{X}} \phi(x)(1 + |x|^r)\mu(dx)$$

for all $\phi \in C_b(\mathscr{X})$ as $N \to \infty$. See Chap. 7 in [4] for more information on these distances.

The notion of N-quantization error is defined in terms of the distance $\mathrm{dist}_{\mathrm{MK,r}}$, as follows. We refer the interested reader to [5] for a more detailed presentation of quantization theory—we have kept the same notation as in [5].

Definition 1 For each probability density ρ on $\mathscr{X}$ s.t. $\rho\mathscr{L}^d \in \mathscr{P}_r(\mathscr{X})$, define[1]

$$V_{N,r}(\rho) := \inf_{\#\mathrm{supp}(\mu) \leq N} \mathrm{dist}_{\mathrm{MK,r}}(\rho\mathscr{L}^d, \mu)^r .$$

Since the purpose of quantization is to approximate absolutely continuous measures by discrete measures, the convergence rate of this approximation process must involve the weak topology, and this is the reason why it is natural to express the N-quantization error in terms of $\mathrm{dist}_{\mathrm{MK,r}}$.

For each ϕ bounded and Lipschitz continuous on $\mathscr{X}$, one has the inequality

$$\begin{aligned} \inf_{\substack{m_1+\ldots+m_N=1 \\ x_k \in \mathscr{X},\, m_k \geq 0}} \left| \sum_{k=1}^N m_k \phi(x_k) - \int_{\mathscr{X}} \phi(y)\rho(y)dy \right| &\leq \mathrm{Lip}(\phi) V_{N,1}(\rho) \\ &\leq \mathrm{Lip}(\phi) V_{N,r}(\rho)^{1/r} , \end{aligned}$$

[1] The Lebesgue measure on $\mathbf{R}^d$ is denoted by $\mathscr{L}^d$ throughout the present paper.

which one can compare with the Koksma inequality recalled above. Notice that the bound above involves $\mathrm{Lip}(\phi)$ instead of $\mathrm{TV}(\phi)$, and $V_{N,r}(\rho)^{1/r}$ instead of the discrepancy of $x_1, \ldots, x_N$. But apart from these differences, both inequalities are obviously of the same nature.

In the sequel, we shall be concerned with the large N behavior of the quantization error, which is given by the following important observation:

$$N^{r/d} V_{N,r}(\rho) \to Q(\rho) := \|\rho\|_{L^{d/(d+r)}(\mathscr{X})} \cdot \inf_{N \geq 1} N^{r/d} V_{N,r}(\mathbf{1}_{[0,1]^d}) \,.$$

In other words, in the large N limit, the quantization error scales as $N^{-r/d}$, and asymptotically depends on the $L^{d/(d+r)}$ norm of ρ only (Theorem 6.2 in [5]).

The set of discrete probability measures used in the definition of $V_{N,r}(\rho)$ is

$$\{\mu \in \mathscr{P}(\mathscr{X}) \text{ s.t. } \#\mathrm{supp}(\mu) \leq N\}$$
$$= \left\{ \sum_{k=1} m_k \delta_{x_k} \ , \ x_k \in \mathscr{X} \ , \ m_k \geq 0 \, , \ \sum_{k=1}^{N} m_k = 1 \right\} .$$

Hence the inf in the definition of $V_{N,r}$ can be obtained by minimizing first on the coefficients m_k, and then on the points x_k.

Minimizing over the coefficients is easy. Given $x_1, \ldots, x_N \in \mathscr{X}$, set

$$F_{N,r}(x_1, \ldots, x_N) := \inf_{\substack{m_1 + \ldots + m_N = 1 \\ m_k \geq 0}} \mathrm{dist}_{\mathrm{MK,r}} \left(\rho \mathscr{L}^d, \sum_{k=1}^{N} m_k \delta_{x_k} \right)^r .$$

(This is the function denoted by $\psi_{N,r}$ in formula (3.4) of [5].) One easily checks that the minimum is attained by choosing

$$m_k := \int_{W(x_k | X_N)} \rho(y) dy \,,$$

where $W(x_k|X_N)$ is the Voronoi cell of x_k in the set of points $X_N := \{x_1, \ldots, x_N\}$, defined as follows:

$$W(x_k|X_N) := \{y \in X_N \ \text{ s.t. } \ |y - x_k| \leq |y - x_j| \text{ for all } j \neq k\} \,.$$

(See Chap. 1, Sect. 1 in [5].) Equivalently, one can recast the function $F_{N,r}$ as

$$F_{N,r}(x_1, \ldots, x_N) = \int_{\mathscr{X}} \min_{1 \leq k \leq N} |y - x_k|^r \rho(y) dy \geq V_{N,r}(\rho) \,.$$

Next we seek information on the optimal system of points $x_1, \ldots, x_N$, in the limit as $N \to \infty$. The following result (Theorem 7.5 in [5]) answers precisely this question, and is therefore very important.

Theorem 1 (Bucklew-Wise 1982) *Let* $(x_{1,N}, \ldots, x_{N,N})$ *be a sequence of* N*-tuples such that*

$$N^{r/d} F_{N,r}(x_{1,N}, \ldots, x_{N,N}) \to Q(\rho) = \lim_{N\to\infty} N^{r/d} V_{N,r}(\rho)\,.$$

Then

$$\frac{1}{N}\sum_{j=1}^{N} \delta_{x_{j,N}} \to \frac{\rho^{d/(d+r)}\mathscr{L}^d}{\displaystyle\int_{\mathscr{X}} \rho(y)^{d/(d+r)}(y)dy}$$

weakly in $\mathscr{P}(\mathscr{X})$ *as* $N \to \infty$.

Remark. The convergence stated in the theorem above is not to be confused with the fact that, by construction, one has

$$\sum_{j=1}^{N} m_{j,N}\delta_{x_{j,N}} \to \rho\mathscr{L}^d$$

weakly in $\mathscr{P}(\mathscr{X})$ as $N \to \infty$, with

$$m_{j,N} := \int_{W(x_{j,N}|X_N)} \rho(y)dy\,.$$

3 The Gradient Flow Approach

The function $F_{N,r}$ is differentiable at each point $(x_1, \ldots, x_N)$ such that $x_j \neq x_k$ if $1 \leq j < k \leq N$, and one has

$$\frac{\partial F_{N,r}}{\partial x_j}(x_1, \ldots, x_N) = -r\int_{W(x_j|X_N)} |y - x_j|^{r-2}(y - x_j)\rho(y)dy\,;$$

see Lemma 4.10 in [5].

The gradient flow of $F_{N,r}$ (for the Euclidean metric of $\mathbf{R}^{dN}$) is the one-parameter group of solutions to the system of ordinary differential equations

$$\begin{aligned}\dot{x}_j &= -\frac{\partial F_{N,r}}{\partial x_j}(x_1, \ldots, x_N)\\ &= r\int_{W(x_j|X_N)} |y - x_j|^{r-2}(y - x_j)\rho(y)dy\,, \quad 1 \leq j \leq N\,.\end{aligned} \tag{1}$$

There is the obvious difficulty that the partial derivatives on the right hand side of the first equality above are not defined everywhere in $\mathbf{R}^{dN}$, but only almost

everywhere in $\mathbf{R}^{dN}$—and more precisely in the complement of the union of the $\frac{1}{2}N(N-1)$ linear manifold of codimension d defined by the equations $x_j \neq x_k$ for $1 \leq j < k \leq N$. Setting

$$\mathscr{Z}_N := \{(x_1, \dots, x_N) \in \mathbf{R}^{dN} \text{ s.t. } x_j \neq x_k \text{ for } 1 \leq j < k \leq N\},$$

one should prove that, for each $(x_1^{in}, \dots, x_N^{in}) \in \mathscr{Z}_N$, the solution to the Cauchy problem for (1), i.e. $t \mapsto (x_1(t), \dots, x_N(t))$, is defined and takes its values in $\mathscr{Z}_N$ for all $t \geq 0$. We shall leave this question aside for the moment.

However, if this is the case, it is natural to look for a Lyapunov function for the differential system (1). As in the case of all gradient flow systems, one has

$$\frac{d}{dt} F_{N,r}(x_1(t), \dots, x_N(t)) = -|\nabla F_{N,r}(x_1(t), \dots, x_N(t))|^2$$

for each solution $t \mapsto (x_1(t), \dots, x_N(t))$ to (1).

This suggests to study the long time limit for solutions to the Cauchy problem for (1) and for all initial data in $\mathscr{Z}_N$. If $F_{N,r}$ was C^1 on $\mathbf{R}^{dN}$ and strictly convex, all trajectories of the gradient flow of $F_{N,r}$ would converge to the optimal $(x_1^*, \dots, x_N^*)$ in the long time limit for all initial data in $\mathscr{Z}_N$, and therefore $F_{N,r}(x_1(t), \dots, x_N(t))$ would converge to the quantization error $V_{N,r}(\rho)$ as $t \to +\infty$.

In view of the Theorem of Bucklew and Wise, it is also natural and interesting to consider the large N limit of the gradient flow system above. One expects the limiting dynamics to be governed by a parabolic system on $\mathbf{R}^d$, which generates a $L^2(\mathbf{R}^d)$-gradient, and it would be interesting to study the large time limit of this infinite dimensional dynamics. This obviously raises the problem of exchanging the order in which the limits as $t \to +\infty$ and as $N \to \infty$ are taken.

However, there are even more basic difficulties in this program. For instance, it seems very hard in general to obtain an explicit parametrization of the Voronoi tessellation of an arbitrary finite subset of $\mathbf{R}^d$, and even harder to control its dynamics under the gradient flow of $F_{N,r}$. In other words, the integration domains $W(x_j|X_N)$ on the right hand side of (1) are in general not very explicit, and this might seriously complicate the task of "passing to limit as $N \to \infty$" in the right hand side of (1). For instance, the number of neighboring cells of $W(x_j|X_N)$ in the Voronoi tessellation of X_N might change as time goes on, so that one should think of (1) as a interacting system of points, where the number of points interacting with $x_j(t)$ may depend both on j and on t. The problem studied here is therefore very different from nearest neighbor interaction models with a fixed number of nearest neighbors, frequently encountered in statistical mechanics. It is also different from classical mean-field models, which apply to long range interaction, and in which each particle interacts with all the other particles in the system. Indeed, most points in the system considered here do not act directly on any given Voronoi cell.

4 The One-Dimensional Case

There is however one particular case where it is easy to compute the Voronoi tessellation explicitly, which is the one-dimensional case. We shall therefore study this case in detail. The content of this section is taken from [6].

4.1 Computing $F_{N,r}$ in the One-Dimensional Setting

Let $0 < x_1 < \cdots < x_N < 1$; denoting

$$x_{1/2} = 0\,, \quad x_{N+1/2} = 1\,, \quad \text{and} \quad x_{k+1/2} = \tfrac{1}{2}(x_k + x_{k+1})\,, \qquad 1 \le k \le N-1\,,$$

one sees easily that the Voronoi tessellation of the finite set $X_N := \{x_1, \ldots, x_N\}$ is given by

$$W(x_k|X_N) = [x_{k-1/2}, x_{k+1/2}]\,, \qquad 1 \le k \le N\,.$$

Accordingly

$$F_{N,r}(x_1, \ldots, x_N) = \sum_{k=1}^{N} \int_{x_{k-1/2}}^{x_{k+1/2}} |y - x_k|^r \rho(y) dy\,.$$

The gradient of $F_{N,r}$ in this case is easily computed, and we arrive at the defining system of ODEs for the Euclidean gradient flow of $F_{N,r}$, i.e. (1) in this special case. With the notation above

$$\dot{x}_k = -r \int_{x_{k-1/2}}^{x_{k+1/2}} |y - x_k|^{r-2}(y - x_k)\rho(y) dy\,, \quad 1 \le k \le N\,.$$

In the special case $r = 2$, one finds

$$\dot{x}_k = -2 \int_{x_{k-1/2}}^{x_{k+1/2}} (y - x_k)\rho(y) dy\,, \quad 1 \le k \le N\,.$$

All this is of course based on the assumption that

$$0 < x_1(t) < \cdots < x_N(t) < 1\,.$$

If $0 < x_1(t) < \cdots < x_{k-1}(t) < x_k(t) = x_{k+1}(t) < x_{k+2}(t) < \cdots < x_N(t) < 1$, then one has $x_k(t) = x_{k+1/2}(t) = x_{k+1}(t)$. Therefore, assuming for simplicity that $\rho > 0$ a.e. on $[0, 1]$,

$$\dot{x}_{k+1}(t) - \dot{x}_k(t) = -r \int_{x_{k+1}(t)}^{x_{k+3/2}(t)} |y - x_{k+1}(t)|^{r-2}(y - x_{k+1}(t))\rho(y)dy + r \int_{x_{k-1/2}(t)}^{x_k(t)} |y - x_k(t)|^{r-2}(y - x_k(t))\rho(y)dy < 0\,.$$

Therefore, $x_{k+1}(t+0) < x_k(t+0)$. After a change in indices, the relaxed condition $0 \le x_1(t) \le \cdots \le x_N(t) \le 1$ can be maintained for all times, at the cost of having to deal with piecewise continuous time derivatives for the x_ks.

4.2 The Slowly Varying Setting

Next we turn to the task of letting $N \to \infty$. The most convenient setting to do so involves the assumption that all the points $x_j(t)$ for $j = 1, \ldots, N$ are "slowly varying" in j for all t. Specifically, we postulate that

$$x_j(t) = X\left(t, \frac{j}{N+1}\right)\,,$$

where

$$X : \mathbf{R}_+ \times \mathbf{R} \ni (t, \theta) \mapsto X(t, \theta) \in \mathbf{R}$$

is smooth (with a level of regularity to be made precise later). The discrete boundary condition

$$x_{1/2}(t) = 0\,, \qquad x_{N+1/2}(t) = 1$$

will be formulated as follows. Obviously, it is natural to postulate that

$$X(t, 0) = 0\,, \quad X(t, 1) = 1\,, \quad \text{and that } \theta \mapsto X(t, \theta) \text{ is increasing on } [0, 1]\,.$$

However, this leaves aside the values of $X(t, \theta)$ for $\theta < 0$ or $\theta > 1$, which are not used in this setting. In fact, it is more convenient to choose a periodic setting for $\partial_\theta X$, i.e.

$$\partial_\theta X(t, \theta + 1) = \partial_\theta X(t, \theta)\,, \quad \theta \in \mathbf{R}\,, \ t \ge 0\,,$$

so that

$$X(t, \theta + 1) = X(t, \theta) + 1\,, \qquad \theta \in \mathbf{R}\,, \quad t \ge 0\,.$$

4.3 The Continuous Functional $\mathscr{F}_r$ and its L^2-Gradient Flow

At this point, we can define a continuous functional, of which $F_{N,r}$ can be regarded as the discretization in the variable θ. Specifically, we set

$$\mathscr{F}_r[X] := C_r \int_0^1 \rho(X(\theta))|\partial_\theta X(\theta)|^{r+1} d\theta\,, \quad \text{with } C_r := \frac{1}{2^r(r+1)}\,,$$

which we consider as defined on

$$\mathscr{E} := \{X \in C^\infty([0,1]) \text{ s.t. } X(0) = 1\,,\ X(1) = 1\}\,.$$

By Taylor's formula

$$F_{N,r}(X(t, \tfrac{1}{N+1}), \ldots, X(t, \tfrac{N}{N+1})) = \frac{\mathscr{F}_r[X(t,\cdot)]}{(N+1)^r} + O\left(\frac{1}{N^{r+1}}\right)\,.$$

This suggests that the Euclidean gradient flow of $F_{N,r}$ is (up to a rescaling of time) the discretization in θ of the $L^2([0,1])$ gradient flow of $\mathscr{F}_r$, defined below.

We begin with the computation of the $L^2([0,1])$ gradient of $\mathscr{F}_r$. Elementary computations show that

$$\begin{aligned}\delta\mathscr{F}_r[X] =& C_r \int_0^1 \rho'(X(\theta))|\partial_\theta X(\theta)|^{r+1}\delta X(\theta) d\theta \\ &+ (r+1)C_r \int_0^1 \rho'(X(\theta))|\partial_\theta X(\theta)|^{r-1}\partial_\theta X(\theta)\partial_\theta \delta X(\theta) d\theta\,.\end{aligned}$$

Integrating by parts and observing that

$$\delta X(0) = \delta X(1) = 0$$

if $X \in \mathscr{E}$, we arrive at the following expression of the functional $L^2([0,1])$-gradient of $\mathscr{F}_r$:

$$\begin{aligned}\frac{\delta\mathscr{F}_r[X]}{\delta X(\theta)} =& C_r\rho'(X(\theta))|\partial_\theta X(\theta)|^{r+1} \\ &- (r+1)C_r\partial_\theta(\rho'(X(\theta))|\partial_\theta X(\theta)|^{r-1}\partial_\theta X(\theta))\,.\end{aligned}$$

Therefore, $L^2([0,1])$-gradient flow of $\mathscr{F}_r$ is defined by the second order PDE

$$\begin{cases} \partial_t X = C_r((r+1)\partial_\theta(\rho(X)|\partial_\theta X|^{r-1}\partial_\theta X) - \rho'(X)|\partial_\theta X|^{r+1})\,, \\ X\big|_{\theta=0} = 0\,, \\ X\big|_{\theta=1} = 1\,. \end{cases} \tag{2}$$

If $\rho \equiv 1$ is the uniform density on $[0, 1]$, one finds a p-Laplacian (with $p = r + 1$) i.e.

$$\begin{cases} \partial_t X = C_r(r+1)\partial_\theta(|\partial_\theta X|^{r-1}\partial_\theta X)\,, \\ X\big|_{\theta=0} = 0\,, \\ X\big|_{\theta=1} = 1\,. \end{cases} \tag{3}$$

Observe that we have left aside in this discussion the condition that $\theta \mapsto X(t,\theta)$ should be increasing from 0 (for $\theta = 0$) to 1 (for $\theta = 1$). This question is reformulated as follows: start from an initial data $X^{in} \in C^2(\mathbf{R})$ such that

$$X^{in}(0) = 0\,, \quad X^{in}(\theta+1) = X^{in}(\theta) + 1\,, \quad \text{and } \partial_\theta X^{in} > 0\,.$$

Is the condition $\partial_\theta X(t,\theta)$ preserved by the flow, i.e. valid for all $\theta \in [0, 1]$?

4.4 The Eulerian Formulation of the Gradient Flow

This last question can be viewed in a slightly different manner. It will be convenient to think of the PDE for X obtained in the previous section as the Lagrangian formulation of the $L^2([0, 1])$-gradient flow of $\mathscr{F}_r$. In the present section, we shall seek the equivalent Eulerian formulation of the same dynamics.

In order to do so, define $f \equiv f(t,x)$ by[2]

$$f(t,\cdot)\mathscr{L}^1 = X(t,\cdot)\#\mathscr{L}^1\,, \qquad \text{or equivalently} \quad f(t, X(t,\theta)) = \frac{1}{\partial_\theta X(t,\theta)}\,.$$

Then, the Eulerian formulation of (2) is the following PDE with unknown f:

$$\begin{cases} \partial_t f = -rC_r\partial_x\left(f\partial_x\left(\dfrac{\rho}{f^{r+1}}\right)\right)\,, \quad x \in \mathbf{R}, \\ f(t, x+1) = f(t,x). \end{cases} \tag{4}$$

To derive (4) from (2), write

$$\int_0^1 \phi(x)\partial_t f(t,x)dx = \frac{d}{dt}\int_0^1 \phi(X(t,\theta))d\theta = \int_0^1 \phi'(X(t,\theta))\partial_t X(t,\theta)d\theta,$$

use the equation for $X(t,\theta)$ to express $\partial_t X(t,\theta)$, substitute $x = X(t,\theta)$ in the resulting expression and integrate by parts. One obtains in this way the weak formulation of (4). This elementary computation is left to the reader.

[2]The notation $T\#m$ designates the push-forward of the measure m by the transformation T.

4.5 Gradient Structure of the Eulerian Formulation (4)

Interestingly, the Eulerian formulation (4) of the $L^2([0,1])$-gradient flow for $\mathscr{F}_r$ defined by (2) also has a gradient structure, which we briefly describe. For each $f > 0$ defined on $\mathbf{R}$, continuous and 1-periodic, we set

$$\mathscr{H}_r[f] := C_r \int_0^1 \frac{\rho(x)}{f(x)^r} dx\,.$$

If $X : \mathbf{R} \to \mathbf{R}$ of class C^1 and satisfying

$$X(0) = 0\,, \quad X(\theta+1) = X(\theta) + 1\,, \quad \partial_\theta X(\theta) > 0, \qquad \theta \in \mathbf{R},$$

is related to f by the formula

$$f\mathscr{L}^1 = X\#\mathscr{L}^1\,, \quad \text{or equivalently} \quad f \circ X = \frac{1}{\partial_\theta X}\,,$$

then

$$\mathscr{H}_r[f] = C_r \int_0^1 \rho(X(\theta))\partial_\theta X(\theta)^{r+1} d\theta = \mathscr{F}_r[X]\,.$$

Now

$$\frac{\delta \mathscr{H}_r[f]}{\delta f(x)} = -rC_r \frac{\rho(x)}{f(x)^{r+1}}\,,$$

so that the PDE (4) takes the form

$$\partial_t f(t,x) = \partial_x \left(f(t,x)\partial_x \frac{\delta \mathscr{H}_r[f]}{\delta f(t,x)} \right)\,.$$

One recognizes in this form of (4) the defining equation for the $\mathrm{dist}_{\mathrm{MK},2}$-gradient flow of $\mathscr{H}_r$ (see Eq. (9.3) in Chap. 9 of [4]).

If $f \equiv f(t,x)$ is the solution of the Eulerian quantization gradient flow equation, we can apply the general prescription valid for all gradient flows and compute the time derivative of the functional $\mathscr{H}_r$ along trajectories of its own gradient flow. One finds that

$$\frac{d}{dt}\mathscr{H}_r[f(t,\cdot)] = -\int_0^1 \left|\frac{\delta \mathscr{H}_r[f]}{\delta f(t,x)}\right|^2 f(t,x)dx = -r^2C_r^2 \int_0^1 \left|\frac{\rho(x)}{f(x)^{r+1}}\right|^2 f(t,x)dx\,.$$

Therefore $t \mapsto \mathscr{H}_r[f(t,\cdot)]$ decreases while $f(t,\cdot) \to f_\infty$ (in some sense to made precise) as $t \to +\infty$, where f_∞ is the function given by the formula

$$f_\infty(x) = Z_r \rho(x)^{1/(1+r)}\,, \qquad Z_r := \frac{1}{\displaystyle\int_0^1 \rho(x)^{1/(1+r)} dx}\,.$$

Since we are in the case $d = 1$, the function f_∞ is precisely the probability density which appears in the Bucklew-Wise theorem.

4.6 Main Results in the One-Dimensional Case

We begin with a comparison principle for the quantization gradient flow in Eulerian variables, which we recast as follows. Set $m := \rho^{1/(1+r)}$ and $u := f/m$; the Eulerian quantization gradient flow equation becomes

$$\partial_t u = m^{-1}\partial_x(m\partial_x H(u))\,, \qquad H(z) := -(r+1)C_r z^{-r}\,. \tag{5}$$

Lemma 1 *If u and v are two solutions of (5), one has*

$$\frac{d}{dt}\int_0^1 (u-v)_+(t,x)m(x)dx \le 0\,.$$

This result is well known in the theory of the porous media equation: see for instance Theorem 3.5 in [7].

Proof Multiply both sides of the equation for $u - v$ by $m\mathrm{sign}_+(H(u) - H(v))$ and integrate in x. Since H is increasing on $(0, +\infty)$, one has

$$\mathrm{sign}_+(H(u) - H(v)) = \mathrm{sign}_+(u - v)\,.$$

and therefore

$$\frac{d}{dt}\int_0^1 (u-v)_+ m dx = -\int_0^1 |\partial_x(H(u) - H(v))|^2 \delta_0(H(u) - H(v))dx \le 0\,.$$

(In order to fully justify this computation in the case where u and v are classical solutions, one needs to replace the Heaviside function sign_+ with some smooth approximation thereof, integrate by parts as indicated above, and finally pass to the limit in the resulting identity.)

With the comparison argument above, one can check in particular that

$$0 < a \le u^{in}(x) \le A < \infty \quad \Rightarrow \quad a \le u(t,x) \le A$$

for all $x \in \mathbf{R}$ and all $t > 0$. Returning to the Lagrangian variables, we conclude that

$$\frac{\inf_{0\le y\le 1}\rho^{1/(1+r)}(y)}{A} \le \partial_\theta X(t,\theta) \le \frac{\sup_{0\le y\le 1}\rho^{1/(1+r)}(y)}{a}$$

for all $\theta \in [0,1]$ and all $t > 0$. In particular, $\partial_\theta X(t,\theta) > 0$ for all $t \ge 0$ and all $\theta \in [0,1]$ if $\rho > 0$ on $[0,1]$.

Our main results for the one-dimensional problem described above are summarized in the following theorem.

Theorem 2 *Let $r = 2$. Assume that $\rho \in C^{3,\alpha}([0,1])$ and that $X^{in} \in C^{4,\alpha}([0,1])$ satisfies the condition*

$$0 < A_0^{-1} \le \partial_\theta X^{in} < A_0\,, \quad X^{in}(0) = 0\,, \ X^{in}(1) = 1\,.$$

Let X be the solution of the L^2-gradient flow equation of $\mathscr{F}_2$, i.e. of (2) (for $r = 2$) with initial condition $X\big|_{t=0} = X^{in}$.

Then there exists $0 < \eta := \eta[A_0, \|X^{in}\|_{C^{4,\alpha}}, \|\rho\|_{C^{3,\alpha}}] \ll 1$, and two constants $C, C' > 0$ such that, if

$$\|\rho'\|_{L^\infty} + \|\rho''\|_{L^\infty} \le \eta\,,$$

the following properties hold:
(a) For each trajectory $(x_j(t))_{1\le j\le N+1}$ of the gradient flow of $F_{N,2}$ satisfying

$$|x_j(0) - X^{in}(\tfrac{j-1/2}{N})| \le \frac{C}{N^2}\,,$$

one has

$$\frac{1}{N}\sum_{j=1}^{N} |x_j(N^3 t) - X(t, \tfrac{j-1/2}{N})|^2 \le \frac{C'}{N^4}\,, \quad t \ge 0\,.$$

(b) There exists $\gamma \equiv \gamma(A_0) > 0$ such that

$$dist_{MK,1}\left(\frac{1}{N}\sum_{j=1}^{N}\delta_{x_j(t)}, Z\rho^{1/3}\mathscr{L}^1\right)$$
$$\le e^{-\gamma t/N^3} + \frac{1}{4N}\|\rho^{-1/3}\|_{L^\infty}\int_0^1 \rho^{1/3}(\theta)d\theta + \frac{\sqrt{C'}}{N^2}\,.$$

Remarks.

(i) The first term on the right hand side of the inequality in (b) measures the distance between the equilibrium and the interpolating density, i.e. the solution at time t/N^3 of the L^2-gradient flow equation for the continuous functional $\mathscr{F}_2$. The second term measures the distance between the equilibrium density and its midpoint discretization, while the third term measures the distance between the discrete and the interpolating densities according to property (a).

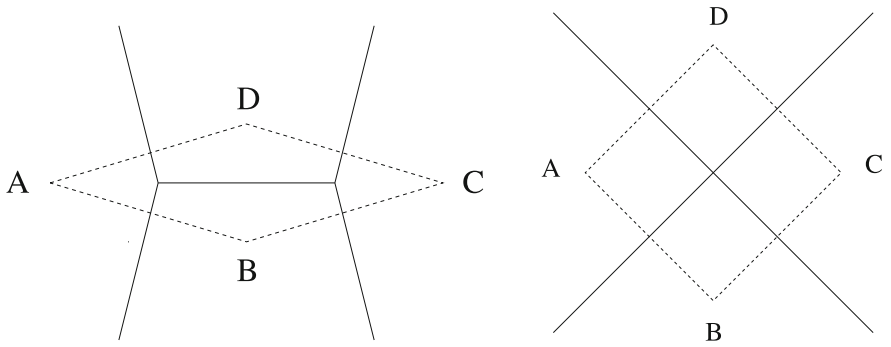

Fig. 1 Consider the case of 4 points A, B, C, D which are the vertices of a lozenge. If the lozenge is not a square, each of the (unbounded) Voronoi cell of A, B, C and D has exactly two neighbors (left). However, as the lozenge is deformed into a square, each one of these Voronoi cells is adjacent to the three other cells (right)

(ii) The condition $\|\rho'\|_{L^\infty} + \|\rho''\|_{L^\infty} \ll 1$ cannot be dispensed with. If one takes $\epsilon \in (0, \frac{1}{8})$

$$\rho = \tfrac{1}{\epsilon}\mathbf{1}_{|2\theta-1|<\epsilon}\,, \quad X(\theta) = \theta\,, \quad Y(\theta) = 1 + |\theta - \tfrac{1}{2}| \text{ for } \tfrac{1}{4} < \theta < \tfrac{3}{4}$$

with Y Lipschitz continuous on $[0, 1]$ such that $Y(0) = Y(1) = 0$, one can see, by a straightforward computation, that $D^2\mathscr{F}_2[X] \cdot (Y, Y) = 2 - \frac{4}{\epsilon}$. Hence $\mathscr{F}_2$ is not convex for ρ so chosen. (In fact, this choice of ρ does not belong to $C^{3,\alpha}([0, 1])$ so that, in order to obtain a counterexample, one needs first to regularize ρ.)

5 The Two-Dimensional Case

In the two-dimensional case, one can see that the dependence of the Voronoi cells in the family $X_N = \{x_1, \ldots, x_N\}$ of their centers is much more involved than in the one-dimension case (where this dependence is completely explicit).

For instance, the number of Voronoi cells adjacent to a given cell may change under smooth deformations of X_N, as shown in the Fig. 1.

This is a strong indication that the gradient flow problem discussed above is much more complex in the two-dimensional case than in the explicit one-dimensional case. From the statistical mechanics point of view, the fact that the number of nearest neighbors to any given center may vary discontinuously with the configuration of centers (and therefore as time increases) makes the problem much more challenging.

By comparison with the discussion above, the style of this section will be much more sketchy. We shall deliberately avoid all lengthy computations, describe the final results and refer the reader to [8] for all missing details. All the results discussed in this section are taken from [8].

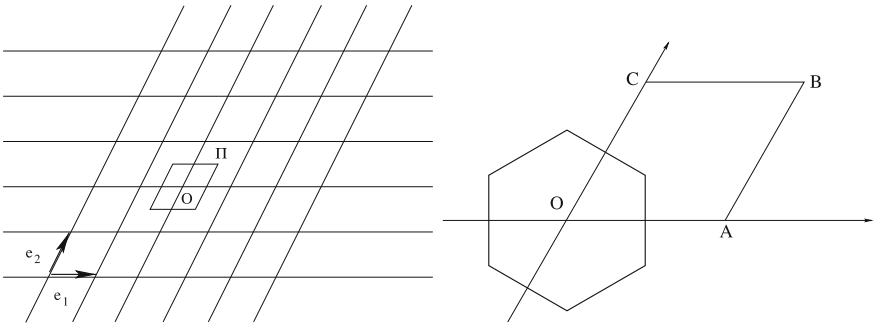

Fig. 2 The lattice Λ and a fundamental domain Π centered at the origin O (left). The Voronoi cell of the origin O (right)—the vectors **OA** and **OC** are e_1 and e_2 respectively. The lozenge $OABC$ is a fundamental domain of the quotient space $\mathbf{R}^2/\Lambda$

First we start from the lattice

$$\Lambda := \mathbf{Z}e_1 \oplus \mathbf{Z}e_2\,, \quad e_1 := (1,0)\,, \quad e_2 := (\tfrac{1}{2}; \tfrac{\sqrt{3}}{2})\,.$$

The Voronoi tessellation of Λ is the set of translates by all the vectors in Λ of the Voronoi cell of the origin, i.e.

$$W(0|\Lambda) = \text{ regular hexagon centered at 0 with side length } \tfrac{\sqrt{3}}{2}\,.$$

Call Π some fundamental domain of $\mathbf{R}^2/\Lambda$ centered at the origin.

There are several reasons for considering the hexagonal tessellation as the reference configuration. First, it is known that the hexagonal lattice solves the quantization problem in the plane for the uniform density and for $r = 1$ (i.e. for the Monge-Kantorovich distance with exponent 1): see for instance [9, 10]. Next, in the case of the hexagonal lattice, each vertex of an hexagon is the center of the circumscribed circle to the triangle of the centers of the three hexagons having this vertex in common. This is a "generic" situation, in the following sense: in the case where there are four adjacent Voronoi cells with one common vertex, the centers of these Voronoi cells must lie on the same circle, which means that these four centers must satisfy one condition (Ptolemy's condition on the lengths of the sides and of the diagonals of the quadrilateral defined by the four centers). This situation is therefore not generic, and therefore not stable under perturbations.

Next we slowly deform the lattice Λ as follows. Let $X \in \mathrm{Diff}(\mathbf{R}^2)$ satisfy

$$\begin{aligned} &X(x+m) = X(x) + m\,, \quad x \in \mathbf{R}^2\,,\ m \in \Lambda\,,\\ &\|DX\|_{L^\infty} \le \eta \ll 1\,. \end{aligned}$$

Henceforth we consider the quantization gradient flow for the uniform density $\rho \equiv 1$ on Π and for the Monge-Kantorovich(-Vasershtein) distance with exponent $r = 2$, starting from the slowly deformed system of lattice points

$$\mathscr{X}_\epsilon := X(\epsilon\Lambda)\,, \quad \epsilon = 1/2n\,,\ n \in \mathbf{N}^*\,.$$

Let Π be a fundamental domain of $\mathbf{R}^2/\Lambda$ centered at 0 as in the Fig. 2, and consider

$$\begin{aligned}\mathscr{F}_{4n^2,2}(\mathscr{X}_\epsilon \cap \Pi) &= \int_\Pi \min_{k\in\mathbf{Z}^2} |y - X(\epsilon k)|^2 dy \\ &= \sum_{k_1,k_2=-n}^{n-1} \int_{W(X(\epsilon k)|\mathscr{X}_\epsilon)} |y - X(\epsilon k)|^2 dy\,.\end{aligned}$$

Lemma 2 *In the limit as $n \to \infty$, one has*

$$n^4 \mathscr{F}_{4n^2,2}(\mathscr{X}_\epsilon \cap \Pi) \to \mathscr{F}[X] = \int_\Pi F(\nabla X(x))dx\,,$$

where the function F is defined on $M_2(\mathbf{R})$ by the formula below.

For each $M \in M_2(\mathbf{R})$

$$F(M) = \tfrac{1}{3} \sum_{\omega\in\{e_1,e_2,e_{12}\}} |M\cdot\omega|^4 \Phi(\omega, M)(3 + \Phi(\omega, M)^2)\,,$$

where $e_{12} = e_2 - e_1$ and

$$\Phi(\omega, M) := \sqrt{\frac{|MR\omega|^2|MR^T\omega|^2}{\frac{3}{4}\det(M)} - 1}$$

for each $\omega \in \mathbf{S}^2$, while

$$R := \begin{pmatrix} \frac{1}{2} & -\frac{\sqrt{3}}{2} \\ \frac{\sqrt{3}}{2} & \frac{1}{2} \end{pmatrix}$$

is the rotation of an angle $\frac{\pi}{3}$.

Next we compute the L^2-gradient of $\mathscr{F}$. Obviously

$$\frac{\delta\mathscr{F}}{\delta X(x)} = -\mathrm{div}_x(\nabla F(\nabla X(x)))\,.$$

It remains to compute ∇F:

$$\nabla F(M) = \tfrac{4}{3} \sum_{\omega \in \{e_1, e_2, e_{12}\}} |M\omega|^2 (3 + \Phi^2) \Phi(\omega, M) M\omega^{\otimes 2} + \sum_{\omega \in \{e_1, e_2, e_{12}\}} |M\omega|^4 \frac{(1 + \Phi^2)^2}{\Phi} (\omega, M) A(\omega, M)^T ,$$

with

$$A(\omega, M) := \frac{R\omega \otimes MR\omega}{|MR\omega|^2} + \frac{R^T\omega \otimes MR^T\omega}{|MR^T\omega|^2} - M^{-1} .$$

Thus, the defining system of PDEs for the L^2-gradient flow of $\mathscr{F}$ takes the form

$$\partial_t X(t, x) = -\frac{\delta \mathscr{F}}{\delta X(t, x)} = \mathrm{div}_x (\nabla F(\nabla X(t, x))) ,$$

to which we add the initial and boundary conditions

$$\begin{cases} X(t, x + m) = X(t, x) + m , \quad x \in \mathbf{R}^2 \text{ and } m \in \Lambda , \\ X\big|_{t=0} = X^{in} . \end{cases}$$

Without loss of generality, we henceforth assume that

$$\int_\Pi X^{in}(x) dx = 0 ; \quad \text{so that } \int_\Pi X(t, x) dx = 0 , \quad \text{for all } t > 0 .$$

Remark. The formula above can be summarized as follows: the quantization of the uniform density $\rho \equiv 1$ for the quadratic Monge-Kantorovich(-Vasershtein) distance is equivalent to "Aristotelian" hyperelasticity[3] with stored energy density F.

Observe that the function Φ involves the $\det(M)$; as a result, the function F is not convex. This is obviously an annoying feature for quantization based on the gradient flow strategy. However, one can say more in the small deformation regime, which we shall discuss in more detail below.

[3] We call "Aristotelian" a mechanical equation based on the axiom that velocity (and not acceleration, as in Newtonian mechanics) is proportional to force. See for instance the following statement: "[…] the medium causes a difference because it impedes the moving thing, most of all if it is moving in the opposite direction, but in a secondary degree even if it is at rest; […] A, then, will move through B in time Γ, and through Δ, which is thinner, in time E (if the length of B is equal to Δ), in proportion to the density of the hindering body. For let B be water and Δ air; then by so much as air is thinner and more incorporeal than water, A will move through Δ faster than through B. […] Then if air is twice as thin, the body will traverse B in twice the time that it does Δ, and the time Γ will be twice the time E". (Aristotle, "Physics", Book IV, Part 8, transl. R. P. Hardie and R. K. Gaye, Clarendon Press, Oxford, 1930).

Elementary computations show that

$$3\sqrt{3}F(I+\tau S) = 10 + 20\tau \mathrm{tr}(S) \\ + \tau^2(14\mathrm{det}(S) + 10(\mathrm{tr}(S))^2 + 3\mathrm{tr}(S^T S)) + O(\tau^3)\,.$$

Define a new function F_0 by the following prescription:

$$F_0(A) := F(A) - \tfrac{20}{3\sqrt{3}}\mathrm{tr}(A-I) - \tfrac{14}{3\sqrt{3}}\mathrm{det}(A-I)\,.$$

Lemma 3 *There exists $r_0 > 0$ and $L > 1$ such that*

$$\mathrm{tr}((A-I)^T(A-I)) \le r_0 \Rightarrow L^{-1}I \le D^2F_0(A) \le LI\,.$$

In addition, for each $X \in Diff(\mathbf{R}^2)$ s.t. $X - I$ is Λ-periodic, one has

$$\mathscr{F}(X) = \int_\Pi F_0(\nabla X)(x)dx\,.$$

Proof By construction,

$$F_0 \in C^2(GL_2(\mathbf{R}))\,, \quad \text{and } D^2F_0(I) \ge \tfrac{2}{\sqrt{3}}I\,.$$

Let $X \in \mathrm{Diff}(\mathbf{R}^2)$ be such that $Y := X - I$ is $\mathscr{L}$-periodic; then

$$F_0(I+\nabla Y) := F(I+\nabla Y) - \tfrac{20}{3\sqrt{3}}\mathrm{div}Y - \tfrac{14}{3\sqrt{3}}\mathrm{det}(\nabla Y)\,.$$

One concludes by observing that

$$\int_\Pi \mathrm{div}(Y)(x)dx = 0$$

and

$$\int_\Pi \mathrm{det}(\nabla Y)(x)dx = \int_\Pi d(Y_1 dY_2) = 0\,,$$

where $Y_1(y)$ and $Y_2(y)$ are the components of $Y(y) \in \mathbf{R}^2$ for all $y \in \mathbf{R}^2$ and d is the exterior derivative.

The results in the lemma can be summarized as follows. Although the function F is not convex, one can replace the minimization problem with deformation energy density F with the same minimization problem with F_0 instead of F, and F_0 is uniformly convex near the identity matrix. With this observation in mind, we arrive at the following results.

Theorem 3 *Assume that* $X^{in} \in Diff(\mathbf{R}^2)$ *satisfies*

$$X^{in} - I \text{ is } \Lambda\text{-periodic and } \int_{\Pi} X^{in}(x)dx = 0\,,$$

together with

$$\|X^{in} - I\|_{W^{s,p}(\Pi)} \leq \eta \ll 1$$

for some $p > 2$ *and* $s > 1 + 2/p$.

Then the Cauchy problem for the L^2*-gradient flow of* $\mathscr{F}$ *has a unique global solution* X *with initial data* X^{in}*, which satisfies, for some* $C, \mu > 0$

$$\|X(t) - I\|_{L^\infty(\Pi)} \leq \|X^{in} - I\|_{L^\infty(\Pi)} e^{-\mu t} \qquad t > 0\,.$$

In other words, under the gradient flow of $\mathscr{F}$, the near-hexagonal Voronoi tessellation of $X^{in}(\Lambda/2n)$ converges to the hexagonal tessellation exponentially fast—as expected since the honeycomb lattice is the optimal configuration of quantizers for the uniform distribution in the plane [9, 10].

6 Final Remarks

There are obviously many fascinating open questions on the quantization problem for regular probability densities in space dimension higher than one.

For instance, in the previous section, we have only addressed the case $\rho \equiv 1$. It would be more satisfying if one could treat the case of a smooth probability density—for instance a "small" (in some sense which remains to be defined precisely) perturbation of the uniform density. In the case of the uniform density addressed above, one knows the optimal configuration of quantizers, which provides the equilibrium state in the PDE system defining the L^2-gradient flow of the continuous functional. In the case of a nonuniform density, the optimal configuration of quantizers is not known in general, and might even be topologically quite complex if the density is not a slowly varying perturbation of the uniform density.

Even in the case of the uniform density studied in the previous section, it could be quite interesting to find the Eulerian formulation of the L^2-gradient flow for $\mathscr{F}$, by analogy with the one-dimensional case. However, this is a much trickier problem. The dynamics of $X(t, \cdot)\#\mathscr{L}^2$ (analogous to the mass density in fluid mechanics) must involve some other Eulerian unknowns (analogous to the velocity field in fluid mechanics), yet to be identified at the time of this writing.

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Semi-Lagrangian Approximation of BGK Models for Inert and Reactive Gas Mixtures

M. Groppi, G. Russo and G. Stracquadanio

Abstract Recent relaxation time-approximation models of BGK-type for the kinetic description of both inert and reacting gas mixtures are reviewed and their main properties are recalled. The models are characterized by only one Maxwellian attractor for each species; such attractors are defined in terms of auxiliary parameters. For their numerical approximation, semi-Lagrangian schemes are proposed. Numerical simulations are presented with the aim of showing the peculiarities of the different BGK models and the performance of the numerical method.

1 Introduction

It is well known that there are several important regimes of gas dynamics in which the proper mathematical tool of investigation is the nonlinear Boltzmann equation. On the other hand, such an equation is quite complex to deal with, and various simpler models have been introduced, among them the most popular and widely used is probably the so-called BGK model [3, 26].

Most of the BGK models have been considered in the case of a single species gas. This seems an important limitation, since even simple applications, relevant for instance to plasma physics or chemically reacting gases, require the possibility to deal with mixtures. Although the extension of the Boltzmann equation to a mixture of gases has been well known for a long time, this is not the case for the BGK

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equation. Considerable troubles are encountered if one tries to extend the BGK model, originally devised for a single species gas, to a gas mixture [10, 25]. Indeed, one faces immediately very basic drawbacks such as loss of positivity of the involved macroscopic fields.

Among the pioneering BGK models for inert mixtures we quote [10, 11, 25]; in particular, the models presented in [11, 25] have an important drawback: when all species are identical, one does not recover the BGK equation for a single gas, that is, they do not satisfy the indifferentiability principle. In [10] a different model overcoming this drawback is proposed, but positivity of temperature is lost. An accurate and detailed discussion on the subject may be found in [2], where the authors propose a simple and very interesting consistent BGK-type model for gas mixtures which overcomes all previous difficulties.

In this paper we review some BGK models for inert [2] and reactive [12, 13, 16] multi-component gaseous flows and describe a numerical strategy for their discretization. In addition, we present the inert version of the model [13], originally proposed for a reacting mixture, and we discuss its properties. The BGK models considered here are characterized by only one Maxwellian attractor for each species; such attractors are defined in terms of auxiliary parameters, which number depends on the features that one wants to reproduce of the corresponding Boltzmann equations.

To solve the BGK equation in an efficient way, in the last years several numerical schemes have been proposed, focusing in particular on procedures capable to capture the limiting behaviour of the solution as a small parameter (Knudsen number) $\varepsilon \to 0$ (the so called asymptotic preserving schemes, AP, see the very recent paper [9] and the references therein). For example, in [22] the authors use IMEX schemes from [20, 21], in which the implicit part is L-stable, thus guaranteeing that the schemes project the numerical solution onto the discrete Maxwellian as $\varepsilon \to 0$. Recently, high-order semi-Lagrangian numerical schemes for the discretization of the BGK equation for a single gas has been proposed by the authors [14, 15]. In this paper we present the extension and application of these high order numerical schemes to BGK-type models which describe the evolution of inert and reactive mixtures of gases. In this context, numerical results had already been obtained in [1], by applying time splitting methods for the simulation of the behaviour of multi-component gaseous flow with simple chemical reactions [16]. One of the advantages of the schemes considered here is that their semi-Lagrangian nature allows us to avoid the classical CFL restriction on the time step; moreover, a higher order than the time splitting scheme has been obtained.

The paper is organized as follows. In Sect. 2 the Boltzmann equations for inert mixtures and for a simple bimolecular reversible chemical reaction are briefly recalled, together with their main properties; in Sect. 3 the BGK model proposed in [2] for inert mixtures and its extension to a chemically reacting mixture [16] are reviewed. Section 4 focuses on BGK models obtained by imposing the fulfillment of the conservations laws: first, the inert version of the BGK model [13] is presented in detail, and then the reactive BGK equations proposed in [13] are recalled. In Sect. 5 the semi-Lagrangian method is introduced and the first and second order method for the

classic one species BGK equation are briefly described; their extension and application to the BGK models for inert and reactive mixtures are presented in Sect. 6. Numerical results are shown in Sect. 7, with the aim of showing the peculiarities of the different BGK models for mixtures, as well as the performance and the accuracy of the proposed numerical methods.

2 Kinetic Boltzmann-Type Equations

For the description of the dynamics of mixtures of gases, even in presence of chemical reactions, extended kinetic equations (of the Boltzmann type) for the evolution of the distribution function f^s of each gases are given by

$$\frac{\partial f^s}{\partial t} + \mathbf{v} \cdot \nabla_x f^s = Q^s, \qquad s = 1, \ldots, L, \tag{1}$$

$$Q^s = I^s + J^s, \quad I^s = \sum_{r=1}^{L} I^{sr},$$

where $I^{sr}[f^s, f^r]$ is the usual elastic scattering collision operator [7] for the binary (s, r) interaction, having the classical form:

$$I^{sr}(f^s, f^r)(\mathbf{x}, \mathbf{v}, t) \iint_{\mathbb{R}^3 \times \mathbb{S}^2} |\mathbf{g}| \sigma_{sr}(|\mathbf{g}|, \chi)[f^s(\mathbf{v}') f^r(\mathbf{v}'_*) - f^s(\mathbf{v}) f^r(\mathbf{v}_*)] \, d\mathbf{v}_* d\boldsymbol{\omega} \,,$$

with $|\mathbf{g}| = |\mathbf{v} - \mathbf{v}_*|$ relative speed, and J^s is the chemical collision operator.

