

Heat Flow in a Periodically Forced, Thermostatted Chain II

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Abstract

We derive a macroscopic heat equation for the temperature of a pinned harmonic chain subject to a periodic force at its right side and in contact with a heat bath at its left side. The microscopic dynamics in the bulk is given by the Hamiltonian equation of motion plus a reversal of the velocity of a particle occurring independently for each particle at exponential times, with rate γ . The latter produces a finite heat conductivity. Starting with an initial probability distribution for a chain of n particles we compute the current and the local temperature given by the expected value of the local energy. Scaling space and time diffusively yields, in the $n \to +\infty$ limit, the heat equation for the macroscopic temperature profile T(t, u), t > 0, $u \in [0, 1]$. It is to be solved for initial conditions T(0, u) and specified $T(t, 0) = T_-$, the temperature of the left heat reservoir and a fixed heat flux J, entering the system at u = 1. |J| equals the work done by the periodic force which is computed explicitly for each n.

Keywords Pinned harmonic chain · Periodic force · Heat equation for the macroscopic temperature · Dirichlet-Neumann type boundary condition · Work into heat

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1 Introduction

The emergence of the heat equation from a microscopic dynamics after a diffusive rescaling of space and time is a challenging mathematical problem in non-equilibrium statistical mechanics [6]. Here we study this problem in the context of conversion of work into heat in a simple model: a pinned harmonic chain. The system is in contact at its left end with a thermal reservoir at temperature T_{-} which acts on the leftmost particle via a Langevin force (Ornstein–Uhlenbeck process). The rightmost particle is acted on by a deterministic periodic force which does work on the system. The work pumps energy into the system with the energy then flowing into the reservoir in the form of heat.

To describe this flow we need to know the heat conductivity of the system. As it is well known, the harmonic crystal has an infinite heat conductivity [19]. To model realistic systems with finite heat conductivity we add to the harmonic dynamics a random velocity reversal. It models in a simple way the various dissipative mechanisms in real systems and produces a finite conductivity (cf. [1, 5]).

In paper [14], which is the first part of the present work, we studied this system in the limit $t \to \infty$, see Sect. 2.1 for rigorous statements of the main results obtained there. In this limit the probability distribution of the phase space configurations is periodic with the period of the external force, see Theorem 2.1 below. We also showed that with a proper scaling of the force and period the averaged temperature profile satisfies the stationary heat equation with an explicitly given heat current. In the present paper we study the time dependent evolution of the system, on the diffusive time scale, starting with some specified initial distribution. We derive a heat equation for the temperature profile of the system.

The periodic forcing generates a Neumann type boundary condition for the macroscopic heat equation, so that the gradient of the temperature at the boundary must satisfy Fourier law with the boundary energy current generated by the work of the periodic forcing (see (2.35) below). On the left side the boundary condition is given by the assigned value T_- , the temperature of the heat bath. As $t \to \infty$ the profile converges to the macroscopic profile obtained in [14].

The energy diffusion in the harmonic chain on a finite lattice, with energy conserving noise and Langevin heat bath at different temperatures at the boundaries, have been previously considered [2–4, 13, 18]. But complete mathematical results, describing the time evolution of the macroscopic temperature profile, have been obtained only for unpinned chains [4, 13].

This article gives the first proof of the heat equation for the pinned chain in a finite interval, and the method can be applied with different boundary conditions (see Remark 2.12). Investigation about energy transport in anharmonic chain under periodic forcing can be found in [10, 11], and very recently in [20]. In the review article [16] we considered various extensions of the present results to unpinned, multidimensional and anharmonic dynamics.

1.1 Structure of the Article

We start Sect. 2 with the precise description of the dynamics of the oscillator chain. Then, as already mentioned, in Sect. 2.1 we give an account of results obtained in [14]. In Sect. 2.2 we formulate our two main theorems: Theorem 2.5 about the limit current generated at the boundary by a periodic force, and Theorem 2.10 about the convergence of the energy profile to the solution of the heat equation with mixed boundary conditions.



In Sect. 3 we obtain a uniform bound on the total energy at any macroscopic time by an entropy argument. As a corollary (cf. Corollary 3.3) we obtain a uniform bound on the time integrated energy current, with respect to the size of the system.

Section 4 contains the proof of the equipartition of energy: Proposition 4.1 shows that the limit profiles of the kinetic and potential energy are equal. Furthermore, we show there the *fluctuation-dissipation relation* ((4.5)). It gives an exact decomposition of the energy currents into a dissipative term (given by a gradient of a local function) and a fluctuation term (given by the generator of the dynamics applied to a local function).