Of course, when only inert mixtures are under investigation, the chemical collision operator is not present ($J^s = 0$). In the case in which gas components may undergo chemical reactions, we will consider a simple four[1] species gas mixture undergoing the reversible chemical reaction

$$A^1 + A^2 \rightleftharpoons A^3 + A^4, \tag{2}$$

according to the kinetic model proposed in [23], where species A^s having mass m^s and energy of chemical bond E^s (with energy gap $\Delta E = E^3 + E^4 - E^1 - E^2 \geq 0$) also interact with any species $r = 1, \ldots, 4$ by elastic scattering. For species 1, the chemical operator reads as

[1] More precisely, throughout this paper the number of species in the mixture will be denoted by L. For inert mixture L can assume whatever positive integer value, whereas $L = 4$ when the chemical reaction is present.

$$J^1(\mathbf{x},\mathbf{v},t) = \int\!\!\int_{\mathbb{R}^3\times\mathbb{S}^2} \Theta\left(|\mathbf{g}|^2 - \frac{2\Delta E}{\mu^{12}}\right)|\mathbf{g}|\sigma_{12}^{34}(|\mathbf{g}|,\chi) \cdot\left[\left(\frac{\mu^{12}}{\mu^{34}}\right)^3 f^3(\mathbf{v}_{12}^{34}) f^4(\mathbf{v}_{*12}^{34}) - f^1(\mathbf{v}) f^2(\mathbf{v}_*)\right] d\mathbf{v}_*\, d\boldsymbol{\omega}$$

(where $\mu^{sr} = m^s m^r/(m^s + m^r)$ is the reduced mass) and the other ones can be obtained by means of suitable permutations of indices, bearing in mind also the microreversibility relation between the involved differential cross sections (for more detail see [23]). The unit step function Θ accounts for the energy threshold in the endothermic reaction.

When no chemical reaction occurs in the mixture of L components, the space of collision invariants is $L+4$ dimensional, and conserved quantities are the mass of each species

$$\int_{\mathbb{R}^3} I^s\, d\mathbf{v} = 0, \qquad s = 1,\ldots,L, \tag{3}$$

as well as the total momentum and total kinetic energy

$$\sum_{s=1}^{L}\int_{\mathbb{R}^3} m^s \mathbf{v} I^s\, d\mathbf{v} = 0, \qquad \sum_{s=1}^{L}\int_{\mathbb{R}^3} \frac{1}{2} m^s |\mathbf{v}|^2 I^s\, d\mathbf{v} = 0.$$

In the four-species chemically reacting mixture described above, the space of collision invariants is 7 dimensional, and conserved quantities are mass in three independent pairs of species, momentum and total (kinetic plus chemical) energy, namely

$$\int (Q^s + Q^r)\, d\mathbf{v} = 0, \qquad (s,r) = (1,3),(1,4),(2,4),$$
$$\sum_{s=1}^{4}\int m_s \mathbf{v} Q^s\, d\mathbf{v} = \mathbf{0}, \ \sum_{s=1}^{4}\int \left(\frac{1}{2} m^s |\mathbf{v}|^2 + E^s\right) Q^s\, d\mathbf{v} = 0.$$

In any case, in a mixture each species exchanges momentum and energy with the others; such exchange rates can be made explicit for Maxwellian molecules in the inert case [2, 7].

As regards equilibria, for an inert L-component mixture, collision equilibria are determined by the $L+4$-parameter family of Maxwellian distributions

$$M^s(\mathbf{v}) = n^s\left(\frac{m^s}{2\pi K T}\right)^{3/2} \exp\left(-\frac{m^s}{2KT}(\mathbf{v}-\mathbf{u})^2\right) \qquad s = 1,\ldots,L, \tag{4}$$

where n^s, $\mathbf{u}$, T stand for number density of species s, mass velocity and temperature of the mixture, respectively, and K is the Boltzmann constant as usual.

In the reactive case described by reaction (2), collision equilibria are a 7-parameter family of Maxwellians (4) with number densities related by the mass action law

$$\frac{n^1 n^2}{n^3 n^4} = \left(\frac{m^1 m^2}{m^3 m^4}\right)^{3/2} \exp\left(\frac{\Delta E}{KT}\right). \tag{5}$$

In the following Sections, BGK models for inert and reacting mixtures are illustrated. We can divide them into two families: the first one is obtained imposing that the BGK equations prescribe the same exchange rates of the Boltzmann level, whereas the second one is devised by imposing that BGK and Boltzmann equations share the same collision invariants. For each family, BGK equations for both inert and reacting mixtures are presented. The structure of each equation of the presented BGK models is exactly the same as the structure of BGK model for simple gas, i.e. with only one Maxwellian attractor for each species; for the case of inert mixtures, a general consistent BGK model that features instead the same structure of the corresponding Boltzmann equations and fulfills all consistency requirements has been very recently proposed and investigated [5].

3 BGK Model Preserving Exchange Rates

In this Section we recall a BGK model whose attractors are obtained by imposing that the exchange rates of each species are exactly the same of the Boltzmann level. First we present the model for inert mixtures [2], then its extension to reactive mixtures [16].

3.1 The BGK Model of Andries, Aoki and Perthame (AAP)

The first consistent BGK model for inert mixtures, satisfying all the main properties of the Boltzmann equations for mixtures, such as positivity, indifferentiability principle and entropy inequality, was introduced in [2]. The key idea is that, instead of approximating each binary collision operator I^{sr} (between species s and r) by a BGK-type relaxation term, only one global operator is introduced for each species s, taking into account interactions with all other species r. The model was built as follows. The relaxation occurs toward a Maxwellian distribution M_s, i.e.

$$\frac{\partial f^s}{\partial t} + \mathbf{v} \cdot \nabla_x f^s = Q^s_{BGK} = \nu_s (M_s - f^s), \quad s = 1, \ldots, L, \tag{6}$$

where f^s is the distribution function of the species s, and M_s is an auxiliary local Maxwellian depending on velocity vector variable $\mathbf{v}$, molecular masses m^s, and disposable parameters[2] n_s, $\mathbf{u}_s$, T_s

[2]For auxiliary parameters a subscript s is used, whereas actual macroscopic fields of the distribution function f^s have a superscript s.

$$M_s = n_s \left(\frac{m^s}{2\pi K T_s} \right)^{3/2} \exp\left(- \frac{m^s}{2KT_s} (\mathbf{v} - \mathbf{u}_s)^2 \right), \quad s = 1, \ldots, L. \tag{7}$$

At last, ν_s represents the inverse of the s-th relaxation time, possibly depending on macroscopic fields, but independent of $\mathbf{v}$. The authors in [2] emphasize that the choice of such a (macroscopic) collision frequencies ν_s is crucial. In particular the model is well defined when

$$\nu_s = \sum_{r=1}^{L} \nu_0^{sr} n^r, \tag{8}$$

where the microscopic collision frequencies ν_0^{sr} are defined by

$$\nu_k^{sr} = 2\pi |\mathbf{g}| \int_0^{\pi} \sigma_{sr}(|\mathbf{g}|, \chi)(1 - \cos\chi)^k \sin\chi d\chi, \qquad k = 0, 1. \tag{9}$$

With this choice of ν_s it can be proved [2] that the positivity of the temperature is ensured. The above auxiliary fields n_s, $\mathbf{u}_s$, T_s are determined from the corresponding actual moments of the distribution functions f^s (namely number density n^s, mass velocity $\mathbf{u}^s$ and temperature T^s of each component) by requiring that the BGK model prescribes the same exchange rates by collisions of the Boltzmann level; such rates can be made explicit in closed analytical form for Maxwellian molecules. By (3) of course $n_s = n^s$ for any s, since $\int_{\mathbb{R}^3} Q^s_{BGK} d\mathbf{v} = n_s - n^s$ must be zero. Following [2], imposing that the Boltzmann equation and its approximate model (6) prescribe the same exchange rates, that is:

$$\int_{\mathbb{R}^3} m^s \mathbf{v} Q^s_{BGK}\, d\mathbf{v} = \int_{\mathbb{R}^3} m^s \mathbf{v} I^s\, d\mathbf{v}, \tag{10}$$

$$\int_{\mathbb{R}^3} \frac{1}{2} m^s |\mathbf{v}|^2 Q^s_{BGK}\, d\mathbf{v} = \int_{\mathbb{R}^3} \frac{1}{2} m^s |\mathbf{v}|^2 I^s\, d\mathbf{v}, \tag{11}$$

we achieve the expressions of the auxiliary fields. Upon introducing the symmetric matrices

$$\xi^{sr} = \xi^{rs} = \nu_1^{sr} \mu_{sr} n^s n^r - \delta^{sr} \sum_{l=1}^{L} \nu_1^{sl} \mu^{sl} n^s n^l,$$

$$\gamma^{sr} = \gamma^{rs} = 3K \nu_1^{sr} \frac{\mu^{sr}}{m^s + m^r} n^s n^r - \delta^{sr} 3K \sum_{l=1}^{L} \nu_1^{sl} \frac{\mu^{sl}}{m^s + m^l} n^s n^l,$$

where δ^{sr} denotes the usual Kronecker symbol, by relations (10)–(11), the parameters determining all attracting Maxwellians M_s read explicitly as

$$\mathbf{u}_s = \frac{1}{m^s n^s}\left[m^s n^s \mathbf{u}^s + \frac{1}{\nu_s}\sum_{r=1}^{L}\xi^{sr}\mathbf{u}^r\right], \tag{12}$$

$$T_s = \frac{2}{3n^s K}\left[n^s\frac{3}{2}KT^s - \frac{1}{2}m^s[n^s|\mathbf{u}_s|^2 - n^s|\mathbf{u}^s|^2] + \frac{1}{\nu_s}\sum_{r=1}^{L}\gamma^{sr}T^r + \right.$$
$$\left. + \frac{1}{\nu_s}\sum_{r=1}^{L}\nu_1^{sr}\frac{\mu^{sr}}{m^s+m^r}n^s n^r(m^s\mathbf{u}^s + m^r\mathbf{u}^r)(\mathbf{u}^r - \mathbf{u}^s)\right]. \tag{13}$$

The above scheme guarantees that the BGK approximation fulfills the main features of the actual collision operator. Obviously, the conservation equations are recovered by construction. Moreover, the main properties, such as indifferentiability principle, H-theorem and entropy inequality are correctly reproduced [2].

3.2 The Extension to a Chemically Reacting Mixture

We recall here the extension of the AAP model to the case of reactive mixture, proposed in [16], with reference to the bimolecular chemical reaction (2). The main structure of this reactive BGK model is similar to (6), (7) and (8). The substantial differences consist in expressions (12) and (13), since now also the chemical exchange rates have to be considered. As a consequence, here the single number densities n^s are not conserved quantities, and therefore also the auxiliary number density of the attracting s-th Maxwellian is different from the one of the actual distribution function f^s. The chemical exchange rates can be made explicit under the assumption of tempered reaction regime, namely when the chemical reaction is moderately slow with respect to elastic scattering. In this case the parameters determining all attracting Maxwellians M_s read explicitly as [16]

$$n_s = n^s + \frac{\lambda^s}{\nu_s}\mathscr{S}, \tag{14}$$

where λ^s are stoichiometric coefficients, $\lambda^1 = \lambda^2 = -\lambda^3 = -\lambda^4 = 1$,

$$m^s n_s \mathbf{u}_s = m^s n^s \mathbf{u}^s + \frac{1}{\nu_s}\sum_{r=1}^{4}\xi^{sr}\mathbf{u}^r + \frac{\lambda^s}{\nu_s}m^s\mathbf{u}\mathscr{S}, \tag{15}$$

$$n_s\frac{3}{2}KT_s = n^s\frac{3}{2}KT^s - \frac{1}{2}m^s[n_s|\mathbf{u}_s|^2 - n^s|\mathbf{u}^s|^2] + \frac{1}{\nu_s}\sum_{r=1}^{4}\gamma^{sr}T^r +$$
$$\frac{1}{\nu_s}\sum_{r=1}^{4}\nu_1^{sr}\frac{\mu^{sr}}{m^s+m^r}n^s n^r(m^s\mathbf{u}^s + m^r\mathbf{u}^r)\cdot(\mathbf{u}^r - \mathbf{u}^s) +$$

$$+\frac{\lambda^s}{\nu_s}\mathscr{S}\left[\frac{M-m^s}{M}KT\left(\frac{\Delta E}{KT}\right)^{3/2}\frac{e^{-\Delta E/KT}}{\Gamma(\frac{3}{2},\frac{\Delta E}{KT})}\right.$$
$$\left.+\frac{1}{2}m^s|\mathbf{u}|^2+\frac{3}{2}KT-\frac{1-\lambda^s}{2}\frac{M-m^s}{M}\Delta E\right], \tag{16}$$

where

$$\mathscr{S}=\nu_{12}^{34}\frac{2}{\sqrt{\pi}}\Gamma\left(\frac{3}{2},\frac{\Delta E}{KT}\right)\left[n^3n^4\left(\frac{m^1m^2}{m^3m^4}\right)^{3/2}e^{\Delta E/KT}-n^1n^2\right], \tag{17}$$
$$\nu_{12}^{34}(|\mathbf{g}|)=2\pi|\mathbf{g}|\int_0^\pi\sigma_{12}^{34}(|\mathbf{g}|,\chi)\sin\chi\,d\chi,$$

Γ denotes an incomplete Gamma function, $M=m^1+m^2=m^3+m^4$.

This BGK model is a robust approximation of the Boltzmann-type kinetic equation describing the reactive mixture under consideration, since it correctly reproduces equilibria (including mass action law) and conservation equations. Such properties are independent from the choice of macroscopic collision frequencies ν_s. Anyway, a suitable evaluation is desired in order to avoid artificial acceleration or slowing down of the relaxation process [16]. To this end, setting $\nu_s=\nu_s^{\mathrm{ME}}+\nu_s^{\mathrm{CH}}$, a reasonable choice for the mechanical contribution ν_s^{ME} is given by formula (8), whereas for the chemical contribution ν_s^{CH}

$$\nu_1^{\mathrm{CH}}=\frac{2}{\sqrt{\pi}}\Gamma\left(\frac{3}{2},\frac{\Delta E}{KT}\right)\nu_{12}^{34}n^2, \tag{18}$$

$$\nu_3^{\mathrm{CH}}=\frac{2}{\sqrt{\pi}}\Gamma\left(\frac{3}{2},\frac{\Delta E}{KT}\right)\left(\frac{\mu^{12}}{\mu^{34}}\right)^{\frac{3}{2}}\exp\left(\frac{\Delta E}{KT}\right)\nu_{12}^{34}n^4 \tag{19}$$

(and analogously for species 2 and 4), where the Gamma function accounts for the presence of the energy threshold.

As regards the H-theorem, an analytical proof using the H function is still lacking in [16], due to the considerable difficulties introduced by the chemical reaction. However, numerical results showed the expected trend for the H-functional of the Boltzmann level

$$H=\sum_{s=1}^{4}\int_{\mathbb{R}^3}f^s\log\left[f^s/(m^s)^3\right]d\mathbf{v}. \tag{20}$$

4 BGK Models Preserving Global Conservations

In this Section we present BGK models in which the fictitious parameters of the attracting Maxwellians are determined by imposing the same conservations of the Boltzmann level. This kind of BGK approach has been first proposed for a four

species mixture, chemically reacting according to (2), and some properties have been studied later in [4, 13]. Here we propose and investigate its version relevant to a L component inert mixtures, then we briefly recall the reactive model.

4.1 Relaxation Model for Inert Mixtures

In the BGK model for inert mixtures recalled in Sect. 3.1, four auxiliary parameters for each of the L species have been introduced, namely $\mathbf{u}_s$ and T_s, $s = 1, \dots, L$ in order to recover the same exchange rates of the Boltzmann level and the correct conservation equations. A different relaxation model can be obtained by imposing the conservation of total momentum and kinetic energy. To this end, we consider a BGK model of the form

$$\frac{\partial f^s}{\partial t} + \mathbf{v} \cdot \nabla_x f^s = \tilde{Q}^s_{BGK} = \nu_s(\tilde{M}_s - f^s), \quad s = 1, \dots, L, \tag{21}$$

where now the attractors $\tilde{M}_s$ are the fictitious Maxwellians

$$\tilde{M}_s = \tilde{n}^s \left(\frac{m^s}{2\pi K \tilde{T}} \right)^{3/2} \exp\left(- \frac{m^s}{2K\tilde{T}} (\mathbf{v} - \tilde{\mathbf{u}})^2 \right), \quad s = 1, \dots, L, \tag{22}$$

defined in terms of 4 (instead of $4L$) auxiliary parameters $\tilde{\mathbf{u}}$ and $\tilde{T}$. The main difference with the previous BGK model is that now the attractors $\tilde{M}_s$ share common fictitious velocities $\tilde{\mathbf{u}}$ and temperature $\tilde{T}$. Once again, the auxiliary macroscopic fields depend on the actual macroscopic fields of f^s and are determined here in such a way that the conservation of momentum and energy are satisfied. Imposing the total conservation of momentum and energy we obtain

$$\sum_{s=1}^{L} \int_{\mathbb{R}^3} m^s \mathbf{v} \tilde{Q}^s_{BGK} \, d\mathbf{v} = 0 \tag{23}$$

or equivalently

$$\sum_{s=1}^{L} \nu_s m^s n^s (\tilde{\mathbf{u}} - \mathbf{u}^s) = 0$$

and for the energy

$$\sum_{s=1}^{L} \int_{\mathbb{R}^3} \frac{1}{2} m^s |\mathbf{v}|^2 \tilde{Q}^s_{BGK} \, d\mathbf{v} = 0 \tag{24}$$

or equivalently

$$\sum_{s=1}^{L} \nu_s \left[\frac{1}{2} m^s n^s |\tilde{\mathbf{u}}|^2 + \frac{3}{2} n^s K \tilde{T} - \frac{1}{2} m^s n^s |\mathbf{u}^s|^2 - \frac{3}{2} n^s K T^s \right] = 0.$$

Therefore, the parameters determining the Maxwellians (22) read explicitly as

$$\tilde{\mathbf{u}} = \frac{\sum_{s=1}^{L} \nu_s m^s n^s \mathbf{u}^s}{\sum_{s=1}^{L} \nu_s m^s n^s}, \tag{25}$$

$$\tilde{T} = \frac{\sum_{s=1}^{L} \nu_s n^s \left[\frac{1}{2} m^s (|\mathbf{u}^s|^2 - |\tilde{\mathbf{u}}|^2) + \frac{3}{2} K T^s \right]}{\frac{3}{2} K \sum_{s=1}^{L} \nu_s n^s}. \tag{26}$$

We prove that the above relaxation model satisfies the consistency property of positivity of temperature; moreover, collision equilibria of the Boltzmann equations for inert mixtures are correctly reproduced and an H-theorem can be proved for the relaxation to equilibrium.

As regards positivity, the following result holds.

Proposition 1 *The auxiliary temperature $\tilde{T}$ in (26) is positive.*

Proof From (26) $\tilde{T} > 0$ if and only if

$$\sum_{s=1}^{L} \nu_s n^s \left[\frac{1}{2} m^s (|\mathbf{u}^s|^2 - |\tilde{\mathbf{u}}|^2) + \frac{3}{2} K T^s \right] > 0,$$

which is equivalent to

$$\sum_{s=1}^{L} \nu_s n^s m^s |\tilde{\mathbf{u}}|^2 < \sum_{s=1}^{L} \nu_s n^s \left[m^s |\mathbf{u}^s|^2 + 3 K T^s \right]$$

$$|\tilde{\mathbf{u}}|^2 < \sum_{s=1}^{L} \alpha_s \left(|\mathbf{u}^s|^2 + 3K \frac{T^s}{m^s} \right),$$

where

$$\alpha_s = \frac{\nu_s n^s m^s}{\sum_{s=1}^{L} \nu_s n^s m^s}, \quad \text{with} \quad \sum_{s=1}^{L} \alpha_s = 1 .$$

One can notice that (25) can be written in the following way

$$\tilde{\mathbf{u}} = \sum_{s=1}^{L} \alpha_s \mathbf{u}^s,$$

therefore the thesis is equivalent to:

$$\left| \sum_{s=1}^{L} \alpha_s \mathbf{u}^s \right|^2 \leq \sum \alpha_s |\mathbf{u}^s|^2 \tag{27}$$

and this inequality can be easily proved using convexity arguments □.

The collision equilibria of (21) are defined by

$$f^s(\mathbf{v}) = \tilde{M}_s(\mathbf{v}) \qquad \forall \mathbf{v} \in \mathbb{R}^3, \qquad s = 1 \dots L \tag{28}$$

from which obviously

$$\mathbf{u}^s = \tilde{\mathbf{u}}, \qquad T^s = \tilde{T}$$

so that equilibrium distributions are Maxwellians at a common mass velocity and temperature, reproducing thus the correct $L + 4$ parameter family of Maxwellians (4) obtained from the Boltzmann equations. For the trend to equilibrium, the following H-theorem can be proved in space homogeneous conditions.

Theorem 1 *Let*

$$H = \sum_{s=1}^{L} \int_{\mathbb{R}^3} f^s \ln(f^s)\, d\mathbf{v}.$$

Then $\dot{H} \leq 0$, *and* $\dot{H} = 0$ *if and only if* $f^s = M^s$.

Proof We have

$$\dot{H} = \sum_{s=1}^{L} \int_{\mathbb{R}^3} \tilde{Q}^s_{BGK} \ln(f^s)\, d\mathbf{v} =$$

$$= \sum_{s=1}^{L} \int_{\mathbb{R}^3} \nu_s (\tilde{M}_s - f^s) \ln(f^s)\, d\mathbf{v}.$$

From conservations (23) and (24) it can be easily seen that

$$\sum_{s=1}^{L} \int_{\mathbb{R}^3} \tilde{Q}^s_{BGK} \ln(\tilde{M}_s)\, d\mathbf{v} = 0.$$

Then we can write

$$\dot{H} = \sum_{s=1}^{L} \int_{\mathbb{R}^3} \tilde{Q}^s_{BGK} [\ln(f^s) - \ln(\tilde{M}_s)]\, d\mathbf{v} = \sum_{s=1}^{L} \int_{\mathbb{R}^3} \nu_s (\tilde{M}_s - f^s) \ln\left(\frac{f^s}{\tilde{M}_s}\right) d\mathbf{v} =$$

$$= \sum_{s=1}^{L} \nu_s \int_{\mathbb{R}^3} \tilde{M}_s \left(1 - \frac{f^s}{\tilde{M}_s}\right) \ln\left(\frac{f^s}{\tilde{M}_s}\right) d\mathbf{v} \leq 0.$$

The last inequality follows from the usual convexity arguments (for the function $(x-1)\ln x$); in addition, the equal sign can be achieved if and only if $f^s = \tilde{M}_s \ \forall s = 1, \ldots, L$, but this is exactly the definition of the collision equilibria (28), and yields then $f^s = M^s$ as unique solution □.

4.2 Extension to the Reactive Case

In this section we recall the reactive version of the BGK model presented in the previous Section. This model follows the same philosophy, namely it pushes the mixture towards auxiliary Maxwellians $\tilde{M}_s$ having the same peculiarities of the true collision equilibria of the Boltzmann equations. With reference to the bimolecular chemical reaction (2), the fictitious Maxwellians $\tilde{M}_s$ are defined in terms of eight fields $\tilde{n}_s$, $s = 1, ..., 4$, $\tilde{u}$, $\tilde{T}$, bound together by the mass action law

$$\frac{\tilde{n}_1 \tilde{n}_2}{\tilde{n}_3 \tilde{n}_4} = \left(\frac{\mu^{12}}{\mu^{34}}\right)^{3/2} \exp\left(\frac{\Delta E}{K\tilde{T}}\right). \tag{29}$$

Imposing conservations of mass, momentum and energy, by easy manipulations, one obtains the fictitius parameters in terms of the variable $\tilde{n}_1$ [13]:

$$\tilde{n}_s = n^s + \lambda^s \frac{\nu_1}{\nu_s}(\tilde{n}_1 - n^1), \qquad s = 2, 3, 4, \tag{30}$$

$$\tilde{\mathbf{u}} = \sum_{s=1}^{4} \nu_s m^s n^s \mathbf{u}^s \Big/ \nu_s m^s n^s \tag{31}$$

$$\tilde{T} = \left[\sum_{s=1}^{4} \nu_s n^s [\frac{1}{2} m^s (|\mathbf{u}^s|^2 - |\tilde{\mathbf{u}}|^2) + \frac{3}{2} K T^s] + \right.$$

$$\left. + \nu_1 \Delta E (\tilde{n}_1 - n^1) \right] \Big/ \left(\frac{3}{2} K \sum_{s=1}^{4} \nu_s n^s \right). \tag{32}$$

Finally, $\tilde{n}_1$ is determined by the mass action law (29) which can be rewritten as a transcendental equation

$$\frac{\nu_3\nu_4\tilde{n}_1[\nu_2 n^2 + \nu_1(\tilde{n}_1 - n^1)]}{\nu_2[\nu_3 n^3 - \nu_1(\tilde{n}_1 - n^1)][\nu_4 n^4 - \nu_1(\tilde{n}_1 - n^1)]} \exp\left(-\frac{\Delta E}{K\tilde{T}(\tilde{n}_1)}\right) = \left(\frac{\mu^{12}}{\mu^{34}}\right)^{3/2} \tag{33}$$

In [13] it has been shown that such equation admits a unique solution, which turns out to be positive. Thus all the unknown auxiliary fields can be uniquely expressed in terms of the actual moments n^s, u^s and T^s.

The fulfillment of the previous conditions implies that the reactive BGK equations yield the correct conservation equations and collision equilibria. Moreover, for the stability of equilibria in space homogeneous conditions, an H-theorem holds [13]; the proof is similar to that of Theorem 1 for the inert case.

5 Lagrangian Formulation of the BGK Equation and Numerical Schemes

In this Section we recall the basic features of semi-Lagrangian schemes used in this paper to numerically simulate the BGK models presented above. The semi-Lagrangian approach allows to avoid the classical CFL restriction on the time step; in this sense the schemes are competitive with the IMEX approach [22], even if, in general, interpolation is required. More details about the numerical method can be found in [14].

With reference to the relaxation equation in one phase space dimension for a single gas, the Lagrangian formulation of the BGK equation is given by the following system:

$$\begin{aligned} &\frac{df}{dt} = \frac{1}{\varepsilon}(M[f] - f), \\ &\frac{dx}{dt} = v, \\ &f(x, v, 0) = f_0(x, v), \quad x(0) = \tilde{x}, \qquad t \geq 0, \quad x, v \in \mathbb{R}, \end{aligned} \tag{34}$$

where the relaxation time ε (inverse of the macroscopic collision frequency) is the Knudsen number, defined as the ratio between the molecular mean free path length and a representative macroscopic length; the Knudsen number can vary in a wide range, from order greater than one (in rarefied regimes) to very small values (in fluid-dynamic regimes).

For simplicity, we assume constant time step Δt and uniform grid in physical and velocity space, with mesh spacing Δx and Δv respectively, and denote the grid points by $t^n = n\Delta t$, $x_i = x_0 + i\Delta x$, $i = 0, \ldots, N_x$, $v_j = j\Delta v$, $j = -N_v, \ldots, N_v$, where $N_x + 1$ and $2N_v + 1$ are the number of grid nodes in space and velocity respectively, so that $[x_0, x_{N_x}]$ is the space domain. We also denote the approximate solution $f(x_i, v_j, t^n)$ by f_{ij}^n.

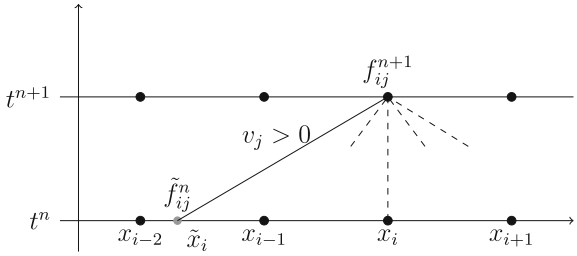

Fig. 1 Representation of the implicit first order scheme. The foot of the characteristic does not lie on the grid, and interpolation is needed to compute $\tilde{f}_{ij}^{n}$

5.1 First Order Scheme

An implicit first order L-stable semi-Lagrangian scheme (Fig. 1) can be achieved in this simple way

$$f_{ij}^{n+1} = \tilde{f}_{ij}^{n} + \frac{\Delta t}{\varepsilon}(M[f]_{ij}^{n+1} - f_{ij}^{n+1}). \tag{35}$$

The quantity $\tilde{f}_{ij}^{n} \simeq f(x_i - v_j \Delta t, v_j, t^n)$ can be computed by suitable reconstruction from $\{f_{\cdot j}^{n}\}$; linear reconstruction will be sufficient for first order scheme, while higher order reconstructions, such as ENO or WENO [6], must be used to achieve high order avoiding oscillations. $M[f]_{ij}^{n+1}$ is the discrete Maxwellian constructed with the macroscopic moments of f^{n+1}:

$$M[f]_{ij}^{n+1} = M[f](x_i, v_j, t^{n+1}) = \frac{\rho_i^{n+1}}{\sqrt{2\pi R T_i^{n+1}}} \exp\left(- \frac{(v_j - u_i^{n+1})^2}{2RT_i^{n+1}} \right),$$

$$\begin{aligned} \rho_i^{n+1} &= \textstyle\sum_{j=-N_v}^{N_v} f_{ij}^{n+1} \Delta v, \\ u_i^{n+1} &= \frac{1}{\rho_i^{n+1}} \textstyle\sum_{j=-N_v}^{N_v} v_j f_{ij}^{n+1} \Delta v, \\ E_i^{n+1} &= \frac{1}{2} \textstyle\sum_{j=-N_v}^{N_v} v_j^2 f_{ij}^{n+1} \Delta v. \end{aligned} \tag{36}$$

From now on, we will denote formulas in (36) with the more compact notation: $(\rho_i^{n+1}, (\rho u)_i^{n+1}, E_i^{n+1}) = m[f_{i\cdot}^{n+1}]$, where, in general, $m[f]$ will indicate the approximated macroscopic moments related to the distribution function f.

Equation (35) is a non linear implicit equation because the Maxwellian depends on f^{n+1} through its moments. To solve the implicit step one can take the moments of Eq. (35); this is obtained at the discrete level multiplying both sides by $\phi_j \Delta v$, where $\phi_j = \{1, v_j, v_j^2\}$ and summing over j as in (36). Then we have

$$\Delta v \sum_j (f_{ij}^{n+1} - \tilde{f}_{ij}^n)\phi_j = \frac{1}{\varepsilon}\Delta v \Delta t \sum_j (M[f]_{ij}^{n+1} - f_{ij}^{n+1})\phi_j,$$

which implies that

$$\sum_j f_{ij}^{n+1}\phi_j = \sum_j \tilde{f}_{ij}^n \phi_j,$$

because, by definition, the Maxwellian at time t^{n+1} has the same moments as f^{n+1} and we assume that Eq. (36) is accurate enough. This in turn gives

$$m[f_{i\cdot}^{n+1}] \simeq m[\tilde{f}_{i\cdot}^n]. \tag{37}$$

Equation (37) could actually be imposed exactly, provided one defines a discrete Maxwellian which depends on the velocity grid spacing and ensures that moments of f^{n+1} are exactly preserved at the discrete level [19]. Such strategy and its generalization to more complex BGK schemes describing gas mixtures will be matter of future work.

Once the Maxwellian at time t^{n+1} is known using the approximated macroscopic moments $m[\tilde{f}_{i\cdot}^n]$, the distribution function f_{ij}^{n+1} can be explicitly computed

$$f_{ij}^{n+1} = \frac{\varepsilon \tilde{f}_{ij}^n + \Delta t M_{ij}^{n+1}}{\varepsilon + \Delta t}. \tag{38}$$

This approach has already been used in [24] and in [22] in the context of Eulerian schemes.

5.2 Second Order BDF Method

The scheme of the previous section corresponds to implicit Euler applied to the BGK model in characteristic form. High order discretization in time at a reasonable computational cost can be obtained by BDF (backward differentiation formula) methods [14, 17].

For the high order numerical approximation of the BGK models presented above, we will make use of the BDF2 scheme to discretize the ordinary differential equations along the characteristics [14]. When a time step Δt is fixed, the scheme reads as (see Fig. 2):

$$\text{BDF2} := \quad f_{i,j}^{n+1} = \frac{4}{3} f_{ij}^{n,1} - \frac{1}{3} f_{ij}^{n-1,2} + \frac{2}{3}\frac{\Delta t}{\varepsilon}(M[f]_{ij}^{n+1} - f_{ij}^{n+1}), \tag{39}$$

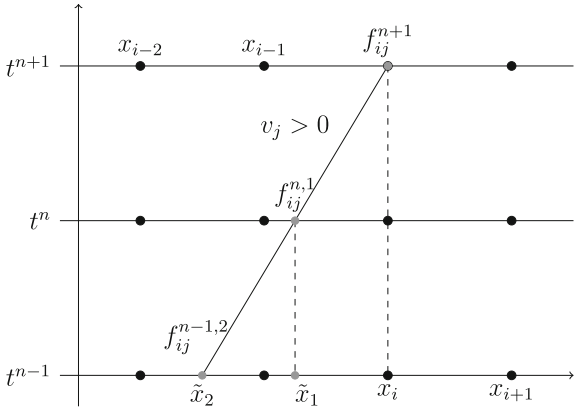

Fig. 2 Representation of the BDF2 scheme. The black circles denote grid nodes, the gray ones the points where interpolation is needed

where $f_{i,j}^{n-(s-1),s} \simeq \tilde{f}(x_i - s v_j \Delta t, v_j, t^{n-(s-1)})$, $s = 1, 2$, can be computed by suitable reconstruction from $\{f_{\cdot j}^{n-(s-1)}\}$; WENO techniques [6] will be used for accurate non oscillatory reconstruction.

Algorithm (BDF2)

- Calculate $f_{ij}^{n-1,2} = \tilde{f}(\tilde{x}_2 = x_i - 2v_j \Delta t, v_j, t^{n-1})$, $f_{ij}^{n,1} = \tilde{f}(\tilde{x}_1 = x_i - v_j \Delta t, v_j, t^n)$ by interpolation from $f_{\cdot j}^{n-1}$ and $f_{\cdot j}^{n}$ respectively;
- Compute the Maxwellian $M[f_{ij}^{n+1}]$ by means of $m[\frac{4}{3} f_{i\cdot}^{n,1} - \frac{1}{3} f_{i\cdot}^{n-1,2}]$ and upgrade the numerical solution f_{ij}^{n+1} using (39).

6 Numerical Approximation of BGK Models for Mixtures

The numerical methods presented in [14] and briefly sketched in the previous Section, based on the semi-Lagrangian formulation, can be extended to the BGK equations for inert and reactive mixtures. We consider 3D (in velocity) problems, in one space dimension and in slab geometry. Under suitable symmetry assumption, it is possible to apply the Chu reduction [8], which allows to transform a 3D (in velocity) equation in a system of two one-dimensional equations.

First of all, we consider the case of inert mixtures. For the sake of simplicity, we fix $L = 4$, and we show the first order numerical scheme applied to the AAP BGK model, described in Sect. 3.1; the discretization of the other relaxation model for inert mixture in Sect. 4.1 is similar.

6.1 First Order Semi-Lagrangian Scheme for the AAP BGK Model

By means of the Chu reduction we transform the starting equations (6) in a system (of double dimension) of 1D equations. Assume axial symmetry with respect to the axis x_1; let us introduce the new unknowns

$$g_1^s(t,x,v) = \int_{\mathbb{R}^2} f^s(t,x,\mathbf{v})\,dv_2dv_3, \quad g_2^s(t,x,v) = \int_{\mathbb{R}^2} (v_2^2+v_3^2) f^s(t,x,\mathbf{v})\,dv_2dv_3, \tag{40}$$

each depending only on one space and one velocity variable $v = v_1$. Multiplication of (6) by 1 and $(v_2^2 + v_3^2)$ and integration with respect to $(v_2, v_3) \in \mathbb{R}^2$ yields then the following system of BGK equations for the unknown vector $g^s = (g_1^s, g_2^s)$, coupled with initial conditions

$$\begin{cases} \dfrac{\partial g_i^s}{\partial t} + v\dfrac{\partial g_i^s}{\partial x} = \nu_s(M_{s,i} - g_i^s), & (t,x,v) \in \mathbb{R}_+ \times \mathbb{R} \times \mathbb{R}, \\ g_i^s(0,x,v) = g_{i,0}^s(x,v), & s = 1,...,4,\ \ i = 1,2. \end{cases} \tag{41}$$

The BGK system (41) describes a relaxation process towards the vector Maxwellians $(M_{s,1}, M_{s,2})$, which is obtained by Chu transform of (7) and has the form

$$(M_{s,1}, M_{s,2}) = \left(M_s, \frac{2KT_s}{m^s} M_s\right),$$

where

$$M_s = n^s \left(\frac{m^s}{2\pi K T_s}\right)^{1/2} \exp\left(-\frac{m^s}{2KT_s}(v-u_s)^2\right), \quad s = 1,\dots,4.$$

To determine the auxiliary parameters u_s and T_s we have to solve (12) and (13). Relations (12) and (13) involve fundamental macroscopic moments of distribution functions f^s, namely n^s, u^s (where u^s stands for u_1^s, being $u^2 = u^3 = 0$) and T^s, which are given in terms of g_1^s and g_2^s as

$$n^s = \int_{\mathbb{R}} g_1^s\,dv, \qquad u^s = \frac{1}{n^s}\int_{\mathbb{R}} v g_1^s\,dv, \tag{42}$$

$$\frac{3KT^s}{m^s} = \frac{1}{n^s}\left[\int_{\mathbb{R}} (v-u^s)^2 g_1^s\,dv + \int_{\mathbb{R}} g_2^s\,dv\right]. \tag{43}$$

We can then apply the first order semi-Lagrangian scheme to each equations of the system (41); it reads as

$$\begin{cases} g_{1,ij}^{s,n+1} = \tilde{g}_{1,ij}^{s,n} + \Delta t \nu_{s,ij}^{n+1} (M_{s,1,ij}^{n+1} - g_{1,ij}^{s,n+1}), \\ g_{2,ij}^{s,n+1} = \tilde{g}_{2,ij}^{s,n} + \Delta t \nu_{s,ij}^{n+1} (M_{s,2,ij}^{n+1} - g_{2,ij}^{s,n+1}), \quad s = 1, ..., 4, \end{cases} \tag{44}$$

where $\tilde{g}_{1,ij}^{s,n} = g_1^s(t^n, x_i - v_j \Delta t, v_j)$ and $\tilde{g}_{2,ij}^{s,n} = g_2^s(t^n, x_i - v_j \Delta t, v_j)$. The main issue is how to solve the implicit equations in (44), where the Maxwellians now depend on the auxiliary fields at time t^{n+1}. The procedure is a quite natural extension of the case of a single gas, and it is here described for readers' convenience.

The auxiliary density can be easily computed by integrating over the kinetic velocity v the first equation of (44) for $s = 1, \ldots, 4$. By easy manipulations and thanks to conservations we obtain $n_i^{s,n+1} = \tilde{n}_i^{s,n}$. Once $n^{s,n+1}$ is known, the collision frequencies ν_s^{n+1} at time t^{n+1} can be evaluated according to (8).

The second task is to compute the fictitious mean velocities u_s^{n+1}. If we multiply by v and then integrate over v the first equation of (44) for $s = 1, ..., 4$ we obtain (omitting the indices i, n, $n+1$ relevant to the discretization)[3]

$$n^s u^s = \tilde{n}^s \tilde{u}^s + \Delta t \, \nu_s (n_s u_s - n^s u^s), \quad s = 1, \ldots, 4, \tag{45}$$

but, since $n_i^{s,n+1} = \tilde{n}_i^{s,n}$, or omitting indices $n^s = \tilde{n}^s$, one obtains

$$u^s = \tilde{u}^s + \Delta t \, \nu_s (u_s - u^s), \quad s = 1, \ldots, 4, \tag{46}$$

then using (12) one has

$$u^s = \tilde{u}^s + \Delta t \, \nu_s \left(\frac{1}{m^s n^s \nu_s} \sum_{r=1}^{4} \xi^{sr} u^r \right), \quad s = 1, \ldots, 4, \tag{47}$$

from which

$$\begin{cases} \left(\xi^{11} - \dfrac{m^1 n^1}{\Delta t} \right) u^1 + \xi^{12} u^2 + \xi^{13} u^3 + \xi^{14} u^4 = -\dfrac{m^1 n^1}{\Delta t} \tilde{u}^1 \\ \xi^{21} u^1 + \left(\xi^{22} - \dfrac{m^2 n^2}{\Delta t} \right) u^2 + \xi^{23} u^3 + \xi^{24} u^4 = -\dfrac{m^2 n^2}{\Delta t} \tilde{u}^2 \\ \xi^{31} u^1 + \xi^{32} u^2 + \left(\xi^{33} - \dfrac{m^3 n^3}{\Delta t} \right) u^3 + \xi^{34} u^4 = -\dfrac{m^3 n^3}{\Delta t} \tilde{u}^3 \\ \xi^{41} u^1 + \xi^{42} u^2 + \xi^{43} u^3 + \left(\xi^{44} - \dfrac{m^4 n^4}{\Delta t} \right) u^4 = -\dfrac{m^4 n^4}{\Delta t} \tilde{u}^4 \end{cases} \tag{48}$$

Thus we have to solve a 4×4 linear system; once the actual mean velocities at time t^{n+1} are obtained, by means of (12) the fictitious mean velocities at time t^{n+1} are updated.

[3]The tilde denotes that we are evaluating the fields on the feet of the characteristics, at time t^n. Without tilde it is understood the time instant t^{n+1}.

Now we have to compute the fictitious temperatures T_s^{n+1}. Thus, computing the species temperatures at time t^{n+1} by using (43) and replacing the marginal distribution function g_1 and g_2 by their expressions given by (44) one obtains (omitting indices $i, n, n+1$):

$$\frac{3n^s K T^s}{m^s} = \frac{3\tilde{n}^s K \tilde{T}^s}{m^s} + \Delta t \nu_s \left(n^s (u_s - u^s)^2 + \frac{3n^s K T_s}{m^s} - \frac{3n^s K T^s}{m^s} \right) \quad s = 1, ...4. \quad (49)$$

Then, by easy manipulation (recalling $n^s = n_s = \tilde{n}^s, \quad s = 1, \dots 4$)

$$T^s - \Delta t \nu_s (T_s - T^s) = \tilde{T}^s + \Delta t \nu_s \frac{m^s}{3K} (u_s - u^s)^2 \quad s = 1, ...4. \quad (50)$$

Now we define

$$\alpha_s = \frac{m^s}{3K} (u_s - u^s)^2,$$

$$\beta_s = \frac{m^s}{3K} [(u_s)^2 - (u^s)^2],$$

$$\gamma_s = \frac{2}{3K} \frac{1}{\nu_s} \sum_{r=1}^{4} \nu_1^{sr} \frac{\mu^{sr}}{m^s + m^r} n^r (m^s u^s + m^r u^r)(u^r - u^s);$$

thus, using (13), Eq. (50) becomes

$$T^s - \frac{2\Delta t}{3n^s K} \sum_{r=1}^{4} \gamma^{sr} T^r = \tilde{T}^s + \Delta t \nu_s (\alpha_s - \beta_s + \gamma_s), \qquad s = 1, \dots, 4. \quad (51)$$

Therefore, to achieve the actual temperature T^s at time t^{n+1} we have to solve the above 4×4 linear system; once the actual temperatures at time t^{n+1} are known, by (13) we are able to update the fictitious temperatures at time t^{n+1}, and we eventually solve the implicit step. In analogous way it is possible to treat the other BGK model (21)–(22) for inert mixtures with relations (25)–(26).

The extension to higher order schemes, once the solution of the implicit step has been fixed, is an easy application of the schemes presented in [14]. Numerical results in Sect. 7 has been obtained using the BDF2 scheme recalled in Sect. 5.2.

6.2 *Sketch of the First Order Semi-Lagrangian Scheme for the Reactive BGK Model*

The solution of the BGK model for reacting mixtures described in Sect. 3.2 leads to additional drawbacks, since also auxiliary number densities n_s have to be taken into account; such parameters are given in terms of the actual macroscopic fields in

Eq. (14), and their expressions are nonlinear due to the exponential factor appearing in the term $\mathscr{S}$ in the Eqs. (14)–(17). Moreover, in this case we do not get three uncoupled linear 4×4 systems, for densities, velocities and temperatures, respectively, as it occurs in the inert case. Indeed, each equation depends on all the twelve actual fields, since all of them are involved in the term (17). As a consequence, the equations cannot be decoupled, and we have to deal with a 12×12 nonlinear system at each node. Solving this nonlinear system by Newton method is impracticable, owing to the very complex expressions of the auxiliary fields (14), (15) and (16). To overcome these difficulties, we adopted an iterative procedure. At the first step $k = 0$, we set

$$\begin{cases} g_{1,ij}^{s,n+1,0} = \tilde{g}_{1,ij}^{s,n} \\ g_{2,ij}^{s,n+1,0} = \tilde{g}_{2,ij}^{s,n}. \end{cases} \tag{52}$$

With this first approximation of $g_{1,ij}^{s,n+1}$ and $g_{2,ij}^{s,n+1}$ we compute a first approximation of the actual fields and therefore of the auxiliary fields at time t^{n+1}. Then we iterate the procedure

$$\begin{cases} g_{1,ij}^{s,n+1,k} = \tilde{g}_{1,ij}^{s,n} + \Delta t \nu_{ij}^{s,n+1,k-1} (M_{1,ij}^{s,n+1,k-1} - g_{1,ij}^{s,n+1,k-1}) \\ g_{2,ij}^{s,n+1,k} = \tilde{g}_{2,ij}^{s,n} + \Delta t \nu_{ij}^{s,n+1,k-1} (M_{2,ij}^{s,n+1,k-1} - g_{2,ij}^{s,n+1,k-1}), \end{cases} \tag{53}$$

until convergence. Fixed a tolerance tol, we stop the iterative procedure when the 2-norm of the difference of two consecutive iterates is smaller than tol for each marginal distribution function g_1^s, g_2^s, $s = 1, ..., 4$.

In a straightforward way we can extend this strategy to higher order schemes. Moreover, these numerical schemes can be also adapted to simulate the reactive BGK model described in Sect. 4.2.

7 Numerical Results

In this Section we present some illustrative tests, aiming at showing the performance of the semi-Lagrangian method applied to the described BGK models for mixtures, and we will point out the main peculiarities of the different BGK models for inert and reactive mixtures presented in this paper. We refer to numerical test proposed in [1] and consider a mixture of four monoatomic gases with the following values of the molecular masses:

$$m_1 = 58.5, \quad m_2 = 18, \quad m_3 = 40, \quad m_4 = 36.5.$$

The numerical values used in our tests have to be considered as dimensionless, and corresponding to arbitrary scales. They have been chosen for illustrative purposes, without any reference to an actual specific problem. However, our reaction scheme can be thought as a rough approximation of bimolecular reversible reactions like $NaCl + H_2O \rightleftharpoons NaOH + HCl$ or $H_2 + Cl \rightleftharpoons HCl + H$.

We present some results for the following Riemann problem for both reactive and non-reactive cases. The collision frequencies for elastic scattering are the same used in [1] and they also do not refer to any actual problem:

$$\begin{aligned} \nu_0^{11} = 500,\ \nu_0^{12} = 600,\ \nu_0^{13} = 200,\ \nu_0^{14} = 700, \\ \nu_0^{22} = 400,\ \nu_0^{23} = 500,\ \nu_0^{24} = 800, \\ \nu_0^{33} = 400,\ \nu_0^{34} = 300, \\ \nu_0^{44} = 600, \end{aligned}$$

with $\nu_0^{sr} = \nu_0^{rs}$ and $\nu_1^{sr} = \nu_0^{sr}$ for $s, r = 1, ..., 4$. The above frequencies will be multiplied by a factor $1/\varepsilon$ in the numerical experiments, where ε is the Knudsen number, to simulate by varying ε different regimes (rarefied or fluid). The chemical collision frequency is $\nu_{12}^{34} = 0$ in the non-reactive case, whereas we set $\nu_{12}^{34} = 100$ in the reactive case. The initial data are chosen as Maxwellians reproducing the following macroscopic fields:

$$(\rho_0, u_0, p_0) = \begin{cases} (1, 0, 5/3), & x < 0.5, \\ (1/8, 0, 1/6), & x > 0.5, \end{cases}$$

$$(\rho_{01}, \rho_{02}, \rho_{03}, \rho_{04}) = \begin{cases} (1/10, 2/10, 3/10, 4/10), & x < 0.5, \\ (1/80, 2/80, 3/80, 4/80), & x > 0.5, \end{cases} \tag{54}$$

$$u_{0i} = 0,\ i = 1, ..., 4\,.$$

The presented results are obtained using the BDF2 scheme, the best performing method thanks to the low number of interpolations required.

In Figs. 3 and 4 we present the result obtained in the inert case. In this case, we set $N_v = 30$, $N_x = 200$, $\Delta t = CFL\ \Delta v / v_{MAX}$, $v \in [-10, 10]$. In all cases presented in the paper $CFL = 2$ has been used, but higher values are possible [14], with larger gain for larger CFL. In addition, the use of CWENO [18] in place of WENO could considerably improve the efficiency of the reconstruction process, since, at variance with standard WENO, CWENO guarantees uniform accuracy for all points inside the domain, with very little overhead. This possibility is left to future investigation. We compare in Fig. 3 the solutions obtained with the two BGK models for inert case presented in Sects. 3.1 and 4.1, respectively. The results are in good agreement with the ones presented in [1]. We can observe that at the final time $t_f = 0.2$, for $\varepsilon = 10^{-1}$ (left column in Fig. 3) the equilibrium is not yet reached and species velocities and temperatures are not yet relaxed to common values. Instead, we can observe that

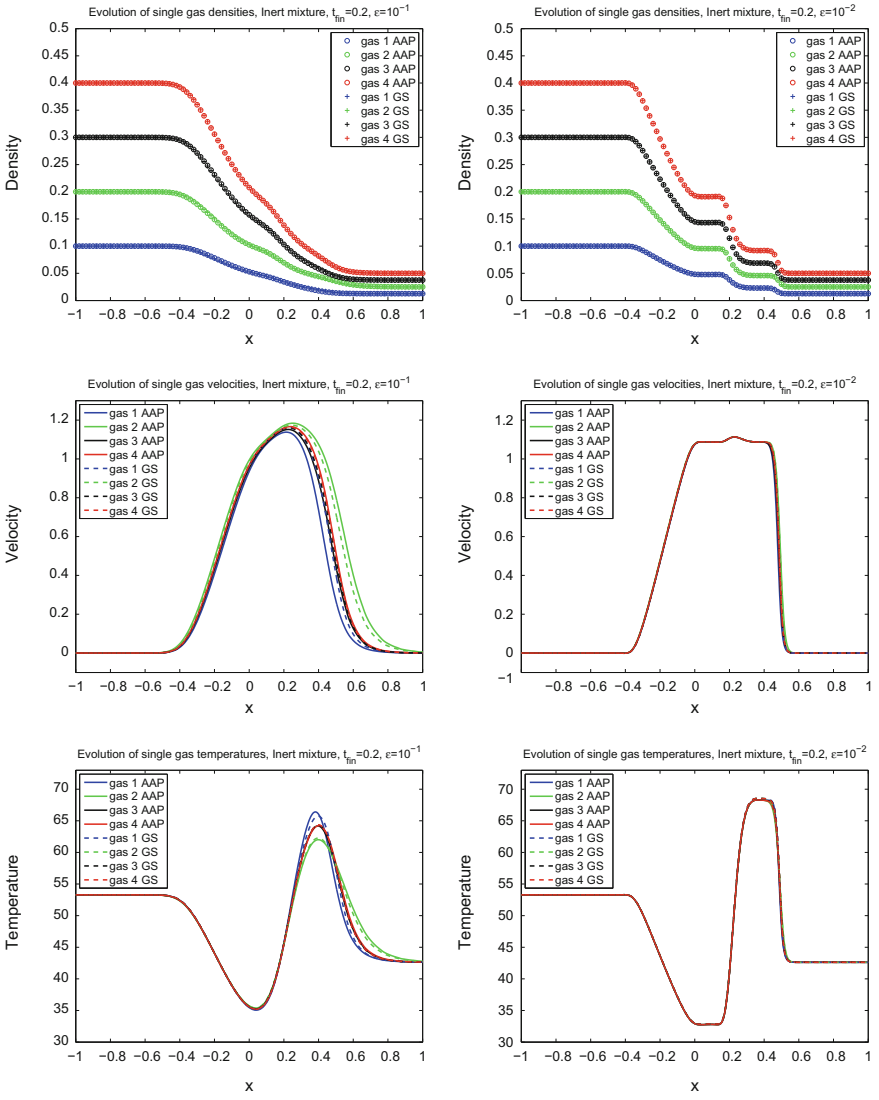

Fig. 3 Inert mixtures. Comparison of the species macroscopic fields, densities, velocities and temperatures, using (54) as initial data, obtained from the numerical approximations of the AAP BGK model and the one presented in Sect. 4.1 (GS model (21)–(22)). Left column $\varepsilon = 10^{-1}$; right column $\varepsilon = 10^{-2}$

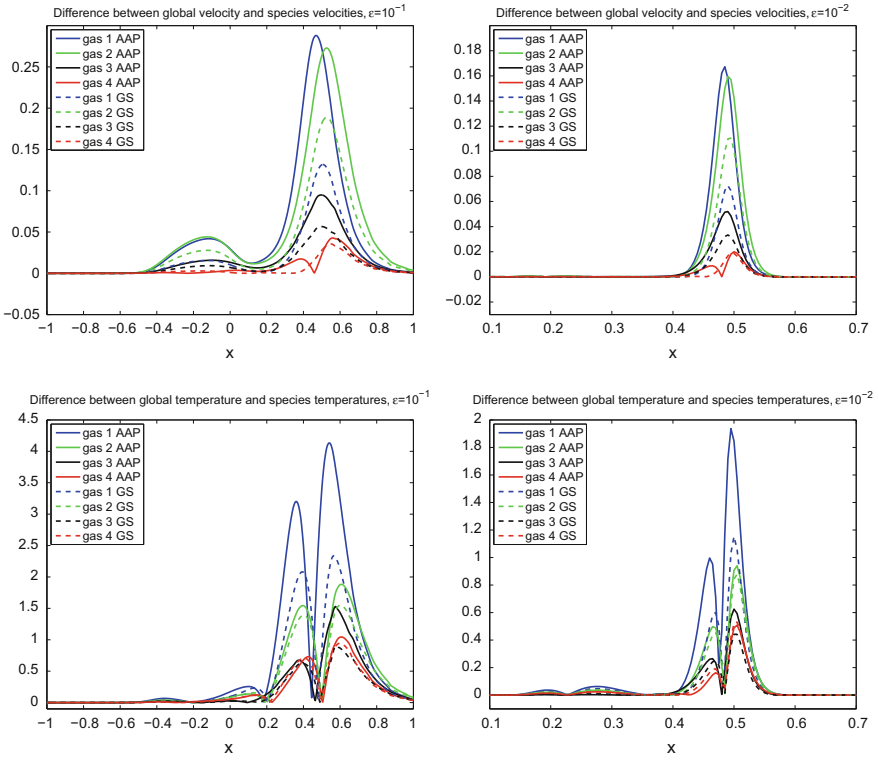

Fig. 4 Inert mixtures. Differences between mixture velocity and species velocities in the top. Differences between mixture temperature and species temperatures below. Left $\varepsilon = 10^{-1}$, right $\varepsilon = 10^{-2}$. We can observe that the differences are smaller for the GS BGK model (21)–(22) than for the AAP BGK model

for $\varepsilon = 10^{-2}$ (right column in Fig. 3) at the same final time we are closer to the equilibrium, namely species velocities and temperatures almost overlap to each other and reproduce the mean velocity and temperature values of the mixture, respectively. Of course, both BGK models give the same number densities, whereas differences can be noticed between the species velocities and temperatures prescribed by the two BGK approaches; such differences are less evident close to the fluid regime (smaller ε). In Fig. 4 the differences between species velocities and temperatures and the global mean velocity and temperature of the mixture are plotted. We can observe that such differences are smaller for the BGK model (21), with respect to the AAP BGK model. This is due to the fact that the BGK model (21) pushes the distribution functions towards the attractors (22), characterized by common velocity and temperature values. On the contrary, the AAP BGK model prescribes relaxation towards attractors with different velocities and temperatures, then species velocities and temperatures equalize later. The differences however tend to disappear when $\varepsilon \to 0$.

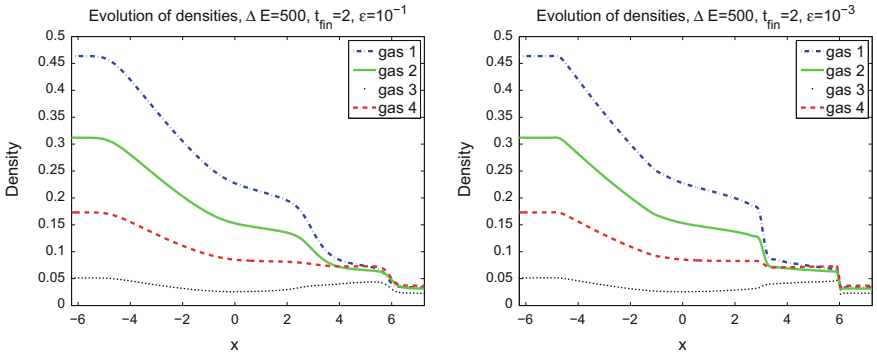

Fig. 5 Reactive mixture. Numerical approximation of the reactive BGK model described in Sect. 3.2; $CFL = 2$, $N_x = 400$, $N_v = 60$, $t_f = 2$. Species densities profiles: top $\varepsilon = 10^{-1}$, low $\varepsilon = 10^{-3}$

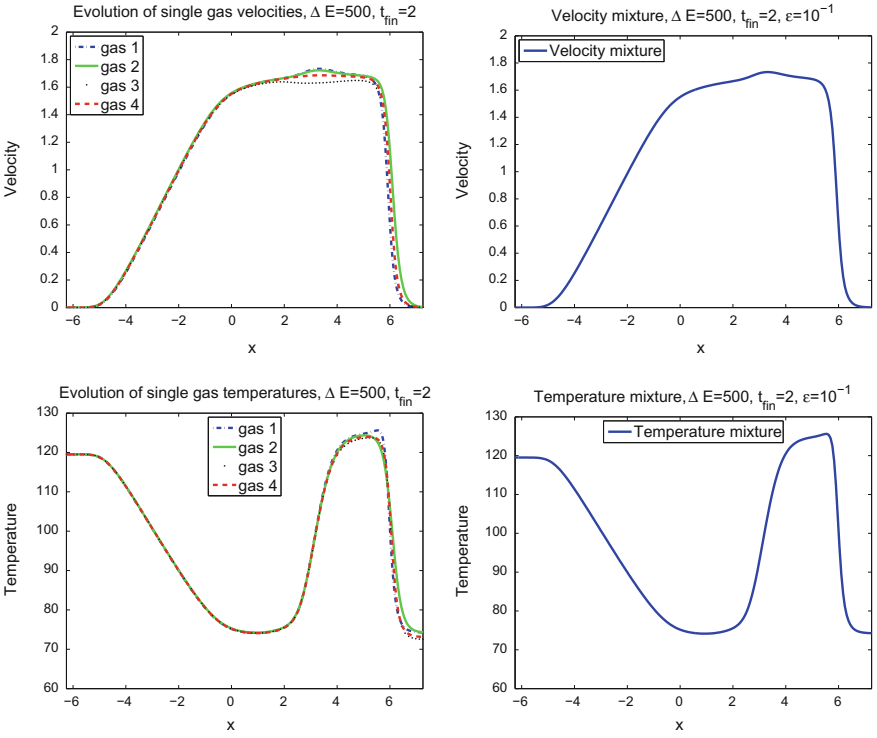

Fig. 6 Reactive mixture. Numerical approximation of the reactive BGK model described in Sect. 3.2; $CFL = 2$, $N_x = 400$, $N_v = 60$, $\varepsilon = 10^{-1}$, $t_f = 2$. Left: species macroscopic fields; right: global macroscopic fields. Top: velocity; below: temperature

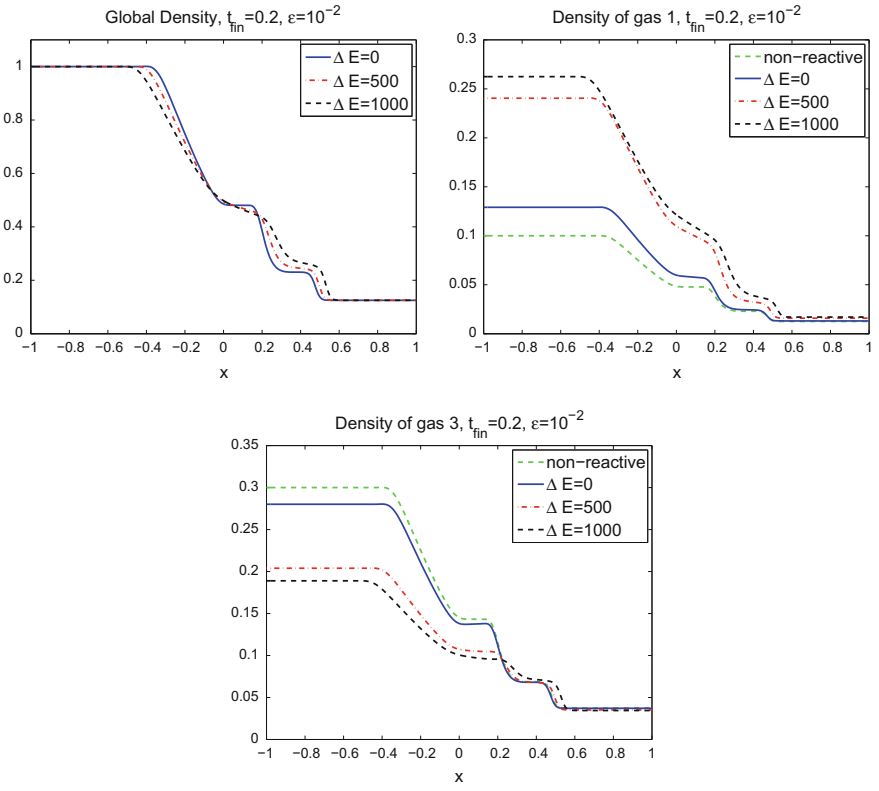

Fig. 7 Reactive mixtures. Numerical approximation of the reactive BGK model described in Sect. 3.2; $CFL = 2$, $N_x = 200$, $N_v = 60$, $\varepsilon = 10^{-2}$, $t_f = 0.2$. Global mass density ρ and density ρ^s, $s = 1, 3$ (gases 1 and 3) for different values of ΔE. The global density when $\Delta E = 0$ overlaps the profile of the non-reactive case

Figures 5 and 6 are relevant to the case of the reactive mixture, with an energy threshold $\Delta E = 500$. The results are obtained from the reactive BGK model described in Sect. 3.2; numerical simulations of the BGK model of subsection 4.2 are scheduled as future work. In Fig. 5 the profiles at time t_f of the species number densities for different values of ε are reported; we can notice significant differences with respect to the inert case (Fig. 3 top), due to the presence of the chemical reaction (2). In Fig. 6 the profiles of velocities and temperature for each gas and for the reacting mixture are reported.

The variations of the profiles of the macroscopic fields for different values of ΔE are shown in Figs. 7 and 8. In Fig. 7 we report the global density ρ and densities ρ^1 and ρ^3 at time $t = 0.2$ for non reactive and reactive cases, with three different choices $\Delta E = 0,\ 500,\ 1000$. The global density of the inert mixture overlap the profile obtained for $\Delta E = 0$, whereas this is not the case for the single components of the gas. The higher ΔE, the greater the variations with respect to the inert case, as

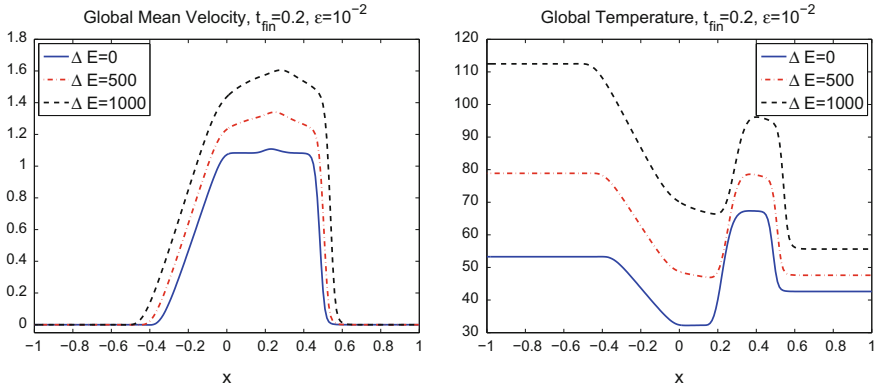

Fig. 8 Reactive mixture. Numerical approximation of the reactive BGK model described in Sect. 3.2; $CFL = 2$, $N_x = 200$, $N_v = 60$, $\varepsilon = 10^{-2}$, $t_f = 0.2$. Global mean velocity u and temperature T for different values of ΔE

Table 1 Relative errors and accuracy order in the approximation of the reactive BGK model described in Sect. 3.2, using BDF2. $CFL = 2$, $\varepsilon = 10^{-1}$. η denotes the average number of iterations

N_x	Global n	Global u	Global T	η
L_1 relative errors				
40	6.5535e-03	3.9862e-01	4.2436e-03	54
80	2.5973e-03	1.7275e-01	1.8118e-03	33
160	6.6116e-04	4.0854e-02	4.3127e-04	21
320	1.3625e-04	8.1096e-03	8.9780e-05	14
640	2.6564e-05	1.4325e-03	1.8282e-05	11
L_1 orders				
80	1.3353	1.2063	1.2278	
160	1.9739	2.0801	2.0708	
320	2.2788	2.3328	2.2641	
640	2.3587	2.5011	2.2960	

expected. The same comment applies to Fig. 8, where we report the profiles of mean velocity and temperature of the mixture for increasing values of ΔE. The results reproduce, with higher order accuracy and without an actual restriction on the CFL number, those in [1] obtained by a splitting technique.

Finally, in Tables 1 and 2 we present the accuracy order obtained using BDF2 scheme for the BGK model presented in Sect. 3.2, for two different values of ε. The test is performed in order to show the efficiency of the iterative procedure (53) used to solve the implicit step. For this test, as smooth initial data we use the Maxwellians reproducing the following initial macroscopic fields

Table 2 Relative errors and accuracy order in the approximation of the reactive BGK model described in Sect. 3.2, using BDF2. $CFL = 2$, $\varepsilon = 10^{-1}$. η denotes the average number of iterations

N_x	Global n	Global u	Global T	η
L_1 relative errors				
40	7.3747e-03	4.3970e-01	4.8548e-03	395
80	3.1298e-03	1.9845e-01	2.1617e-03	218
160	1.2041e-03	7.0644e-02	7.5636e-04	120
320	3.3898e-04	1.8127e-02	2.2317e-04	68
640	7.1701e-05	3.0637e-03	5.3147e-05	40
L_1 orders				
80	1.2365	1.1477	1.1673	
160	1.3782	1.4901	1.5150	
320	1.8286	1.9624	1.7610	
640	2.2411	2.5648	2.0701	

$$n_0^s(x) = \frac{1}{m^s}, \qquad T_0^s(x) = \frac{4}{\sum_{s=1}^4 n_0^s(x)},$$

$$u_0^s(x) = \frac{s}{\sigma_s}\left[\exp\left(-\left(\sigma_s x - 1 + \frac{s}{3}\right)^2\right) - 2\exp\left(-\left(\sigma_s x + 3 - \frac{s}{10}\right)^2\right)\right],$$

$s = 1, ..., 4$, where $\sigma_s = (10, 13, 16, 19)$. We use $CFL = 2$, $N_v = 30$, $tol = 10^{-8}$ as tolerance to stop the iterations. In Tables 1 and 2 η denotes the average number of iterations performed during each time step; the relative errors are computed taking the differences between two solutions obtained by two different meshes, N_x and $2N_x$. The number of iterations depends on the magnitude of the collision frequencies and on the time step Δt; it increases as such magnitude increases, and decreases as $\Delta t \to 0$. Thus, for not too large CFL numbers we can simulate the fluid regime (high magnitude of ν_s) with a reasonable number of iterations without increasing the computational cost with respect to the inert case.

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Hydrostatic Limit and Fick's Law for the Symmetric Exclusion with Long Jumps

Byron Jiménez Oviedo and Arthur Vavasseur

Abstract Hydrostatic behavior and Fick's law for the one dimensional exclusion process with long jumps in contact with infinite reservoirs at different densities are derived. The jump rate is described by a transition probability p which is proportional to $|\cdot|^{-(\gamma+1)}$ for $\gamma > 2$. The reservoirs add or remove particles with rate proportional to $\kappa N^{-\theta}$, where $\kappa > 0$ and $\theta = 2 - \gamma$. The behavior of the solution of the hydrostatic equation is also studied.

1 Introduction

In this work we consider the symmetric exclusion process with long jumps on $\Lambda_N := \{1, \dots, N-1\}$ in contact with infinitely many stochastic reservoirs. Each pair of sites of the bulk $\{x, y\} \subset \Lambda_N$ carries a Poisson process of intensity one. The Poisson processes associated to different bonds are independent. If the clock associated to $\{x, y\}$ rings, particles at the sites are exchanged with rate $p(y-x)$, if one of the site is empty and the other one is not. Otherwise nothing happens. In the dynamics at the left boundary each pair of sites $\{x, y\}$ with $x \in \Lambda_N$ and $y \in \mathbb{Z}_-$ carries a Poisson process of intensity one, all being independent. If the clock associated to the bound $\{x, y\}$ rings, then a particle can get into (resp. get out from) the bulk from (resp. to) the left reservoir at rate $\alpha \frac{\kappa}{N^\theta} p(z)$ (resp. $(1-\alpha)\frac{\kappa}{N^\theta} p(z)$) where $z = y - x$ is the size of the jump, if the site at x is empty (resp. occupied). The right reservoir acts in the same way, except that α is replaced by β in the jump rates given above. We can also interpret that particles can be created (resp. annihilated) at all the sites x in the bulk with one of the rates $r_N^-(x/N)\alpha\kappa/N^\theta$ or $r_N^+(x/N)\beta\kappa/N^\theta$ (resp. $r_N^-(x/N)(1-\alpha)\kappa/N^\theta$ or $r_N^+(x/N)(1-\beta)\kappa/N^\theta$) where $r_N^\pm$ are given in Sect. 2.

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We are interested in the case where $p(\cdot)$ has a heavy tail proportional to $|\cdot|^{-(\gamma+1)}$ for $\gamma > 2$. The case $\gamma < 2$ is study in [1], in this case is obtained a non local operator (fractional version of the Laplacian) instead the usual Laplacian (Fig. 1).

The presence of a slow or fast boundary depending on θ and κ can strongly affect the macroscopic behavior of the system. In [2] it is given a complete characterization of the hydrodynamic behavior of the process described above: there are five different macroscopic phases, depending on $\theta \in \mathbb{R}$. Moreover, we can see that hydrostatic limit for $\theta \neq 2-\gamma$ can be obtained easily. For that reason, the hydrostatic behavior, form and properties of the stationary solution in the case $\theta = 2-\gamma$ deserve to be treated.

Then, the aim of this work is to complete the stationary scenario given in [2]. We show that the stationary density profile is a stationary solution of a reaction-diffusion equation with Dirichlet boundary conditions:

$$\begin{cases} -\frac{\sigma^2}{2}\,\Delta\bar{\rho}^{\kappa}(u) + \dfrac{\kappa c_\gamma}{\gamma}\left\{\dfrac{\bar{\rho}^{\kappa}(u)-\alpha}{u^{\gamma}} + \dfrac{\bar{\rho}^{\kappa}(u)-\beta}{(1-u)^{\gamma}}\right\} = 0, \quad u \in (0,1), \\ \bar{\rho}^{\kappa}(0) = \alpha, \quad \bar{\rho}^{\kappa}(1) = \beta \end{cases}$$

(see Sect. 2 for the definition of σ and c_γ). As a consequence of the hydrostatic limit, we get Fick's law of particles transport, which says that the flux goes from regions of high concentration to regions of low concentration, with a magnitude that is proportional to the concentration gradient.

It is also part of this work to give a series of properties of the profile. Namely, we prove that this profile is increasing, convex on $[0, \frac{1}{2}]$ and concave on $[\frac{1}{2}, 1]$. Those facts follow directly from a description of the dependence of the profile on the parameter κ that we prove thanks to an adaptation of the maximum principle. In a second step, we will see that those properties give a precise description of the behavior of the profile near the boundary, which will allow us to improve the regularity given by the existence theory (Fig. 2).

The outline of this paper is as follows. In Sect. 2 we describe the model precisely the model, we introduce the hydrodynamic equations and state the results. In Sect. 3 we deal with hydrostatic limit and Fick's law. Finally, Sect. 4 is devoted to present the behavior of the solution of the hydrostatic equation.

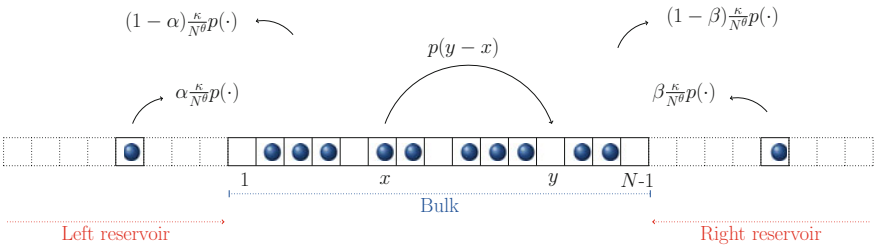

Fig. 1 Exclusion process with long jumps and infinitely extended reservoirs

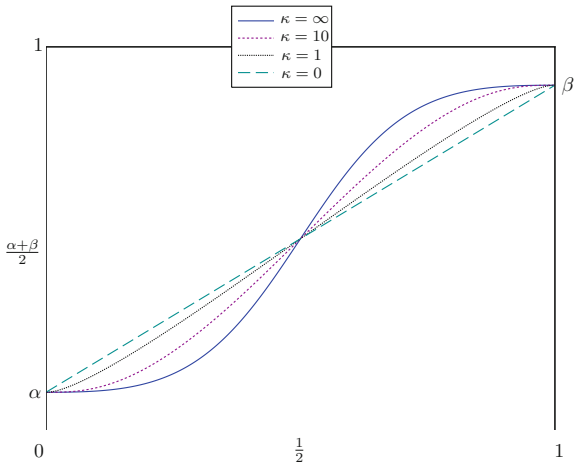

Fig. 2 Profiles of the solution of the hydrostatic equations

2 Notation and Results

2.1 The Model

For an integer $N \geq 2$ let $\Lambda_N = \{1, \dots, N-1\}$ and $\Omega_N = \{0,1\}^{\Lambda_N}$. Fix $\gamma > 2$. Let $p(\cdot)$ be a probability on $\mathbb{Z}$ defined by

$$p(z) = c_\gamma \frac{\mathbf{1}_{z\neq 0}}{|z|^{\gamma+1}}$$

where $c_\gamma^{-1} = 2\zeta_{\gamma+1}$($\zeta_s$ is the Riemann zeta function defined for $s > 1$). We denote $m = \sum_{z\geq 0} zp(z)$. Note that $p(\cdot)$ has mean zero due to its symmetry, that is: $\sum_{z\in\mathbb{Z}} zp(z) = 0$. The latter allows us to write the variance of $p(\cdot)$ as $\sigma^2 := \sum_{z\in\mathbb{Z}} z^2 p(z)$, which is finite since $\gamma > 2$.

Fix $0 \leq \alpha \leq \beta \leq 1$ and $\kappa > 0$. We consider the symmetric long jumps exclusion process on Λ_N with infinitely many stochastic reservoirs with density α at all negative integer sites $j \leq 0$ and with density β at all integer sites $j \geq N$ (see [2] for more details about the model). The intensity of the reservoirs is regulated by a parameter $\kappa N^{-\theta}$ where $\theta = 2 - \gamma$. This process is a Markov process with configuration space Ω_N. A typical configuration is described as an element $\eta = \{\eta_x\}_{x\in\Lambda_N}$ in Ω_N, so that for $x \in \Lambda_N$, $\eta_x = 0$ means that the site x is vacant while $\eta_x = 1$ means that the site x is occupied.

The process is characterized by its infinitesimal generator

$$L_N = L_N^0 + \kappa N^{-\theta}\left[L_N^\ell + L_N^r\right],$$

where the generator L_N^0 corresponds to the bulk dynamics and generators L_N^ℓ and L_N^r corresponding to non-conservative boundary dynamics. The action of L_N on functions $f : \Omega_N \to \mathbb{R}$ is given by

$$\begin{aligned}(L_N^0 f)(\eta) &= \frac{1}{2}\sum_{x,y\in\Lambda_N} p(x-y)[f(\eta^{xy}) - f(\eta)],\\ (L_N^\ell f)(\eta) &= \sum_{\substack{x\in\Lambda_N\\ y\le 0}} p(x-y)c_x(\eta;\alpha)[f(\eta^x) - f(\eta)],\\ (L_N^r f)(\eta) &= \sum_{\substack{x\in\Lambda_N\\ y\ge N}} p(x-y)c_x(\eta;\beta)[f(\eta^x) - f(\eta)],\end{aligned} \tag{1}$$

where

$$(\eta^{xy})_z = \begin{cases}\eta_z, & z\neq x,y,\\ \eta_y, & z=x,\\ \eta_x, & z=y.\end{cases} \qquad (\eta^x)_z = \begin{cases}\eta_z, & z\neq x,\\ 1-\eta_x, & z=x,\end{cases}$$

and for any $x \in \Lambda_N$ and any $\eta \in \Omega_N$ we have that

$$c_x(\eta;\alpha) = [\eta_x(1-\alpha) + (1-\eta_x)\alpha]$$

and

$$c_x(\eta;\beta) = [\eta_x(1-\beta) + (1-\eta_x)\beta].$$

Given $x \in \Lambda_N \cup \{N\}$ and a configuration η, we denote by $W_x(\eta)$ the current over the value $x - \frac{1}{2}$ which is defined as the rate of particles crossing $x - \frac{1}{2}$ from the left to the right minus the rate of particles crossing $x - \frac{1}{2}$ from the right to the left. Then, the current can be written as

$$\begin{aligned}W_x(\eta) = &\sum_{\substack{1\le y\le x-1\\ x-1<z\le N-1}} p(z-y)(\eta_y - \eta_z)\\ &+\kappa N^{-\theta}\Bigg[\sum_{\substack{x\le z\le N-1\\ y\le 0}} p(z-y)(\alpha-\eta_z) - \sum_{\substack{1\le y\le x-1\\ z\ge N}} p(z-y)(\beta-\eta_y)\Bigg]\\ &=: W_x^0(\eta) + \kappa N^{-\theta} W_x^{\ell,r}(\eta).\end{aligned}$$

We will often omit the dependence of W_x on η. Note that for any $x \in \Lambda_N$ we have that $L_N\eta_x$ is equal to

$$\sum_{y\in\Lambda_N} p(y-x)[\eta_y - \eta_x] + \kappa N^{-\theta}\Big[\sum_{y\le 0} p(y-x)(\alpha-\eta_x) + \sum_{y\ge N} p(y-x)(\beta-\eta_x)\Big].$$

Now note that $W_x - W_{x+1}$ is equal to

$$\sum_{\substack{1\le y\le x-1\\ x-1<z\le N-1}} p(z-y)(\eta_y-\eta_z) - \sum_{\substack{1\le y\le x\\ x+1<z\le N-1}} p(z-y)(\eta_y-\eta_z)$$

$$\kappa N^{-\theta}\Big[\sum_{\substack{x\le z\le N-1\\ y\le 0}} p(z-y)(\alpha-\eta_z) - \sum_{\substack{x+1\le z\le N-1\\ y\le 0}} p(z-y)(\alpha-\eta_z)\Big]$$

$$\kappa N^{-\theta}\Big[\sum_{\substack{1\le y\le x\\ z\ge N}} p(z-y)(\beta-\eta_y) - \sum_{\substack{1\le y\le x-1\\ z\ge N}} p(z-y)(\beta-\eta_y)\Big].$$

Thus, it is not difficult to see the microscopic continuity equation

$$L_N\eta_x = -\nabla W_x := -(W_{x+1} - W_x).$$

Let us denote by $\{\eta(t)\}_{t\ge 0}$ the Markov process associated to the generator L_N speeded up by N^2, i.e. the process with generator N^2L_N. For $\rho\in(0,1)$, we denote by ν_ρ the Bernoulli product measure in Ω_N with density ρ, that is, the measure whose marginals satisfy $\nu_\rho(\eta_x=1) = 1-\nu_\rho(\eta_x=0) = \rho$. The irreducible Markov process generated by L_N has a unique invariant measure that we will denote by $\bar{\mu}_N$ and $f_{N,\rho}$ will denote its density with respect to the measure ν_ρ. If $\alpha=\beta=\rho$ then $\bar{\mu}_N = \nu_\rho$. To simplify the notation of the expectation with respect to $\bar{\mu}_N$ (resp. ν_ρ) we will often use the notation $\int_{\Omega_N} f(\eta)d\bar{\mu}_N(\eta) = \langle f\rangle_N$ $\Big(\text{resp. } \int_{\Omega_N} f(\eta)d\nu_\rho(\eta) = \langle f\rangle_\rho\Big)$.

2.2 Hydrostatic Equation

In this section we will define the partial differential equation that the empirical density solves in the thermodynamic limit $N\to\infty$. For that purpose we need to introduce some notation and definitions. First, we abbreviate the Hilbert space $L^2([0,1]^d, h(u)du)$ for $d=1,2$, by $L^2_h([0,1]^d)$ and we denote its inner product by $\langle\cdot,\cdot\rangle_h$ and the corresponding norm by $\|\cdot\|_h$. When $h\equiv 1$ we simply write $L^2([0,1]^d)$, $\langle\cdot,\cdot\rangle$ and $\|\cdot\|$. The set $C^\infty([0,1]^d)$ denotes the set of restrictions of smooth functions on $\mathbb{R}$ to $[0,1]^d$. The supremum norm is denoted by $\|\cdot\|_\infty$. We denote by $C_c^\infty((0,1)^d)$ the set of all smooth real-valued functions defined in $(0,1)^d$ with compact support included in $(0,1)^d$. We denote by Δ the Laplacian operator: $\Delta = \sum_{i=1}^d \partial^2_{u_i}$. The semi inner-product $\langle\cdot,\cdot\rangle_1$ is defined on the set $C^\infty([0,1]^d)$ by $\langle F,G\rangle_1 = \int_{[0,1]^d}\sum_{i=1}^d(\partial_{u_i}F)(u)\,(\partial_{u_i}G)(u)\,du$. The corresponding semi-norm is denoted by $\|\cdot\|_1$.

Definition 1 The Sobolev space $\mathcal{H}^1([0,1]^d)$ is the Hilbert space defined as the completion of $C^\infty([0,1]^d)$ for the norm

$$\|\cdot\|^2_{\mathcal{H}^1} := \|\cdot\|^2 + \|\cdot\|^2_1.$$

Its elements elements coincide a.e. with continuous functions (see [5]). The completion of $C_c^\infty((0,1)^d)$ for this norm is denoted by $\mathcal{H}_0^1([0,1]^d)$. This is a Hilbert space whose elements coincide a.e. with continuous functions vanishing at the boundary of $[0,1]^d$. On $\mathcal{H}_0^1$, the two norms $\|\cdot\|_{\mathcal{H}^1}$ and $\|\cdot\|_1$ are equivalent. We also define the spaces $\mathcal{H}_h^1 := \mathcal{H}^1 \cap L_h^2$ and $\mathcal{H}_{0,h}^1 := \mathcal{H}_0^1 \cap L_h^2$.

In order to simplify notation in Definition 2 below and in the rest of the paper we define the functions $r_N^\pm : [0,1] \to \mathbb{R}$ such that for $x \in \Lambda_N$ as follows: at the points $\frac{x}{N}$ the are defined as

$$r_N^-(\tfrac{x}{N}) = \sum_{y \geq x} p(y), \quad r_N^+(\tfrac{x}{N}) = \sum_{y \leq x-N} p(y), \tag{2}$$

with $r_N^\pm(0) = r_N^\pm(\frac{1}{N})$ and $r_N^\pm(1) = r_N^\pm(\frac{N-1}{N})$. At the remaining points, they are defined by linear interpolation. Let us consider the functions $r^\pm : (0,1) \to \mathbb{R}_+$ defined by $r^-(u) = c_\gamma \gamma^{-1} u^{-\gamma}$ and $r^+(u) = c_\gamma \gamma^{-1}(1-u)^{-\gamma}$. By Lemma 3.3 of [3] we know that

$$\lim_{N\to\infty} N^\gamma r_N^\pm(u) = r^\pm(u) \tag{3}$$

uniformly in any compact set included in $(0,1)$. We also introduce the functions $V_1(u) = r^-(u) + r^+(u)$ and $V_0(u) = \alpha r^-(u) + \beta r^+(u)$.

We are ready to define weak solutions of the partial differential equation which we will deal with.

Definition 2 Let $\sigma > 0$ and $\kappa > 0$. We say that $\bar\rho^\kappa : [0,1] \to [0,1]$ is a weak solution of the stationary reaction-diffusion equation with Dirichlet boundary conditions

$$\begin{cases} -\frac{\sigma^2}{2}\Delta\bar\rho^\kappa(u) + \kappa V_1(u)\Big\{\bar\rho^\kappa(u) - \bar\rho^\infty(u)\Big\} = 0, \quad u \in (0,1), \\ \bar\rho^\kappa(0) = \alpha, \quad \bar\rho^\kappa(1) = \beta, \end{cases} \tag{4}$$

where $\bar\rho^\infty(u) = \dfrac{V_0(u)}{V_1(u)}$, if

(i) $\bar\rho^\kappa \in \mathcal{H}^1([0,1])$.

(ii) $\int_0^1 \left\{ \frac{(\alpha-\bar\rho^\kappa(u))^2}{u^\gamma} + \frac{(\beta-\bar\rho^\kappa(u))^2}{(1-u)^\gamma} \right\} du < \infty$.

(iii) For any function $G \in C_c^\infty((0,1))$ we have that

$$-\langle\bar\rho^\kappa, \tfrac{\sigma^2}{2}\Delta G\rangle + \kappa\langle\bar\rho^\kappa, G\rangle_{V_1} - \kappa\langle V_0, G\rangle = 0. \tag{5}$$

Remark 1 Even though equation given in the introduction and the Eq. 4 are the same, we have decided to write the last one in this way because in Theorem 3 we will see that many properties of the weak solution $\bar\rho^\kappa$ will be related with properties satisfied by $\bar\rho^\infty$.

Remark 2 Observe that items (i) and (ii) of the previous definition imply that $\bar{\rho}^\kappa(0) = \alpha$ and $\bar{\rho}^\kappa(1) = \beta$. Indeed, first note that from (i) we have $\bar{\rho}^\kappa \in \mathcal{H}^1([0,1])$ then by Morrey's inequality (see e.g. [6]) we have that $\bar{\rho}^\kappa$ is $\frac{1}{2}$-Hölder in $[0,1]$. Now, take $\varepsilon \in (0,1)$ and note that

$$\begin{aligned} &\lim_{\varepsilon\to 0} \varepsilon^{\gamma-1} \int_\varepsilon^1 \frac{(\alpha - \bar{\rho}^\kappa(0))^2}{u^\gamma} du \\ &\leq \lim_{\varepsilon\to 0} 2\varepsilon^{\gamma-1} \int_\varepsilon^1 \frac{(\alpha - \bar{\rho}^\kappa(u))^2 + (\bar{\rho}^\kappa(u) - \bar{\rho}^\kappa(0))^2}{u^\gamma} du. \end{aligned} \tag{6}$$

In the last inequality we used the fact that $(a+b)^2 \leq 2a^2 + 2b^2$. Then from the fact that $\bar{\rho}^\kappa$ is $\frac{1}{2}$-Hölder in $[0,1]$ and item (ii) we conclude that $(\alpha - \bar{\rho}^\kappa(0))^2 = 0$ and we are done. Showing that $\bar{\rho}^\kappa(1) = \beta$ is completely analogous.

Remark 3 Since $\bar{\rho}^\infty$ is a continuous function such that

$$\int_0^1 \left\{ \frac{(\alpha - \bar{\rho}^\infty(u))^2}{u^\gamma} + \frac{(\beta - \bar{\rho}^\infty(u))^2}{(1-u)^\gamma} \right\} du < \infty$$

and $\bar{\rho}^\infty(0) = \alpha$ and $\bar{\rho}^\infty(1) = \beta$, it is easy to see that from item (i) and item (ii) in Definition 2 we have that $\bar{\rho}^\kappa - \bar{\rho}^\infty \in \mathcal{H}^1_{0,V_1}([0,1])$.

Proposition 1 *There exists a unique weak solution of (4).*

Proof First note that we can rewrite (5) as

$$-\langle \varphi^\kappa, \tfrac{\sigma^2}{2}\Delta G\rangle + \kappa\langle \varphi^\kappa, G\rangle_{V_1} = \langle \bar{\rho}^\infty, \tfrac{\sigma^2}{2}\Delta G\rangle, \tag{7}$$

where $\varphi^\kappa(u) = \bar{\rho}^\kappa(u) - \bar{\rho}^\infty(u)$. Let $a^\kappa : \mathcal{H}^1_{0,V_1}([0,1]) \times \mathcal{H}^1_{0,V_1}([0,1]) \to \mathbb{R}$ be a bilinear form defined as

$$a^\kappa(\varphi, \varrho) = \langle \varphi, \varrho\rangle_1 + \kappa\langle \varphi, \varrho\rangle_{V_1},$$

for functions $\varphi, \varrho \in \mathcal{H}^1_{0,V_1}([0,1])$. We claim that a^κ is coercive. Indeed

$$a^\kappa(\varphi,\varphi) = \|\varphi\|_1^2 + \kappa\|\varphi\|_{V_1}^2 \geq \min\{1, \kappa V_1(\tfrac{1}{2})\}\|\varphi\|_{\mathcal{H}^1}^2$$

and trivially we have that $a^\kappa(\varphi,\varphi) \geq \kappa\|\varphi\|_{V_1}^2$. By using the Cauchy-Schwarz inequality we get that

$$|a^\kappa(\varphi,\varrho)| \leq \|\varphi\|_1\|\varrho\|_1 + \kappa\|\varphi\|_{V_1}\|\varrho\|_{V_1}.$$

The latter allows to conclude that the bilinear form a^κ is also continuous. Now we consider the linear form $I_{\bar{\rho}^\infty} : \mathcal{H}^1_{0,V_1}([0,1]) \to \mathbb{R}$ defined by $I_{\bar{\rho}^\infty}(\varphi) = -\frac{\sigma^2}{2}\langle \bar{\rho}^\infty, \varphi\rangle_1$.

This linear form is continuous. Indeed, first note that $\bar{\rho}^{\infty} \in C^2([0,1])$. Using the Cauchy-Schwarz inequality we get that

$$|I_{\bar{\rho}^{\infty}}(\varphi)| \leq \tfrac{\sigma^2}{2} \|\bar{\rho}^{\infty}\|_1 \|\varphi\|_1.$$

On the other hand, using integration by parts and the Cauchy-Schwarz inequality we have that

$$|I_{\bar{\rho}^{\infty}}(\varphi)| = \tfrac{\sigma^2}{2} |\langle \Delta \bar{\rho}^{\infty} V_1^{-1/2}, V_1^{1/2} \varphi \rangle| \leq \tfrac{\sigma^2}{2} \|\Delta \bar{\rho}^{\infty} V_1^{-1/2}\| \|\varphi\|_{V_1}.$$

Now we can apply Lax-Milgram's Theorem to guarantee that there exists a unique function $\varphi^{\kappa} \in \mathcal{H}^1_{0,V_1}([0,1])$, which satisfies (7) for any function $G \in C_c^{\infty}((0,1))$. Then, in order to conclude the proof it is enough to take $\rho^{\kappa}(u) = \varphi^{\kappa}(u) + \bar{\rho}^{\infty}(u)$ which clearly satisfies Definition 2.

Remark 4 Although the proof of the previous proposition has been given for $\kappa > 0$, the result is also true for $\kappa = 0$. We can see this, trivially taking $\bar{\rho}^0(u) = (\beta - \alpha)u + \alpha$.

Lemma 1 *Let $\bar{\rho}^{\kappa}$ be the unique weak solution of (4). Then we have that $\bar{\rho}^{\kappa}(u) + \bar{\rho}^{\kappa}(1-u) = \alpha + \beta$, for all $u \in (0,1)$.*

Proof Note that $\alpha + \beta - \bar{\rho}^{\kappa}(1-u)$ is a weak solution of (4). Then, by uniqueness of these solutions, we have that $\bar{\rho}^{\kappa}(u) = \alpha + \beta - \bar{\rho}^{\kappa}(1-u)$ for all $u \in (0,1)$.

In other words, Lemma 1 says that the graph of $\bar{\rho}^{\kappa}$ has rotational symmetry with respect to the point $(\frac{1}{2}, \frac{\alpha+\beta}{2})$.

2.3 Statement of Results

The first result is the following law of large numbers for the empirical density under the stationary measure $\bar{\mu}_N$.

Theorem 1 (Hydrostatic) *For any continuous function $G : [0,1] \to \mathbb{R}$ and for any $\delta > 0$*

$$\lim_{N \to \infty} \bar{\mu}_N \left[\eta : \left| \frac{1}{N-1} \sum_{x \in \Lambda_N} G(\tfrac{x}{N}) \eta_x - \int_0^1 G(u) \bar{\rho}^{\kappa}(u) du \right| > \delta \right] = 0,$$

where $\bar{\rho}^{\kappa}$ is the unique weak solution of (4).

The "Fick's law" is our second result.

Theorem 2 (Fick's law) *For all* $v \in (0, 1)$ *the following Fick's law holds*

$$\lim_{N\to\infty} N\langle W_{[vN]}\rangle_N = -\frac{\sigma^2}{2}\partial_v\bar{\rho}^\kappa(v) + \kappa\int_v^1(\alpha-\bar{\rho}^\kappa(u))r^-(u)du - \kappa\int_0^v(\beta-\bar{\rho}^\kappa(u))r^+(u)du, \tag{8}$$

where $\bar{\rho}^\kappa$ *is the unique weak solution of (4).*

Our last result is about the behavior of the weak solution of (4).

Theorem 3 *Let* $\bar{\rho}^\kappa$ *be the unique solution of (4). Then,*

(i) $\bar{\rho}^\kappa$ *increases on* $[0, 1]$*, it is convex on* $[0, \frac{1}{2}]$ *and concave on* $[\frac{1}{2}, 1]$*. Moreover,* $\bar{\rho}^\kappa(\frac{1}{2}) = \frac{\alpha+\beta}{2}$ *and* $(\beta-\alpha) \le (\bar{\rho}^\kappa)'(\frac{1}{2}) \le \gamma(\beta-\alpha)$.

(ii) If $\kappa < \iota$ *and* $\bar{\rho}^\kappa$, $\bar{\rho}^\iota$ *are the respective solutions of* (4) *then we have*

- $\bar{\rho}^0(u) > \bar{\rho}^\kappa(u) > \bar{\rho}^\iota(u) > \bar{\rho}^\infty(u)$ *if* $u \in (0, \frac{1}{2})$,
- $\bar{\rho}^0(u) < \bar{\rho}^\kappa(u) < \bar{\rho}^\iota(u) < \bar{\rho}^\infty(u)$ *if* $u \in (\frac{1}{2}, 1)$.

(iii) $\bar{\rho}^\kappa \in C^2([0,1]) \cap C^\infty((0,1))$*, its behavior at the boundary is precisely described:*

$$\bar{\rho}^\kappa(u) \underset{u\to 0}{=} \alpha + (\beta-\alpha)u^\gamma + o(u^\gamma)$$

and

$$\bar{\rho}^\kappa(u) \underset{u\to 1}{=} \beta - (\beta-\alpha)(1-u)^\gamma + o\left((1-u)^\gamma\right).$$

Note that in the general case $\gamma > 2$, the regularity of $\bar{\rho}^\kappa$ on $[0, 1]$ is optimal: if $2 \le n < \gamma < n+1$, $\bar{\rho}^\kappa$ can not be in $C^{n+1}([0,1])$ by item (iii) of Theorem 3. The function $\bar{\rho}^\kappa$ can possibly be a smooth function on $[0, 1]$ only if γ is an integer number. It is easy to see that $\bar{\rho}^\kappa$ depends linearly on the boundary conditions. Since κ and σ^2 can be associated in a single parameter, Corollary 1 in Theorem 3 ends the description of the dependence of $\bar{\rho}^\kappa$ in all the parameters. Moreover, in Corollary 1, we also prove that

$$\bar{\rho}^\kappa \in C([0,1]) \cap C^\infty((0,1)), \tag{9}$$

independently of Theorem 3 and this result will be useful in the proof of such Theorem.

Remark 5 Observe that the expression at the right hand side of (8) does not depend on v. Indeed, taking the derivative with respect to v, the right hand side of (8) vanishes thanks to (4). Thus, we have that

$$\lim_{N\to\infty} N\langle W_1\rangle_N = \kappa\int_0^1(\alpha-\bar{\rho}^\kappa(u))r^-(u)du. \tag{10}$$

Using item (iii) of Theorem 3, we can see that the expression at the right hand side of (10) is finite.

3 Hydrostatic Limit and Fick's Law

In this section we prove Theorems 1 and 2. Let $\mathcal{M}_d^+, d = 1, 2$, be the space of positive measures on $[0, 1]^d$ with total mass bounded by 1 equipped with the weak topology. For any $\eta \in \Omega^N$ the empirical measures $\pi^N(\eta) \in \mathcal{M}_1^+$ (resp. $\hat{\pi}^N(\eta) \in \mathcal{M}_2^+$) is defined by

$$\pi^N(\eta) = \frac{1}{N-1} \sum_{x=1}^{N-1} \eta_x \delta_{x/N} \quad \left(\text{resp. } \hat{\pi}^N(\eta) = \frac{1}{(N-1)^2} \sum_{x,y=1}^{N-1} \eta_x \eta_y \delta_{(x/N, y/N)} \right)$$

where δ_u (resp. $\delta_{(u,v)}$) is the Dirac mass on $u \in [0, 1]$ (resp. $(u, v) \in [0, 1]^2$). Let $\mathbb{P}^N$ be the law on $\mathcal{M}_1^+ \times \mathcal{M}_2^+$ induced by $(\pi^N, \hat{\pi}^N) : \Omega^N \to \mathcal{M}_1^+ \times \mathcal{M}_2^+$ when Ω^N is equipped with the non-equilibrium stationary state $\bar{\mu}_N$. To simplify notations, we denote $\pi^N(\eta)$ (resp. $\hat{\pi}^N(\eta)$) by π^N (resp. $\hat{\pi}^N$) and the action of $\pi \in \mathcal{M}_d^+$ on a continuous function $G : [0, 1]^d \to \mathbb{R}$ by $\langle \pi, G \rangle = \int_{[0,1]^d} G(u)\pi(du)$.

Our goal is to prove that every limit point $\mathbb{P}^*$ of the sequence $\{\mathbb{P}^N\}_{N \geq 2}$ is concentrated on the set of measures $(\pi, \hat{\pi})$ of $\mathcal{M}_1^+ \times \mathcal{M}_2^+$ such that π (resp. $\hat{\pi}$) is absolutely continuous with respect to the Lebesgue measure on $[0, 1]$ (resp. $[0, 1]^2$) and whose density $\bar{\rho}^\kappa$ (resp. $\bar{\rho}^\kappa(u)\bar{\rho}^\kappa(v)$) is a weak solution of (4).

Lemma 2 *The sequence $\{\mathbb{P}^N\}_{N \geq 2}$ is tight. Let $\mathbb{P}^*$ be a limit point of the sequence $\{\mathbb{P}^N\}_{N \geq 2}$. Then $\mathbb{P}^*$ is concentrated on absolutely continuous measures $(\pi(du), \hat{\pi}(du\,dv)) = (\pi(u)du, \pi(u)\pi(v)du\,dv)$. The density π is a positive function in $\mathcal{H}^1([0, 1])$ and satisfies $\int_0^1 \left\{ \frac{(\alpha - \pi(u))^2}{u^\gamma} + \frac{(\beta - \pi(u))^2}{(1-u)^\gamma} \right\} du < \infty$.*

Proof Since $\mathcal{M}_d^+$ is compact in the weak topology we have that the sequence $\{\mathbb{P}^N\}_{N \geq 2}$ is tight on $\mathcal{M}_d^+$ (see e.g [4]). $\mathbb{P}^*$ is concentrated on absolutely continuous measures because the process allows one particle per site. Since $\hat{\pi}^N$ is a product measure whose marginals are given by π^N, by weak convergence, we have that $\hat{\pi}(u, v) = \pi(u)\pi(v)$ for any $(u, v) \in [0, 1]^2$.

The proof that the density $\pi \in \mathcal{H}^1([0, 1])$ and satisfies $\int_0^1 \left\{ \frac{(\alpha - \pi(u))^2}{u^\gamma} + \frac{(\beta - \pi(u))^2}{(1-u)^\gamma} \right\} du < \infty$ is similar to the one done in Sect. 6 in [2] and the fact that $\bar{\mu}_N$ is stationary measure.

Let $\mathbb{P}^*$ be a limit point of the sequence $\{\mathbb{P}^N\}_{N \geq 2}$ whose existence follows from the previous Lemma. Hereinafter, we assume without lost of generality that $\{\mathbb{P}^N\}_{N \geq 2}$ converges to $\mathbb{P}^*$.

Lemma 3 *Let $G : \mathbb{R} \to \mathbb{R}$ be a two times continuously differentiable function. Then we have*

$$\limsup_{N \to \infty} \sup_{x \in \Lambda_N} \left| N^2 \sum_{y \in \mathbb{Z}} (G(\tfrac{y+x}{N}) - G(\tfrac{x}{N}))p(y) - \frac{\sigma^2}{2} \Delta G(\tfrac{x}{N}) \right| = 0.$$

Proof The proof can be found in [2].

Lemma 4 *Let $\bar{\rho}^{\kappa}$ be the unique weak solution of (4). For any F, G in $C_c^{\infty}([0,1])$ we have*

$$\int_{[0,1]^2} \left\{ F(u)\left[-\tfrac{\sigma^2}{2}\Delta G(v) + \kappa G(v)V_1(v)\right] + G(v)\left[-\tfrac{\sigma^2}{2}\Delta F(u) + \kappa F(u)V_1(u)\right]\right\} I^{\kappa}(u,v)dudv = 0 \tag{11}$$

where

$$I^{\kappa}(u,v) = \mathbb{E}^*\left[(\pi(u) - \bar{\rho}^{\kappa}(u))\,(\pi(v) - \bar{\rho}^{\kappa}(v))\right]. \tag{12}$$

Proof We have that

$$\begin{aligned} N^2 L_N(\langle \pi^N, G\rangle) =& \frac{1}{1-N}\sum_{x\in\Lambda_N}\left[N^2\sum_{y\in\mathbb{Z}}\left(G(\tfrac{y+x}{N}) - G(\tfrac{x}{N})\right)p(y)\right]\eta_x \\ &+ \frac{\kappa N^{\gamma}}{N-1}\sum_{x\in\Lambda_N} G(\tfrac{x}{N})\left[r_N^-(\tfrac{x}{N})(\alpha-\eta_x) + r_N^+(\tfrac{x}{N})(\beta-\eta_x)\right]. \end{aligned} \tag{13}$$

Taking the expectation with respect to $\bar{\mu}_N$ on both sides of (13), by stationarity the left hand side vanishes. By using Lemma 3, (3) and weak convergence we have that

$$\mathbb{E}^*\left[\int_0^1 \left\{-\tfrac{\sigma^2}{2}\Delta G(u) + \kappa G(u)V_1(u)\right\}\pi(u)du\right] - \kappa\int_0^1 V_0(u)G(u)du = 0. \tag{14}$$

By a similar argument done in Lemma 4.6 in [3] we get

$$\begin{aligned} &\mathbb{E}^*\left[\int_{[0,1]^2}\left\{F(u)(-\tfrac{\sigma^2}{2}\Delta G(v) + \kappa V_1(v)G(v))\right\}\pi(u)\pi(v)dudv\right] \\ &+\mathbb{E}^*\left[\int_{[0,1]^2}\left\{G(v)(-\tfrac{\sigma^2}{2}\Delta F(u) + \kappa V_1(u)F(u))\right\}\pi(u)\pi(v)dudv\right] \\ &-\mathbb{E}^*\left[\kappa\int_{[0,1]^2}\{F(u)G(v)V_0(v)\,\pi(u) + F(u)G(v)V_0(u)\pi(v)\}\,dudv\right] = 0 \end{aligned} \tag{15}$$

Let $\bar{\rho}^{\kappa}$ be the unique weak solution of (4). Then we have

$$\int_0^1 \left\{-\tfrac{\sigma^2}{2}\Delta G(u) + \kappa V_1(u)G(u)\right\}\bar{\rho}^{\kappa}(u)du - \kappa\int_0^1 G(u)V_0(u)\,du = 0, \tag{16}$$

for all $G \in C_c^{\infty}((0,1))$. By using (14) we can get that

$$
\begin{aligned}
&- \mathbb{E}^* \left[\int_{[0,1]^2} \left\{ F(u)(-\tfrac{\sigma^2}{2} \Delta G(v) + \kappa V_1(v) G(v)) \right\} \pi(v) \bar{\rho}^\kappa(u) du dv \right] \\
&+ \kappa \int_{[0,1]^2} F(u) G(v) V_0(v)\, \bar{\rho}^\kappa(u) du dv = 0
\end{aligned} \tag{17}
$$

and

$$
\begin{aligned}
&- \mathbb{E}^* \left[\int_{[0,1]^2} \left\{ G(v)(-\tfrac{\sigma^2}{2} \Delta F(u) + \kappa V_1(u) F(u)) \right\} \pi(u) \bar{\rho}^\kappa(v) du dv \right] \\
&+ \kappa \int_{[0,1]^2} F(u) G(v) V_0(u)\, \bar{\rho}^\kappa(v) du dv = 0.
\end{aligned} \tag{18}
$$

Now, from (16) we can get the following equations

$$
\begin{aligned}
&- \mathbb{E}^* \left[\int_{[0,1]^2} \left\{ F(u)(-\tfrac{\sigma^2}{2} \Delta G(v) + \kappa V_1(v) G(v)) \right\} \pi(u) \bar{\rho}^\kappa(v) du dv \right] \\
&+ \mathbb{E}^* \left[\kappa \int_{[0,1]^2} F(u) G(v) V_0(v)\, \pi(u) du dv \right] = 0,
\end{aligned} \tag{19}
$$

$$
\begin{aligned}
&- \mathbb{E}^* \left[\int_{[0,1]^2} \left\{ G(v)(-\tfrac{\sigma^2}{2} \Delta F(u) + \kappa V_1(u) F(u)) \right\} \pi(v) \bar{\rho}^\kappa(u) du dv \right] \\
&+ \mathbb{E}^* \left[\kappa \int_{[0,1]^2} F(u) G(v) V_0(u)\, \pi(v) du dv \right] = 0,
\end{aligned} \tag{20}
$$

$$
\begin{aligned}
&\int_{[0,1]^2} \left\{ F(u)(-\tfrac{\sigma^2}{2} \Delta G(v) + \kappa V_1(v) G(v)) \right\} \bar{\rho}^\kappa(v) \bar{\rho}^\kappa(u) du dv \\
&- \kappa \int_{[0,1]^2} F(u) G(v) V_0(v)\, \bar{\rho}^\kappa(u) du dv = 0
\end{aligned} \tag{21}
$$

and

$$
\begin{aligned}
&\int_{[0,1]^2} \left\{ G(v)(-\tfrac{\sigma^2}{2} \Delta F(u) + \kappa V_1(u) F(u)) \right\} \bar{\rho}^\kappa(u) \bar{\rho}^\kappa(v) du dv \\
&- \kappa \int_{[0,1]^2} F(u) G(v) V_0(u)\, \bar{\rho}^\kappa(v) du dv = 0.
\end{aligned} \tag{22}
$$

Now using Eqs. (15), (17)–(22), then it follows (11).

Let us consider the following definition needed in the proof of Theorem 1.

Definition 3 We say that $\bar{I}^\kappa : [0,1]^2 \to [0,1]$ is a weak solution of

$$
\begin{cases}
-\frac{\sigma^2}{2} \Delta \bar{I}^\kappa(u,v) + \kappa \bar{I}^\kappa(u,v) \hat{V}(u,v) = 0, \quad (u,v) \in (0,1)^2, \\
\bar{I}^\kappa(u,v) = 0, \quad (u,v) \in \partial [0,1]^2
\end{cases} \tag{23}
$$

where $\hat{V}(u,v) = V_1(u) + V_1(v)$, if

(i) $\bar{I}^\kappa \in \mathcal{H}^1_{0,\hat{V}}([0,1]^2)$.

(ii) For any function $G \in C_c^\infty((0,1)^2)$ we have that

$$-\langle \bar{I}^\kappa, \tfrac{\sigma^2}{2}\Delta G\rangle + \kappa\langle \bar{I}^\kappa, G\rangle_{\hat{V}} = 0. \tag{24}$$

Lemma 5 *The unique weak solution of (23) is the constant function equal to zero.*

Proof The proof is omitted since is similar to the one of Proposition 1.

3.1 Proof of Theorem 1

Let $\bar{\rho}^\kappa(u)$ the unique weak solution of (4) and recall the definition of the function $I^\kappa : [0,1]^2 \to \mathbb{R}$ introduced in Lemma 4. We want to prove that I^κ is a weak solution of (23). First, we claim that $I^\kappa \in \mathcal{H}^1_{0,\hat{V}}([0,1]^2) = \mathcal{H}^1_0([0,1]^2) \cap L^2_{\hat{V}}([0,1]^2)$. Indeed, since $\bar{\rho}^\kappa, \pi \in \mathcal{H}^1([0,1])$ (see Definition 2 and Lemma 2) then we have $I^\kappa \in \mathcal{H}^1_0([0,1]^2)$. In order to show that $I^\kappa \in L^2_{\hat{V}}([0,1]^2)$, note that $\int_{[0,1]^2}(I^\kappa(u,v))^2\hat{V}(u,v)dudv$ is less that

$$\mathbb{E}^*\left[\int_{[0,1]^2} P^2(u,v)\hat{V}(u,v)dudv\right] \le 2\mathbb{E}^*\left[\int_{[0,1]^2} P^2(u,v)V_1(v)dudv\right], \tag{25}$$

where $P(u,v) = (\pi(u) - \bar{\rho}^\kappa(u))\,(\pi(v) - \bar{\rho}^\kappa(v))$ and in the last inequality we performed a change of variables. Note that the term on the right hand side of (25) is bounded from above by

$$4\mathbb{E}^*\left[\int_0^1 (\pi(u) - \bar{\rho}^\kappa(u))du \int_0^1 \left((\pi(v) - \bar{\rho}^\infty(v))^2 + (\bar{\rho}^\infty(v) - \bar{\rho}^\kappa(v))^2\right) V_1(v)dv\right]. \tag{26}$$

We know that π, $\bar{\rho}^\kappa$ satisfy items (i) and (ii) then by Remarks 2 and 3 we have that (26) is finite. Therefore we get that $I^\kappa \in L^2_{\hat{V}}([0,1]^2)$. Now, by Lemma 4 we have that the function I^κ is a weak solution of (23) (note that in Definition 3 the test function can be taken as the product of two test functions on $C_c^\infty((0,1))$). By Lemma 5 we have that $I^\kappa \equiv 0$. Whence we conclude that $I^\kappa(u,u) = 0$ for all $u \in (0,1)$ or equivalently $\mathbb{P}^*$ almost surely $\pi = \bar{\rho}^\kappa$. This conclude the proof of Theorem 1. □

An important step in the proof of Theorem 2 is to use stationarity of $\bar{\mu}_N$ which give an upper bound of the average current.

Lemma 6 *Fix $N \ge 2$. There exists a constant $C > 0$ such that $\langle W_1\rangle_N \le CN^{-1}$.*

Proof By stationarity of $\bar{\mu}_N$ we have that $\langle W_1 \rangle_N$ is equal to

$$\frac{1}{N-1}\sum_{x=1}^{N-1}\langle W_x\rangle_N = \frac{1}{N-1}\sum_{x=1}^{N-1}\langle W_x^0\rangle_N + \frac{\kappa N^{-\theta}}{N-1}\sum_{x=1}^{N-1}\langle W_x^{\ell,r}\rangle_N = (I)+(II).$$

Let us first consider (I). By using a similar argument as in Lemma 4.1 of [3] we have that $|I| \leq \frac{2}{N-1}\sum_{x=1}^{N-2} x^2 p(x) \leq \sigma^2 (N-1)^{-1}$. The last inequality is obtained using the fact that p has finite variance.

For (II) we first use Fubini's theorem which permits to rewrite For (II) as

$$\frac{\kappa}{N^{\theta+1}}\sum_{x=1}^{N-1} x r_N^-(\tfrac{x}{N})(\alpha - \langle \eta_x\rangle_N) + \frac{\kappa}{N^{\theta+1}}\sum_{x=1}^{N-1}(N-1-x) r_N^+(\tfrac{x}{N})(\langle \eta_x\rangle_N - \beta).$$

We will just analyse the first term on the right hand side of the latter expression, because analogous arguments can be done for the other one. Fix $a \in (0, \frac{1}{2})$. Note that the absolute value of the term at the right hand side in last expression is bounded from above by

$$\frac{\kappa}{N^{\theta+1}}\left(\sum_{x=1}^{[aN]-1} x r_N^-(\tfrac{x}{N})|\alpha - \langle \eta_x\rangle_N| + 2\sum_{x=[aN]}^{N-1} x r_N^-(\tfrac{x}{N})\right).$$

Using (3) there exists a constant $C > 0$ such that

$$\frac{2\kappa}{N^{\theta+1}}\sum_{x=[aN]}^{N-1} x r_N^-(\tfrac{x}{N}) \leq C N^{-1}. \tag{27}$$

Since the measure $\bar{\mu}_N$ is invariant, by writing $\langle L_N \eta_x\rangle_N = 0$, it is easy to see that

$$\langle \eta_x\rangle_N - \alpha = \frac{\sum_{y\in\Lambda_N} p(x,y)(\langle \eta_y\rangle_N - \alpha) + \frac{\kappa}{N^\theta}(\beta-\alpha) r_N^+\left(\frac{x}{N}\right)}{\sum_{y\in\Lambda_N} p(x,y) + \frac{\kappa}{N^\theta} r_N^+\left(\frac{x}{N}\right) + \frac{\kappa}{N^\theta} r_N^-\left(\frac{x}{N}\right)}. \tag{28}$$

By neglecting terms in the denominator and bounding from above $|\langle \eta_y\rangle_N - \alpha|$ by 2, then for any $x \in \{1, \cdots, [aN]-1\}$ we have that

$$|\langle \eta_x\rangle_N - \alpha| \leq \frac{N^\theta}{c_\gamma \kappa} + \gamma^{-1}(\beta-\alpha)\,(N-[aN])^{-\gamma}.$$

Then, using last bound and the fact that $\gamma > 2$, we have

$$\frac{\kappa}{N^{\theta+1}}\sum_{x=1}^{[aN]-1} xr_N^-(\tfrac{x}{N})|\alpha-\langle\eta_x\rangle_N| \le \left(\frac{c_\gamma\zeta_{\gamma-1}}{\gamma}+\frac{2^\gamma\kappa(\beta-\alpha)c_\gamma\zeta_{\gamma-1}}{\gamma^2}\right)N^{-1}.$$

It is clear by last bound that there exist a constant $C>0$ such that

$$\left|\frac{\kappa}{N^{\theta+1}}\sum_{x=1}^{N-1} xr_N^-(\tfrac{x}{N})(\alpha-\langle\eta_x\rangle_N)\right| \le CN^{-1},$$

and we are done.

3.2 *Proof of Theorem 2*

For any $\delta>0$ we define the function $G_\delta\in C_c^\infty((0,1))$ such that $0\le G_\delta(u)\le 1$ and $G_\delta(u)=1$ for $u\in[\delta,1-\delta]$. By stationarity of $\bar{\mu}_N$ and (1) we have that

$$\begin{aligned}N\langle W_{[vN]}\rangle_N=\sum_{x=1}^N\langle W_x\rangle_N&=\sum_{x=1}^N G_\delta(\tfrac{x}{N})\langle W_x\rangle_N+\sum_{x=1}^N(1-G_\delta(\tfrac{x}{N}))\langle W_x\rangle_N\\&=\sum_{x=1}^N G_\delta(\tfrac{x}{N})\Big(\langle W_x^0\rangle_N+\frac{\kappa}{N^\theta}\langle W_x^{\ell,r}\rangle_N\Big)+O(\delta),\end{aligned}$$

where in the last equality we used the definition of G_δ and the fact that $\langle W_1\rangle_N=O(N^{-1})$ (see Lemma 6 above). We first consider the term in last expression with $\frac{\kappa}{N^\theta}\langle W_x^{\ell,r}\rangle_N$. Since G_δ has compact support included in $(0,1)$ and the fact that $\theta=2-\gamma$, we use (3) and Riemann sum to get easily that

$$\begin{aligned}\lim_{N\to\infty}\frac{\kappa}{N^2}\sum_{x\in\Lambda_N}G_\delta(\tfrac{x}{N})\langle N^\gamma W_x^{\ell,r}\rangle_N=\kappa\int_0^1 G_\delta(v)\Bigg[\int_v^1(\alpha-\bar{\rho}^\kappa(u))r_N^-(u)du\\-\int_0^v(\beta-\bar{\rho}^\kappa(u))r_N^+(u)du\Bigg]dv.\end{aligned}$$

On the other hand, in the case $x-1\le N-x$ we can write W_x^0 as

$$\begin{aligned}&\sum_{y=1}^{x-1}\sum_{z=x}^{y+x-1}p(z-y)[\eta_y-\eta_z]+\sum_{y=1}^{x-1}\sum_{z=y+x}^{N-1}p(z-y)[\eta_y-\eta_z]\\&=\sum_{j=1}^{x-1}p(j)\sum_{k=1}^{j}[\eta_{x-j+k-1}-\eta_{x+k-1}]+\sum_{y=1}^{x-1}\sum_{z=y+x}^{N-1}p(z-y)[\eta_y-\eta_z].\end{aligned}$$

In the last expression we used Fubini's Theorem and change of variables. Similarly, in the case $N - x \leq x - 1$ we can write W_x^0 as

$$\sum_{z=x}^{N-1} \sum_{y=z+x-N}^{x-1} p(z-y)[\eta_y - \eta_z] + \sum_{z=x}^{N-1} \sum_{y=1}^{z+x-N-1} p(z-y)[\eta_y - \eta_z]$$
$$= \sum_{j=1}^{N-x} p(j) \sum_{k=1}^{j} [\eta_{x-j+k-1} - \eta_{x+k-1}] + \sum_{z=x}^{N-1} \sum_{y=1}^{z+x-N-1} p(z-y)[\eta_y - \eta_z].$$

Thus we can write $\langle W_x^0 \rangle_N$ as

$$\sum_{j=1}^{m_x} p(j) \sum_{k=1}^{j} [\langle \eta_{x-j+k-1} \rangle_N - \langle \eta_{x+k-1} \rangle_N] + \langle S(m_x) \rangle_N, \tag{29}$$

where $m_x = \min\{x-1, N-x\}$ and

$$S(m_x) = \begin{cases} \displaystyle\sum_{y=1}^{m_x} \sum_{z=y+x}^{N-1} p(z-y)[\eta_y - \eta_z], \ \textit{if } m_x = x-1, \\ \displaystyle\sum_{z=x}^{N-1} \sum_{y=1}^{z-m_x-1} p(z-y)[\eta_y - \eta_z], \ \textit{if } m_x = N-x. \end{cases}$$

By using Riemann's sum we get that $\left| \sum_{x \in \Lambda_N} G_\delta(\frac{x}{N}) \langle S(m_x) \rangle_N \right| \leq N^{2-\gamma}$. Now we can write the sum $\sum_{x \in \Lambda_N} G_\delta(\frac{x}{N}) \left(\langle W_x^0 \rangle_N - \langle S(m_x) \rangle_N \right)$ as

$$\sum_{j=1}^{a_N} j p(j) \sum_{k=1}^{j} \frac{1}{N} \sum_{x=j+1}^{N-j} G_\delta(\tfrac{x}{N}) \frac{\left[\langle \eta_{x-j+k-1} \rangle_N - \langle \eta_{x+k-1} \rangle_N \right] N}{j} \tag{30}$$

where $a_N = \left[\frac{N-1}{2} \right]$. Recall that $\frac{\sigma^2}{2} = \sum_{j=1}^{\infty} j^2 p(j)$. Thus, taking $N \to \infty$ and using Riemann's sum, we get that (30) is equal to $\frac{\sigma^2}{2} \int_0^1 G_\delta(v) \partial_v \bar{\rho}^\kappa(v) dv$. Since the expression at the right hand side of (8) does not depend on v we have that

$$\frac{\sigma^2}{2} \partial_v \bar{\rho}^\kappa(v) + \kappa \int_v^1 (\alpha - \bar{\rho}^\kappa(u)) r_N^-(u) du - \kappa \int_0^v (\beta - \bar{\rho}^\kappa(u)) r_N^+(u) du \int_0^1 G_\delta(v) dv,$$

Thus we can deduce the Fick's Law claimed in Theorem 2 taking $\delta \to 0$.

4 Proof of Theorem 3

In this section we present some properties of the weak solution of (4) given in Theorem 3 which will give us an idea of its behavior. We first notice that (4) implies that $(\bar{\rho}^\kappa)''$ and $\bar{\rho}^\kappa - \bar{\rho}^\infty$ share the same sign. It will be very useful in the proof of Theorem 3 and for that reason, many properties of $\bar{\rho}^\kappa$ will be related to the ones satisfied by $\bar{\rho}^\infty$. We now set up those properties in the following lemma.

Lemma 7 *Setting* $\bar{\rho}^\infty(u) = \alpha\frac{(1-u)^\gamma}{u^\gamma+(1-u)^\gamma} + \beta\frac{u^\gamma}{u^\gamma+(1-u)^\gamma}$, $\bar{\rho}^\infty$ *has the following property*

(i) $\bar{\rho}^\infty(u)$ *is a solution of* (4) *when* $\sigma = 0$.
(ii) $\bar{\rho}^\infty(u) + \bar{\rho}^\infty(1-u) = \alpha + \beta$.
(iii) $(\bar{\rho}^\infty)'(u) = \gamma(\beta-\alpha)\frac{(1-u)^{\gamma-1}u^{\gamma-1}}{(u^\gamma+(1-u)^\gamma)^2}$, *in particular* $\bar{\rho}^\infty$ *is increasing.*
(iv) $\bar{\rho}^\infty$ *is convex on* $[0, 1/2]$ *and concave on* $[1/2, 1]$.

Proof The computations which lead to prove (i)–(iii) are clear, since we have an explicit expression for $\bar{\rho}^\infty$. From (iii), we get that $\frac{(\bar{\rho}^\infty)''(u)}{\beta-\alpha}$ is equal to

$$\gamma(\gamma-1)\frac{u^{\gamma-2}(1-u)^{\gamma-2}}{(u^\gamma+(1-u)^\gamma)^2}(1-2u) + 2\gamma^2\frac{u^{\gamma-1}(1-u)^{\gamma-1}}{(u^\gamma+(1-u)^\gamma)^3}((1-u)^{\gamma-1} - u^{\gamma-1}),$$

for all $u \in (0, 1)$. Then we check that last two terms are both positive for $u \in (0, 1/2)$ and both negative for $u \in (1/2, 1)$.

In items (iii) and (iv) of Lemma 7, we recognize the properties that we will prove for $\bar{\rho}^\kappa$. We now start the proof of the properties listed in Theorem 3. The methods used in the proof of item (iii) are quite different from the ones used for the first two items. Thus, we have decided to split the proof in two parts in order to make it easier to read.

Proof of item (i) **and** (ii) **of Theorem** 3.

We split the proof in four steps.
First step: *Position of* $\bar{\rho}^\kappa$ *with respect to* $\bar{\rho}^\infty$.

We first prove the inequalities in item (ii) of Theorem 3 between $\bar{\rho}^\kappa$ and $\bar{\rho}^\infty$ by contradiction. According to Lemmas 1 and 7, $\bar{\rho}^\kappa(\frac{1}{2}) = \bar{\rho}^\infty(\frac{1}{2}) = \frac{\alpha+\beta}{2}$ and thanks to the boundary condition $\bar{\rho}^\kappa(0) = \bar{\rho}^\infty(1) = \alpha$, then on both sides $(\bar{\rho}^\kappa - \bar{\rho}^\infty)(0) = (\bar{\rho}^\infty - \bar{\rho}^\infty)(\frac{1}{2}) = 0$. We now take $\hat{u}$, a minimizer of $(\bar{\rho}^\kappa - \bar{\rho}^\infty)$ on $[0, \frac{1}{2}]$. If $\hat{u}$ belongs to $(0, \frac{1}{2})$, then

$$(\bar{\rho}^\kappa - \bar{\rho}^\infty)''(\hat{u}) \geq 0 \quad \text{while} \quad (\bar{\rho}^\kappa - \bar{\rho}^\infty)(\hat{u}) \leq 0. \tag{31}$$

Thanks to (4), $(\bar{\rho}^\kappa)''(\hat{u}) \leq 0$ and according to Lemma 7, $(\bar{\rho}^\infty)''(\hat{u}) > 0$, then $(\bar{\rho}^\kappa - \bar{\rho}^\infty)''(\hat{u}) < 0$ which contradicts (31). On $(0, \frac{1}{2})$, it allows us to deduce $(\bar{\rho}^\kappa - \bar{\rho}^\infty) >$

$\min\{(\bar{\rho}^\kappa - \bar{\rho}^\infty)(0); (\bar{\rho}^\kappa - \bar{\rho}^\infty)(\frac{1}{2})\} = 0$. The opposite inequality on $(\frac{1}{2}, 1)$ can easily be deduced from Lemma 1 and item (ii) of Lemma 7. Finally we have

$$\bar{\rho}^\kappa(u) > \bar{\rho}^\infty(u) \,\forall u \in (0, \tfrac{1}{2}), \;\; \bar{\rho}^\kappa(u) < \bar{\rho}^\infty(u) \,\forall u \in (\tfrac{1}{2}, 1). \tag{32}$$

Second step: Position of $\bar{\rho}^\kappa$ related to $\bar{\rho}^\iota$.

The proof is very similar to the previous one, we just point out the difference. As previously we take $\hat{u}$ a minimizer of $(\bar{\rho}^\kappa - \bar{\rho}^\iota)$ on $[0, \frac{1}{2}]$. If $\hat{u}$ belongs to $(0, \frac{1}{2})$, then $(\bar{\rho}^\kappa - \bar{\rho}^\iota)(\hat{u}) \leq 0$ while $(\bar{\rho}^\kappa - \bar{\rho}^\iota)''(\hat{u}) \geq 0$. We have by (4)

$$(\bar{\rho}^\iota)''(\hat{u}) = \frac{2\iota}{\sigma^2} V_1(\hat{u})(\bar{\rho}^\iota(\hat{u}) - \bar{\rho}^\infty(\hat{u})) \leq \frac{2\iota}{\sigma^2} V_1(\hat{u})(\bar{\rho}^\kappa(\hat{u}) - \bar{\rho}^\infty(\hat{u})) < (\bar{\rho}^\kappa)''(\hat{u}).$$

(note that we need to know that $\bar{\rho}^\kappa(u) - \bar{\rho}^\infty(u) < 0$). As previously, we get $(\bar{\rho}^\kappa - \bar{\rho}^\iota)''(\hat{u}) < 0$ which is a contradiction. We deduce $(\bar{\rho}^\kappa - \bar{\rho}^\iota) > 0$ on $(0, \frac{1}{2})$. Using Lemma 1 again, we finally get

$$\bar{\rho}^\kappa(u) > \bar{\rho}^\iota(u) \,\forall u \in (0, \tfrac{1}{2}), \;\; \bar{\rho}^\kappa(u) < \bar{\rho}^\iota(u) \,\forall u \in (\tfrac{1}{2}, 1). \tag{33}$$

Third step: *Proof of* (ii).

On $[0, \frac{1}{2}]$ we have proved that $\bar{\rho}^\kappa$ is strictly convex. Recall that $\bar{\rho}^0$ is a linear function given by

$$\bar{\rho}^0(u) = (\beta - \alpha)u + \alpha. \tag{34}$$

Since $\bar{\rho}^\kappa(0) = \bar{\rho}^0(0)$ and $\bar{\rho}^\kappa(\frac{1}{2}) = \bar{\rho}^0(\frac{1}{2})$, we deduce by convexity that $\bar{\rho}^0 > \bar{\rho}^\kappa$ on $(0, \frac{1}{2})$. Using Lemma 1 again, we get

$$\bar{\rho}^0(u) > \bar{\rho}^\kappa(u) \,\forall u \in (0, \tfrac{1}{2}), \;\; \bar{\rho}^0(u) < \bar{\rho}^\kappa(u) \,\forall u \in (\tfrac{1}{2}, 1). \tag{35}$$

Putting (32), (33) and (35) together, we have proved item (ii) of Theorem 3.

Fourth step: *Proof of* (i).

According to (32) and (4), it is clear that $(\bar{\rho}^\kappa)'$ increases on $[0, \frac{1}{2}]$ and decreases on $[\frac{1}{2}, 1]$. The convexity and the concavity of $\bar{\rho}^\kappa$ on these sets is established. Since $(\bar{\rho}^\kappa)'' \leq 0$ on $[\frac{1}{2}, 1)$, $(\bar{\rho}^\kappa)'(u)$ goes to a limit $\ell \in \mathbb{R} \cup \{-\infty\}$ when u goes to 1. By (32), for all u in $[\frac{1}{2}, 1]$, we also have $\bar{\rho}^\kappa(u) \leq \bar{\rho}^\infty(u) \leq \beta = \bar{\rho}^\kappa(1)$, then ℓ cannot be negative. Using Lemma 1 to deduce what happens in 0, we have

$$\lim_{u \to 0} (\bar{\rho}^\kappa)'(u) = \lim_{u \to 1} (\bar{\rho}^\kappa)'(u) = \ell \in \mathbb{R}_+. \tag{36}$$

From the variations of $(\bar{\rho}^\kappa)'$, we deduce that $(\bar{\rho}^\kappa)'(u) \geq \ell \geq 0$ on $[0, 1]$.

According to Lemmas 1 and 7 and the expression (34), it is clear that we have $\bar{\rho}^{\infty}\left(\frac{1}{2}\right) = \bar{\rho}^{\kappa}\left(\frac{1}{2}\right) = \bar{\rho}^{0}\left(\frac{1}{2}\right) = \frac{\alpha+\beta}{2}$. For all u in $[\frac{1}{2}, 1]$ we have established $\bar{\rho}^{0} \leq \bar{\rho}^{\kappa} \leq \bar{\rho}^{\infty}$, by item (iii) in Lemma 7 and (34), we deduce that

$$(\beta - \alpha) = (\bar{\rho}^{0})'\left(\tfrac{1}{2}\right) \leq (\bar{\rho}^{\kappa})'\left(\tfrac{1}{2}\right) \leq (\bar{\rho}^{\infty})'\left(\tfrac{1}{2}\right) = \gamma(\beta - \alpha).$$

It ends the proof of item (i) of Theorem 3. □

We end by investigating the behavior of $\bar{\rho}^{\kappa}$ at the boundary.

Proof of item (iii) **of Theorem** 3. According to (36), it is clear that $\bar{\rho}^{\kappa} \in C^1([0, 1])$ with $(\bar{\rho}^{\kappa})'(0) = (\bar{\rho}^{\kappa})'(1) = \ell$. Using the first order Taylor approximation of $\bar{\rho}^{\kappa}$ around 0, we get from (4) that

$$\begin{aligned}(\bar{\rho}^{\kappa})''(u) &\underset{u\to 0}{=} \frac{2c_\gamma \kappa}{\gamma\sigma^2}\left(\frac{\ell u + o(u)}{u^\gamma} + \frac{\alpha - \beta + \ell u + o(u)}{(1-u)^\gamma}\right) \\ &\underset{u\to 0}{=} \frac{2c_\gamma \kappa \ell u^{1-\gamma}}{\gamma\sigma^2} + o\left(u^{1-\gamma}\right).\end{aligned}$$

Since $\gamma > 2$, we deduce that $(\bar{\rho}^{\kappa})''$ is integrable in 0 if and only if $\ell = 0$. If not, we have $\lim_{u\to 0}(\bar{\rho}^{\kappa})'(u) = +\infty$ which is wrong by (36). We have proved

$$\lim_{u\to 0}(\bar{\rho}^{\kappa})'(u) = \lim_{u\to 1}(\bar{\rho}^{\kappa})'(u) = 0. \tag{37}$$

According to Lemma 1, we just have to investigate the behaviour of $\bar{\rho}^{\kappa}$ arround 1. One can check that $\bar{\rho}^{\kappa} - \beta$ is still a solution of (4) for the boundary conditions $(\alpha - \beta, 0)$, therefore we will just consider the case where $\alpha < \beta = 0$. We point out that in this situation $\bar{\rho}^{\kappa}$ and $\bar{\rho}^{\infty}$ are non positive because of item (i) of Theorem 3. From those restrictions we get $\bar{\rho}^{\infty}(u) \underset{u\to 1}{\sim} \alpha(1-u)^\gamma$ and $V_1(u) \underset{u\to 1}{\sim} \frac{\alpha c_\gamma \gamma^{-1}}{\bar{\rho}^{\infty}(u)}$. According to (4), it leads us to

$$(\bar{\rho}^{\kappa})''(u) \underset{u\to 1}{\sim} \frac{2\alpha c_\gamma \kappa}{\gamma\sigma^2}\left(\frac{\bar{\rho}^{\kappa}(u) - \rho_\infty(u)}{\rho_\infty(u)}\right). \tag{38}$$

Then, the description we seek can be rephrase as $\bar{\rho}^{\kappa}(u) \underset{u\to 1}{=} \bar{\rho}^{\infty}(u) + o(\bar{\rho}^{\infty}(u))$ and it is equivalent to $\lim_{u\to 1}(\bar{\rho}^{\kappa})''(u) = 0$. Since we do not have any clear information about $(\bar{\rho}^{\kappa})'''$, the proof is more complex, we briefly explain our strategy. In a first step, using (37), we prove that we can find u_1 as close as desired to 1 such that $\frac{\bar{\rho}^{\kappa}(u_1)}{\bar{\rho}^{\infty}(u_1)} \leq (1+\varepsilon)$. In a second step, we set up some useful inequality satisfied in a neighborhood of 1 and take u_1 in that neighborhood. In a third step, we establish a bound on the size of any interval of $[u_1, 1)$ where $\frac{\bar{\rho}^{\kappa}}{\bar{\rho}^{\infty}} > (1+\varepsilon)$. In the last step, we prove that this bound is tight enough to establish $1 \leq \frac{\bar{\rho}^{\kappa}(u)}{\bar{\rho}^{\infty}(u)} \leq (1+\varepsilon)^4$ on $[u_1, 1)$.

First step: *Proof of* $\liminf_{u\to 1} \frac{\bar{\rho}^{\kappa}(u)}{\bar{\rho}^{\infty}(u)} = 1$.

We first suppose that $\liminf_{u\to 0}(\bar{\rho}^{\kappa})''(u) \neq 0$. According to item (i) of Theorem 3, $(\bar{\rho}^{\kappa})''$ is positive on $(0, \frac{1}{2})$. Then, we can find $M > 0$ such that $(\bar{\rho}^{\kappa})''(u) \geq M$ in a

neighborhood of 0. In other words for $n = 0$, there exists $\varepsilon, M > 0$ such that for all $u \in (0, \varepsilon)$ we have

$$(\bar{\rho}^{\kappa})''(u) \geq \frac{M}{u^{n(\gamma-2)}}. \tag{39}$$

Thanks to (37), $(\bar{\rho}^{\kappa})'(0) = 0$. If (39) is satisfied for $0 \leq n < \frac{1}{\gamma-2}$, we integrate it two times, since $\bar{\rho}^{\kappa}(0) = \alpha$ we get for any $u \in (0, \varepsilon)$ that

$$\bar{\rho}^{\kappa}(u) \geq \alpha + Cu^{2-n(\gamma-2)}$$

where $C := M\,[(1 - n(\gamma - 2))(2 - n(\gamma - 2))]^{-1}$. Using (4), we have that for all $u \in (0, \varepsilon)$,

$$(\bar{\rho}^{\kappa})''(u) \geq \frac{2c_{\gamma}\kappa}{\gamma\sigma^2}\left(\frac{Cu^{2-n(\gamma-2)}}{u^{\gamma}} + \frac{\alpha + Cu^{2-n(\gamma-2)} - \beta}{(1-u)^{\gamma}}\right) \underset{u\to 0}{\sim} \frac{2c_{\gamma}\kappa C}{\gamma\sigma^2}\frac{1}{u^{(n+1)(\gamma-2)}}.$$

Then, changing M for $\frac{c_{\gamma}\kappa C}{\gamma\sigma^2}$ and taking potentially ε a bit smaller, it is clear that (39) is also satisfied for $n + 1$. Finally, we take $m < \frac{1}{\gamma-2} \leq m + 1$ such that (39) is satisfied for $n = m + 1$ by induction. Since $(m + 1)(\gamma - 2) \geq 1$ we deduce that $(\bar{\rho}^{\kappa})''$ is not integrable in $[0, \varepsilon]$ and this contradicts (37). We have proved that $\liminf_{u\to 0}(\bar{\rho}^{\kappa})''(u) = 0$ and using Lemma 1 we deduce that $\limsup_{u\to 1}(\bar{\rho}^{\kappa})''(u) = 0$. According to (38), since $\alpha < 0$, we get $\liminf_{u\to 1}\frac{\bar{\rho}^{\kappa}(u)}{\bar{\rho}^{\infty}(u)} = 1$.

Second step: *Required inequality satisfied in a neighborhood of* 1.

According to Lemma 7, we have

$$\bar{\rho}^{\infty}(u) \underset{u\to 1}{\sim} \alpha(1-u)^{\gamma}, \quad (\bar{\rho}^{\infty})'(u) \underset{u\to 1}{\sim} -\gamma\alpha(1-u)^{\gamma-1}. \tag{40}$$

We now fix $\varepsilon > 0$ and we set $A = \frac{2\gamma^2(1+\varepsilon)\sigma^2}{\kappa c_{\gamma}\varepsilon}$. From (40) and (38), we can find $\lambda > 0$ such that for all $u \in (\lambda, 1)$, we have the following inequalities

$$\text{(i) } (\bar{\rho}^{\kappa})''(u) \leq \left(\frac{\alpha c_{\gamma}\kappa}{\gamma\sigma^2}\right)\frac{\bar{\rho}^{\kappa}(u)-\bar{\rho}^{\infty}(u)}{\bar{\rho}^{\infty}(u)} \leq 0 \qquad \text{(ii) } (\bar{\rho}^{\infty})'(u) \leq -2\gamma\alpha(1-u)^{\gamma-1}$$
$$\text{(iii) } \frac{\bar{\rho}^{\infty}(u)}{(1+\varepsilon)} \geq \alpha(1-u)^{\gamma} \geq (1+\varepsilon)\bar{\rho}^{\infty}(u) \text{ (iv) } \left(\frac{1}{1-A(1-u)^{\gamma-2}}\right)^{\gamma} \leq (1+\varepsilon). \tag{41}$$

Since $\liminf_{u\to 1}\frac{\bar{\rho}^{\kappa}(u)}{\bar{\rho}^{\infty}(u)} = 1$, we can find $u_1 \in (\lambda, 1)$ such that $\frac{\bar{\rho}^{\kappa}(u_1)}{\bar{\rho}^{\infty}(u_1)} \leq (1 + \varepsilon)$.

Third step: *bound on the length of any interval of* $[u_1, 1)$ *where* $\frac{\bar{\rho}^{\kappa}}{\bar{\rho}^{\infty}} > (1 + \varepsilon)$.

We now suppose that we can find $\hat{u} \in (u_1, 1)$ such that $\bar{\rho}^{\kappa}(\hat{u}) < (1 + \varepsilon)\bar{\rho}^{\infty}(\hat{u}) \leq 0$. We set

$$\underline{u} = \min\left\{v \in (u_1, \hat{u}) \,|\, \forall u \in (v, \hat{u}]\, \frac{\bar{\rho}^\kappa(u)}{\bar{\rho}^\infty(u)} > (1+\varepsilon)\right\}. \tag{42}$$

By continuity, it is clear that $\bar{\rho}^\kappa(\underline{u}) = (1+\varepsilon)\bar{\rho}^\infty(\underline{u})$. Thus we have for all $h \in [0, \hat{u} - \underline{u}]$, that

$$\frac{\bar{\rho}^\kappa(\underline{u}+h) - \bar{\rho}^\kappa(\underline{u})}{h} \leq \frac{(1+\varepsilon)(\bar{\rho}^\infty(\underline{u}+h) - \bar{\rho}^\infty(\underline{u}))}{h}$$

taking $h \to 0$ we get

$$(\bar{\rho}^\kappa)'(\underline{u}) \leq (1+\varepsilon)(\bar{\rho}^\infty)'(\underline{u}).$$

By definition of $\underline{u}$ and by (41)-(i), for all $v \in [\underline{u}, \hat{u}]$ we have

$$(\bar{\rho}^\kappa)''(v) \leq \frac{\alpha c_\gamma \kappa}{\gamma\sigma^2}\left(\frac{\bar{\rho}^\kappa(v) - \bar{\rho}^\infty(v)}{\bar{\rho}^\infty(v)}\right) \leq \frac{\varepsilon\alpha c_\gamma \kappa}{\gamma\sigma^2} \leq 0. \tag{43}$$

We now integrate (43) on $[\underline{u}, \hat{u}]$ and apply (41)-(ii) to get

$$\begin{aligned}(\bar{\rho}^\kappa)'(\hat{u}) &= (\bar{\rho}^\kappa)'(\underline{u}) + \int_{\underline{u}}^{\hat{u}} (\bar{\rho}^\kappa)''(s)ds \leq (1+\varepsilon)(\bar{\rho}^\infty)'(\underline{u}) + \frac{\varepsilon\alpha c_\gamma\kappa}{\gamma\sigma^2}(\hat{u} - \underline{u}) \\ &\leq -2(1+\varepsilon)\gamma\alpha(1-\underline{u})^{\gamma-1} + \frac{\varepsilon\alpha c_\gamma\kappa}{\gamma\sigma^2}(\hat{u} - \underline{u}).\end{aligned}$$

Since $(\bar{\rho}^\kappa)'$ is positive, we get

$$\hat{u} - \underline{u} \leq \underbrace{\frac{2\gamma^2(1+\varepsilon)\sigma^2}{\kappa c_\gamma \varepsilon}}_{=A}(1-\underline{u})^{\gamma-1}. \tag{44}$$

Fourth step: *proof of* $\frac{\bar{\rho}^\kappa}{\bar{\rho}^\infty} \leq (1+\varepsilon)^4$ *on* $[u_1, 1)$ *and conclusion.*

Take $\hat{u} \in [u_1, 1)$, if $\frac{\bar{\rho}^\kappa(\hat{u})}{\bar{\rho}^\infty(\hat{u})} \leq (1+\varepsilon)$, then it is obviously smaller than $(1+\varepsilon)^4$.
If not, taking $\underline{u}$ defined by (42), since $\bar{\rho}^\kappa$ increases and $\bar{\rho}^\infty$ is negative, applying (41)-(iii), we first get

$$\begin{aligned}\frac{\bar{\rho}^\kappa(\hat{u})}{\bar{\rho}^\infty(\hat{u})} &\leq \frac{\bar{\rho}^\kappa(\underline{u})}{\bar{\rho}^\infty(\hat{u})} \leq \frac{\bar{\rho}^\kappa(\underline{u})}{\bar{\rho}^\infty(\underline{u})}\frac{\bar{\rho}^\infty(\underline{u})}{\bar{\rho}^\infty(\hat{u})} \leq (1+\varepsilon)^3\frac{\alpha(1-\underline{u})^\gamma}{\alpha(1-\hat{u})^\gamma} \\ &\leq (1+\varepsilon)^3\left(\frac{1}{1-(\hat{u}-\underline{u})/(1-\underline{u})}\right)^\gamma.\end{aligned}$$

Thanks to (44), $\frac{\hat{u}-\underline{u}}{1-\underline{u}} \leq A(1-\underline{u})^{\gamma-2}$. Since the mapping $x \mapsto \left(\frac{1}{1-x}\right)^\gamma$ increases on $(-\infty, 1)$, (41)-(iv) allows us to deduce

$$\frac{\bar{\rho}^{\kappa}(\hat{u})}{\bar{\rho}^{\infty}(\hat{u})} \leq (1+\varepsilon)^3 \left(\frac{1}{1 - A(1-\underline{u})^{\gamma-2}} \right)^{\gamma} \leq (1+\varepsilon)^4.$$

According to Theorem 3-(ii), we also have $\frac{\bar{\rho}^{\kappa}}{\bar{\rho}^{\infty}} \geq 1$ on $(\frac{1}{2}, 1)$. Finally we have proved $\lim_{u\to 1} \frac{\bar{\rho}^{\kappa}(u)}{\bar{\rho}^{\infty}(u)} = 1$. Using (38) and (40), we get

$$\lim_{u\to 1} (\bar{\rho}^{\kappa})''(u) = 0 \text{ and } \bar{\rho}^{\kappa}(u) \underset{u\to 1}{=} \alpha(1-u)^{\gamma} + o((1-u)^{\gamma}).$$

If $\beta \neq 0$, considering $\bar{\rho}^{\kappa} - \beta$, we get $\bar{\rho}^{\kappa}(u) \underset{u\to 1}{=} \beta + (\alpha - \beta)(1-u)^{\gamma} + o((1-u)^{\gamma})$. We deduce the similar property when u goes to 0 by Lemma 1. □

Corollary 1 *The solution $\bar{\rho}^{\kappa}$ is unique in $C([0,1])$ and the mapping $\kappa \mapsto \bar{\rho}^{\kappa}$ is continuous from $[0, +\infty]$ to $C([0,1])$.*

Proof ***Step 1***: *uniqueness*. Previously, we have proved in Proposition 1 that there was a unique solution $\bar{\rho}^{\kappa}$ of (4) such that

$$\bar{\rho}^{\kappa} - \bar{\rho}^{\infty} \in \mathcal{H}^1_{0,V_1}([0,1]).$$

It is well known that $\mathcal{H}^1_0([0,1]) \hookrightarrow C^{1/2}([0,1])$ (see [6]), since we also have $\bar{\rho}^{\infty} \in C^2([0,1])$, it is clear that $\bar{\rho}^{\kappa} \in C([0,1])$.

From now until the end of this first step, we just consider $\bar{\rho}^{\kappa}$ as a weak solution of (4) such that $\bar{\rho}^{\kappa} \in C([0,1])$. From (4), the weak second derivative $\Delta\bar{\rho}^{\kappa}$ is continuous on $(0,1)$. Therefore, it is enough to deduce that $\Delta\bar{\rho}^{\kappa}$ is actually a classical second derivative, the argument is standard, we briefly explain how we proceed. We fix $\varepsilon > 0$. For $\tau < \varepsilon$ we define $\bar{\rho}^{\kappa,\tau} = \bar{\rho}^{\kappa} * (\frac{1}{\tau}\theta(\frac{\cdot}{\tau}))$ where θ is an even non negative smooth function supported in $(-1,1)$ such that $\int \theta(u)du = 1$. The function $\bar{\rho}^{\kappa,\tau}$ is smooth and well defined on $[2\varepsilon, 1-2\varepsilon]$ and its second derivative is $(\Delta\bar{\rho}^{\kappa}) * (\frac{1}{\tau}\theta(\frac{\cdot}{\tau}))$. For all x in $[2\varepsilon, 1-2\varepsilon]$ we have

$$(\bar{\rho}^{\kappa} - \bar{\rho}^{\kappa,\tau})(x) = \int_{-1}^{1} (\bar{\rho}^{\kappa}(x) - \bar{\rho}^{\kappa}(x - \tau y))\theta(y)dy$$

and it allows us to deduce

$$\|\bar{\rho}^{\kappa} - \bar{\rho}^{\kappa,\tau}\|_{L^{\infty}([2\varepsilon,1-2\varepsilon])} \leq \sup_{|h|\leq\tau} \|\bar{\rho}^{\kappa} - \bar{\rho}^{\kappa}(\cdot + h)\|_{L^{\infty}([2\varepsilon,1-2\varepsilon])} \xrightarrow[\tau\to 0]{} 0$$

by uniform continuity of $\bar{\rho}^{\kappa}$ on $[\varepsilon, 1-\varepsilon]$. Using the same argument for $(\bar{\rho}_{\kappa,\tau})''$, we deduce that $\bar{\rho}^{\kappa,\tau}$ and $(\bar{\rho}^{\kappa,\tau})''$ converge, respectively, to $\bar{\rho}^{\kappa}$ and $\Delta\bar{\rho}^{\kappa}$ in $L^{\infty}([2\varepsilon, 1-2\varepsilon])$ as τ goes to 0. Since $C^2([2\varepsilon, 1-2\varepsilon])$ is a Banach space for that convergence, we conclude that $\bar{\rho}^{\kappa} \in C^2([2\varepsilon, 1-2\varepsilon])$ and its weak and classical second derivative are both $\Delta\bar{\rho}^{\kappa}$ given by (4).

Letting ε go to 0 we get that $\bar{\rho}^{\kappa} \in C^2((0,1))$. Thanks to (4), by induction we get immediately

$$\bar{\rho}^{\kappa} \in C([0,1]) \cap C^{\infty}((0,1)). \tag{45}$$

One can check that in the proof of Theorem 3 we have only used (45). It is easy to check that the regularity and behavior of $\bar{\rho}^{\kappa}$ near the boundary given in (iii) of Theorem 3 are enough to ensure $\bar{\rho}^{\kappa} - \bar{\rho}^{\infty} \in \mathcal{H}^1_{0,V_1}([0,1])$. By Proposition 1 we deduce that the solutions are unique in $C([0,1])$.

Step 2: *continuity*. Take $\{\kappa_n\}_{n\in\mathbb{N}}$ monotonic such that $\kappa_n \xrightarrow[n\to\infty]{} \kappa \in [0,+\infty]$. According to item (ii) of Theorem 3, for all u in $[0,1]$, the mapping $\iota \mapsto \bar{\rho}^{\iota}(u)$ is monotonic and bounded, then $\{\bar{\rho}^{\kappa_n}(u)\}_{n\in\mathbb{N}}$ is also monotonic and bounded for all u, thus it converges. We set $\hat{\rho}(u) := \lim_{n\to\infty} \bar{\rho}^{\kappa_n}(u) \quad \forall u \in [0,1]$. According to item (i) of Theorem 3, for all $n \in \mathbb{N}$ we have

$$||(\bar{\rho}^{\kappa_n})'||_{L^\infty([0,1])} = (\bar{\rho}^{\kappa_n})'(\tfrac{1}{2}) \leq \gamma(\beta - \alpha).$$

By the Arzela-Ascoli Theorem, we can find a subsequence $\{n(k)\}_{k\in\mathbb{N}}$ such that $||\bar{\rho}_{\kappa_{n(k)}} - \hat{\rho}||_{L^\infty([0,1])}$ goes to 0. For all u, since $\{\bar{\rho}^{\kappa_n}(u)\}_{n\in\mathbb{N}}$ is monotonic and convergent, if $m > n$ we have $|\bar{\rho}_{\kappa_m}(u) - \hat{\rho}(u)| \leq |\bar{\rho}_{\kappa_n}(u) - \hat{\rho}(u)|$. Taking the supremum on all $u \in [0,1]$, we deduce that $\left\{||\bar{\rho}^{\kappa_n} - \hat{\rho}||_{L^\infty([0,1])}\right\}_{n\in\mathbb{N}}$ decreases. We get

$$\lim_{n\to\infty} ||\bar{\rho}^{\kappa_n} - \hat{\rho}||_{L^\infty([0,1])} = 0. \tag{46}$$

In order to conclude, we just have to identify $\hat{\rho}$. When $\kappa = +\infty$, we come back to item (i) of Theorem 3. It allows us to deduce that for all n, we have the uniform estimate $||(\bar{\rho}^{\kappa_n})''||_{L^1([0,1])} = 2(\bar{\rho}^{\kappa_n})'(\frac{1}{2}) \leq 2\gamma(\beta - \alpha)$. Dividing (4) by $\kappa_n V_1$, we get that $||\bar{\rho}^{\kappa_n} - \bar{\rho}^{\infty}||_{L^1(0,1)}$ is bounded from above by

$$\frac{\sigma^2}{2\kappa_n} \left|\left|\frac{1}{V_1}\right|\right|_{L^\infty(0,1)} ||(\bar{\rho}^{\kappa_n})''||_{L^1(0,1)} \leq \frac{\sigma^2}{2\kappa_n} 2^{\gamma+1}\gamma(\beta - \alpha) \xrightarrow[n\to\infty]{} 0.$$

By uniqueness of the limit in the distribution space, we deduce from (46) that $\hat{\rho} = \bar{\rho}^{\infty}$.

When κ belongs to $[0,+\infty)$, we end proving that $\hat{\rho}$ is the unique solution of (4). Take $\varepsilon > 0$ and $K_\varepsilon = [\varepsilon, 1-\varepsilon]$. Combining the uniform convergence of $(\bar{\rho}^{\kappa_n})_n$ given by (46) and (4), it is clear that $(\bar{\rho}^{\kappa_n})''$ converges to $\frac{2\kappa}{\sigma^2} V_1(\hat{\rho} - \bar{\rho}^{\infty})$ in $L^\infty(K_\varepsilon)$. Since $C^2(K_\varepsilon)$ is a Banach space for the norm $f \mapsto ||f||_{L^\infty(K_\varepsilon)} + ||f''||_{L^\infty(K_\varepsilon)}$, we deduce that $\hat{\rho} \in C^2(K_\varepsilon)$ and its second derivative is $\hat{\rho}''(u) = \frac{2\kappa}{\sigma^2} V_1(u)(\hat{\rho}(u) - \bar{\rho}^{\infty}(u))$. Letting ε go to 0 and getting the boundary conditions from (46), we deduce that $\hat{\rho}$ is the unique solution of (4) for the limit parameter κ.

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Hydrodynamic Analysis of Sound Wave Propagation in a Reactive Mixture Confined Between Two Parallel Plates

Denize Kalempa, Adriano W. Silva and Ana Jacinta Soares

Abstract The aim of this work is to study the problem of sound wave propagation through a binary mixture undergoing a reversible chemical reaction of type $A + A \rightleftharpoons B + B$, when the mixture is confined between two flat, infinite and parallel plates. One plate is stationary, whereas the other oscillates harmonically in time and constitutes an emanating source of sound waves that propagate in the mixture. The boundary conditions imposed in our problem correspond to assume that the plates are impenetrable and that the mixture chemically react at the surface plates, reaching the chemical equilibrium instantaneously. The reactive mixture is described by the Navier-Stokes equations derived from the Boltzmann equation in a chemical regime for which the chemical reaction is in its final stage. Explicit expressions for transport coefficients and chemically production rates are supplemented by the kinetic theory. Starting from this setting, we study the dynamics of the sound waves in the reactive mixture in the low frequency regime and investigate the influence of the chemical reaction on the properties of interest in the considered problem. We then compute the amplitude and phase profiles of the relevant macroscopic quantities, showing how they vary in the reactive flow between the plates in dependence on several factors, as the chemical activation energy, concentration of products and reactants, as well as oscillation speed parameter.

Keywords Sound propagation · Chemically reactive mixtures · Kinetic theory Navier-Stokes equations

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1 Introduction

The mathematical modelling of sound wave propagation in a rarefied medium and the correct description of the properties of interest in terms of both the rarefaction degree of the medium and the sound frequency of the wave is a topic of great relevance in several fields. This subject appears in many applied situations of modern engineering, associated with porous nanomaterials, vibrating micro-devices, near-vacuum systems, acoustic measurements, propagation of noise and many other problems.

These facts have motivated many scientific contributions, both theoretical and numerical [1–11]. In particular, theoretical works and numerical simulations can provide some guidance in experimental studies and design of many devices, and can help to predict the acoustic behaviour in many systems.

From the mathematical point of view, the modelling of sound wave propagation is based on the Navier-Stokes equations when a regime of continuum flow and low oscillation frequencies is considered. However, when the systems approach the micro scale or when high oscillation frequencies are taken into account, other regimes should be considered for which the Navier-Stokes equations become not valid and the Boltzmann equation is used to capture the rarefaction effects or to treat the boundary Knudsen layer [5, 11].

Various problems have been studied in several regimes of propagation, considering a one-component gas or a mixture of inert gases, either occupying a semi-infinite space [11–13] or confined between two parallel plates [1, 5, 9, 10]. In particular, Ref. [5] addresses the problem of sound propagation in a monoatomic gas confined between source and receptor of sound waves over a wide range of gas rarefaction and sound frequency regimes. The results presented in Ref. [5] show many interesting features concerning, in particular, how the sound waves reflected from the receptor influence the solution of the problem when the distance between both plates is varying.

On the other hand, some problems associated to sound wave propagation have also been investigated in the context of chemically reactive mixtures [3, 6, 14–18]. The results indicate that the sound propagation can be considerably influenced by the chemical reaction.

However, the presence of the chemical reaction introduces additional complexities and, in general, one considers some simplifications in order to solve the sound wave problem. For instance, in Refs. [3, 14, 15] the problem is formulated in an unbounded domain, so that no boundary conditions are involved, assuming that the mixture fields are the sum of an equilibrium value plus an harmonic wave of small amplitude. In Refs. [14, 15, 17, 18], an Eulerian mixture is considered and the transport effects are absent, so that only the effects of chemical reactions on sound propagation are considered. In Ref. [6], a binary mixture confined between two parallel plates is considered and the gaseous particles can react chemically at one wall only, with infinitely fast chemical reaction so that the gaseous particles reach the equilibrium instantaneously and the flow between the boundaries is non-reactive.

The problems described in the latter reference have motivated the study developed in the present paper, and we give here a further contribution for the sound wave propagation problem within a chemically reactive mixture.

We consider a binary mixture confined between source and receptor, in the presence of a chemical reaction of type $A + A \rightleftharpoons B + B$, which is typical of isomers [19]. Our approach is based on the Navier-Stokes equations with temperature jump and velocity impenetrable conditions at both source and receptor of sound waves. A chemical regime for which the chemical reaction is in its final stage is assumed.

Since there are no papers regarding the temperature jump in reactive gas mixtures, the temperature jump coefficient for a single gas is used here. This choice is motivated by two facts. First, both constituents have the same molecular mass, as a consequence of the mass conservation during the chemical reaction, so that they are identical in mechanical sense. Second, the chemical reaction is in its final stage, so that chemical transformations become less frequent and the deviations from the chemical equilibrium are small. Therefore, in the context of the present problem, this simplification does not seem to be so restrictive. In fact, it is well known that for a mixture with a small ratio of molecular masses, the temperature jump coefficient does not differ significantly from that for a single gas, see paper [12]. However, it is our future research plan to determine the temperature jump coefficient for a more general reactive gas mixture, resorting to an appropriate model in kinetic theory for the description of the reactive mixture.

Starting from this setting, we study the sound wave propagation in the reactive mixture in the low frequency regime and investigate both the influence of the chemical reaction and the effects of the reflected waves from the receptor on the relevant macroscopic quantities. We perform some numerical computations to investigate how the amplitudes and phases vary in dependence of several parameters, as the chemical activation energy, concentration of products and reactants (exothermic or endothermic dominant reaction), distance between source and receptor and oscillation speed parameter.

2 Description of the Mixture

We consider a binary mixture of monoatomic gases whose constituents, denoted by A and B, undergo a reversible chemical reaction of symmetric type represented by

$$A + A \rightleftharpoons B + B. \tag{1}$$

Both constituents have the same molecular mass m and the same molecular diameter d. The molar fraction of each species in the mixture is defined as

$$x_A = \frac{n_A}{n_A + n_B}, \qquad x_B = 1 - x_A, \tag{2}$$

where n_α (α = A, B) denotes the number density of species α in the mixture, with $n = n_A + n_B$ the total number density of the mixture.

The constituents have different binding energies ε_A and ε_B, so that we introduce the heat of the chemical reaction defined as the binding energy difference between reactants and products of the forward reaction,

$$E = 2(\varepsilon_A - \varepsilon_B). \tag{3}$$

Observe that the forward reaction in (1) is exothermic when $E > 0$, whereas it is endothermic when $E < 0$.

The hydrodynamic model describing the considered mixture is that of the reactive Navier-Stokes equations [3, 19] formed by the balance equations for the number densities n_A of the reactants and n_B of the products, together with the conservation equations for the momentum and total energy of the whole mixture. The transport coefficients involved in the description of the mixture are the shear viscosity μ, diffusion D, thermal diffusion ratio κ_T and thermal conductivity λ.

The interaction among the constituents due to the chemical reaction (1) is specified by the chemical production rate $\mathscr{T}$, which plays an important role in the model. In the present analysis, the reaction rate is explicitly obtained from the kinetic theory of reactive mixtures, as it will be explained in Sect. 4. The concentration of each constituent in the reactive mixture is measured by the corresponding number density n_α ($\alpha = A, B$).

For sake of brevity, we omit here the full system of reactive Navier-Stokes equations, since they will be introduced in its one-dimensional form in Sect. 4.

3 Statement of the Problem

We assume that the mixture is quiescent in equilibrium conditions, confined between two flat, infinite and parallel plates, located at $x' = 0$ and $x' = L'$, where x' is the first space coordinate of a 3-dimensional orthogonal reference frame $Ox'y'z'$.

Both plates are kept at the same uniform temperature, which is the equilibrium temperature T_0 of the mixture. The plate located at $x' = L'$ is at rest, whereas the one located at $x' = 0$ oscillates harmonically in time, in the x'-direction, i.e. in the direction orthogonal to its own plane, with angular frequency ω and velocity

$$U_p(t) = \Re\left(U e^{-i\omega t}\right), \tag{4}$$

where $\Re$ denotes the real part of a complex number, i is the imaginary unit and $U \in \mathbb{R}$ represents the constant amplitude of the oscillating velocity. We assume that U is very small when compared to the characteristic molecular speed v_m of the mixture, that is

$$U \ll v_m, \qquad v_m = \sqrt{\frac{2k_B T_0}{m}}, \tag{5}$$

where k_B is the Boltzmann constant, T_0 is the equilibrium temperature of the mixture and m is the molecular mass of the species.

Perturbations. According to this description, the oscillating plate ($x' = 0$) constitutes an emanating source of sound waves that propagate in the x'-direction and slightly deviate the properties of the reactive mixture from the equilibrium state. On the other hand, the stationary plate ($x' = L'$) behaves as a receptor of sound waves and can significantly change the flow due to the influence of the reflected waves from the plate. The sound waves generated by the oscillating plate disturb the number densities n_α and mean velocities v_α of the constituents ($\alpha = A, B$), as well as the mass density ρ, temperature T, pressure p and heat flux q of the mixture. We assume that all mixture properties depend harmonically on time and introduce the following expansions of the state variables around an equilibrium state,

$$\begin{aligned} n_\alpha(t, x') &= n_{\alpha 0} + \Re[\overline{n}_\alpha(x')\, e^{-i\omega t}], \\ v_\alpha(t, x') &= \Re[\overline{v}_\alpha(x')\, e^{-i\omega t}], \\ \rho(t, x') &= \rho_0 + \Re[\overline{\rho}(x')\, e^{-i\omega t}], \\ v(t, x') &= \Re[\overline{v}(x')\, e^{-i\omega t}], \\ T(t, x') &= T_0 + \Re[\overline{T}(x')\, e^{-i\omega t}]. \end{aligned} \tag{6}$$

Here, the quantities $n_{\alpha 0}$, ρ_0, T_0 are constant and refer to the thermodynamical equilibrium state of the reactive mixture, so that the number densities n_{A0}, n_{B0} of the constituents and the temperature T_0 of the mixture are constrained to the mass action law of the model, see [19], that is

$$\exp\left(-\frac{E}{k_B T_0}\right) = \left(\frac{n_{A0}}{n_{B0}}\right)^2, \tag{7}$$

where E is the reaction heat defined in (3). Furthermore, the quantities $\overline{n}_\alpha(x')$, $\overline{v}_\alpha(x')$, $\overline{\rho}(x')$, $\overline{v}(x')$, $\overline{T}(x')$ appearing in expansions (6) represent the complex spatial perturbations of the corresponding state variables.

Under these conditions, a linearized theory based on the reactive Navier-Stokes equations is appropriate to describe the dynamics and the chemical kinetics of the perturbed variables (6), in particular to describe the spatial evolution of the perturbation amplitudes.

Relevant parameters. The relevant parameters in this description are the rarefaction parameter, δ, which is inversely proportional to the well known Knudsen number [20], and the oscillation parameter, θ, defined by

$$\delta = \frac{L' p_0}{\eta v_m}, \qquad \theta = \omega\tau, \tag{8}$$

where L' is the distance between the plates, already introduced, v_m is given in (5), p_0 is the equilibrium pressure of the mixture, η the shear viscosity of the mixture and τ represents the effective mean free time between successive molecular collisions.

Note that the oscillation parameter θ is defined as in [3] and corresponds to the ratio of the oscillation frequency to the collision frequency.

For convenience, the dimensionless x-coordinate is introduced as

$$x = \frac{x'\omega}{v_m}, \tag{9}$$

and, as a consequence, the dimensionless distance between the plates is written as $L = \delta\theta$. Since our mathematical setting corresponds to the hydrodynamic regime, large values for δ and small values for θ are considered, i.e. $\delta \gg 1$ and $\theta \ll 1$.

Boundary conditions. The interaction of the reactive mixture with the surface plates is described by the boundary conditions to be imposed to our differential equations. We assume that both plates are impenetrable, so that the mixture accommodates its bulk velocity to the velocity of the plates. In fact, at the stationary plate ($x = L$), the mixture instantaneously relax to a resting state and its bulk velocity vanishes at this boundary. At the oscillatory plate ($x = 0$), the mixture instantaneously accommodates its bulk velocity to the velocity of the plate, as a consequence of the oscillatory movement of the plate itself. Therefore, from (4) and (6), the boundary conditions for the spatial part of the mixture bulk velocity are given as

$$\overline{v}(x)|_{x=0} = U, \qquad \overline{v}(x)|_{x=L} = 0. \tag{10}$$

Concerning the temperature, jump conditions at source and receptor are employed, so that from (6) we have

$$\overline{T}|_{x=0} = T_0 + \zeta_T \theta \left.\frac{\partial \overline{T}}{\partial x}\right|_{x=0}, \qquad \overline{T}|_{x=L} = T_0 - \zeta_T \theta \left.\frac{\partial \overline{T}}{\partial x}\right|_{x=L}, \tag{11}$$

where ζ_T is the temperature jump coefficient, see papers [8, 12, 21–23].

As explained and motivated in the Introduction, we will use, in this work, the temperature jump coefficient for a single gas, namely $\zeta_T = 1.954$, see [5, 12], as an approximation of the corresponding coefficient in the considered binary reactive mixture.

4 Hydrodynamic Equations for the Reactive Mixture

Starting from a kinetic description in terms of a Boltzmann equation for the considered binary reactive mixture, the macroscopic field equations of the reactive flow can be derived in the hydrodynamic limit at Navier-Stokes level. This derivation has been addressed in paper [24] for the reactive mixture considered in our work.

Basic fields and macroscopic equations. The basic fields of the mixture are the particle number densities n_A of the reactants and n_B of products, the velocity v and temperature T of the mixture. For the problem under consideration, the balance equations for these fields can be written in the following form (see paper [3])

$$\frac{\partial n_\alpha}{\partial t} + \frac{\partial}{\partial x'}(n_\alpha v_\alpha) = \lambda_\alpha \mathscr{T}, \quad \alpha = A, B, \tag{12}$$

$$\rho \frac{\partial v}{\partial t} + \rho v \frac{\partial v}{\partial x'} + \frac{\partial P_{xx}}{\partial x'} = 0, \tag{13}$$

$$\frac{3}{2}\frac{p}{T}\left(\frac{\partial T}{\partial t} + v\frac{\partial T}{\partial x'}\right) + \frac{\partial q}{\partial x'} - \frac{E}{2}\frac{\partial}{\partial x'}\Big[n_A(v_A - v)\Big] + P_{xx}\frac{\partial v}{\partial x'} = \frac{E}{2}\mathscr{T}, \tag{14}$$

where $\mathscr{T}$ represents the reaction production term due to the chemical reaction, λ_α is the stoichiometric coefficient of each constituent, with $\lambda_A = -\lambda_B = -1$. Moreover, the symbol E stands for the chemical reaction heat introduced in (3). Finally, plain symbols refer to the whole mixture and have the usual meaning in kinetic theory and fluid mechanics [19], in particular $p = nk_BT$ is the mixture pressure, q the heat flux and P_{xx} the first component of the pressure tensor.

The constitutive relations for the field equations (12–14) have been derived in paper [24] in the form

$$\textit{Fick law} \qquad v_A - v = -\frac{D}{n_A}\left(\frac{n_B}{n}\frac{\partial n_A}{\partial x'} - \frac{n_A}{n}\frac{\partial n_B}{\partial x'} + \frac{n}{T}\kappa_T\frac{\partial T}{\partial x'}\right) \tag{15}$$

$$\textit{Newton law} \qquad P_{xx} = p - \frac{4}{3}\eta\frac{\partial v}{\partial x'} \tag{16}$$

$$\textit{Fourier law} \qquad q = -\lambda\frac{\partial T}{\partial x'} + \left(\frac{E}{2} + \frac{n}{n_A n_B}p\,\kappa_T\right)n_A(v_A - v) \tag{17}$$

$$\textit{Reaction rate law} \qquad \mathscr{T} = \ell\,\frac{\mathscr{A}}{k_BT} \tag{18}$$

where D, η and λ are the coefficients of diffusion, shear viscosity and thermal conductivity, respectively, κ_T is the thermal diffusion ratio, ℓ the coefficient of the forward reaction rate and $\mathscr{A}$ the chemical affinity of the forward reaction given by

$$\mathscr{A} = E + 2k_BT\ln\left(\frac{n_A}{n_B}\right). \tag{19}$$

Equations (12–14) with their constitutive conditions (15–18) represent the closed set of Navier-Stokes equations for the binary reactive mixture considered here. Such equations have been derived in paper [24] from a kinetic theory dynamics and therefore explicit expressions have been obtained in the quoted paper for the transport coefficients D, η, λ, κ_T and reaction rate coefficient ℓ.

5 Analysis of Sound Propagation in the Reactive Mixture

The linearized equations for the problem in question are obtained by inserting the representation (6) into both the balance equations (12)–(14) and the constitutive relations (15)–(18), keeping only linear terms of the field deviations. The resulting set of equations describes the spatial evolution of the complex perturbation of the state variables, and is written as follows.

$$-i\omega\overline{n}_A + x_A n_0 \frac{d\overline{v}}{dx'} - Dx_B \frac{d^2\overline{n}_A}{dx'^2} + Dx_A \frac{d^2\overline{n}_B}{dx'^2} - D\frac{n_0}{T_0}\kappa_T \frac{d^2\overline{T}}{dx'^2} = -\frac{2\ell_0}{n_0}\left(\frac{\overline{n}_A}{x_A} - \frac{\overline{n}_B}{x_B}\right), \tag{20}$$

$$-i\omega\overline{n}_B + x_B n_0 \frac{d\overline{v}}{dx'} - Dx_A \frac{d^2\overline{n}_B}{dx'^2} + Dx_B \frac{d^2\overline{n}_A}{dx'^2} + D\frac{n_0}{T_0}\kappa_T \frac{d^2\overline{T}}{dx'^2} = \frac{2\ell_0}{n_0}\left(\frac{\overline{n}_A}{x_A} - \frac{\overline{n}_B}{x_B}\right), \tag{21}$$

$$-i\omega m n_0 \overline{v} + k_B T_0 \frac{d\overline{n}}{dx'} + k_B n_0 \frac{d\overline{T}}{dx'} - \frac{4}{3}\eta \frac{d^2\overline{v}}{dx'^2} = 0, \tag{22}$$

$$-\frac{3}{2}i\omega k_B n_0 \overline{T} - \lambda \frac{d^2\overline{T}}{dx'^2} - \frac{k_B T_0}{x_A}\kappa_T D \frac{d^2\overline{n}_A}{dx'^2} + \frac{k_B T_0}{x_B}\kappa_T D \frac{d^2\overline{n}_B}{dx'^2} + n_0 k_B T_0 \frac{d\overline{v}}{dx'} - \frac{n_0 k_B}{x_A x_B} D\kappa_T^2 \frac{d^2\overline{T}}{dx'^2} = \frac{E\ell_0}{n_0}\left(\frac{\overline{n}_A}{x_A} - \frac{\overline{n}_B}{x_B}\right), \tag{23}$$

where ℓ_0 is the dimensionless coefficient of the forward reaction rate, given by

$$\ell_0 = -4x_A n_0^2 d^2 s^2 \sqrt{\frac{\pi k_B T_0}{m}} \exp\left(-\frac{\varepsilon_f}{k_B T_0}\right), \tag{24}$$

with s being the steric factor and ε_f the activation energy of the forward chemical reaction. Moreover, we use here the notation x_α for the equilibrium molar fraction of species α in the mixture, $x_\alpha = n_{\alpha 0}/n_0$ ($\alpha = A, B$), and x_A, x_B are related to the reaction heat through the mass action law (7). Accordingly, the forward chemical reaction reaction is exothermic if $x_A < 0.5$, whereas it is endothermic if $x_A > 0.5$.

After some algebraic manipulation, the system of equations (20–23) is reduced to two differential equations for the bulk velocity of species A and B as

$$A_1 \frac{d^4\overline{v}_A}{dx'^4} + B_1 \frac{d^2\overline{v}_A}{dx'^2} + C_1 \overline{v}_A = 0, \qquad A_2 \frac{d^4\overline{v}_B}{dx'^4} + B_2 \frac{d^2\overline{v}_B}{dx'^2} + C_2 \overline{v}_B = 0 \tag{25}$$

where A_i, B_i, C_i, for $i = 1, 2$, are known coefficients depending on the transport coefficients and equilibrium quantities as follows

$$
\begin{aligned}
A_1 &= -\lambda\left(\frac{iT_0}{\omega}+\frac{4\eta}{3k_Bn_0}\right),\\
B_1 &= \frac{5}{2}k_Bn_0T_0-2i\eta\omega-\frac{\rho_0}{k_Bn_0}i\lambda\omega+\frac{k_Bn_0T_0}{x_A}\kappa_T+\frac{E\ell_0}{x_Ax_BT_0}\left(\frac{iT_0}{\omega}+\frac{4\eta}{3k_Bn_0}\right)\kappa_T,\\
C_1 &= \frac{3}{2}\rho_0\omega^2+\frac{E\ell_0}{x_AD}+\frac{E\ell_0}{x_Ax_BT_0}\frac{\rho_0}{k_Bn_0}\,i\omega\kappa_T,
\end{aligned}
\tag{26}
$$

and

$$
\begin{aligned}
A_2 &= A_1,\\
B_2 &= \frac{5}{2}k_Bn_0T_0-2i\eta\omega-\frac{\rho_0}{k_Bn_0}i\lambda\omega-\frac{k_Bn_0T_0}{x_B}\kappa_T+\frac{E\ell_0}{x_Ax_BT_0}\left(\frac{iT_0}{\omega}+\frac{4\eta}{3k_Bn_0}\right)\kappa_T,\\
C_2 &= \frac{3}{2}\rho_0\omega^2-\frac{E\ell_0}{x_BD}+\frac{E\ell_0}{x_Ax_BT_0}\frac{\rho_0}{k_Bn_0}\,i\omega\kappa_T.
\end{aligned}
\tag{27}
$$

For convenience, the equations given by (25) are written in a dimensionless form by referring them to the dimensionless x-coordinate (9) and by introducing the following dimensionless macroscopic fields

$$
n^* = \frac{\overline{n}}{n_0}\frac{v_m}{U}, \qquad n_\alpha^* = \frac{\overline{n}_\alpha}{n_0}\frac{v_m}{U}, \qquad v^* = \frac{\overline{v}}{U}, \tag{28}
$$

$$
v_\alpha^* = \frac{\overline{v}_\alpha}{U}, \qquad T^* = \frac{\overline{T}}{T_0}\frac{v_m}{U}, \qquad P_{xx}^* = \frac{\overline{P}_{xx}}{P_0}\frac{v_m}{U}. \tag{29}
$$

Such fields measure the deviation of the macroscopic fields introduced in (6) with respect to corresponding equilibrium values. Furthermore, the dimensionless transport coefficients are introduced as

$$
\eta^* = \frac{\eta}{\eta_I}, \quad \lambda^* = \frac{\lambda}{\lambda_I}, \quad D^* = \frac{D}{D_I}, \tag{30}
$$

where η_I, λ_I, D_I are the first-order approximation to the coefficients of shear viscosity, thermal conductivity and diffusion of an inert gas of hard-spheres with diameter d, given by (see, again, paper [24])

$$
\eta_I = \frac{5}{16}\frac{1}{d^2}\sqrt{\frac{mk_BT_0}{\pi}}, \quad \lambda_I = \frac{75}{64}\frac{k_B}{d^2}\sqrt{\frac{k_BT_0}{\pi m}}, \quad D_I = \frac{177}{464}\frac{1}{n_0d^2}\sqrt{\frac{k_BT_0}{\pi m}}. \tag{31}
$$

Table 1 shows the values of the transport coefficients in the reactive mixture, for different values of the dimensionless activation energy $\varepsilon^* = \varepsilon_f/k_BT_0$ and molar fraction x_A specifying the exothermic ($x_A < 0.5$) or endothermic ($x_A > 0.5$) character of the forward reaction. Observe that high values of the activation energy mean that the energy barrier that the particles must overcome in order to react chemically is to high, so that only few particles react chemically. In particular, the case $\varepsilon^* = 20$

Table 1 Dimensionless transport coefficients for different values of the forward activation energy ε^* and reactants molar fraction x_A. The data is obtained with the results derived in paper [24]

ε^*	x_A	D^*	η^*	λ^*	κ_T
2	0.1	0.9843	0.9800	0.9674	0.0077
	0.3	0.9462	0.9039	0.8904	0.0225
	0.7	0.7301	0.7814	0.7308	−0.1088
	0.9	0.5136	0.7309	0.4559	−0.2671
5	0.1	0.9994	0.9979	0.9973	0.0004
	0.3	0.9979	0.9872	0.9863	0.0012
	0.7	0.9865	0.9573	0.9529	−0.0065
	0.9	0.9318	0.9845	0.9027	−0.0305
10	0.1	0.9999	0.9999	0.9999	0
	0.3	0.9999	0.9998	0.9998	0
	0.7	0.9999	0.9991	0.9990	0
	0.9	0.9997	0.9987	0.9984	−0.0002
20	0.1	0.9999	0.9999	0.9999	0
	0.3	0.9999	0.9999	0.9999	0
	0.7	0.9999	0.9999	0.9999	0
	0.9	0.9999	0.9999	0.9999	0

represents a limiting situation of this type in which the effects of the chemical reaction becomes almost negligible and the values of the dimensionless transport coefficients D^*, η^*, λ^* approach the unity and κ_T vanishes, as shown in Table 1.

We also specify the effective mean free time τ between successive molecular collisions and introduce both the exponential factor Δ of the Arrhenius law and the dimensionless reaction heat $\mathscr{E}$, given by

$$\tau = \frac{4}{5}\frac{\eta_I}{k_B n_0 T_0}, \qquad \Delta = x_A^2 s^2 \exp\left(-\frac{\varepsilon_f}{k_B T_0}\right), \qquad \mathscr{E} = \frac{E}{k_B T_0}. \tag{32}$$

Therefore, the dimensionless equations read

$$A_1' \frac{d^4 v_A^*}{dx^4} + B_1' \frac{d^2 v_A^*}{dx^2} + C_1' v_A^* = 0, \qquad A_2' \frac{d^4 v_B^*}{dx^4} + B_2' \frac{d^2 v_B^*}{dx^2} + C_2' v_B^* = 0 \tag{33}$$

where

$$
\begin{aligned}
A_1' &= -\frac{25}{32} i\theta\lambda^* - \frac{125}{96}\theta^2\lambda^*\eta^*, \\
B_1' &= \frac{5}{6} - \frac{5}{6} i\theta\eta^* - \frac{25}{16} i\theta\lambda^* + \frac{1}{3x_A}\kappa_T - \frac{\mathscr{E}^*\Delta}{3x_A x_B}\left(\frac{i}{\theta} + \frac{5}{3}\eta^*\right), \\
C_1' &= 1 - \frac{232}{531}\frac{\mathscr{E}\Delta}{x_A\theta^2 D^*} - \frac{2}{3} i \frac{\mathscr{E}\Delta}{x_A x_B \theta}\kappa_T,
\end{aligned}
\tag{34}
$$

and

$$
\begin{aligned}
A_2' &= A_1', \\
B_2' &= \frac{5}{6} - \frac{5}{6} i\theta\eta^* - \frac{25}{16} i\theta\lambda^* - \frac{1}{3x_B}\kappa_T - \frac{\mathscr{E}^*\Delta}{3x_A x_B}\left(\frac{i}{\theta} + \frac{5}{3}\eta^*\right), \\
C_2' &= 1 + \frac{232}{531}\frac{\mathscr{E}\Delta}{x_B\theta^2 D^*} - \frac{2}{3} i \frac{\mathscr{E}\Delta}{x_A x_B \theta}\kappa_T.
\end{aligned}
\tag{35}
$$

The analytic solutions of the equations given by (33) are

$$
\begin{aligned}
v_A^*(x) &= a_1 \mathrm{e}^{ik_{1A}x} + b_1 \mathrm{e}^{-ik_{1A}x} + c_1 \mathrm{e}^{ik_{2A}x} + d_1 \mathrm{e}^{-ik_{2A}x}, \\
v_B^*(x) &= a_2 \mathrm{e}^{ik_{1B}x} + b_2 \mathrm{e}^{-ik_{1B}x} + c_2 \mathrm{e}^{ik_{2B}x} + d_2 \mathrm{e}^{-ik_{2B}x},
\end{aligned}
\tag{36}
$$

where the complex wave numbers k_{1A}, k_{2A}, k_{1B} and k_{2B} read

$$
k_{1A} = \sqrt{\frac{B_1' - \sqrt{B_1'^2 - 4A_1'C_1'}}{2A_1'}}, \qquad k_{2A} = \sqrt{\frac{B_1' + \sqrt{B_1'^2 - 4A_1'C_1'}}{2A_1'}}, \tag{37}
$$

$$
k_{1B} = \sqrt{\frac{B_2' - \sqrt{B_2'^2 - 4A_2'C_2'}}{2A_2'}}, \qquad k_{2B} = \sqrt{\frac{B_2' + \sqrt{B_2'^2 - 4A_2'C_2'}}{2A_2'}}. \tag{38}
$$

The constants a_j, b_j, c_j and d_j $(j = 1, 2)$ are determined via the set of algebraic equations obtained from the boundary conditions (10) and (11). Note that, since v_A^* and v_B^* are known from (36), (37 and 38), all the other moments (28–29) of the mixture can be obtained from the set of linearized balance equations (20–23). In particular, the temperatures T_A^* and T_B^*, whose expressions are used in the boundary condition (11), are written as follows

$$
T_A^* = t_{11}\frac{dv_A^*}{dx} + t_{12}\frac{d^3v_A^*}{dx^3}, \qquad T_B^* = t_{21}\frac{dv_B^*}{dx} + t_{22}\frac{d^3v_B^*}{dx^3}, \tag{39}
$$

where

$$t_{11} = -\frac{2}{3}\frac{i\mathscr{E}\Delta}{x_A x_B \theta \xi}\left(1 - \frac{2i\Delta}{x_B\theta}\right) + \frac{2}{3}\frac{\mathscr{E}\Delta}{x_B\theta} - \frac{25}{8}\lambda^*\theta - \frac{59}{58}\frac{D^*\kappa_T^2\theta}{x_A x_B} - \frac{2}{3}i\,,$$

$$t_{12} = \frac{59}{116}\frac{iD^*\kappa_T\theta}{x_A x_B}\left(\frac{1}{\xi} - \frac{2i\Delta}{x_B\theta\xi} + ix_A + i\kappa_T + \frac{5}{3}\kappa_T\eta^*\theta\right) - \frac{25}{16}\lambda^*\theta\left(1 - \frac{5}{3}i\eta^*\theta\right),$$

$$t_{21} = -\frac{4}{3}\frac{i\mathscr{E}\Delta^2}{x_A x_B^2\theta^2\xi} + \frac{2}{3}\frac{\mathscr{E}\Delta}{x_B\theta} - \frac{25}{8}\lambda^*\theta - \frac{59}{58}\frac{D^*\kappa_T^2\theta}{x_A x_B} - \frac{2}{3}i\,,$$

$$t_{22} = \frac{59}{116}\frac{iD^*\kappa_T\theta}{x_A x_B}\left(\frac{1}{\xi} - \frac{2i\Delta}{x_B\theta\xi} + ix_A + i\kappa_T + \frac{5}{3}\kappa_T\eta^*\theta\right) - \frac{25}{16}\lambda^*\theta\left(1 - \frac{5}{3}i\eta^*\theta\right).$$

Here, we have introduced the notation $\xi = i + \dfrac{2\Delta}{x_A x_B \theta}$.

6 Results and Discussion

Usually, in acoustics, the quantity measured in experiments is the pressure difference in the direction of sound propagation, P^*_{xx} in our notation. The attenuation coefficient and phase speed are then determined by using the experimental data measured at the receptor. In the context of a chemically reactive mixture, the temperature deviation from equilibrium, T^* in our notation, is another important indicator of the effects induced by the chemical reaction.

Therefore, we use the solution obtained in the previous section to determine the amplitudes and phases of the macroscopic fields and focus our attention on the pressure difference P^*_{xx} and temperature deviation T^*.

Since such quantities are complex, they can be represented in the form

$$P^*_{xx}(x) = A_P(x)\exp\left[i\varphi_P(x)\right], \qquad T^*(x) = A_T(x)\exp\left[i\varphi_T(x)\right], \tag{40}$$

where $A_P(x)$, $A_T(x)$ are the amplitudes and $\varphi_P(x)$, $\varphi_T(x)$ are the corresponding phases. These amplitudes and phases give a measure of the deviation of the macroscopic properties of the gas mixture from the corresponding values in equilibrium. They were calculated as functions of the rarefaction δ and oscillation θ parameters, the molar fraction x_A of the reactants and activation energy ϵ_f of the chemical reaction.

Figures 1 and 2 show the profiles of the amplitude and phase of the pressure difference P^*_{xx} when $x_A = 0.3$ (exothermic reaction), $\delta = 10$ and $\theta = 0.1, \theta = 0.01$. Figures 3 and 4 show the profiles of the amplitude and phase of the temperature deviation T^* when $x_A = 0.3$ (exothermic reaction), $\delta = 10$ and $\theta = 0.1, \theta = 0.01$.

Figures 5, 6, 7 and 8 show the same quantities P^*_{xx} and T^* for the endothermic reaction corresponding to $x_A = 0.7$.

Note that, since $L = \delta\theta$ is the distance between the source and receptor, the situations considered in the figures correspond to a variation in the distance between the plates. Therefore, to analyse how the distance between the plates influence the

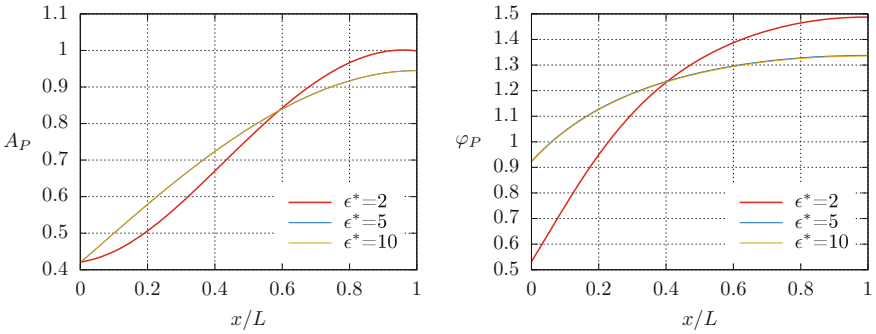

Fig. 1 Amplitude (left) and phase (right) of the pressure difference P^*_{xx} when the exothermic reaction dominates ($x_A = 0.3$), for $\delta = 10$ and $\theta = 0.1$

amplitude and phase of P^*_{xx} and T^*, we can compare the plots given in Figs. 1 and 2, 3 and 4, 5 and 6, 7 and 8, respectively. As one can see from the figures, the closer the receptor, the larger the influence of the reflected waves from the receptor on the properties of the gas flow, as expected, since the sound waves are less attenuated when the distance between the plates is smaller. This feature is observed for both exothermic (Figs. 1, 2, 3 and 4) and endothermic (Figs. 5, 6, 7 and 8) reactions.

Moreover, in the limit of high activation energy, $\epsilon^* = 10$, the mixture tends to a non-reactive configuration, so that the effects of the chemical reaction on the macroscopic properties of the mixture can be inferred by comparing the profiles for $\epsilon^* = 2$, $\epsilon^* = 5$ with those for $\epsilon^* = 10$. We can see that only in the situation $\epsilon^* = 2$, the profiles of the plotted quantities are significantly different from those corresponding to a non-reactive gas. These results should be analysed together with the values of the transport coefficients presented in Table 1. Accordingly, we can see that, regarding the influence of the chemical reaction on the solution of the problem, such influence is rather significant when also the transport coefficients show a larger deviation from the corresponding values in the inert mixture, that is, when the dimensionless values shown in Table 1 are not so close to the unity.

Another aspect that can be recognizable from the figures is that the amplitudes and phases of P^*_{xx} and T^* are larger when the reaction is endothermic (Figs. 5, 6, 7 and 8). This behaviour is in agreement with the results obtained in Refs. [3, 15], in the sense that, in Refs. [3, 15], it is shown that, for low oscillation frequencies, the attenuation of the sound waves are smaller for the endothermic reaction than for the exothermic one.

Observe that, combining the results shown in Figs. 1, 2, 3, 4, 5, 6, 7 and 8 with the values of the transport coefficients presented in Table 1, we can infer that the transport coefficients also contribute to increase the amplitudes and phases of P^*_{xx} and T^* when the reaction is endothermic, since Table 1 shows that the deviation of the reactive transport coefficients from the corresponding inert values is larger for the endothermic reaction than for the exothermic one.

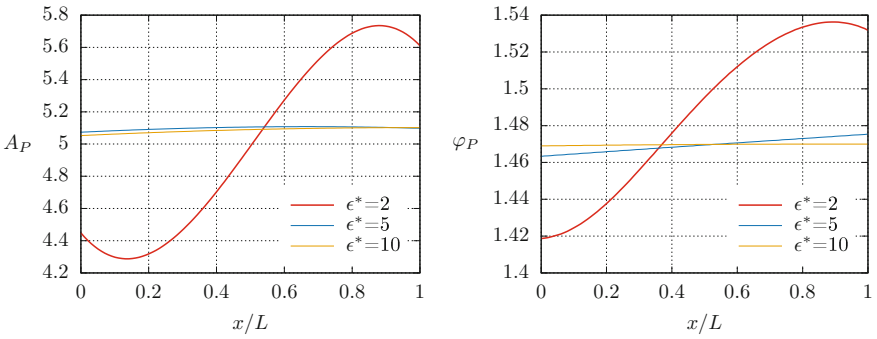

Fig. 2 Amplitude (left) and phase (right) of the pressure difference P^*_{xx} when the exothermic reaction dominates ($x_A = 0.3$), for $\delta = 10$ and $\theta = 0.01$

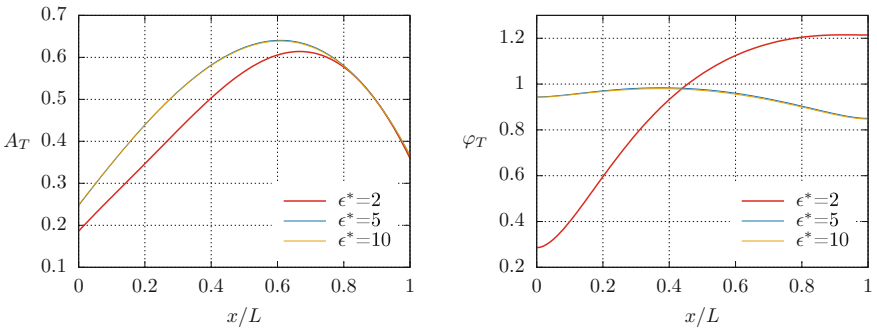

Fig. 3 Amplitude (left) and phase (right) of the pressure difference T^* when the exothermic reaction dominates ($x_A = 0.3$), for $\delta = 10$ and $\theta = 0.1$

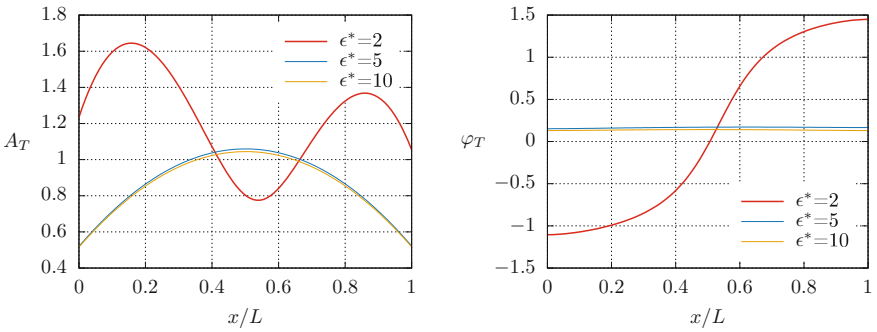

Fig. 4 Amplitude (left) and phase (right) of the temperature deviation difference T^* when the exothermic reaction dominates ($x_A = 0.3$), for $\delta = 10$ and $\theta = 0.01$

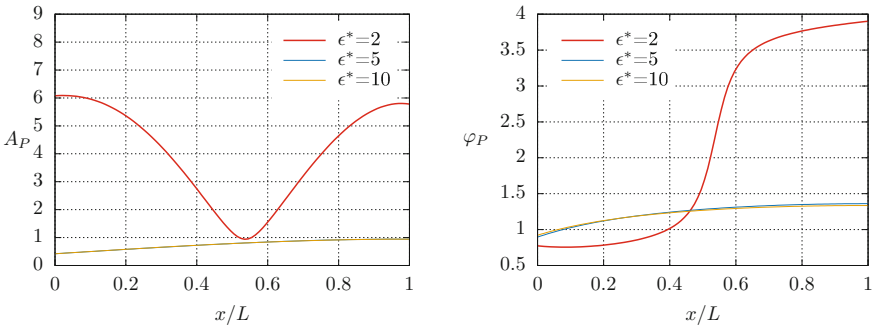

Fig. 5 Amplitude (left) and phase (right) of the pressure difference P^*_{xx} when the endothermic reaction dominates ($x_A = 0.7$), for $\delta = 10$ and $\theta = 0.1$

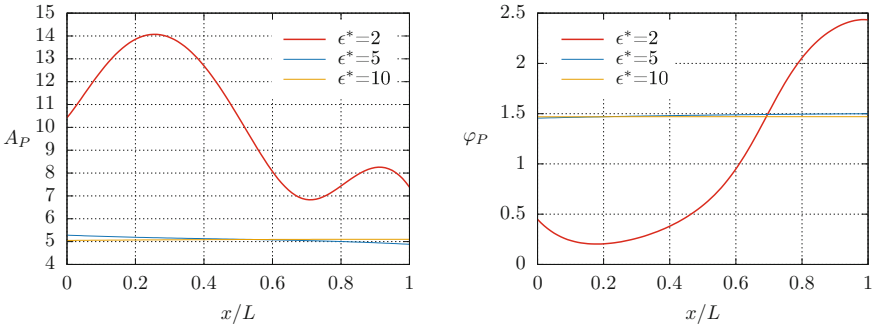

Fig. 6 Amplitude (left) and phase (right) of the pressure difference P^*_{xx} when the endothermic reaction dominates ($x_A = 0.7$), for $\delta = 10$ and $\theta = 0.01$

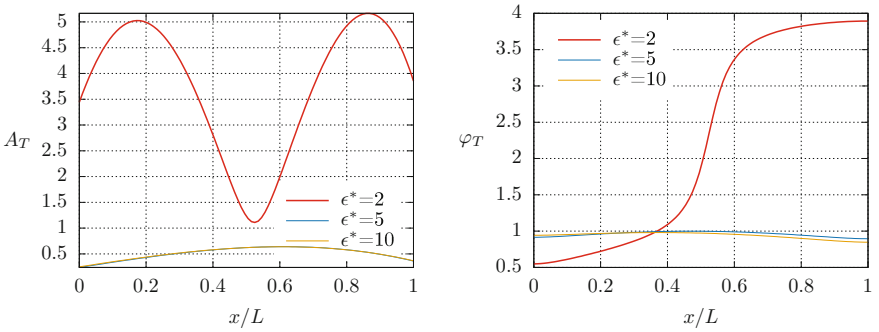

Fig. 7 Amplitude (left) and phase (right) of the pressure difference T^* when the endothermic reaction dominates ($x_A = 0.7$), for $\delta = 10$ and $\theta = 0.1$

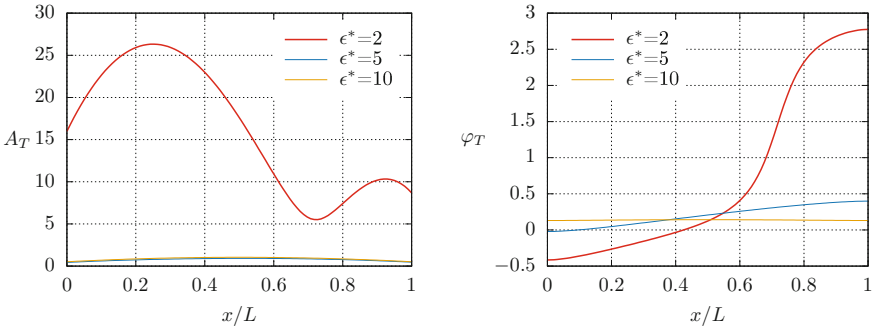

Fig. 8 Amplitude (left) and phase (right) of the temperature deviation difference T^* when the endothermic reaction dominates ($x_A = 0.7$), for $\delta = 10$ and $\theta = 0.01$

7 Final Remarks and Future Plans

In this paper we have analysed the sound wave propagation through a binary mixture undergoing a reversible chemical reaction of symmetric type. The mixture is confined between two flat, infinite and parallel plates, one of them is stationary whereas the other one oscillates harmonically in time and constitutes an emanating source of sound waves that propagate in the mixture. The mathematical problem was studied in the low frequency regime, using the Navier-Stokes equations with chemically reaction rate derived from the kinetic theory of reactive mixtures, assuming temperature jump and velocity impenetrable conditions at both plates.

The main objective of our study was to investigate the influence of the chemical reaction on the properties of interest in the considered problem and how the sound waves reflected from the receptor influence the solution of the problem when the distance between both plates is varying and when the dominant chemical reaction is of exothermic or endothermic type.

To the best of our knowledge, similar sound wave propagation problems have been studied only in the context of non-reactive systems, and no results are known for chemically reactive mixtures and, thus, our analysis in this paper gives the first contribution in this direction. However, the presence of the chemical reaction, combined with the type of boundary conditions, brings additional complexities in the sound wave propagation problem, and we have introduced a simplified assumption for what concerns the temperature jump coefficient appearing in the boundary conditions, as it was explained and motivated in the Introduction.

In our opinion, this simplification is not so restrictive in the context of the present problem, however, if we consider a general mixture with a more complex chemical reaction, the temperature jump coefficient should be determined resorting to an appropriate model of the kinetic theory for chemically reactive mixtures. This development is the subject of a future work.

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Porous Medium Model in Contact with Slow Reservoirs

Renato de Paula, Patrícia Gonçalves and Adriana Neumann

Abstract We analyse the hydrodynamic limit of the porous medium model in contact with slow reservoirs which is given by a porous medium equation with Dirichlet, Robin or Neumann boundary conditions depending on the range of the parameter that rules the slowness of the reservoirs.

Keywords Porous medium model · Hydrodynamic limit
Porous medium equation · Boundary conditions

1 Introduction

We address the hydrodynamic behavior of the porous medium model in contact with slow reservoirs which is given by the porous medium equation with various boundary conditions. Before describing the particle system of interest, let us present the porous medium equation with boundary conditions that appears in this article.

We start by the classical Porous Medium Equation (in short PME), which is the equation

$$\partial_t \rho = \Delta(\rho^M),$$

where $\rho = \rho_t(u)$ is a function from $[0, \infty] \times \mathbb{R}^d$ to $[0, \infty]$, $\Delta = \sum_{j=1}^{d} \partial^2_{u_j}$ and $M \in \mathbb{N}\backslash\{1\}$. Above the notation $\rho_t(u)$ does not mean the time derivative of ρ in t it is simply

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the value of ρ at (t, u). In a sense it is the simplest possible nonlinear version of the heat equation. Note that when $M = 1$ this equation is the heat equation. The PME can be rewritten in divergence form as $\partial_t \rho = \nabla(D(\rho)\nabla\rho)$, where $D(\rho) = M\rho^{M-1}$ is the diffusion coefficient and it goes to zero as $\rho \to 0$, so that the PME is a degenerate parabolic equation.

One of the most important properties of the PME given above is that its solutions can be compactly supported at each fixed time or, in physical terms, they have a finite speed of propagation. This is in strong contrast with the solutions of the classical heat equation since a nonnegative solution of the heat equation is always positive on its domain. For a reference on the mathematical properties of this equation we refer to [8] and references therein.

There are many physical applications, where this equation appears in a natural way to describe processes involving diffusion or heat transfer. Maybe the most well known of them is the description of the flow of an isentropic gas through a porous medium, see [7]. Another important application refers to heat radiation in plasmas, see [10]. Beyond these contexts where the PME is applied, there exists also, see [5, 8, 9], the description of the density of an ideal gas flowing isothermally through a homogeneous porous medium (it corresponds to the choice $M = 2$ above).

In this article we consider the one-dimensional boundary-value problem to the PME in a spatial domain $[0, 1] \subset \mathbb{R}$ with $M = 2$. We consider Dirichlet, Robin and Neumann boundary conditions, i.e. the following equations:

$$\begin{cases} \partial_t \rho_t(u) = \Delta\,(\rho_t(u))^2 \\ \rho_t(0) = \rho^-, \quad \rho_t(1) = \rho^+ \end{cases} \quad \text{and} \quad \begin{cases} \partial_t \rho_t(u) = \Delta\,(\rho_t(u))^2 \\ \partial_u(\rho_t(0))^2 = \kappa_-(\rho_t(0) - \rho^-) \\ \partial_u(\rho_t(1))^2 = \kappa_+(\rho^+ - \rho_t(1)) \end{cases},$$

where $\rho^-, \rho^+ \in (0, 1)$ and $\kappa_-, \kappa_+ \in [0, \infty)$. The equation on the left-hand side of last display has Dirichlet boundary conditions, the one on the right-hand side has Robin boundary conditions and if in that equation we take $\kappa_- = \kappa_+ = 0$, we get Neumann boundary conditions. A consequence of the degeneracy of these equations is that (depending on the initial condition) we do not have classical solutions of the problems above, see Chap. 5 of [9]. The solutions that we will obtain from the particle system are not classical solutions, and for that reason we just need to require the initial condition $\rho_0 : [0, 1] \to [0, 1]$ to be a measurable function. Therefore we need to introduce an appropriate concept of generalized solution of the equation. There are different ways of defining generalized solutions of partial differential equations. The weak formulation is obtained by multiplying the equation by suitable test functions, integrating by parts some or all the terms and using the boundary conditions. One also needs to ask from the solution a regularity that allows the weak formulation to make sense. In this case, we say that the solution is a weak solution. The definitions for weak solution of the equations above are given in Definitions 2 and 3. The integral equations (8) and (10) that appear in the definition of the weak solution are exactly

what we obtain when we study the hydrodynamic limit for the Porous Medium Model (in short PMM) in contact with slow reservoirs.

The hydrodynamic limit is the derivation of a macroscopic equation which rules the space-time evolution of some quantity of interest from an underlying microscopic stochastic model, the latter being an interacting particle system. More precisely, the hydrodynamic limit says that the time evolution of the spatial density of particles converges (as a scaling parameter, that we denote by n, is sent to ∞) to the solution of a macroscopic equation, which is called *hydrodynamic equation*.

The PMM in contact with slow reservoirs is given by a collection of interacting particles on the discrete set $\Sigma_n = \{1, \dots, n-1\}$ under the exclusion rule that states that there can be at most one particle at each site of Σ_n. A configuration of particles is an element of $\{0, 1\}^{\Sigma_n}$ and for each site $x \in \Sigma_n$ the occupation variable $\eta(x) \in \{0, 1\}$, where $\eta(x) = 0$ means that x is an empty site and $\eta(x) = 1$ means that x is an occupied site. The evolution in time is then given by a continuous time Markov process during which the jump of a particle from a site x to an empty nearest neighbor site y in Σ_n occurs at a rate $c(x; y; \eta)$ to be prescribed later on. The choice $c(x; y; \eta) = 1$ corresponds to the Symmetric Simple Exclusion Process (SSEP) and, as it is very well known, leads to the heat equation under diffusion coefficient $D(\rho) = 1$. In order to get a degenerate diffusion coefficient, we impose at the level of the rates $c(x; y; \eta)$ a local constraint stating that the jump of a particle between the sites x and $x + 1$ is allowed if and only if, there exists at least one particle in one of the two sites $x - 1$ and $x + 2$. From this constraint we see that configurations with few particles and such that the distance between two consecutive particles is bigger than 2 are not evolving under this dynamics, and we call these configurations the *blocked* configurations. One way of getting rid of these configurations is to superpose this dynamics with a SSEP dynamics on the bulk, that is, we perturb slightly the dynamics in such a way that the blocked configurations are destroyed and the macroscopic hydrodynamic behavior still evolves according to the PME. We also superpose this dynamics with a Glauber dynamics at the end points $x = 1$ and $x = n - 1$ which represents a contact with reservoirs. We want to tune the reservoirs to make them slow with respect to the rest of the dynamics by scaling the rates in the parameter n. Therefore, we consider that particles can enter the system (or be created) at the site $x = 1$ with rate $m\alpha n^{-\theta}$ or leave the system (or be removed) from the site $x = 1$ with rate $m\gamma n^{-\theta}$. For the right reservoir the dynamics is completely analogous but the entrance (or creation) rate is given by $m\beta n^{-\theta}$ and the exit (annihilation) rate is given by $m\delta n^{-\theta}$. From here on, we fix the parameters $\alpha, \beta, \gamma, \delta \in (0, 1)$, $m > 0$ and $\theta \geq 0$, see Fig. 1. The introduction of these reservoirs breaks down the conservation on the number of particles since there is a mass transfer between the reservoirs (which have different densities) and the bulk.

In [5] the authors considered the PMM in $\mathbb{Z}$ without the superposition with the Glauber dynamics and they proved that the hydrodynamic limit is given by the PME on $\mathbb{R}$ for any value of $M \geq 2$. Here, for simplicity, we restrict to the case $M = 2$ but we note that the extension to other values of M can be obtained by imposing the rates as given in [5].

In [1] the authors showed that for the SSEP in Σ_n in contact with slow reservoirs the hydrodynamic limit is given by the heat equation in $[0, 1]$ with similar boundary conditions to the ones described above. The works of [1, 5] inspired and motivated us to study the PMM in contact with slow reservoirs and the results presented here are a combination of the results of those two articles. More precisely, our hydrodynamic equation is the PME on $[0, 1]$ with boundary conditions, which depends on the range of θ. For $0 \leq \theta < 1$, we obtain the PME with Dirichlet boundary conditions which fixes the value of the density as being $\rho^- = \frac{\alpha}{\alpha+\gamma}$ and $\rho^+ = \frac{\beta}{\beta+\delta}$, respectively, at the points $u = 0$ and $u = 1$. For $\theta = 1$, the boundary dynamics is slowed enough so that the boundary conditions of Dirichlet type are replaced by a type of Robin boundary conditions. These Robin boundary conditions state that the current at the boundary is fixed and it is equal to the difference of the density between the bulk and the boundary. Here we obtain the Robin boundary conditions with $\kappa_- = m(\alpha + \gamma)$ and $\kappa_+ = m(\beta + \delta)$. Finally, for $\theta > 1$, the boundary is sufficiently slowed so that the Robin boundary conditions are replaced by Neumann boundary conditions stating that macroscopically there is no flux of particles from the boundary reservoirs. We would like to stress that we do not present a complete rigorous proof of the hydrodynamic limit since some replacements lemmas that are needed in order to recover the weak solutions of the corresponding hydrodynamic equations, are not presented in this article and are left for a future work. All we claim is that once these replacement lemmas are shown then the hydrodynamic limit follows.

Here follows an outline of this article. In Sect. 2 we present the model, the main definitions and we state the hydrodynamic limit. In Sect. 3 we present a heuristic argument to derive the hydrodynamic equations from the PMM for each range of θ by the use of Dynkin's formula. In Sect. 4 we prove tightness for the sequence of processes of interest and in Sect. 5 we prove some of the auxiliary results that are needed along the text.

2 Statement of Results

2.1 The Model

The dynamics of the PMM in contact with slow reservoirs can be described as follows. We fix a scaling parameter $n \geq 1$, a parameter $0 < a < 2$ and we consider the model evolving on the discrete space $\Sigma_n = \{1, \ldots, n-1\}$ which we call the bulk. To each bond $\{x, x+1\}$, with $x = 1, \ldots, n-2$, we associate one Poisson process $N_{x,x+1}(t)$ with parameter $\eta(x-1) + \eta(x+2) + n^{a-2}$. Note that for $x = 1$ and $x = n-1$ above we use the convention

$$\eta(0) = \rho^-, \quad \eta(n) = \rho^+, \tag{1}$$

where

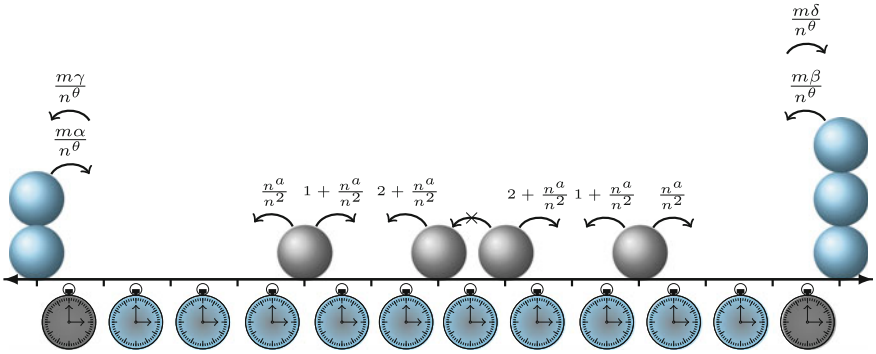

Fig. 1 The perturbed porous medium model in contact with slow reservoirs

$$\rho^- = \frac{\alpha}{\alpha+\gamma} \quad \text{and} \quad \rho^+ = \frac{\beta}{\beta+\delta}, \tag{2}$$

and $\alpha, \beta, \gamma, \delta \in (0, 1)$. We observe that, for $\gamma = 1 - \alpha$, $\rho^- = \alpha$ and for $\delta = 1 - \beta$, $\rho^+ = \beta$. Now we artificially add two end points at the bulk, namely, we add the sites $x = 0$ and $x = n$, and we also add extra Poisson processes at the bonds $\{0, 1\}$ and $\{n - 1, n\}$. Each one of these bonds is associated with two Poisson processes: $N_{0,1}(t)$ with parameter $m\alpha n^{-\theta}(1 - \eta(1))$, $N_{1,0}(t)$ with parameter $m\gamma n^{-\theta}\eta(1)$, $N_{n,n-1}(t)$ with parameter $m\beta n^{-\theta}(1 - \eta(n - 1))$ and $N_{n-1,n}(t)$ with parameter $m\delta n^{-\theta}\eta(n - 1)$. All the Poisson processes are independent, and we call them exponential clocks (since the law of the time between arrivals of a Poisson process is exponential). Above $\alpha, \beta, \gamma, \delta \in (0, 1)$, $m > 0$ and $\theta \geq 0$ is a parameter that rules the slowness of the boundary dynamics. Now that the clocks are fixed we can explain the dynamics. If a clock rings for the bond $\{x, x + 1\}$ in the bulk, the particles at the sites of the bond exchange positions with a rate that depends on whether there is a particle at site $x - 1$ and a particle at site $x + 2$. Now if the clock rings for the bond at the boundary as, for example, from the Poisson process $N_{0,1}(t)$ then a particle gets into the bulk to site 1 if and only if there is no particle at the site 1, otherwise nothing happens. If the clock rings from the Poisson process $N_{1,0}(t)$ and there is a particle at site 1, then it exits from the bulk. At the right boundary we have a very similar dynamics as the one just described. Note that the higher the value of θ the slower is the dynamics at the boundaries. For a display of the description of the dynamics just given see Fig. 1.

In this article we want to analyse the PMM with a superposed SSEP dynamics on the bulk. To properly define our dynamics, let $\{\eta_t\}_{t\geq 0}$ denote a Markov process with state space $\Omega_n := \{0, 1\}^{\Sigma_n}$. If $\eta \in \Omega_n$, then we call η a configuration of particles. If $\eta(x) = 0$ it means that the site $x \in \Sigma_n$ is vacant while $\eta(x) = 1$ means that the site x is occupied. This Markov process can be fully characterized in terms of its infinitesimal generator L_n given by

$$L_n = L_P + n^{a-2}L_S + L_B,$$

where $0 < a < 2$, L_P is the generator of the PMM, L_S is the generator of the SSEP and L_B is the generator of the boundary dynamics, which act on local functions $f : \Omega_n \to \mathbb{R}$ as

$$\begin{aligned}
(L_P f)(\eta) &= \sum_{x=1}^{n-2} [c_{x,x+1}(\eta) + c_{x+1,x}(\eta)][f(\eta^{x,x+1}) - f(\eta)], \\
(L_B f)(\eta) &= \tfrac{m}{n^\theta}[\alpha(1-\eta(1)) + \gamma\eta(1)][f(\eta^1) - f(\eta)] \\
&\quad + \tfrac{m}{n^\theta}[\beta(1-\eta(n-1)) + \delta\eta(n-1)][f(\eta^{n-1}) - f(\eta)], \\
(L_S f)(\eta) &= \sum_{x=1}^{n-2} [\eta(x)(1-\eta(x+1)) + \eta(x+1)(1-\eta(x))][f(\eta^{x,x+1}) - f(\eta)]
\end{aligned} \tag{3}$$

with

$$\eta^{x,y}(z) = \begin{cases} \eta(z), \ z \neq x, y, \\ \eta(y), \ z = x, \\ \eta(x), \ z = y \end{cases}, \quad \eta^x(z) = \begin{cases} \eta(z), \ z \neq x, \\ 1 - \eta(x), \ z = x, \end{cases} \tag{4}$$

$$c_{x,x+1}(\eta) = \eta(x)(1-\eta(x+1))(\eta(x-1) + \eta(x+2)), \ \ c_{x+1,x}(\eta) = c_{x,x+1}(\eta^{x,x+1}),$$

for $x \in \{1, \ldots, n-2\}$. Above, the parameters $\theta \geq 0$, $m > 0$, $\alpha, \beta, \gamma, \delta \in (0,1)$. If one defines

$$\kappa_- = m(\alpha + \gamma) \ \text{ and } \ \kappa_+ = m(\beta + \delta), \tag{5}$$

then the infinitesimal generator at the boundary can be rewritten as

$$\begin{aligned}
(L_B f)(\eta) &= \tfrac{\kappa_-}{n^\theta}[\rho^-(1-\eta(1)) + (1-\rho^-)\eta(1)][f(\eta^1) - f(\eta)] \\
&\quad + \tfrac{\kappa_+}{n^\theta}[\rho^+(1-\eta(n-1)) + (1-\rho^+)\eta(n-1)][f(\eta^{n-1}) - f(\eta)].
\end{aligned} \tag{6}$$

We are going to consider the process speeded up in the diffusive time scale tn^2 so that from here on, we consider the Markov process $\{\eta_{tn^2}\}_{t \geq 0}$ which has infinitesimal generator $n^2 L_n$. Note that above L_S is multiplied by a function n^{a-2} and since we want to observe the same macroscopic density behavior given by the dynamics of $L_P + L_B$, we have to restrict ourselves to the case $0 < a < 2$.

Note that our dynamics is given by an irreducible finite-state Markov process so that there exists only one invariant measure. We remark that if $\rho := \rho^+ = \rho^-$ then the Bernoulli product measure with parameter ρ is reversible and, as a consequence, it is invariant for the perturbed process, since it is invariant for each of the process L_P, L_S and L_B. We leave the details of this fact to the reader.

2.2 Hydrodynamic Equations

In order to state the hydrodynamic limit, we need to introduce some notations and definitions. For an interval $\mathcal{I}$ in $\mathbb{R}$ and integers m and n, we denote by $C^{m,n}([0,T]\times\mathcal{I})$ the set of functions defined on $[0,T]\times\mathcal{I}$ that are m times differentiable on the first variable and n times differentiable on the second variable (with continuous derivatives), and $C_0^{m,n}([0,T]\times[0,1])$ denotes the set of functions $G\in C^{m,n}([0,T]\times[0,1])$ such that $G_s(0)=G_s(1)=0$, for all $s\in[0,T]$. Denote by $\langle\cdot,\cdot\rangle$ the inner product in $L^2([0,1])$ and by $\|\cdot\|_{L^2}$ the corresponding norm.

The semi inner-product $\langle\cdot,\cdot\rangle_1$ is defined on the set $C^\infty([0,1])$ by

$$\langle G,H\rangle_1=\int_0^1(\partial_u G)(u)\,(\partial_u H)(u)\,du.$$

The corresponding semi-norm is denoted by $\|\cdot\|_1$.

Definition 1 The Sobolev space $\mathcal{H}^1$ on $[0,1]$ is the Hilbert space defined as the completion of $C^\infty([0,1])$ for the norm $\|\cdot\|^2_{\mathcal{H}^1}:=\|\cdot\|^2_{L^2}+\|\cdot\|^2_1$. The space $L^2(0,T;\mathcal{H}^1)$ is the set of measurable functions $f:[0,T]\to\mathcal{H}^1$ such that $\int_0^T\|f_s\|^2_{\mathcal{H}^1}ds<\infty$.

Definition 2 Let $\rho^-,\rho^+\in(0,1)$ and $g:[0,1]\to[0,1]$ be 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

$$\begin{cases}\partial_t\rho_t(u)=\Delta\,(\rho_t(u))^2, & (t,u)\in[0,T]\times(0,1),\\ \rho_t(0)=\rho^-, \quad \rho_t(1)=\rho^+, & t\in[0,T],\\ \rho_0(\cdot)=g(\cdot),\end{cases}\tag{7}$$

if the following conditions hold:

1. $\rho\in L^2(0,T;\mathcal{H}^1)$;
2. ρ satisfies the integral equation:

$$\begin{aligned}\langle\rho_t,G_t\rangle-\langle g,G_0\rangle-\int_0^t\langle\rho_s,(\partial_s G_s+\rho_s\Delta G_s)\rangle\,ds\\ +\int_0^t\{(\rho^+)^2\partial_u G_s(1)-(\rho^-)^2\partial_u G_s(0)\}\,ds=0,\end{aligned}\tag{8}$$

for all $t\in[0,T]$ and any function $G\in C_0^{1,2}([0,T]\times[0,1])$.

Definition 3 Let $\kappa_-,\kappa_+\geq 0$, $\rho^-,\rho^+\in(0,1)$ and $g:[0,1]\to[0,1]$ be 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

$$\begin{cases} \partial_t \rho_t^{\kappa}(u) = \Delta\,(\rho_t(u))^2, \quad (t,u) \in [0,T] \times (0,1), \\ \partial_u(\rho_t(0))^2 = \kappa_-(\rho_t(0) - \rho^-), \quad t \in [0,T], \\ \partial_u(\rho_t(1))^2 = \kappa_+(\rho^+ - \rho_t(1)), \quad t \in [0,T], \\ \rho_0(\cdot) = g(\cdot), \end{cases} \tag{9}$$

if the following conditions hold:

1. $\rho \in L^2(0,T;\mathcal{H}^1)$;
2. ρ satisfies the integral equation:

$$\begin{aligned} &\langle \rho_t, G_t\rangle - \langle g, G_0\rangle - \int_0^t \langle \rho_s, (\partial_s G_s + \rho_s \Delta G\rangle\, ds \\ &+ \int_0^t \{(\rho_s(1))^2 \partial_u G_s(1) - (\rho_s(0))^2 \partial_u G_s(0)\}\, ds \\ &- \int_0^t \{G_s(0)\kappa_-(\rho^- - \rho_s(0)) + \kappa_+ G_s(1)(\rho^+ - \rho_s(1))\}\, ds = 0, \end{aligned} \tag{10}$$

for all $t \in [0,T]$ and any function $G \in C^{1,2}([0,T] \times [0,1])$.

Remark 1 For $\kappa_- = \kappa_+ = 0$ we obtain above Neumann boundary conditions.

Remark 2 We believe that the partial differential equations given above have a unique weak solution in the sense given in the previous definition. The result might be proved in the literature but we did not find exactly the uniqueness result in the case of the precise boundary conditions given above.

Remark 3 The stationary solution of (7) is given on $u \in (0,1)$ by

$$\bar{\rho}(u) = \sqrt{((\rho^+)^2 - (\rho^-)^2)u + (\rho^-)^2},$$

and, for $\kappa_+ \neq \kappa_-$, the stationary solution of (9) is given on $u \in (0,1)$ by

$$\bar{\rho}(u) = \sqrt{au + b},$$

where $a = \kappa_-(\sqrt{b} - \rho^-)$ and $\sqrt{b}$ is solution of

$$[\kappa_+^2 - \kappa_-^2]b + \sqrt{b}\kappa_-[2(\kappa_+\rho^+ + \kappa_-\rho^-) + \kappa_+^2] - [\kappa_-\rho^-\kappa_+^2 + (\kappa_+\rho^+ + \kappa_-\rho^-)^2] = 0.$$

The solution of the previous equation is given by

$$\sqrt{b} = \frac{-\kappa_-(2(\kappa_+\rho^+ + \kappa_-\rho^-) + \kappa_+^2) \pm \sqrt{\Theta}}{2[\kappa_+^2 - \kappa_-^2]},$$

where

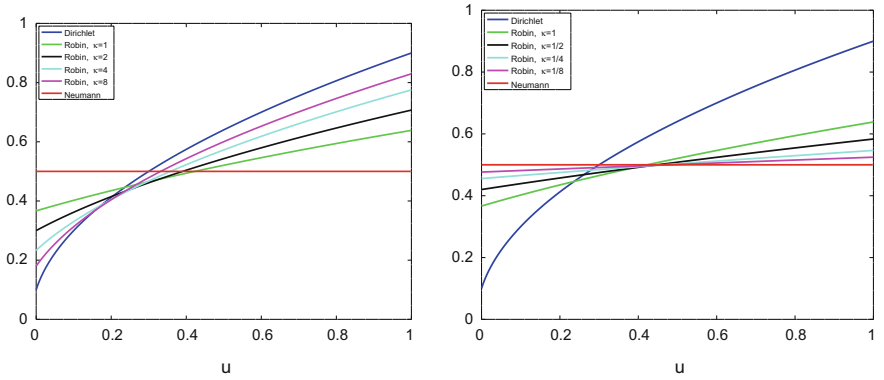

Fig. 2 Stationary solutions when $\kappa_- = \kappa_+ = \kappa$

$$\Theta = \kappa_+^2\Big(4(\kappa_+\rho^+ + \kappa_-\rho^-)^2 + 4\kappa_+\kappa_-(\kappa_+\rho^- + \kappa_-\rho^+) + \kappa_-^2\kappa_+^2\Big).$$

Observe that when $\kappa_- = 0 \neq \kappa_+$, then $\bar{\rho}(u) = \rho^+$, and when $\kappa_+ = 0 \neq \kappa_-$, then $\bar{\rho}(u) = \rho^-$. We also note that when $\kappa_- = \kappa_+ = \kappa$, we have

$$a = \frac{\kappa((\rho^+)^2 - (\rho^-)^2)}{2(\rho^+ + \rho^-) + \kappa} \quad \text{and} \quad b = \Big(\frac{(\rho^+ + \rho^-)^2 + \rho^-\kappa}{2(\rho^+ + \rho^-) + \kappa}\Big)^2.$$

We also remark that when $\kappa = 0$ the solution above is simply given by $\bar{\rho}(u) = \frac{\rho^+ + \rho^-}{2}$. Below we present the graphs of these stationary solutions, namely for the choice $\kappa_- = \kappa_+ = \kappa$. In the figure below, we take different values of κ, increasing values of κ on the left-hand side and decreasing values of κ on the right-hand side, to see the dependence of the stationary solutions on the parameter κ.

Observe that on the left-hand (resp. right-hand) side of Fig. 2 we can see that for the Robin case, as we increase (resp. decrease) the value of κ, the stationary solution is getting closer to the stationary solution corresponding to the Dirichlet (resp. Neumann) case. We believe that, as happens in [4], the convergence of the time dependent weak solution (that we denote now by ρ^κ) in the Robin case converges (in a suitable topology) to the weak solution of Definition 2 (resp. Definition 3 when $\kappa_- = \kappa_+ = 0$) when $\kappa \to +\infty$ (resp. $\kappa \to 0$). We leave the rigorous proof of this problem for a future work.

2.3 *Hydrodynamic Limit*

Let $\mathcal{M}^+$ 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 $\pi^n(\eta, du)$ on $[0, 1]$ by

$$\pi^n(\eta, du) = \frac{1}{n} \sum_{x \in \Sigma_n} \eta(x) \delta_{\frac{x}{n}}(du), \tag{11}$$

where δ_a is a Dirac mass on $a \in [0, 1]$. We define $\pi_t^n(\eta, du) := \pi^n(\eta_{tn^2}, du)$, where η_t has been defined in Sect. 2.1. For a test 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 which is equal to

$$\langle \pi_t^n, G \rangle = \frac{1}{n} \sum_{x \in \Sigma_n} G(\tfrac{x}{n}) \eta_{tn^2}(x).$$

Fix $T > 0$ and $\theta \geq 0$. Let μ_n be an initial measure on Ω_n. We denote by $\mathbb{P}_{\mu_n}$ the probability measure in the Skorohod space $\mathcal{D}([0, T], \Omega_n)$ induced by the Markov process $\{\eta_{tn^2}\}_{t \geq 0}$ and the initial measure μ_n and we denote by $\mathbb{E}_{\mu_n}$ the expectation with respect to $\mathbb{P}_{\mu_n}$. Let $\{\mathbb{Q}_n\}_{n \geq 1}$ be the sequence of probability measures on $\mathcal{D}([0, T], \mathcal{M}^+)$ induced by the Markov processes $\{\pi_t^n\}_{t \geq 0}$ and by $\mathbb{P}_{\mu_n}$.

Let $g : [0, 1] \to [0, 1]$ be a measurable function. We say that a sequence of probability measures $\{\mu_n\}_{n \geq 1}$ in Ω_n is associated with the profile $g(\cdot)$ if for any continuous function $G : [0, 1] \to \mathbb{R}$ and every $\delta > 0$

$$\lim_{n \to \infty} \mu_n \left(\left| \frac{1}{n} \sum_{x \in \Sigma_n} G\left(\tfrac{x}{n}\right) \eta(x) - \int_0^1 G(u) g(u) du \right| > \delta \right) = 0. \tag{12}$$

Theorem 1 *Let $g : [0, 1] \to [0, 1]$ be a measurable function and let $\{\mu_n\}_{n \geq 1}$ be a sequence of probability measures on Ω_n associated with $g(\cdot)$. Then, the sequence $\{\mathbb{Q}_n\}_{n \geq 1}$ is tight and any limit point $\mathbb{Q}$ satisfies*

$$\mathbb{Q}(\pi_\cdot : \pi_t(du) = \rho_t(u) du, \forall t \in [0, T]) = 1,$$

where

- *for $\theta < 1$, $\rho_t(\cdot)$ is a weak solution of (7);*
- *for $\theta = 1$, $\rho_t(\cdot)$ is a weak solution of (9) with κ_- and κ_+ defined in (5);*
- *for $\theta > 1$, $\rho_t(\cdot)$ is a weak solution of (9) with $\kappa_- = \kappa_+ = 0$.*

The method of proof of last theorem is classical and relies on first showing tightness of the sequence of measures $\{\mathbb{Q}_n\}_{n \geq 1}$, which we postpone to Sect. 4. From this it follows that the sequence $\{\mathbb{Q}_n\}_{n \geq 1}$ has limit points. Then, the next step is to characterize the limit points by showing that they are concentrated on trajectories of measures that are absolutely continuous with respect to the Lebesgue measure (we do not present the proof of this result since it is a simple consequence of the fact that our dynamics is of exclusion type, see Sect. 2 of Chap. 4 of [6]). Moreover, we also have to show that the density is a weak solution of the corresponding hydrodynamic equation. We do not prove rigorously this result, but in the next section

we present a heuristic argument in order to derive the density as a weak solution of the corresponding hydrodynamic equation. In Sect. 5 we present the proofs of some replacement lemmas that are needed along the argument. If we had uniqueness of weak solutions in the sense given above, then we would conclude that the limit point is unique so that $\{\mathbb{Q}_n\}_{n\geq 1}$ weakly converges to this limit point.

3 Discrete Versions of Weak Solutions

As mentioned above, in Sect. 4 we will prove that $\{\mathbb{Q}_n\}_{n\geq 1}$ has limits points. Let $\mathbb{Q}^*$ be one of these limit points. From Sect. 2 of Chap. 4 of [6], this limit point is supported on trajectories of measures that are absolutely continuous with respect to the Lebesgue measure, that is: $\mathbb{Q}^*(\pi_\cdot : \pi_t(du) = \rho_t(u)du) = 1$. We call to the function $\rho_t(\cdot)$, appearing inside last probability, the density profile. In principle this function could be random, but here we *heuristically* prove that $\rho_t(\cdot)$ is a weak solution of the hydrodynamic equation. Fix a function $G \in C^{1,2}([0,T]\times[0,1])$. We know by Dynkin's formula, see Lemma A1.5.1 of [6], that

$$M_t^n(G) = \langle \pi_t^n, G_t\rangle - \langle \pi_0^n, G_0\rangle - \int_0^t (\partial_s + n^2 L_P + n^a L_S + n^2 L_B)\langle \pi_s^n, G_s\rangle\, ds \tag{13}$$

is a martingale with respect to the natural filtration $\{\mathcal{F}_t\}_{t\geq 0} = \{\sigma(\eta_s) : s \leq t\}_{t\geq 0}$. Note that $\partial_s\langle \pi_s^n, G_s\rangle = \langle \pi_s^n, \partial_s G_s\rangle$, for any function $G \in C^{1,2}([0,T]\times[0,1])$ and, macroscopically, this extra term will give rise to the term involving $\partial_s G$ in (8) and (10). Since this term does not have any information about the dynamics of the model, and for simplicity of the presentation, we consider here test functions G only space-dependent, that is $G \in C^2([0,1])$. Then in (13) the ∂_s can be suppressed. Let us compute now the other term. From a simple computation, we have, for $\eta \in \Omega_n$ and for $x \in \Sigma_n$, that $L_n\eta(x) = j_{x-1,x}(\eta) - j_{x,x+1}(\eta)$, where the instantaneous current $j_{x,x+1}(\eta)$ is given by

$$\begin{cases} j_{0,1}(\eta) = \frac{m}{n^\theta}(\alpha - (\alpha+\gamma)\eta(1)), \\ j_{x,x+1}(\eta) = \tau_x h(\eta) - \tau_{x+1}h(\eta) \ \text{ for } \ x \in \{1,\dots,n-2\}, \\ j_{n-1,n}(\eta) = \frac{m}{n^\theta}((\beta+\delta)\eta(n-1) - \beta), \end{cases} \tag{14}$$

where

$$\tau_x h(\eta) = \eta(x-1)\eta(x) + \eta(x)\eta(x+1) - \eta(x-1)\eta(x+1) + n^{a-2}\eta(x). \tag{15}$$

Now, from another simple computation we have that $n^2 L_n\langle \pi_s^n, G\rangle$ is equal to

$$\begin{aligned}
&\frac{1}{n}\sum_{x=1}^{n-1}\Delta_n G(\tfrac{x}{n})\tau_x h(\eta_{sn^2}) \\
&+\nabla_n^+ G(0)\tau_1 h(\eta_{sn^2}) + nG(\tfrac{1}{n})\tfrac{m}{n^\theta}\big(\alpha-(\alpha+\gamma)\eta_{sn^2}(1)\big) \\
&-\nabla_n^- G(1)\tau_{n-1} h(\eta_{sn^2}) + nG(\tfrac{n-1}{n})\tfrac{m}{n^\theta}\big(\beta-(\beta+\delta)\eta_{sn^2}(n-1)\big),
\end{aligned} \tag{16}$$

where for $x \in \Sigma_n$

$$\begin{aligned}
\Delta_n G(x) &= n^2(G(x-1/n) - 2G(x) + G(x+1/n)), \\
\nabla_n^+ G(x) = n(G(x+1/n) - G(x)) \quad &\text{and} \quad \nabla_n^- G(x) = n(G(x) - G(x-1/n)).
\end{aligned}$$

From the computations above and since the function G is time independent, the martingale $M_t^n(G)$ is equal to

$$\begin{aligned}
&\langle \pi_t^n, G\rangle - \langle \pi_0^n, G\rangle - \int_0^t \frac{1}{n}\sum_{x=1}^{n-1}\Delta_n G(\tfrac{x}{n})\tau_x h(\eta_{sn^2})ds \\
&- \int_0^t \nabla_n^+ G(0)\tau_1 h(\eta_{sn^2})ds + \int_0^t \nabla_n^- G(1)\tau_{n-1} h(\eta_{sn^2})ds \\
&- m\frac{n}{n^\theta}\int_0^t \Big(G(\tfrac{1}{n})(\alpha-(\alpha+\gamma)\eta_{sn^2}(1)) + G(\tfrac{n-1}{n})(\beta-(\beta+\delta)\eta_{sn^2}(n-1))\Big)ds.
\end{aligned} \tag{17}$$

Above we used (1). Since $|\Delta_n G(\frac{x}{n})| \le 2\|G''\|_\infty, |\nabla_n^+ G(0)| \le 2\|G'\|_\infty, |\nabla_n^- G(1)| \le 2\|G'\|_\infty$, and $|\eta_{sn^2}(x)| \le 1$, for all $s \ge 0$ and $x \in \Sigma_n$, the terms that come from the SSEP jumps vanish when $n \to \infty$. From here on we ignore them and we look only at the other terms.

Let us now consider the case $\theta < 1$. From Theorem 2 of Sect. 5.2, it is easy to see that we can replace in the expression above $\eta_{sn^2}(1)$ by ρ^- (resp. $\eta_{sn^2}(n-1)$ by ρ^+). Moreover, since in this regime we take G vanishing at the boundary, see the space of test functions in (8), last expression can be written as

$$\begin{aligned}
M_t^n(G) = \langle \pi_t^n, G\rangle - \langle \pi_0^n, G\rangle - \int_0^t \frac{1}{n}\sum_{x=1}^{n-1}\Delta_n G(\tfrac{x}{n})\tau_x h(\eta_{sn^2})ds \\
- \int_0^t \Big(\nabla_n^+ G(0)(\rho^-)^2 - \nabla_n^- G(1)(\rho^+)^2\Big)ds + O(n^{-\theta}).
\end{aligned} \tag{18}$$

As usual, see [3], the notations O, o and $\sim$ have the following meaning: *For functions φ and ψ depending on a parameter n, which tend to infinity and $\psi > 0$, we write*

$$\left.\begin{array}{c}\varphi = O(\psi)\\ \varphi = o(\psi)\\ \varphi \sim \psi\end{array}\right\} \quad \text{if} \quad \frac{\varphi}{\psi} \quad \left\{\begin{array}{c}\text{remains bounded}\\ \to 0\\ \to 1.\end{array}\right.$$

Note that the term $O(n^{-\theta})$ in (18) comes from last integral in (17), where we use the fact that G is a function vanishing at the boundary and that $|\eta_{sn^2}(x)| \leq 1$, for all $s \geq 0$ and $x \in \Sigma_n$.

From Theorem 4 of Sect. 5.2, we have that

$$M_t^n(G) = \langle \pi_t^n, G\rangle - \langle \pi_0^n, G\rangle - \int_0^t \frac{1}{n}\sum_{x=1}^{n-1} \Delta_n G(\tfrac{x}{n})(\overrightarrow{\eta}^{\varepsilon n}_{sn^2}(x))^2 ds$$
$$- \int_0^t \nabla_n^+ G(0)(\rho^-)^2 - \nabla_n^- G(1)(\rho^+)^2 ds + O(n^{-\theta}) + o(1).$$

The sense of convergence for the term $o(1)$ is the one stated in Theorem 4. Above, $\overrightarrow{\eta}^{\varepsilon n}_{sn^2}(x)$ is the empirical density in the box of size εn, which is given on $x \in \Sigma_n$ by

$$\overrightarrow{\eta}^{\varepsilon n}_{sn^2}(x) = \frac{1}{\varepsilon n}\sum_{y=x+1}^{x+\varepsilon n} \eta_{sn^2}(y). \tag{19}$$

Above and below εn should be understood as $\lfloor \varepsilon n \rfloor$. Note that $\overrightarrow{\eta}^{\varepsilon n}_{sn^2}(x) = \langle \pi^n_{sn^2}, \iota^x_\varepsilon\rangle$, where

$$\iota^x_\varepsilon(u) = \tfrac{1}{\varepsilon}\mathbf{1}_{(\frac{x}{n}, \frac{x}{n}+\varepsilon)}(u).$$

Then, *heuristically*, we have that $\langle \pi^n_{sn^2}, \iota^x_\varepsilon\rangle$ converges, when $n \to \infty$, to

$$\langle \pi_s, \iota^x_\varepsilon\rangle = \int_0^1 \rho_s(u)\iota^x_\varepsilon(u)\, du,$$

where $\rho_s(\cdot)$ is the density profile. Finally, we take, the limit when $\varepsilon \to 0$ and we obtain that $\langle \pi_s, \iota^x_\varepsilon\rangle$ converges to $\rho_s(\frac{x}{n})$. From the observation above we say that $\overrightarrow{\eta}^{\varepsilon n}_{sn^2}(x) \sim \rho_s(\frac{x}{n})$.

By the computations of Sect. 4 we see that $\mathbb{E}_{\mu_n}[M_t^n(G)]$ vanishes as $n \to \infty$. Then, taking the limit $n \to \infty$ and $\varepsilon \to 0$, in the last display we obtain:

$$0 = \langle \rho_t, G\rangle - \langle \rho_0, G\rangle - \int_0^t \langle \Delta G, (\rho_s)^2\rangle\, ds - \int_0^t \partial_u G(0)(\rho^-)^2 - \partial_u G(1)(\rho^+)^2 ds,$$

from where we see (8).

Remark 4 Note that above we used (1). If we had assumed that $\eta(0)$ is any positive constant, let us call it r, then in the second line of (17) we would have

$$\int_0^t \nabla_n^+ G(0)\big(\eta_{sn^2}(1)r + \eta_{sn^2}(1)\eta_{sn^2}(2) - \eta_{sn^2}(2)r + n^{a-2}\eta_{sn^2}(1)\big) ds.$$

Note that last integrand function only comes from the bulk dynamics. Now to get the Dirichlet boundary conditions as above, we would have to prove that we can replace

$\eta(1)$ by $\eta(2)$, which can be done by a similar argument to the one of Theorem 4 and then we can use Theorem 2 of Sect. 5.2, to replace $\eta_{sn^2}(1)$ by ρ^-. This could give us some freedom to take other rates for the bulk dynamics. Here we stick to the choice (1).

Now we consider $\theta = 1$ and we take a test function G which is twice differentiable. In this case we have

$$M_t^n(G) = \langle \pi_t^n, G\rangle - \langle \pi_0^n, G\rangle - \int_0^t \frac{1}{n}\sum_{x=1}^{n-1} \Delta_n G(\tfrac{x}{n})\tau_x h(\eta_{sn^2})ds$$
$$- \int_0^t \nabla_n^+ G(0)\tau_1 h(\eta_{sn^2})ds + \int_0^t \nabla_n^- G(1)\tau_{n-1} h(\eta_{sn^2})ds$$
$$- m\int_0^t G(\tfrac{1}{n})(\alpha - (\alpha+\gamma)\eta_{sn^2}(1)) + G(\tfrac{n-1}{n})(\beta - (\beta+\delta)\eta_{sn^2}(n-1))ds.$$

Now, we note that by Theorem 3 of Sect. 5.2, and since, as seen above, $\overrightarrow{\eta}^{\varepsilon n}_{sn^2}(x) \sim \rho_s(\frac{x}{n})$, taking the limit in $n \to \infty$ and $\varepsilon \to 0$ in last expression, we obtain

$$0 = \langle \rho_t, G\rangle - \langle \rho_0, G\rangle - \int_0^t \langle \Delta G, (\rho_s)^2\rangle\, ds$$
$$- \int_0^t \partial_u G(0)(\rho_s(0))^2 - \partial_u G(1)(\rho_s(1))^2 ds$$
$$- m\int_0^t G(0)(\alpha - (\alpha+\gamma)\rho_s(0)) + G(1)(\beta - (\beta+\delta)\rho_s(1))\, ds,$$

from where we see (10) for κ_- and κ_+ as defined in (5).

Finally, when $\theta > 1$ we take the same space of test functions as in the case $\theta = 1$, but since $\theta > 1$ the last term on the right-hand side of (17) vanishes as $n \to \infty$. Moreover, since Theorems 3 and 4 of Sect. 5.2 hold, when taking the limit in $n \to \infty$ and $\varepsilon \to 0$ in (17) we obtain

$$0 = \langle \rho_t, G\rangle - \langle \rho_0, G\rangle - \int_0^t \langle \Delta G, (\rho_s)^2\rangle\, ds$$
$$- \int_0^t \partial_u G(0)(\rho_s(0))^2 - \partial_u G(1)(\rho_s(1))^2 ds,$$

which corresponds to (10) for $\kappa_- = \kappa_+ = 0$.

4 Tightness

Proposition 1 *The sequence of measures* $\{\mathbb{Q}_n\}_{n\geq 1}$ *is tight with respect to the Skorohod topology of* $\mathcal{D}([0,T],\mathcal{M}^+)$.

Proof In order to prove the tightness of $\{\pi_t^n\}_{0\leq t\leq T}$ it is enough to show tightness of the real-valued process $\{\langle \pi_t^n, G\rangle\}_{0\leq t\leq T}$ for $G\in C([0,1])$. In fact, see Proposition 4.1.6 of [6], it is enough to show that for each $\varepsilon>0$

$$\lim_{\gamma\to 0}\limsup_{n\to\infty}\mathbb{P}_{\mu_n}\left(\sup_{|t-s|\leq\gamma}|\langle\pi_t^n,G\rangle-\langle\pi_s^n,G\rangle|>\varepsilon\right)=0. \tag{20}$$

By Proposition 4.1.7 of [6], it is enough to show that (20) holds for functions G in a dense subset of $C([0,1])$ with respect to the uniform topology. Note that from (13) we have that

$$\begin{aligned}
&\mathbb{P}_{\mu_n}\left(\sup_{|t-s|\leq\gamma}|\langle\pi_t^n,G\rangle-\langle\pi_s^n,G\rangle|>\varepsilon\right)\\
\leq&\mathbb{P}_{\mu_n}\left(\sup_{|t-s|\leq\gamma}|M_t^n(G)-M_s^n(G)|>\frac{\varepsilon}{2}\right)\\
+&\mathbb{P}_{\mu_n}\left(\sup_{|t-s|\leq\gamma}\left|\int_s^t n^2L_n\langle\pi_r^n,G\rangle dr\right|>\frac{\varepsilon}{2}\right)\\
\leq&\frac{2}{\varepsilon}\mathbb{E}_{\mu_n}\left(\sup_{|t-s|\leq\gamma}|M_t^n(G)-M_s^n(G)|\right)+\frac{2}{\varepsilon}\mathbb{E}_{\mu_n}\left(\sup_{|t-s|\leq\gamma}\left|\int_s^t n^2L_n\langle\pi_r^n,G\rangle dr\right|\right),
\end{aligned} \tag{21}$$

where in the last step we used the Chebyshev's inequality. So, by (20) and (21) to show that the sequence is tight it is enough to prove that

$$\lim_{\gamma\to 0}\limsup_{n\to+\infty}\mathbb{E}_{\mu_n}\left(\sup_{|t-s|\leq\gamma}\left|M_t^n(G)-M_s^n(G)\right|\right)=0, \tag{22}$$

and

$$\lim_{\gamma\to 0}\limsup_{n\to+\infty}\mathbb{E}_{\mu_n}\left(\sup_{|t-s|\leq\gamma}\left|\int_s^t n^2L_n\langle\pi_r^n,G\rangle dr\right|\right)=0. \tag{23}$$

The proof is divided in 2 cases: $\theta\geq 1$ and $\theta\in[0,1)$.

Tightness for $\theta\geq 1$. In this case we use the dense subset $C^2([0,1])$ of $C([0,1])$. We will start proving (22). To this end, note that by Doob's and Hölder's inequalities, we have that

$$\mathbb{E}_{\mu_n}\left(\sup_{|t-s|\le\gamma}|M_t^n(G)-M_s^n(G)|\right)\le 2\mathbb{E}_{\mu_n}\left(\sup_{0\le t\le T}|M_t^n(G)|\right)$$
$$\le 2\mathbb{E}_{\mu_n}\left(\left(\sup_{0\le t\le T}|M_t^n(G)|\right)^2\right)^{\frac{1}{2}}\le 4\mathbb{E}_{\mu_n}\left(|M_T^n(G)|^2\right)^{\frac{1}{2}}$$
$$=4\mathbb{E}_{\mu_n}\left(\langle M^n(G)\rangle_T\right)^{\frac{1}{2}},$$

where the second inequality follows from Doob's inequality and the fact that $(M_t^n(G))^2-\int_0^t B_s^n(G)ds$ is a mean zero martingale. Above $\langle M^n(G)\rangle_t=\int_0^t B_s^n(G)\,ds$ is the quadratic variation of $M_t^n(G)$ and

$$B_s^n(G)=n^2[L_n\langle\pi_s^n,G\rangle^2-2\langle\pi_s^n,G\rangle L_n\langle\pi_s^n,G\rangle]. \tag{24}$$

We now prove that the quadratic variation of $M_t^n(G)$ converges to zero uniformly in $t\in[0,T]$, when $n\to\infty$. Since the rates $c_{x,x+1}$ are bounded from above, for all $x\in\{1,\dots,n-2\}$, a simple computation shows that

$$B_s^n(G)\le C\Big(\frac{1}{n}\|(G')^2\|_\infty+C(\alpha,\gamma,\beta,\delta)\frac{m}{n^\theta}\|G^2\|_\infty+n^{a-3}\|(G')^2\|_\infty\Big), \tag{25}$$

from where we get that

$$\lim_{n\to\infty}\left|\int_0^t B_s^n(G)ds\right|=0,$$

for $\theta\ge 1$. This proves (22). We note that, in fact, the proof above works for any $\theta>0$ but not for $\theta=0$ since the bound in (25) does not vanish when $n\to+\infty$. In any case, below we present a proof which works out for any $\theta<1$ since in this case we will use compactly supported functions. Now we will prove (23). Recall (16). By the mean value theorem and since $|\eta_{sn^2}(x)|\le 1$ for any $x\in\{0,\cdots,n\}$ and $s\in[0,T]$, we have that

$$\begin{aligned}&\left|\Delta_n G(\tfrac{x}{n})\tau_x h(\eta_{tn^2})\right|\le 2\|G''\|_\infty,\\ &c_1(t,G)\le\|G'\|_\infty+n^{1-\theta}m\|G\|_\infty,\\ &c_{n-1}(t,G)\le\|G'\|_\infty+n^{1-\theta}m\|G\|_\infty,\end{aligned} \tag{26}$$

where $c_1(t,G)$ (resp. $c_{n-1}(t,G)$) corresponds to the term on the second and third (resp. fourth and fifth) lines of (16). So, since $\theta\ge 1$, by (16) and (26) we have that

$$\lim_{\gamma\to 0}\limsup_{n\to\infty}\mathbb{E}_{\mu_n}\left(\sup_{|t-s|\le\gamma}\left|\int_s^t n^2L_n\langle\pi_r^n,G\rangle dr\right|\right)$$
$$\le\lim_{\gamma\to 0}\limsup_{n\to\infty}\left(2\|G''\|_\infty+2\|G'\|_\infty+2mn^{1-\theta}\|G\|_\infty\right)\gamma=0.$$

This proves (23).

Tightness for $\theta \in [0, 1)$. If we try to apply the same strategy used for $\theta \geq 1$, we will run into trouble trying to control the modulus of continuity of $\int_0^t n^2 L_B \langle \pi_s^n, G\rangle ds$, because this expression can explode with n. However, since this expression depends on the value of $G(\frac{1}{n})$ and $G(\frac{n-1}{n})$, they vanish if the test function G has compact support in $(0, 1)$. Therefore, we can reuse the computations for $\theta \geq 1$ to show that (22) and (23) are still valid when $G \in C_c^2(0, 1)$. The problem here is that (22) and (23) need to be valid for $G \in C(0, 1)$. To accomplish that, we take a function $G \in C^1[0, 1] \subset L^1[0, 1]$, and we take a sequence of functions $\{G_k\}_{k\geq 0} \in C_c^2(0, 1)$ converging to G with respect to the L^1-norm as $k \to \infty$. Now, since

$$\begin{aligned}
&\mathbb{P}_{\mu_n}\left(\sup_{|t-s|\leq\gamma} |\langle \pi_t^n, G\rangle - \langle \pi_s^n, G\rangle| > \varepsilon\right)\\
\leq &\mathbb{P}_{\mu_n}\left(\sup_{|t-s|\leq\gamma} |\langle \pi_t^n, G_k\rangle - \langle \pi_s^n, G_k\rangle| > \frac{\varepsilon}{2}\right)\\
+&\mathbb{P}_{\mu_n}\left(\sup_{|t-s|\leq\gamma} |\langle \pi_t^n, G - G_k\rangle - \langle \pi_s^n, G - G_k\rangle| > \frac{\varepsilon}{2}\right)
\end{aligned}$$

and G_k has compact support, from the computation above, it remains only to check that the last probability vanishes as $n \to \infty$, then $k \to \infty$ and $\gamma \to 0$. For that purpose, we use the fact that

$$|\langle \pi_t^n, G - G_k\rangle - \langle \pi_s^n, G - G_k\rangle| \leq \frac{2}{n} \sum_{x\in\Sigma_n} \left|(G - G_k)\left(\tfrac{x}{n}\right)\right|,$$

and we use the estimate

$$\begin{aligned}
\frac{1}{n} \sum_{x\in\Sigma_n} \left|(G - G_k)\left(\tfrac{x}{n}\right)\right| &\leq \sum_{x\in\Sigma_n} \int_{\frac{x}{n}}^{\frac{x+1}{n}} \left|(G - G_k)\left(\tfrac{x}{n}\right) - (G - G_k)(q)\right| dq\\
&\quad + \int_0^1 |(G - G_k)(q)| dq\\
&\leq \frac{1}{n}\|(G - G_k)'\|_\infty + \int_0^1 |(G - G_k)(q)| dq.
\end{aligned}$$

We conclude the result by taking first the lim sup in $n \to \infty$ and then in $k \to \infty$, and using the fact that $C^1([0, 1])$ is a dense subset of $C([0, 1])$.

5 Auxiliary Results

In this section we state all the replacement lemmas that are used along Sect. 3, but we only prove in details the replacement lemma needed for the boundary terms in the case $\theta < 1$ to get Dirichlet boundary conditions. Before stating the results we give some words on the argument. First we replace our general measure μ_n (which satisfies (12)) by a reference measure $\nu^n_{\rho(\cdot)}$ that is Bernoulli product and is defined in (27). Depending on the range of the parameter θ, some conditions will have to be imposed on the profile $\rho(\cdot)$. We note however that since we can control the entropy of μ_n with respect to this product measure, the choice on the type of profile does not impose any extra condition on the starting measure μ_n. Second, we will make use of the Feynman–Kac formula and we will have to control the error between the Dirichlet form of the process, defined in (28), and the quantity D_n defined in (29). We remark that D_n is the Dirichlet form that we would obtain in case the reference measure is reversible with respect to the exchange and the flip dynamics. Since the reference measure that we consider below is not invariant for all these transformations, some errors appear which have to vanish in the limit. This is the purpose of the next subsection.

5.1 Dirichlet Forms

Let $\rho : [0, 1] \to [0, 1]$ be a measurable profile and let $\nu^n_{\rho(\cdot)}$ be the Bernoulli product measure on Ω_n with marginals given by

$$\nu^n_{\rho(\cdot)}\{\eta(x) = 1\} = \rho(\tfrac{x}{n}). \tag{27}$$

For a probability measure μ on Ω_n and a density $f : \Omega_n \to \mathbb{R}$ with respect to μ, the Dirichlet form of the process is defined as

$$\langle f, -L_n f\rangle_\mu = \langle f, -L_P f\rangle_\mu + \langle f, -L_B f\rangle_\mu + n^{a-2}\langle f, -L_S f\rangle_\mu, \tag{28}$$

where

$$\langle f, g\rangle_\mu = \sum_{\eta\in\Omega_n} f(\eta)g(\eta)\,\mu(\eta),$$

for all functions $f, g : \Omega_n \to \mathbb{R}$. Below we will also make use of the following quantities:

$$D_n(\sqrt{f}, \mu) := D_P(\sqrt{f}, \mu) + D_B(\sqrt{f}, \mu) + n^{a-2}D_S(\sqrt{f}, \mu), \tag{29}$$

where

$$D_P(\sqrt{f},\mu) := \sum_{x=1}^{n-2} D_P^x(\sqrt{f},\mu),$$

with

$$D_P^x(\sqrt{f},\mu) = \int \big[c_{x,x+1}(\eta)+c_{x+1,x}(\eta)\big]\Big[\sqrt{f(\eta^{x,x+1})}-\sqrt{f(\eta)}\Big]^2 d\mu, \tag{30}$$

$$D_{\mathbb{S}}(\sqrt{f},\mu) = \sum_{x=1}^{n-2}\int \big[\eta(x)+\eta(x+1)\big]^2\Big[\sqrt{f(\eta^{x,x+1})}-\sqrt{f(\eta)}\Big]^2 d\mu, \tag{31}$$

and

$$D_B(\sqrt{f},\mu) = \tfrac{m}{n^\theta}\Big(I_1^{\alpha,\gamma}(\sqrt{f},\mu)+I_{n-1}^{\beta,\delta}(\sqrt{f},\mu)\Big), \tag{32}$$

where $I_1^{\alpha,\gamma}$ and $I_{n-1}^{\beta,\delta}$ have the following expression

$$I_x^{a,c}(\sqrt{f},\mu) = \int [a(1-\eta(x))+c\,\eta(x)]\big[\sqrt{f(\eta^x)}-\sqrt{f(\eta)}\big]^2 d\mu, \tag{33}$$

for $a\in\{\alpha,\beta\}$, $c\in\{\gamma,\delta\}$ and $x\in\{1,n-1\}$. Our goal in this section consists in showing that when $\mu=\nu^n_{\rho(\cdot)}$, the Dirichlet form of the process (defined in (28)) is bounded from above by $D_n(\sqrt{f},\nu^n_{\rho(\cdot)})$, where f is a density with respect to $\nu^n_{\rho(\cdot)}$, plus an error that we can control. Since we have to consider the model for different regimes of θ, we will make use of different profiles $\rho(\cdot)$ when $\theta<1$ and when $\theta\geq 1$. Let $C:=C(\alpha,\beta,\gamma,\delta,\rho)>0$ be a constant which is independent of f and n. We claim that:

- for $\theta<1$ and for $\rho:[0,1]\to[0,1]$ a Lipschitz profile such that

$$\rho^- = \tfrac{\alpha}{\alpha+\gamma} = \rho(0)\leq\rho(u)\leq\rho(1) = \tfrac{\beta}{\beta+\delta} = \rho^+,$$

  and which is locally constant at the boundary, the following bound holds

$$\langle L_n\sqrt{f},\sqrt{f}\rangle_{\nu^n_{\rho(\cdot)}} \leq -\frac{1}{4}D_n(\sqrt{f},\nu^n_{\rho(\cdot)})+O(\tfrac{1}{n}). \tag{34}$$

- for $\theta\geq 1$ and for $\rho:[0,1]\to[0,1]$ a constant profile equal to, for example, ρ^-, the following bound holds

$$\langle L_n\sqrt{f},\sqrt{f}\rangle_{\nu^n_{\rho(\cdot)}} \leq -\frac{1}{4}D_n(\sqrt{f},\nu^n_{\rho(\cdot)})+O(\tfrac{1}{n^\theta}).$$

To prove the claim, we recall first the following lemma from [2]:

Lemma 1 *Let f be a density with respect to a finite positive measure μ on Ω_n and for $x, y \in \Sigma_n$ let $a_{x,y}(\eta)$ be a positive local function. Then, we have that*

$$\begin{aligned}
&\int a_{x,y}(\eta)\big[\sqrt{f(\eta^{x,y})} - \sqrt{f(\eta)}\big]\ \sqrt{f(\eta)}\, d\mu \\
&\leq -\frac{1}{4}\int a_{x,y}(\eta)\left[\sqrt{f(\eta^{x,y})} - \sqrt{f(\eta)}\right]^2 d\mu \\
&+ \frac{1}{16}\int \frac{1}{a_{x,y}(\eta)}\left[a_{x,y}(\eta) - a_{x,y}(\eta^{x,y})\frac{\mu(\eta^{x,y})}{\mu(\eta)}\right]^2\left[\sqrt{f(\eta^{x,y})} + \sqrt{f(\eta)}\right]^2 d\mu.
\end{aligned} \tag{35}$$

The same is true if $a_{x,y}$ is replaced by local functions a_x and $\eta^{x,y}$ by η^x.

We observe that the previous lemma is stated in [2] asking the measure μ to be a probability measure. In fact, the result of the lemma is true with the more general condition stated above and this is the one that suits our purposes.

The claim follows easily from this lemma. Let us start with the L_P dynamics and we take $\mu := \nu^n_{\rho(\cdot)}$. Note that, by definition we have that

$$\langle L_P\sqrt{f}, \sqrt{f}\rangle_{\nu^n_{\rho(\cdot)}} = \sum_{x=1}^{n-2}\int a_{x,x+1}(\eta)\left[\sqrt{f(\eta^{x,x+1})} - \sqrt{f(\eta)}\right]\sqrt{f(\eta)}\, d\nu^n_{\rho(\cdot)}, \tag{36}$$

where $a_{x,x+1}(\eta) := c_{x,x+1}(\eta) + c_{x+1,x}(\eta)$. Define $\Omega^x_n := \{\eta \in \Omega_n;\ a_{x,x+1}(\eta) \neq 0\}$. Now, use Lemma 1, (30) and note that $a_{x,x+1}(\eta) = a_{x,x+1}(\eta^{x,x+1})$ to bound each term of the sum above by $-\frac{1}{4}D^x_P(\sqrt{f}, \nu^n_{\rho(\cdot)})$ plus

$$\frac{1}{16}\int_{\Omega^x_n} a_{x,x+1}(\eta)\left[1 - \frac{\nu^n_{\rho(\cdot)}(\eta^{x,x+1})}{\nu^n_{\rho(\cdot)}(\eta)}\right]^2\left[\sqrt{f(\eta^{x,x+1})} + \sqrt{f(\eta)}\right]^2 d\nu^n_{\rho(\cdot)}.$$

Since $a_{x,x+1}(\eta) \leq c_1$ and $\left(\frac{\nu^n_{\rho(\cdot)}(\eta^{x,x+1})}{\nu^n_{\rho(\cdot)}(\eta)} - 1\right)^2 \leq c_2\Big(\rho\big(\frac{x}{n}\big) - \rho\big(\frac{x+1}{n}\big)\Big)^2$, for some constants $c_1 = c_1(\alpha, \beta, \gamma, \delta) > 0$ and $c_2 = c_2(\rho) > 0$, then the right-hand side of (36) is bounded from above by

$$-\frac{1}{4}D_P(\sqrt{f}, \nu^n_{\rho(\cdot)}) + C\sum_{x=1}^{n-2}\Big(\rho\big(\tfrac{x}{n}\big) - \rho\big(\tfrac{x+1}{n}\big)\Big)^2,$$

because f is a density with respect to $\nu^n_{\rho(\cdot)}$. Above $C = C(\alpha, \beta, \gamma, \delta, \rho)$. Now we look at the bulk dynamics from L_S, and the same proof as above shows that

$$\langle L_S\sqrt{f}, \sqrt{f}\rangle_{\nu^n_{\rho(\cdot)}} \leq -\frac{n^{a-2}}{4}D_S(\sqrt{f}, \nu^n_{\rho(\cdot)}) + C\sum_{x=1}^{n-2}\Big(\rho\big(\tfrac{x}{n}\big) - \rho\big(\tfrac{x+1}{n}\big)\Big)^2.$$

Finally, we look at the L_B dynamics. We claim that for $\theta \geq 0$ fixed, there exists a constant $C > 0$ (independent of f and n) such that

$$\begin{aligned}\langle L_B\sqrt{f}, \sqrt{f}\rangle_{\nu^n_{\rho(\cdot)}} \leq -\tfrac{1}{4} D_B(\sqrt{f}, \nu^n_{\rho(\cdot)}) + C\tfrac{m}{n^\theta}\big[(\alpha+\gamma)\rho(\tfrac{1}{n}) - \alpha\big]^2 \\ + C\tfrac{m}{n^\theta}\big[(\beta+\delta)\rho(\tfrac{n-1}{n}) - \beta\big]^2,\end{aligned} \tag{37}$$

for any density f with respect to $\nu^n_{\rho(\cdot)}$. Since L_B is the sum of two terms we just present the proof for one of them, namely the term which involves α and γ, but for the other one it is completely analogous. To prove the result it is enough to note that from Lemma 1 and (32), we have that

$$\begin{aligned}&\int \tfrac{m}{n^\theta}\big[\alpha(1-\eta(1)) + \gamma\eta(1)\big]\left[\sqrt{f(\eta^1)} - \sqrt{f(\eta)}\right]\sqrt{f(\eta)}\, d\nu^n_{\rho(\cdot)} \\ &\leq -\frac{1}{4} D_B(\sqrt{f}, \nu^n_{\rho(\cdot)}) \\ &+ \frac{m}{16\, n^\theta}\int \frac{1}{a_1(\eta)}\left[a_1(\eta) - a_1(\eta^1)\tfrac{\nu^n_{\rho(\cdot)}(\eta^1)}{\nu^n_{\rho(\cdot)}(\eta)}\right]^2\left[\sqrt{f(\eta^1)} + \sqrt{f(\eta)}\right]^2 d\nu^n_{\rho(\cdot)},\end{aligned}$$

where $a_1(\eta) := \alpha(1-\eta(1)) + \gamma\eta(1)$. By a simple computation we see that there exists a constant $c_3 = c_3(\alpha, \gamma, \rho) > 0$ such that

$$\frac{1}{a_1(\eta)}\left[a_1(\eta) - a_1(\eta^1)\tfrac{\nu^n_{\rho(\cdot)}(\eta^1)}{\nu^n_{\rho(\cdot)}(\eta)}\right]^2 \leq c_3\big[(\alpha+\gamma)\rho(\tfrac{1}{n}) - \alpha\big]^2,$$

uniformly on $\eta \in \Omega_n$. Finally, using the fact that f is a density with respect to $\nu^n_{\rho(\cdot)}$, and repeating the argument for the term which involves β and δ, we conclude (37). Putting together all the estimates that we have obtained we see that there exists a constant $\tilde{C} = \tilde{C}(\alpha, \gamma, \beta, \delta, \rho)$ such that

$$\begin{aligned}\langle L_n\sqrt{f}, \sqrt{f}\rangle_{\nu^n_{\rho(\cdot)}} \leq -\frac{1}{4} D_n(\sqrt{f}, \nu^n_{\rho(\cdot)}) + \tilde{C}\sum_{x=1}^{n-2}\Big(\rho(\tfrac{x}{n}) - \rho(\tfrac{x+1}{n})\Big)^2 \\ + \tilde{C}\tfrac{m}{n^\theta}\big[(\alpha+\gamma)\rho(\tfrac{1}{n}) - \alpha\big]^2 \\ + \tilde{C}\tfrac{m}{n^\theta}\big[(\beta+\delta)\rho(\tfrac{n-1}{n}) - \beta\big]^2.\end{aligned} \tag{38}$$

From the previous bound it is quite easy to see that the claim follows.

5.2 Replacement Lemmas

We start this section by proving the next lemma which is an adaptation of Lemma 5.5 of [2].

Lemma 2 *Let $\varphi : \Omega \to \Omega$ be a positive and bounded function which does not depend on the value of the configuration η at the site 1. For any density f with respect to $\nu^n_{\rho(\cdot)}$ and any positive constant A, there exists a constant $C := C(\varphi) > 0$ such that*

$$\Big|\langle\varphi(\eta)(\alpha-(\alpha+\gamma)\eta(1)),\, f\rangle_{\nu^n_{\rho(\cdot)}}\Big| \le C\Big(\tfrac{1}{4A} I_1^{\alpha,\gamma}(\sqrt{f},\nu^n_{\rho(\cdot)}) + \tfrac{A}{4} + \Big|(\alpha+\gamma)\rho(\tfrac{1}{n})-\alpha\Big|\Big).$$

The same result holds if α (resp. γ) is replaced by β (resp. δ) and $\eta(1)$ is replaced with $\eta(n-1)$ and in that case the function φ does not depend on the value of the configuration η at the site $n-1$.

Proof By summing and subtracting appropriate terms, we have that

$$\begin{aligned}
&|\langle\varphi(\eta)(\alpha-(\alpha+\gamma)\eta(1)),\, f\rangle_{\nu^n_{\rho(\cdot)}}| \\
&\qquad \le \frac{1}{2}\left|\int \varphi(\eta)(\alpha-(\alpha+\gamma)\eta(1))[f(\eta)-f(\eta^1)]\, d\nu^n_{\rho(\cdot)}\right| \\
&\qquad + \frac{1}{2}\left|\int \varphi(\eta)(\alpha-(\alpha+\gamma)\eta(1))[f(\eta)+f(\eta^1)]\, d\nu^n_{\rho(\cdot)}\right|.
\end{aligned}$$

From Young's inequality and Lemma 5.2 of [2], the first term at the right side of last display is bounded from above by

$$\begin{aligned}
&\frac{A}{4}\int \frac{(\varphi(\eta)(\alpha-(\alpha+\gamma)\eta(1)))^2}{a_1(\eta)}\left(\left[\sqrt{f(\eta^1)}\right]+\left[\sqrt{f(\eta)}\right]\right)^2 d\nu^n_{\rho(\cdot)} + \frac{I_1^{\alpha,\gamma}(\sqrt{f},\nu^n_{\rho(\cdot)})}{4A} \\
&\le C_1\Big(\frac{A}{4}+\frac{I_1^{\alpha,\gamma}(\sqrt{f},\nu^n_{\rho(\cdot)})}{4A}\Big),
\end{aligned}$$

where $a_1(\eta) = \alpha(1-\eta(1)) + \gamma\eta(1)$. Above A is a positive constant. In last inequality we used the fact that $\varphi(\cdot)$ is bounded. Now we treat the remaining term. Let $\bar{\eta}$ denote the configuration η removing its value at 1. For the remaining term we do the following estimates:

$$\begin{aligned}
&\frac{1}{2}\Big|\sum_{\bar{\eta}}\big(-\gamma\varphi(\bar{\eta})(f(1,\bar{\eta})+f(0,\bar{\eta}))\nu^n_{\rho(\cdot)}(\eta(1)=1) \\
&+\alpha\varphi(\bar{\eta})(f(0,\bar{\eta})+f(1,\bar{\eta}))\nu^n_{\rho(\cdot)}(\eta(1)=0)\big)\,\nu^n_{\rho(\cdot)}(\bar{\eta})\Big| \\
&\quad = \frac{1}{2}\Big|\sum_{\bar{\eta}}\Big(\alpha-(\alpha+\gamma)\rho(\tfrac{1}{n})\Big)\varphi(\bar{\eta})(f(0,\bar{\eta})+f(1,\bar{\eta}))\nu^n_{\rho(\cdot)}(\bar{\eta})\Big| \\
&\le C_2\Big|\alpha-(\alpha+\gamma)\rho(\tfrac{1}{n})\Big|\sum_{\bar{\eta}}\Big(\rho(\tfrac{1}{n})f(1,\bar{\eta})\nu^n_{\rho(\cdot)}(\bar{\eta})+\Big(1-\rho(\tfrac{1}{n})\Big)f(0,\bar{\eta})\nu^n_{\rho(\cdot)}(\bar{\eta})\Big) \\
&\quad = C_2\Big|\alpha-(\alpha+\gamma)\rho(\tfrac{1}{n})\Big|\sum_{\eta\in\Omega_n} f(\eta)\nu^n_{\rho(\cdot)}(\eta) = C_2\Big|\alpha-(\alpha+\gamma)\rho(\tfrac{1}{n})\Big|.
\end{aligned}$$

The notation $f(j,\bar{\eta})$ means that we are computing $f(\eta)$ with $\eta(1)=j$ with $j\in\{0,1\}$. Above we used the fact that the profile is bounded below and above by a constant and the fact that f is a density. This finishes the proof taking $C=C_1\vee C_2$.

Theorem 2 *Let $\varphi:\Omega\to\Omega$ be a positive and bounded function which does not depend on the value of the configuration η at the site 1. Fix $\theta<1$. For any $t\in[0,T]$ we have that*

$$\limsup_{n\to+\infty}\mathbb{E}_{\mu_n}\left[\left|\int_0^t\varphi(\eta_{sn^2})(\alpha-(\alpha+\gamma)\eta_{sn^2}(1))ds\right|\right]=0. \tag{39}$$

The same is true replacing α by β, γ by δ and 1 by $n-1$. In last case, the function $\varphi:\Omega\to\Omega$ does not depend on the value of the configuration η at the site $n-1$.

Proof We consider a Lipschitz profile $\rho:[0,1]\to[0,1]$ such that

$$\rho^-=\tfrac{\alpha}{\alpha+\gamma}=\rho(0)\le\rho(u)\le\rho(1)=\tfrac{\beta}{\beta+\delta}=\rho^+,$$

and $\nu^n_{\rho(\cdot)}$ is given by (27). Note that the expectation in the statement of the theorem can be written as $\int\mathbb{E}_\eta\left[\left|\int_0^t\varphi(\eta_{sn^2})(\alpha-(\alpha+\gamma)\eta_{sn^2}(1))ds\right|\right]d\mu_n$. Now we use the entropy inequality and the last expectation is bounded from above, for any $B>0$, by

$$\frac{H(\mu_n|\nu^n_{\rho(\cdot)})}{Bn}+\frac{1}{Bn}\log\int e^{B\mathbb{E}_\eta\left[\left|\int_0^t\varphi(\eta_{sn^2})(\alpha-(\alpha+\gamma)\eta_{sn^2}(1))ds\right|\right]}d\nu^n_{\rho(\cdot)}, \tag{40}$$

and at this point we use Jensen's inequality and we bound the previous display by

$$\frac{H(\mu_n|\nu^n_{\rho(\cdot)})}{Bn}+\frac{1}{Bn}\log\int\mathbb{E}_\eta\left[e^{Bn\left|\int_0^t\varphi(\eta_{sn^2})(\alpha-(\alpha+\gamma)\eta_{sn^2}(1))ds\right|}\right]d\nu^n_{\rho(\cdot)}, \tag{41}$$

which is equal to

$$\frac{H(\mu_n|\nu^n_{\rho(\cdot)})}{Bn}+\frac{1}{Bn}\log\mathbb{E}_{\nu^n_{\rho(\cdot)}}\left[e^{Bn\left|\int_0^t\varphi(\eta_{sn^2})(\alpha-(\alpha+\gamma)\eta_{sn^2}(1))ds\right|}\right]. \tag{42}$$

Since $e^{|x|}\le e^x+e^{-x}$ and

$$\limsup_{n\to+\infty}n^{-1}\log(a_n+b_n)=\max\{\limsup_{n\to+\infty}n^{-1}\log(a_n),\limsup_{n\to+\infty}n^{-1}\log(b_n)\},$$

we can remove the absolute value inside the exponential in (42). Now, using the explicit form for the entropy we have that

$$H(\mu_n|\nu^n_{\rho(\cdot)}) = \sum_{\eta\in\Omega_n} \mu_n(\eta)\log\left(\frac{\mu_n(\eta)}{\nu^n_{\rho(\cdot)}(\eta)}\right) \leq \sum_{\eta\in\Omega_n} \mu_n(\eta)\log\left(\frac{1}{\nu^n_{\rho(\cdot)}(\eta)}\right)$$
$$\leq n\log\left(\rho^- \wedge (1-\rho^+)\right) \leq nC_{\alpha,\beta,\gamma,\delta}. \tag{43}$$

By (43) and Feynman–Kac's formula we can estimate (42) from above by

$$\frac{C_{\alpha,\beta,\gamma,\delta}}{B} + t\sup_f \left\{\langle\varphi(\eta)(\alpha-(\alpha+\gamma)\eta(1)),\, f\rangle_{\nu^n_{\rho(\cdot)}} + \frac{n}{B}\langle L_n\sqrt{f},\sqrt{f}\rangle_{\nu^n_{\rho(\cdot)}}\right\}, \tag{44}$$

where the supremum is carried over all the densities f with respect to $\nu^n_{\rho(\cdot)}$. By Lemma 2 with the choice $A = 4Bn^{\theta-1}mC^{-1}$ we have that

$$\left|\langle\varphi(\eta)(\alpha-(\alpha+\gamma)\eta(1)),\, f\rangle_{\nu^n_{\rho(\cdot)}}\right| \leq \frac{n}{4B}D_B(\sqrt{f},\nu^n_{\rho(\cdot)}) + \frac{4Bn^\theta}{nm} + C\left|(\alpha+\gamma)\rho(\tfrac{1}{n})-\alpha\right|.$$

From (38) and the inequality above, the term on the right-hand side of (44), is bounded from above by

$$\frac{4Bn^\theta}{nm} + C\left|(\alpha+\gamma)\rho(\tfrac{1}{n})-\alpha\right| + \frac{1}{B}\tilde{C}\sum_{x=1}^{n-2}\left(\rho(\tfrac{x}{n})-\rho(\tfrac{x+1}{n})\right)^2$$
$$+\tilde{C}\frac{m}{n^\theta}\left[(\alpha+\gamma)\rho(\tfrac{1}{n})-\alpha\right]^2 + \tilde{C}\frac{m}{n^\theta}\left[(\beta+\delta)\rho(\tfrac{n-1}{n})-\beta\right]^2. \tag{45}$$

Above $\tilde{C} = C(\alpha,\gamma,\beta,\delta,\rho)$. Taking $n\to\infty$ on last term and using the fact that ρ is Lipschitz, that $\rho(0) = \frac{\alpha}{\alpha+\gamma}$ and $\rho(1) = \frac{\beta}{\beta+\delta}$, we have that these terms vanish since $\theta < 1$. To finish we send $B\to+\infty$ and we are done.

Now we state the other replacement lemmas that are needed in order to close the martingales of Sect. 3. We start with the replacement lemma that is needed to recover the Robin boundary conditions and below we state the replacement lemma that is needed in order to obtain the diffusion term in all the partial differential equations.

Theorem 3 *Fix $\theta \geq 1$. For $x = 1$ and $x = n-1$; and for any $t\in[0,T]$, we have*

$$\limsup_{\varepsilon\to 0}\limsup_{n\to+\infty}\mathbb{E}_{\mu_n}\left[\left|\int_0^t\left(\eta_{sn^2}(x) - \overrightarrow{\eta}^{\varepsilon n}_{sn^2}(x)\right)ds\right|\right] = 0,$$

$\overrightarrow{\eta}^{\varepsilon n}_{sn^2}(x)$ where was defined in (19).

Theorem 4 *For any $\theta\geq 0$, $G\in C^2([0,1])$ and for any $t\in[0,T]$, we have*

$$\limsup_{\varepsilon\to 0}\limsup_{n\to+\infty}\mathbb{E}_{\mu_n}\left[\left|\int_0^t\frac{1}{n}\sum_{x=1}^{n-1}G(\tfrac{x}{n})\left[\tau_x h(\eta_{sn^2}) - (\overrightarrow{\eta}^{\varepsilon n}_{sn^2}(x))^2\right]ds\right|\right] = 0,$$

where $\tau_x h$ is defined in (15) and $\overrightarrow{\eta}^{\varepsilon n}_{sn^2}(x)$ where was defined in (19).

We do not present in this paper the proof of the two previous results but we note that they will be rigorously proved in a coming paper where we combine the results of [1, 5] to this setting. Since the two previous replacement lemmas are concerned with the bulk dynamics, we have first to eliminate configurations with few particles and then adapt the arguments of [1] to the configurations which have at least three particles so that they can move other particles which, in principle, are blocked by the bulk dynamics.

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On the Fibonacci Universality Classes in Nonlinear Fluctuating Hydrodynamics

G. M. Schütz

Abstract We present a lattice gas model that without fine tuning of parameters is expected to exhibit the so far elusive modified Kardar–Parisi–Zhang (KPZ) universality class. To this end, we review briefly how non-linear fluctuating hydrodynamics in one dimension predicts that all dynamical universality classes in its range of applicability belong to an infinite discrete family which we call Fibonacci family since their dynamical exponents are the Kepler ratios $z_i = F_{i+1}/F_i$ of neighbouring Fibonacci numbers F_i, including diffusion ($z_2 = 2$), KPZ ($z_3 = 3/2$), and the limiting ratio which is the golden mean $z_\infty = (1 + \sqrt{5})/2$. Then we revisit the case of two conservation laws to which the modified KPZ model belongs. We also derive criteria on the macroscopic currents to lead to other non-KPZ universality classes.

1 Introduction

It is well-known that in one dimension transport in stationary states is usually anomalous even when the microscopic interactions are short-ranged and noise is uncorrelated [16]. This property manifests itself in transport coefficients that diverge, usually algebraically, with system size. This is in contrast to normal (i.e., diffusive) transport where the transport coefficients are material-dependent constants.

If for n globally conserved quantities N_α (such as mass, energy, etc.) with densities $\bar\rho_\alpha$ the large-scale behaviour of the spatio-temporal fluctuations in the system is dominated by the long wave length modes $\rho_\alpha(x, t)$ of these conserved densities then anomalous behaviour is prominently captured also by the spatio-temporal correlations of the normal modes $\phi_\alpha(x, t) = \sum_\beta R_{\alpha\beta}(\rho_\beta(x, t) - \bar\rho_\beta)$. The normal modes are linear combinations of the fluctuation fields $\rho_\beta(x, t)$ of the n conserved quantities centered around their mean $\bar\rho_\beta$ defined in an orthonormal eigenbasis in which the center of mass of the modes travel with the so-called collective velocity v_α. Here the coefficients $R_{\alpha\beta}$ depend on the mean densities $\bar\rho_\beta$. Anomalous scaling properties

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manifest themselves by non-Gaussian dynamical universality classes with dynamical exponents $z_\alpha \neq 2$, including the celebrated Kardar–Parisi–Zhang (KPZ) universality class where $z = 3/2$ [12, 27], or another universality class with $z = 3/2$ [1, 2, 18, 26].

If all collective velocities v_α are different the theory of nonlinear fluctuating hydrodynamics (NLFH) [26] predicts that, in a comoving frame with collective velocity v_α, the normalized dynamical structure function of mode α, i.e., the stationary correlation function $S_\alpha(x,t) := \langle\, \phi_\alpha(x,t)\phi_\alpha(0,0)\,\rangle$, has a scaling limit of the form $S_\alpha(x,t) = t^{-1/z_\alpha} f_\alpha((x - v_\alpha t)/(\lambda_\alpha t)^{z_\alpha})$. Here $f_\alpha(\cdot)$ is a *universal* scaling function that does not depend depend on the microscopic details of the interaction. Non-universal are the scale factors λ_α as well as the collective velocities and the coefficients $R_{\alpha\beta}$ that all depend on the stationary densities $\bar\rho_\alpha$ and the stationary currents $\bar j^\alpha(\bar\rho_1, \ldots, \bar\rho_n)$ associated with the conserved quantities. For diffusion the scaling function is a Gaussian, while for the KPZ universality class one has the Prähofer-Spohn function [22].[1]

Thus the main quantities of interest in the study of spatio-temporal fluctuations in one space dimension are the dynamical exponents z_α and the scaling functions $f_\alpha(\cdot)$. They determine the dynamical universality class that a given microscopic model belongs to. Remarkably, it was found [20] that the possible dynamical exponents are either sequences of the Kepler ratios $z_i = F_{i+1}/F_i$ of neighbouring Fibonacci numbers F_i beginning with $z_2 = 2 = 2/1$ or with $z_3 = 3/2$, or the golden mean $z_\infty = (1 + \sqrt{5})/2$ which is the limiting value $i \to \infty$ of the Kepler sequence. For two conservation laws the dynamical exponents $z_2 = 2$ and $z_3 = 3/2$ as well as a pair of golden mean modes may appear [19, 28], while for $n > 2$ conservation laws Kepler ratios up to z_{n+1} are possible. Also the corresponding scaling functions have been determined, with one exception, which is the so-called modified Kardar–Parisi–Zhang universality class [28] for which, however, until now no generic microscopic model has been proposed.

In the following we briefly review the reasoning that leads to these predictions. We follow mainly the arguments put forward in Refs. [21, 26] which lead, via mode coupling theory, to the conclusion that the dynamical universality class of a mode can be deducted from the above-mentioned macroscopic stationary current-density relation $\bar j^\alpha(\bar\rho_1, \ldots, \bar\rho_n)$ through the so-called mode-coupling matrices (Sect. 2). Then we revisit the case of two conservation laws studied in some detail already in [19] and [28]. In Sect. 3 we construct a microscopic lattice gas model that, without fine-tuning of parameters, is predicted to be in the modified Kardar–Parisi–Zhang universality class. Finally, in Sect. 4, we present in a "consumer-friendly" fashion the criteria on the currents $\bar j^\alpha(\bar\rho_1, \ldots, \bar\rho_n)$ under which only non-KPZ universality classes appear in systems with two conservation laws.

[1] If some collective velocities are equal then the crucial assumption of spatial separation of the normal modes at large times breaks down. The predictions of NLFH for this case have not been studied yet in great detail.

2 Nonlinear Fluctuating Hydrodynamics

2.1 Notation and General Properties of Fluctuations

In order to fix ideas we consider discrete microscopic models that evolve in continuous time t and that have n locally conserved quantities. By this we mean the following. Let $\mathbb{S}$ be some set, Λ denote a contiguous set of integers, and $\eta_k \in \mathbb{S}$ with $k \in \Lambda$ be the local state variable. The index k denotes a lattice site or a particle in a chain, depending on the type of model one has in mind. A microscopic configuration at time t is thus given by $\eta(t) = \{\eta_k(t) : k \in \Lambda\}$.[2] The generator of the dynamics is denoted by $\mathscr{L}$. The translation operator is denoted by $\mathscr{T}$ and defined by the property $\mathscr{T}(\eta_k) = \eta_{k+1}$, and similar for functions of the local state variables. We assume the dynamics to be translation invariant, i.e., $\mathscr{T}\mathscr{L} = \mathscr{L}\mathscr{T}$, with the identification $\eta_k \equiv \eta_{k+L}$ if Λ is the integer torus.

In order to introduce conservation laws consider a cylinder function $\xi_0^\alpha(\eta)$ where $\alpha \in \{1, \ldots, n\}$ and define $\xi_k^\alpha(\eta) := \mathscr{T}^k(\xi_0^\alpha(\eta))$. We shall assume that (i) the $\xi_k^\alpha(\eta)$ satisfy the discrete continuity equations

$$\mathscr{L}(\xi_k^\alpha(\eta)) = j_{k-1}^\alpha(\eta) - j_k^\alpha(\eta) \tag{1}$$

for all α, (ii) only the $\xi_k^\alpha(\eta)$ have this property, and (iii) that also the so-called microscopic currents $j_k^\alpha(\eta)$ are cylinder functions. We shall drop the dependence of the conserved quantities ξ_k^α and currents j_k^α on the configuration η.

Following [11, 30] we postulate that there exists a family of translation invariant grand-canonical measures parametrized by fugacities φ^α which are translation invariant and invariant under the dynamics generated by $\mathscr{L}$. Expectations under this measure with fixed values φ^α are denoted by $\langle \cdot \rangle$. In particular, we introduce the stationary conserved densities $\bar{\rho}_\alpha := \langle \xi_k^\alpha \rangle$ and the stationary currents $\bar{j}^\alpha := \langle j_k^\alpha \rangle$. The first and second derivatives of the currents $\bar{j}^\alpha$ w.r.t. the densities $\bar{\rho}_\beta$, $\bar{\rho}_\gamma$ are denoted by $\bar{j}_\beta^\alpha$ and $\bar{j}_{\beta\gamma}^\alpha$.

The dynamical structure matrix $\bar{\mathbf{S}}_k(t)$ is defined by the matrix elements

$$\bar{S}_k^{\alpha\beta}(t) := \langle \left(\xi_k^\alpha(t) - \bar{\rho}_\alpha\right)\left(\xi_0^\beta(0) - \bar{\rho}_\beta\right) \rangle. \tag{2}$$

The compressibility matrix $\mathbf{K} = \sum_k \bar{\mathbf{S}}_k(t)$ is the covariance matrix of the conserved quantities which is independent of time due to the conservation laws (1). The current Jacobian $\mathbf{J}$ is the matrix with matrix elements $J_{\alpha\beta} = \bar{j}_\beta^\alpha$ and the Hessians $\mathbf{H}^\alpha$ have matrix elements $H_{\beta\gamma}^\alpha = \bar{j}_{\beta\gamma}^\alpha$. The n-dimensional unit matrix is denoted by $\mathbb{1}$. Transposition of a matrix is denoted by the superscript T.

[2] When the time t is irrelevant we drop the dependence on t.

We make the mild (but essential !) assumptions on the invariant measure that for all α, β one has $K_{\alpha\beta} < \infty$ and $\lim_{k\to\infty} k\langle \left(\xi_0^\alpha - \bar{\rho}_\alpha\right) j_k^\beta \rangle = 0$ [11]. These hypotheses imply the Onsager-type current symmetry

$$\frac{\partial \bar{j}^\beta}{\partial \phi^\alpha} = \frac{\partial \bar{j}^\alpha}{\partial \phi^\beta} \tag{3}$$

for all α, β.[3] In particular, the chain rule implies [26]

$$\mathbf{JK} = (\mathbf{JK})^T. \tag{4}$$

The current symmetry (3) ensures that the current Jacobian has real eigenvalues which we denote by v_α. It should be noted that the assumption of locality of the conserved quantity and the associated current as well as the finite number n of conservation laws also rules out models with infinitely many and non-local conservation laws. Nevertheless, some of the phenomenology of such models seems to be similar to the finite and local case [15]. Some models with non-decaying correlations exhibit phase separation [3, 13, 23].

Throughout this work we shall assume complete absence of degeneracy of the eigenvalues v_α. Then one can always write $\mathbf{V} := \mathbf{RJR}^{-1} = \mathrm{diag}(v_1, \ldots, v_n)$. By convention we choose the normalization

$$\mathbf{RKR}^T = \mathbb{1}. \tag{5}$$

The eigenmodes are defined to be the transformed fluctuation fields $\phi_k^\alpha(t) := \sum_\beta R_{\alpha\beta}\bar{\rho}_k^\beta(t)$. They give rise to the normal form of the dynamical structure matrix

$$\mathbf{S}_k(t) := \mathbf{R}\bar{\mathbf{S}}_k(t)\mathbf{R}^T \tag{6}$$

which satisfies $\sum_k \mathbf{S}_k(t) = \mathbb{1}$ for all t. The conservation law, translation invariance and the mild decay of stationary correlations as assumed for the invariant measure yields the exact relation $d/dt \sum_k k\mathbf{S}_k(t) = \mathbf{V}$ for all t.

We point out that the dynamical structure functions $S_k^{\alpha\beta}(t)$ have an alternative meaning as describing the relaxation of a microscopic perturbation of the invariant measure at the origin $k = 0$ [19]. As the perturbation evolves in time, it separates into distinct density peaks, one for each mode α. The eigenvalues v_α are the center-of-mass velocities of these perturbations. The variance w.r.t. k of the diagonal structure function $S_k^{\alpha\alpha}(t)$ describes, on lattice scale, the spatial spreading of mode α.

[3] It seems to have gone unnoticed that, quite remarkably, this symmetry relates a purely static property of the invariant measure (the covariances $K_{\alpha\beta}$) with the microscopic dynamics which give rise to the currents $\bar{j}^\alpha$. This restricts severely the possible microscopic dynamics for which a given measure can be invariant.

2.2 Nonlinear Fluctuating Hydrodynamics

In the hydrodynamic limit where the "lattice" spacing tends to zero we denote the scaling limits of the density by $\rho_\alpha(x,t)$, $\bar{\rho}_\alpha(x,t)$, and $\phi_\alpha(x,t)$ resp. Under Eulerian scaling one expects from the law of large numbers and local stationarity [14] that the discrete continuity equation (1) gives rise to the system of conservation laws $\partial_t \rho_\alpha(x,t) + \partial_x j_\alpha(x,t) = 0$ where the currents $j_\alpha(x,t)$ depend on x and t only through the local densities $\rho_\alpha(x,t)$ via the stationary current-density relation.[4] Thus one can write $j_\alpha(x,t) = j_\alpha(\rho_1(x,t), \ldots, \rho_n(x,t))$ which gives

$$\partial_t \rho_\alpha(x,t) + \sum_\beta J_{\alpha\beta}(\rho_1(x,t), \ldots, \rho_n(x,t))\partial_x \rho_\beta(x,t) = 0. \tag{7}$$

Non-degeneracy of $\mathbf{J}$ implies that this nonlinear system of conservation laws is strictly hyperbolic. Obviously, the constant functions $\rho_\alpha(x,t) = \bar{\rho}_\alpha$ form a translation invariant stationary solution.

In order to study fluctuations one expands around a fixed stationary solution and adds to the current a phenomenological diffusion term with diffusion matrix $\tilde{\mathbf{D}}(\bar{\rho}_1, \ldots, \bar{\rho}_n)$ and Gaussian white noise $\tilde{\zeta}^\alpha(x,t)$ with an amplitude that is usually taken to satisfy the fluctuation-dissipation theorem. Renormalization group arguments suggest that only terms up to second order in the density expansion are relevant. Third order terms may lead to logarithmic corrections to the fluctuations, but only if the second-order term vanishes. All higher order terms vanish in the scaling limit of large x and large t [5]. Thus, omitting arguments, one arrives at the non-linear fluctuating hydrodynamics equation [26]

$$\partial_t \bar{\rho}_\alpha(x,t) + \partial_x \left[\sum_\beta \hat{J}_{\alpha\beta} \bar{\rho}_\beta(x,t) + \frac{1}{2} \sum_{\beta\gamma} \bar{\rho}_\beta(x,t) H^\alpha_{\beta\gamma} \bar{\rho}_\gamma(x,t) + \tilde{\zeta}_\alpha(x,t) \right] = 0 \tag{8}$$

with linear current operator $\hat{J}_{\alpha\beta} = J_{\alpha\beta} - \tilde{D}_{\alpha\beta}\partial_x$.

In terms of the eigenmodes one has

$$\partial_t \phi_\alpha(x,t) + \partial_x \left[\sum_\beta \hat{V}_{\alpha\beta} \partial_x \phi_\beta(x,t) + \sum_{\beta\gamma} \phi_\beta(x,t) G^\alpha_{\beta\gamma} \phi_\gamma(x,t) + \zeta_\alpha(x,t) \right] = 0 \tag{9}$$

with $\hat{V}_{\alpha\beta} = v_\alpha \delta_{\alpha\beta} - D_{\alpha\beta}\partial_x$ where $\mathbf{D} = \mathbf{R}\tilde{\mathbf{D}}\mathbf{R}^{-1}$, the symmetric mode coupling matrices

[4] We stress that for more than one conservation law this expectation is mathematically very difficult to prove. Not only is on macroscopic level existence and uniqueness of global solutions in time a major open problem in pde theory, but also the derivation of the hydrodynamic limit after the occurrence shocks, which is a generic property of hyperbolic systems of conservation laws, is largely an open problem, with some results only for the Leroux system [9].

$$\mathbf{G}^\alpha = \frac{1}{2}\sum_\lambda R_{\alpha\lambda}(\mathbf{R}^{-1})^T \mathbf{H}^\lambda \mathbf{R}^{-1}, \tag{10}$$

and transformed noise $\zeta_\alpha(x,t) = \sum_\lambda R_{\alpha\lambda}\tilde{\zeta}_\lambda(x,t)$ with covariance $\langle\, \zeta_\alpha(x,t)\zeta_\beta(x',t')\,\rangle = 2D_{\alpha\beta}\delta(x-x')\delta(t-t')$. One recognizes in (9) a system of coupled noisy Burgers equations which with the substitution $\bar{\rho}_\alpha(x,t) = \partial_x h_\alpha(x,t)$ turns into a system of coupled KPZ equations [6, 7, 10, 25].

2.3 Mode Coupling Theory

Following [26] one writes the stochastic pde (9) in discretized form $\phi_\alpha(x,t) \to \phi_\alpha(n,t)$ with $n \in \mathbb{Z}$ in terms of a generator $L = L_0 + L_1$ where L_0 represents the linear part involving $\hat{\mathbf{V}}$ and L_1 represents the non-linear part involving the mode-coupling matrices $\mathbf{G}^\alpha$. This yields $S_{\alpha\beta}(n,t) = \langle\, \phi_\beta(0,0)\mathrm{e}^{Lt}\phi_\alpha(n,0)\,\rangle$ and therefore

$$\frac{\mathrm{d}}{\mathrm{d}t}S_{\alpha\beta}(n,t) = \langle\, \phi_\beta(0,0)\mathrm{e}^{Lt}L_0\phi_\alpha(n,0)\,\rangle + \langle\, \phi_\beta(0,0)\left(\mathrm{e}^{Lt}L_1\phi_\alpha(n,0)\right)\rangle. \tag{11}$$

The discretization of the generator is chosen such that a product of mean-zero Gaussian measures for the $\phi_\alpha(n) \equiv \phi_\alpha(n,0)$ is invariant under the stochastic evolution.

We insert the identity $\mathrm{e}^{Lt} = \mathrm{e}^{L_0 t} + \int_0^t \mathrm{d}s\, \mathrm{e}^{L_0(t-s)}L_1\mathrm{e}^{Ls}$ into the second term on the r.h.s. of (11). The first contribution involving only the linear evolution vanishes since by closer inspection one realizes that one is left with the expectation of cubic terms which are zero. The second contribution involves higher order correlators which due to the Gaussian measure can be factorized into pair correlations using the Wick rule. Finally, one replaces the bare evolution $\mathrm{e}^{L_0(t-s)}$ by the interacting evolution $\mathrm{e}^{L(t-s)}$ and takes the continuum limit. One arrives at the mode coupling equation [26]

$$\begin{aligned}\partial_t S_{\alpha\beta}(x,t) = &-v_\alpha\partial_x S_{\alpha\beta}(x,t) + \sum_\gamma D_{\alpha\gamma}\partial_x^2 S_{\gamma\beta}(x,t)\\ &+ \int_0^t \mathrm{d}s \int_{-\infty}^{\infty}\mathrm{d}y\, \partial_y^2 \sum_\gamma M_{\alpha\gamma}(y,s)S_{\gamma\beta}(x-y,t-s)\end{aligned} \tag{12}$$

with the memory term

$$M_{\alpha\gamma}(y,s) = 2\sum_{\mu\mu'\nu\nu'} G^\alpha_{\mu\nu}G^\gamma_{\mu'\nu'}S_{\mu\mu'}(y,s)S_{\nu\nu'}(y,s). \tag{13}$$

Next we recall that in the strictly hyperbolic case all modes drift with different velocities. Hence after time t their centers of mass are a distance of order t apart. On the other hand, the broadening of the peaks is expected to grow sublinearly.

Hence, eventually the offdiagonal terms $S_{\alpha\beta}(x,t)$ die out and can be neglected. With $S_\alpha(x,t) \equiv S_{\alpha\alpha}(x,t)$ the mode-coupling equations thus reduce to

$$\partial_t S_\alpha(x,t) = -v_\alpha \partial_x S_\alpha(x,t) + D_{\alpha\alpha}\partial_x^2 S_\alpha(x,t) + \int_0^t \mathrm{d}s \int_{-\infty}^{\infty} \mathrm{d}y\, \partial_y^2 M_{\alpha\alpha}(y,s) S_\alpha(x-y,t-s) \tag{14}$$

with the memory term

$$M_{\alpha\alpha}(y,s) = 2\sum_{\mu\nu} \left(G^\alpha_{\mu\nu}\right)^2 S_\mu(y,s) S_\nu(y,s). \tag{15}$$

2.4 Fibonacci Universality Classes

It was found in [20, 21] that the mode coupling equations (14) have scaling solutions which can be obtained in explicit form after Fourier and Laplace transformation. In order to classify the solutions we recall the recursive definition of the Fibonacci numbers $F_{n+1} = F_n + F_{n-1}$ with $F_1 = F_2 = 1$ and introduce the set $\mathbb{I}_\alpha := \{\beta : G^\alpha_{\beta\beta} \neq 0\}$ of modes β that give rise to a non-linear term in the time-evolution of mode α.

Theorem 1 (Refs. [20, 21]) *Let $u = pt^{1/z_\alpha}$ with dynamical exponent $z_\alpha > 1$. Then (1) In Fourier representation $\hat{S}_\alpha(p,t) := \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{\infty} \mathrm{d}x\, \mathrm{e}^{-ipx} S_\alpha(x,t)$ the mode coupling equation (14) with memory term (15) has for finite $|u|$ the scaling solution*

$$\lim_{t\to\infty} \mathrm{e}^{iv_\alpha pt} \hat{S}_\alpha(p,t) = \hat{f}_\alpha(u) \tag{16}$$

where

- *Case 1: For modes α such that $\mathbb{I}_\alpha = \emptyset$ one has $z_\alpha = 2$ and $\hat{f}_\alpha(u) = \frac{1}{\sqrt{2\pi}} \mathrm{e}^{-D_\alpha u^2}$ (diffusive universality class).*
- *Case 2: For modes α such that $\mathbb{I}_\alpha \neq \emptyset$ and $\alpha \notin \mathbb{I}_\alpha$ the dynamical exponents satisfy the nonlinear recursion $z_\alpha = \min_{\beta\in\mathbb{I}_\alpha} \left[\left(1 + \frac{1}{z_\beta}\right)\right]$ and the scaling function is given by $\hat{f}_\alpha(u) = \frac{1}{\sqrt{2\pi}} \mathrm{e}^{-E_\alpha |u|^{z_\alpha} \left[1 - iA_\alpha \tan\left(\frac{\pi z_\alpha}{2}\right) u/|u|\right]}$ with explicit real constants $E_\alpha > 0$, $A_\alpha \in [-1,1]$ given in [21] (Lévy universality class).*
- *Case 3: If $\alpha \in \mathbb{I}_\alpha$ then $z_\alpha = 3/2$. (a) If there is no diffusive mode $\beta \in \mathbb{I}_\alpha$, then $\hat{f}_\alpha(u) = \hat{f}^{MCT}_{KPZ}(u)$ given in [21] (KPZ universality class). (b) If there is at least one diffusive mode $\beta \in \mathbb{I}_\alpha$, then $\hat{f}_\alpha(u) = \hat{f}^{MCT}_{mKPZ}(u)$ given in [21] (modified KPZ universality class).*

(2) The non-linear recursion for the dynamical exponents in case 2 has as unique solution the sequence of Kepler ratios of Fibonacci numbers $z_i = F_{i+1}/F_i$, starting from $z_3 = 3/2$ (if at least one diffusive mode $\beta \in \mathbb{I}_\alpha$), or $z_4 = 5/3$ (if no diffusive mode but at least one KPZ mode $\beta \in \mathbb{I}_\alpha$) or else the golden mean $z_i = (1+\sqrt{5})/2$ for all modes i.

Remark 1 The subballistic scaling $z_\alpha > 1$ is motivated by the locality of interactions, conservation laws and currents. Since all dynamical exponents that can appear are Kepler ratios of neighbouring Fibonacci numbers we call the whole family of universality classes comprising diffusion, Lévy, KPZ and modified KPZ the *Fibonacci universality classes*.

The main ingredients in the proof of item (a) are strict hyperbolicity and power counting of the leading singularities in the Fourier-Laplace representation of the mode-coupling equation. Item (b) follows from the recursion of the Fibonacci numbers by a judiciously chosen ordering of the modes belonging to case 2.

We stress that the theorem deals with the function $S_\alpha(x,t)$ satisfying the mode coupling equations (14). There is no general rigorous result how this function relates to the true scaling limit of the dynamical structure function $S_k^{\alpha\alpha}(t)$. However, in the diffusive case 1 one expects the Gaussian scaling function to be the true scaling limit, up to possible logarithmic corrections. For specific models there are numerical [18–20] and mathematically rigorous results [1, 2] that suggest that the true scaling form in case 2 is indeed generally a Lévy distribution. However, the coefficients A_α, E_α arising from the mode-coupling equations are not believed to correspond to the true values. The scaling limit of $S_\alpha(x,t)$ has a closed expression in Fourier-Laplace representation also in case 3. However, for the case of a single conservation law (the usual KPZ universality class) it is known that this scaling function, studied in detail in [4, 8], is not exact but rather given by the Prähofer-Spohn scaling function [22]. Correspondingly, one does not expect the scaling forms $\hat{f}_{KPZ}^{MCT}(u)$ and $\hat{f}_{mKPZ}^{MCT}(u)$ solving the mode coupling equations (14) to exact either.

With these provisos Theorem 1 shows that, according to the mode coupling theory reviewed above, the dynamical universality classes of all modes are fully determined by whether or not the diagonal elements of the mode coupling matrices vanish. This in turn is fully determined by the stationary current-density density relation. Thus, as long as mode-coupling theory is valid, one can read off from this macroscopic stationary quantity alone the dynamical universality classes of all modes.

3 Two-Lane Lattice Gas for the Modified KPZ Universality Class

The modified KPZ universality class [28] arises for $G_{11}^1 = G_{22}^1 = 0$ and $G_{11}^2 \neq 0$, $G_{22}^2 \neq 0$, see case 3b) in Theorem 1. However, so far no microscopic model with this property has been proposed. Here we present a two-lane lattice gas that belongs to case 3b) in Theorem 1 for all values of the conserved densities without fine-tuning of model parameters. This model consists of two coupled one-dimensional lattice gases without self-interaction, but where the jump rates between sites k and $k+1$ of the particles of one gas depend on the number of particles of the other gas on the same pair of sites. It is convenient to describe this a model as a two-lane lattice gas

model in the spirit of the multi-lane exclusion processes of Popkov and Salerno [17], but without requiring exclusion.

We denote the number of particles on site k on lane i as particles of type by n_k^i. Thus the local state variable is the pair $\eta_k = (n_k^1, n_k^2) \in \mathbb{N}_0^2$. We introduce the parameters

$$r_i = \frac{1}{2}(w_i + f_i), \quad \ell_i = \frac{1}{2}(w_i - f_i), \quad g^{\pm} = \frac{1}{2}(\alpha \pm \gamma) \tag{17}$$

with strictly positive constants $w_i, \alpha > 0$, and $|f_i| \leq w_i$, $|\gamma| \leq \alpha$. We also define the mean pair occupation numbers

$$\bar{n}_k^i = \frac{1}{2}\left(n_k^i + n_{k+1}^i\right). \tag{18}$$

Informally, the stochastic dynamics is then defined as follows. A particle on lane 1 jumps independently of all other particles on lane 1 after an exponential waiting time from site k to site $k+1$ of lane 1 with rate $r^1(\bar{n}_k^2) = r_1 + g^+\bar{n}_k^2$ and from site $k+1$ to k with rate $\ell^1(\bar{n}_k^2) = \ell_1 + g^-\bar{n}_k^2$. Likewise, particles on lane 2 jump with rates $r^2(\bar{n}_k^1) = r_2 + g^+\bar{n}_k^1$ and from site $k+1$ to k and with rate $\ell^2(\bar{n}_k^1) = \ell_2 + g^-\bar{n}_k^1$. Thus w_i are the "bare" jump rates (i.e., in the absence of interaction), f_i are the bare jump biases, α is the interaction strength and γ is the interaction asymmetry.

With the updated state variable

$$\eta_l^{i;k,k'} = \begin{cases} n_k^i - 1 & \text{if } l = k \\ n_{k'}^i + 1 & \text{if } l = k' \\ n_k^i & \text{else} \end{cases} \tag{19}$$

the generators for independent random walkers read

$$(\mathscr{L}_i f)(\eta) = \sum_k \left[r_i \left(f(\eta^{i;k,k+1}) - f(\eta) \right) + \ell_i \left(f(\eta^{i;k+1,k}) - f(\eta) \right) \right]. \tag{20}$$

The interaction between the lanes is given by the generator

$$\begin{aligned} (\mathscr{L}_I f)(\eta) = \sum_k \Big\{ & \bar{n}_k^2 \left[g^+ f(\eta^{1;k,k+1}) + g^- f(\eta^{1;k+1,k}) - (g^+ + g^-) f(\eta) \right] \\ & + \bar{n}_k^1 \left[g^+ f(\eta^{2;k,k+1}) + g^- f(\eta^{2;k+1,k}) - (g^+ + g^-) f(\eta) \right] \Big\}. \end{aligned} \tag{21}$$

The generator of the full interacting process is then

$$\mathscr{L} = \mathscr{L}_1 + \mathscr{L}_2 + \mathscr{L}_I. \tag{22}$$

The interaction between the lanes does not change the invariant measure of the non-interacting part. Thus one arrives at

Proposition 1 *For parameters $\bar\rho_{1,2} \geq 0$ the product measure with factorized Poisson marginals*

$$\mu(\eta_k) = \frac{\bar\rho_1^{n_k^1}\mathrm{e}^{-\bar\rho_1}}{(n_k^1)!}\,\frac{\bar\rho_1^{n_k^2}\mathrm{e}^{-\bar\rho_2}}{(n_k^2)!} \tag{23}$$

for the occupation at site k is a translation invariant measure of the process defined by the generator (22).

Proof We prove the proposition for the finite torus $\Lambda = \{1, \ldots, L\}$ with L sites in the quantum operator formalism [24, 29]. Since (23) is invariant for the non-interacting part $\mathscr{L}_1 + \mathscr{L}_2$ of the generator one needs to prove only invariance under $\mathscr{L}_I$. For $n \in \mathbb{N}_0$ let $|\, n \,\rangle$ be the infinite-dimensional vector with components $(|\, n \,\rangle)_i = \delta_i$ and define the tensor vectors $|\, n^1, n^2 \,\rangle = |\, n^1 \,\rangle \otimes |\, n^2 \,\rangle$. Furthermore, define the matrices $\mathbf{1}$, $a^\pm$ and $\hat n$ by $a^+|\, n \,\rangle = |\, n+1 \,\rangle$, $a^-|\, n \,\rangle = n|\, n-1 \,\rangle$, $\hat n|\, n \,\rangle = n|\, n \,\rangle$, $\mathbf{1}|\, n \,\rangle = n|\, n \,\rangle$ and also the tensor products $a^{1,\pm} = a^\pm \otimes \mathbf{1}$, $a^{2,\pm} = \mathbf{1} \otimes a^\pm$, $\hat n^1 = \hat n \otimes \mathbf{1}$, $\hat n^2 = \mathbf{1} \otimes \hat n$, $\mathbf{1}_{12} = \mathbf{1} \otimes \mathbf{1}$ and $X_k = \mathbf{1}_{12}^{\otimes(k-1)} \otimes X \otimes \mathbf{1}_{12}^{\otimes(L-k)}$ where X is any of the two-fold tensor products just defined. The matrix form H_I of the generator $\mathscr{L}_I$ is then given by $H_I = \sum_k (g_k^1 + g_k^2)$ with

$$g_k^1 = -\frac{1}{2}\left\{\left(\hat n_k^2 + \hat n_{k+1}^2\right)\left[g^+\left(a_k^{1,-}a_{k+1}^{1,+} - \hat n_k^1\right) + g^-\left(a_k^{1,+}a_{k+1}^{1,-} - \hat n_{k+1}^1\right)\right]\right\} \tag{24}$$

$$g_k^2 = -\frac{1}{2}\left\{\left(\hat n_k^1 + \hat n_{k+1}^1\right)\left[g^+\left(a_k^{2,-}a_{k+1}^{2,+} - \hat n_k^2\right) + g^-\left(a_k^{2,+}a_{k+1}^{2,-} - \hat n_{k+1}^2\right)\right]\right\}. \tag{25}$$

Let $|\, \bar\rho \,\rangle = \mathrm{e}^{-\bar\rho}\sum_{n=0}^\infty \bar\rho^n/(n!)|\, n \,\rangle$ and $|\, \bar\rho_1, \bar\rho_2 \,\rangle = (|\, \bar\rho_1 \,\rangle \otimes |\, \bar\rho_2 \,\rangle)^{\otimes L}$ for $\bar\rho_{1,2} \geq 0$. One has $a_k^{\alpha,+}|\, \bar\rho_1, \bar\rho_2 \,\rangle = \hat n_k^\alpha/\bar\rho_\alpha$ and $a_k^{\alpha,-}|\, \bar\rho_1, \bar\rho_2 \,\rangle = \bar\rho_\alpha|\, \bar\rho_1, \bar\rho_2 \,\rangle$ [24]. It follows that

$$\left(a_k^{\alpha,-}a_{k+1}^{\alpha,+} - \hat n_k^\alpha\right)|\, \bar\rho_1, \bar\rho_2 \,\rangle = \left(\hat n_{k+1}^\alpha - \hat n_k^\alpha\right)|\, \bar\rho_1, \bar\rho_2 \,\rangle \tag{26}$$

$$\left(a_k^{\alpha,+}a_{k+1}^{\alpha,-} - \hat n_{k+1}^\alpha\right)|\, \bar\rho_1, \bar\rho_2 \,\rangle = \left(\hat n_k^\alpha - \hat n_{k+1}^\alpha\right)|\, \bar\rho_1, \bar\rho_2 \,\rangle \tag{27}$$

and therefore

$$g_k^1|\, \bar\rho_1, \bar\rho_2 \,\rangle = -\frac{\gamma}{2}\left(\hat n_k^2 + \hat n_{k+1}^2\right)\left(\hat n_{k+1}^1 - \hat n_k^1\right)|\, \bar\rho_1, \bar\rho_2 \,\rangle \tag{28}$$

$$g_k^2|\, \bar\rho_1, \bar\rho_2 \,\rangle = -\frac{\gamma}{2}\left(\hat n_k^1 + \hat n_{k+1}^1\right)\left(\hat n_{k+1}^2 - \hat n_k^2\right)|\, \bar\rho_1, \bar\rho_2 \,\rangle. \tag{29}$$

The telescopic property of the lattice sum then yields $H_I|\, \bar\rho_1, \bar\rho_2 \,\rangle = 0$. □

In Proposition 1 the parameters $\bar\rho_i = \langle\, n_k^i \,\rangle$ are the conserved stationary densities and one finds immediately the compressibility matrix $\mathbf{K}$ with matrix elements $K_{\alpha\beta} = \bar\rho_\alpha\delta_{\alpha\beta}$. From the definition (22) of the generator one computes the microscopic currents defined up to an irrelevant constant by the discrete continuity equation (1). The factorization of the invariant measure then yields the stationary current-density relation

$$\bar j^1(\bar\rho_1, \bar\rho_2) = \bar\rho_1(f_1 + \gamma\bar\rho_2), \quad \bar j^2(\bar\rho_1, \bar\rho_2) = \bar\rho_2(f_2 + \gamma\bar\rho_1). \tag{30}$$

Remarkably, the stationary currents depend only on the hopping biases $f_{1,2}$ and the interaction asymmetry γ, not on the interaction strength α.[5]

The main result is the following.

Theorem 2 *Define the quantities*

$$\Delta := \sqrt{(f_1 - f_2 + \gamma(\bar{\rho}_2 - \bar{\rho}_1))^2 + 4\gamma^2 \bar{\rho}_1 \bar{\rho}_2} \tag{31}$$

$$\xi := \frac{\Delta - (f_2 - f_1 + \gamma(\bar{\rho}_1 - \bar{\rho}_2))}{2\gamma\sqrt{\bar{\rho}_1 \bar{\rho}_2}}, \quad y := \frac{f_2 - f_1 + \gamma(\bar{\rho}_1 - \bar{\rho}_2)}{2\gamma\sqrt{\bar{\rho}_1 \bar{\rho}_2}}. \tag{32}$$

For all bare hopping rates $w_{1,2}$, $f_{1,2}$, all strictly positive densities $\bar{\rho}_{1,2}$, and all non-zero interaction parameters α, γ, the current Jacobian of the process defined by (22) with invariant measure given in Proposition 1 is non-degenerate and has eigenvalues

$$v_\pm = \frac{1}{2}\left(f_1 + f_2 + \gamma(\bar{\rho}_1 + \bar{\rho}_2) \pm \Delta\right). \tag{33}$$

The mode coupling matrices (10) where mode 1 (2) has collective velocity v_+ (v_-) are given by

$$\mathbf{G}^\alpha = -g_\alpha \begin{pmatrix} -1 & y \\ y & 1 \end{pmatrix} \tag{34}$$

with

$$g_1 = \bar{\rho}_1 \sqrt{\frac{\gamma^3 \xi}{\Delta^3}} (\gamma(\bar{\rho}_1 + \bar{\rho}_2) + \Delta + f_2 - f_1) \tag{35}$$

$$g_2 = \bar{\rho}_2 \sqrt{\frac{\gamma^3 \xi}{\Delta^3}} (\gamma(\bar{\rho}_1 + \bar{\rho}_2) - (\Delta + f_2 - f_1)). \tag{36}$$

Remark 2 For $\gamma = 0$ one has $g_1 = g_2 = 0$ for all f_1, f_2, $\bar{\rho}_1$, $\bar{\rho}_2$ so that both modes are diffusive with drift velocities $f_{1,2}$. For interaction asymmetry $\gamma > 0$ and strictly positive densities the drift velocities of the two modes are different even for equal individual bare hopping asymmetries $f_1 = f_2$.

Remark 3 For $\gamma > 0$ and strictly positive densities one has $g_1 \neq 0$ for all f_1, f_2. On the other hand, $g_2 \neq 0$ if and only if $f_1 \neq f_2$. Thus according to case 3 of Theorem 1 one expects that for any $\gamma > 0$ and strictly positive densities $\bar{\rho}_{1,2}$ both modes are KPZ if $f_1 \neq f_2$ whereas for equal asymmetries $f_1 = f_2$ mode 1 is modified KPZ and mode 2 is diffusive, without fine-tuning of parameters.

Remark 4 The offdiagonal elements of the mode coupling matrices vanish for $\bar{j}_1^1 = \bar{j}_2^2$, which is equivalent to $f_1 - f_2 = \gamma(\bar{\rho}_1 - \bar{\rho}_2)$.

[5]The product measure (23) remains invariant also for different interaction strength $\alpha_1 \neq \alpha_2$ which leaves the currents unchanged. However, equal interaction asymmetry is required.

Proof The proof of Theorem 2 is computational. From the current-density relation (30) one obtains the current Jacobian

$$\mathbf{J} = \begin{pmatrix} f_1 + \gamma\bar{\rho}_2 & \gamma\bar{\rho}_1 \\ \gamma\bar{\rho}_2 & f_2 + \gamma\bar{\rho}_1 \end{pmatrix}. \tag{37}$$

Solving the eigenvalue equation proves (33). With

$$u = \sqrt{\frac{\bar{\rho}_1}{\bar{\rho}_2}} \tag{38}$$

the diagonalizing matrix defined by

$$\mathbf{V} := \mathbf{R}\mathbf{J}\mathbf{R}^{-1} = \begin{pmatrix} v_+ & 0 \\ 0 & v_- \end{pmatrix}. \tag{39}$$

is computed to be

$$\mathbf{R} = \begin{pmatrix} x_+ & x_+\xi^{-1}u \\ -x_-\xi^{-1}u^{-1} & x_- \end{pmatrix} \tag{40}$$

with $\det(\mathbf{R}) = x_+x_-(1+\xi^{-2})$ and with free parameters $x_\pm$. The parameters $x_\pm$ are fixed by the normalization condition (5). One finds

$$x_+ = \frac{1}{\sqrt{\bar{\rho}_1(1+\xi^{-2})}} = \sqrt{\frac{\gamma\xi}{\delta u}}, \quad x_- = \frac{1}{\sqrt{\bar{\rho}_2(1+\xi^{-2})}} = \sqrt{\frac{\gamma\xi u}{\delta}}. \tag{41}$$

For the Hessians one finds

$$\mathbf{H}^1 = \mathbf{H}^2 = \gamma \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix} =: H \tag{42}$$

and therefore

$$(\mathbf{R}^{-1})^T \mathbf{H} \mathbf{R}^{-1} = 2\gamma\bar{\rho}_1\bar{\rho}_2 \frac{\gamma}{\delta} \begin{pmatrix} 1 & -y \\ -y & -1 \end{pmatrix}. \tag{43}$$

The definition (10) then yields (34). □

4 Criterion for Lévy Universality Classes for Systems with Two Conservation Laws

In the case of two conservation laws we denote the universality classes of the two modes by a pair $(\cdot,\cdot)$ where the possible entries are D for diffusion ($z = 2$), $\frac{3}{2}L$ for

the Lévy universality class with $z = 3/2$ and GM for the Lévy universality class with the golden mean $z = (1 + \sqrt{5})/2$.

4.1 Diagonalization of the Current Jacobian

Let

$$\mathbf{J} = \begin{pmatrix} \bar{j}_1^1 & \bar{j}_2^1 \\ \bar{j}_1^2 & \bar{j}_2^2 \end{pmatrix} \tag{44}$$

be a current Jacobian. The two eigenvalues of $\mathbf{J}$ are

$$v_\pm = \frac{1}{2}\left(\bar{j}_1^1 + \bar{j}_2^2 \pm \Delta\right) \tag{45}$$

with

$$\Delta = \sqrt{(\bar{j}_1^1 - \bar{j}_2^2)^2 + 4\bar{j}_2^1 \bar{j}_1^2}. \tag{46}$$

We consider only the strictly hyperbolic case $\Delta > 0$. The diagonalizer R with the property (39) reads

$$\mathbf{R} = \begin{pmatrix} x_+ & x_+ \frac{2\bar{j}_2^1}{\Delta + (\bar{j}_1^1 - \bar{j}_2^2)} \\ -x_- \frac{2\bar{j}_1^2}{\Delta + (\bar{j}_1^1 - \bar{j}_2^2)} & x_- \end{pmatrix} \tag{47}$$

with constants $x_\pm$ satisfying $x_+ x_- \neq 0$ and to be chosen such that $\mathbf{R}$ has well-defined limits $\bar{j}_2^1 \to 0$ or $\bar{j}_1^2 \to 0$.

4.2 Non-KPZ Universality Classes

According to cases 1 and 2 in Theorem 1 mode coupling theory predicts two non-KPZ universality classes for $G_{11}^1 = G_{22}^2 = 0$ and specifically

- (DD) if and only if $G_{22}^1 = G_{11}^2 = 0$
- $(D, \frac{3}{2}L)$ if and only if $G_{22}^1 = 0$, $G_{11}^2 \neq 0$
- $(\frac{3}{2}L, D)$ if and only if $G_{22}^1 \neq 0$, $G_{11}^2 = 0$
- (GM, GM) if and only if $G_{22}^1 \neq 0$, $G_{11}^2 = 0$.

The diagonal elements of the mode coupling matrices have been computed explicitly in [19], albeit in a form that does not directly express them in terms of the current-density relation. Moreover, the expressions in [19] depend on the normalization factors $x_\pm$ in (47) fixed by (5), which, however, is irrelevant with regard to whether a diagonal element is zero or not and therefore irrelevant to the question which universality class one expects. A more "user-friendly" form that expresses the

conditions on the various allowed universality classes directly in terms of the current derivatives is the following result.

Theorem 3 *Let* $\mathbf{J}$ *be a current Jacobian and* $\mathbf{G}^\alpha$ *be mode coupling matrices as defined in (10). Then one has the generic non-KPZ conditions* $G^1_{22} = G^2_{11} = 0$ *if and only if*

$$\bar{j}^2_1 \left(2\bar{j}^1_{12} + \bar{j}^2_{22}\right) + \bar{j}^1_2 \bar{j}^2_{11} - \bar{j}^1_{11} \left(\bar{j}^2_2 - \bar{j}^1_1\right) = 0 \tag{48}$$

$$\bar{j}^1_2 \left(2\bar{j}^2_{12} + \bar{j}^1_{11}\right) + \bar{j}^2_1 \bar{j}^1_{22} + \bar{j}^2_{22} \left(\bar{j}^2_2 - \bar{j}^1_1\right) = 0 \tag{49}$$

and the specific conditions

$$(D,D) \Leftrightarrow \bar{j}^2_1 \bar{j}^1_{22} + \bar{j}^1_2 \bar{j}^1_{11} = \bar{j}^2_1 \bar{j}^2_{22} + \bar{j}^1_2 \bar{j}^2_{11} = 0 \tag{50}$$

for two diffusive modes,

$$(D, \frac{3}{2}L) \Leftrightarrow \left(\bar{j}^2_1\right)^2 \bar{j}^1_{22} + \bar{j}^1_2 \bar{j}^2_1 \bar{j}^1_{11} = \frac{1}{2}\left(\bar{j}^1_1 - \bar{j}^2_2 - \delta\right)\left(\bar{j}^2_1 \bar{j}^2_{22} + \bar{j}^1_2 \bar{j}^2_{11}\right) \tag{51}$$

$$(\frac{3}{2}L, D) \Leftrightarrow \left(\bar{j}^2_1\right)^2 \bar{j}^1_{22} + \bar{j}^1_2 \bar{j}^2_1 \bar{j}^1_{11} = \frac{1}{2}\left(\bar{j}^1_1 - \bar{j}^2_2 + \delta\right)\left(\bar{j}^2_1 \bar{j}^2_{22} + \bar{j}^1_2 \bar{j}^2_{11}\right) \tag{52}$$

for the mixed case with one diffusive and one 3/2-Lévy mode, and

$$(GM,GM) \Leftrightarrow \left(\bar{j}^2_1\right)^2 \bar{j}^1_{22} + \bar{j}^1_2 \bar{j}^2_1 \bar{j}^1_{11} \neq \frac{1}{2}\left(\bar{j}^1_1 - \bar{j}^2_2 \pm \delta\right)\left(\bar{j}^2_1 \bar{j}^2_{22} + \bar{j}^1_2 \bar{j}^2_{11}\right) \tag{53}$$

for two golden mean Lévy modes.

Remark 5 Specific examples with concrete parameter values for each case can be found in [19, 28].

Proof We invert (10) to find $2R^T G^\alpha R = R_{\alpha 1} H^1 + R_{\alpha 2} H^2$. Requiring the generic non-KPZ conditions $G^1_{22} = G^2_{11} = 0$ and using that the mode coupling matrices and the Hessians are symmetric leads to six independent equations involving the current derivatives. In term of the parameters

$$u = \sqrt{\frac{\bar{j}^1_2}{\bar{j}^2_1}}, \quad \xi = \frac{\Delta - \left(\bar{j}^2_2 - \bar{j}^1_1\right)}{2\sqrt{\bar{j}^1_2 \bar{j}^2_1}}, \quad y = \frac{\bar{j}^2_2 - \bar{j}^1_1}{2\sqrt{\bar{j}^1_2 \bar{j}^2_1}} \tag{54}$$

they read

$$\xi u^{-1}\bar{j}^1_{11} + \bar{j}^2_{11} = 2G^1_{22}\frac{(x_-)^2}{x_+u\xi^{-1}}\left(\frac{u^{-1}}{\xi}\right)^2 - 4G^1_{12}x_-u^{-2} \tag{55}$$

$$\xi u^{-1}\bar{j}^1_{12} + \bar{j}^2_{12} = -2G^1_{22}\frac{(x_-)^2}{x_+u\xi^{-1}}\frac{u^{-1}}{\xi} - 4G^1_{12}x_-u^{-1}\frac{1-\xi^2}{2\xi} \tag{56}$$

$$\xi u^{-1}\bar{j}^1_{22} + \bar{j}^2_{22} = 2G^1_{22}\frac{(x_-)^2}{x_+u\xi^{-1}} + 4G^1_{12}x_- \tag{57}$$

$$\frac{u^{-1}}{\xi}\bar{j}^1_{11} - \bar{j}^2_{11} = -2G^2_{11}\frac{\left(x_+u\xi^{-1}\right)^2}{x_-}\left(\xi u^{-1}\right)^2 + 4G^2_{12}x_+u\xi^{-1}u^{-2} \tag{58}$$

$$\frac{u^{-1}}{\xi}\bar{j}^1_{12} - \bar{j}^2_{12} = -2G^2_{11}\frac{\left(x_+u\xi^{-1}\right)^2}{x_-}\xi u^{-1} + 4G^2_{12}x_+u\xi^{-1}u^{-1}\frac{1-\xi^2}{2\xi} \tag{59}$$

$$\frac{u^{-1}}{\xi}\bar{j}^1_{22} - \bar{j}^2_{22} = -2G^2_{11}\frac{\left(x_+u\xi^{-1}\right)^2}{x_-} - 4G^2_{12}x_+u\xi^{-1}. \tag{60}$$

Since G^1_{12} and G^2_{12} are arbitrary, we can introduce arbitrary new constants

$$A = \frac{-4G^1_{12}x_- + 4G^2_{12}x_+u\xi^{-1}}{\xi^{-1}+\xi}, \quad B = \frac{-4G^1_{12}x_-\xi^{-1} - 4G^2_{12}x_+u\xi^{-1}\xi}{\xi^{-1}+\xi} \tag{61}$$

so that the six non-KPZ equations become

$$\bar{j}^1_{11} = u^{-1}\left(\frac{2G^1_{22}\frac{(x_-)^2}{x_+u\xi^{-1}}\xi^{-2} - 2G^2_{11}\frac{\left(x_+u\xi^{-1}\right)^2}{x_-}\xi^2}{\xi^{-1}+\xi} + A\right) \tag{62}$$

$$\bar{j}^1_{12} = \frac{-2G^1_{22}\frac{(x_-)^2}{x_+u\xi^{-1}}\xi^{-1} - 2G^2_{11}\frac{\left(x_+u\xi^{-1}\right)^2}{x_-}\xi}{\xi^{-1}+\xi} + A\frac{1-\xi^2}{2\xi} \tag{63}$$

$$\bar{j}^1_{22} = u\left(\frac{2G^1_{22}\frac{(x_-)^2}{x_+u\xi^{-1}} - 2G^2_{11}\frac{\left(x_+u\xi^{-1}\right)^2}{x_-}}{\xi^{-1}+\xi} - A\right) \tag{64}$$

$$\bar{j}^2_{11} = u^{-2}\left(\frac{2G^1_{22}\frac{(x_-)^2}{x_+u\xi^{-1}}\xi^{-3} + 2G^2_{11}\frac{\left(x_+u\xi^{-1}\right)^2}{x_-}\xi^3}{\xi+\xi^{-1}} + B\right) \tag{65}$$

$$\bar{j}^2_{12} = u^{-1}\left(-\frac{2G^1_{22}\frac{(x_-)^2}{x_+u\xi^{-1}}\xi^{-2} - 2G^2_{11}\frac{\left(x_+u\xi^{-1}\right)^2}{x_-}\xi^2}{\xi+\xi^{-1}} + B\frac{1-\xi^2}{2\xi}\right) \tag{66}$$

$$\bar{j}^2_{22} = \frac{2G^1_{22}\frac{(x_-)^2}{x_+u\xi^{-1}}\xi^{-1} + 2G^2_{11}\frac{\left(x_+u\xi^{-1}\right)^2}{x_-}\xi}{\xi+\xi^{-1}} - B. \tag{67}$$

Now we use the fact that $\xi^{\pm 1} = \sqrt{1+y^2} \mp y$ to write

$$1 = \xi^{\pm 2} \pm 2y\xi^{\pm 1}, \quad \xi^{\pm 3} = \xi^{\pm 1} \mp 2y\xi^{\pm 2}. \tag{68}$$

Defining

$$C = \frac{2\left(\frac{G^1_{22}(x_-)^2}{x_+ u\xi} - \frac{G^2_{11}(x_+u)^2}{x_-}\right)}{\xi + \xi^{-1}}, \quad D = \frac{2\left(\frac{G^1_{22}(x_-)^2}{x_+ u} + \frac{G^2_{11}(x_+u)^2}{x_-\xi}\right)}{\xi + \xi^{-1}} \tag{69}$$

this yields

$$\frac{2G^1_{22}\frac{(x_-)^2}{x_+u\xi^{-1}} - 2G^2_{11}\frac{\left(x_+u\xi^{-1}\right)^2}{x_-}}{\xi + \xi^{-1}} = C - 2yD \tag{70}$$

$$\frac{2G^1_{22}\frac{(x_-)^2}{x_+u\xi^{-1}}\xi^{-3} + 2G^2_{11}\frac{\left(x_+u\xi^{-1}\right)^2}{x_-}\xi^3}{\xi + \xi^{-1}} = D + 2yC. \tag{71}$$

Thus the six non-KPZ conditions can be recast in the form

$$\bar{j}^1_{11} = u^{-1}(C + A) \tag{72}$$
$$\bar{j}^1_{12} = -D + yA \tag{73}$$
$$\bar{j}^1_{22} = u(C - 2yD - A) \tag{74}$$
$$\bar{j}^2_{11} = u^{-2}(D + 2yC + B) \tag{75}$$
$$\bar{j}^2_{12} = u^{-1}(-C + yB) \tag{76}$$
$$\bar{j}^2_{22} = D - B. \tag{77}$$

Next we choose the arbitrary functions as

$$A = u\bar{j}^1_{11} - C, \quad B = D - \bar{j}^2_{22} \tag{78}$$

to obtain

$$\bar{j}^1_{12} = -(D + yC) + yu\bar{j}^1_{11} \tag{79}$$
$$\bar{j}^1_{22} = 2u(C - yD) - u^2\bar{j}^1_{11} \tag{80}$$
$$\bar{j}^2_{11} = 2u^{-2}(D + yC) - u^{-2}\bar{j}^2_{22} \tag{81}$$
$$\bar{j}^2_{12} = -u^{-1}(C - yD) - yu^{-1}\bar{j}^2_{22}. \tag{82}$$

With the short-hands

$$F_1 = 2u(C - yD), \quad F_2 = 2(D + yC) \tag{83}$$

these equations take the form

$$2\bar{j}^1_{12} + \bar{j}^2_{22} + u^2\bar{j}^2_{11} - 2uy\bar{j}^1_{11} = 0 \tag{84}$$
$$2\bar{j}^2_{12} + \bar{j}^1_{11} + u^{-2}\bar{j}^1_{22} + 2u^{-1}y\bar{j}^2_{22} = 0 \tag{85}$$
$$\bar{j}^1_{22} + u^2\bar{j}^1_{11} = F_1 \tag{86}$$
$$\bar{j}^2_{22} + u^2\bar{j}^2_{11} = F_2. \tag{87}$$

Next we observe

$$F_1 = u\left(2G^1_{22}\frac{(x_-)^2}{x_+u\xi^{-1}}\xi^{-1} - 2G^2_{11}\frac{\left(x_+u\xi^{-1}\right)^2}{x_-}\xi\right) \tag{88}$$
$$F_2 = 2G^1_{22}\frac{(x_-)^2}{x_+u\xi^{-1}}\xi^{-2} + 2G^2_{11}\frac{\left(x_+u\xi^{-1}\right)^2}{x_-}\xi^2. \tag{89}$$

Thus, by setting the respective diagonal elements $G^\alpha_{\beta\beta}$ to zero,

$$(D, D) : G^1_{22} = G^2_{11} = 0 \Rightarrow F_1 = F_2 = 0 \tag{90}$$
$$(D, \frac{3}{2}L) : G^1_{22} = 0, G^2_{11} \neq 0 \Rightarrow F_1 = -\xi^{-1}uF_2 \neq 0 \tag{91}$$
$$(\frac{3}{2}L, D) : G^1_{22} \neq 0, G^2_{11} = 0 \Rightarrow F_1 = \xi uF_2 \neq 0 \tag{92}$$
$$(GM, GM) : G^1_{22} \neq 0, G^2_{11} \neq 0 \Rightarrow F_1 \neq \pm u\xi^{\pm 1}F_2. \tag{93}$$

In terms of the derivatives one has

$$uy = \frac{\bar{j}^2_2 - \bar{j}^1_1}{2\bar{j}^2_1}, \quad u^{-1}y = \frac{\bar{j}^2_2 - \bar{j}^1_1}{2\bar{j}^1_2} \tag{94}$$
$$u\xi = \frac{\delta - \left(\bar{j}^2_2 - \bar{j}^1_1\right)}{2\bar{j}^2_1}, \quad u\xi^{-1} = \frac{\delta + \left(\bar{j}^2_2 - \bar{j}^1_1\right)}{2\bar{j}^2_1}, \tag{95}$$

which yields the conditions (48)–(53) as stated in the theorem. Conversely, one proves that the required diagonal elements vanish by assuming the conditions to be valid and using the definition (10) of the mode coupling matrices. □

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