The fluctuation-dissipation relation (4.5) and equipartition of energy (4.1) are two of the ingredients for the proof of the main Theorem 2.10. The third component is a local equilibrium result for the limit covariance of the positions integrated in time. It is formulated in Proposition 5.1, for the covariances in the bulk, and in Proposition 5.2, for the boundaries. The local equilibrium property allows to identify correctly the thermal diffusivity in the proof of Theorem 2.10, see Sect. 5.

The technical part of the argument is presented in the appendices: the proof of the local equilibrium is given in Appendix D, after the analysis of the time evolution of the matrix for the time integrated covariances of positions and momenta, carried out in Appendix C. Both in Appendix C and Appendix D we use results proven in [14], when possible. Appendix B contains the proof of the current asymptotics (Theorem 2.5), that involves only the dynamics of the averages of the configurations. Appendix E contains the proof of the uniqueness of measured valued solutions of the Dirichlet-Neumann initial-boundary problem for the heat equation, satisfied by the limiting energy profile. Finally, in Appendix F we present an argument for the relative entropy inequality stated in Proposition 3.1.

2 Description of the Model

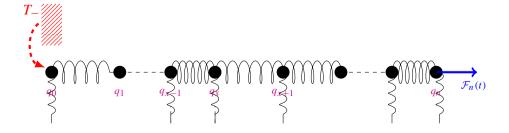
We consider a pinned chain of n+1-harmonic oscillators in contact on the left with a Langevin heat bath at temperature T_- , and with a periodic force acting on the last particle on the right. The configuration of particle positions and momenta are specified by

$$(\mathbf{q}, \mathbf{p}) = (q_0, \dots, q_n, p_0, \dots, p_n) \in \Omega_n := \mathbb{R}^{n+1} \times \mathbb{R}^{n+1}.$$
 (2.1)

We should think of the positions q_x as relative displacement from a point, say x in a finite lattice $\{0, 1, ..., n\}$. The total energy of the chain is given by the Hamiltonian: $\mathcal{H}_n(\mathbf{q}, \mathbf{p}) := \sum_{x=0}^n \mathcal{E}_x(\mathbf{q}, \mathbf{p})$, where the energy of particle x is defined by

$$\mathcal{E}_{x}(\mathbf{q}, \mathbf{p}) := \frac{p_{x}^{2}}{2} + \frac{1}{2}(q_{x} - q_{x-1})^{2} + \frac{\omega_{0}^{2}q_{x}^{2}}{2}, \quad x = 0, \dots, n,$$
 (2.2)

where $\omega_0 > 0$ is the pinning strength. We adopt the convention that $q_{-1} := q_0$.





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The microscopic dynamics of the process $\{(\mathbf{q}(t), \mathbf{p}(t))\}_{t\geq 0}$ describing the total chain is given in the bulk by

$$\dot{q}_{x}(t) = p_{x}(t), \quad x \in \{0, \dots, n\}, d p_{x}(t) = \left(\Delta q_{x}(t) - \omega_{0}^{2} q_{x}(t)\right) dt - 2p_{x}(t) dN_{x}(\gamma t), \quad x \in \{1, \dots, n-1\}$$
(2.3)

and at the boundaries by

$$dp_{0}(t) = \left(q_{1}(t) - q_{0}(t) - \omega_{0}^{2}q_{0}(t)\right)dt - 2\gamma p_{0}(t)dt + \sqrt{4\gamma T_{-}}d\widetilde{w}_{-}(t),$$

$$dp_{n}(t) = \left(q_{n-1}(t) - q_{n}(t) - \omega_{0}^{2}q_{n}(t)\right)dt + \mathcal{F}_{n}(t)dt - 2p_{n}(t)dN_{n}(\gamma t). \tag{2.4}$$

Here Δ is the Neumann discrete laplacian, corresponding to the choice $q_{n+1} := q_n$ and $q_{-1} = q_0$, see (A.1) below. Processes $\{N_x(t), x = 1, ..., n\}$ are independent Poisson of intensity 1, while $\widetilde{w}_-(t)$ is a standard one dimensional Wiener process, independent of the Poisson processes. Parameter $\gamma > 0$ regulates the intensity of the random perturbations and the Langevin thermostat. We have choosen the same parameter in order to simplify notations, it does not affect the results concerning the macroscopic properties of the dynamics.

We assume that the forcing $\mathcal{F}_n(t)$ is given by

$$\mathcal{F}_n(t) = \frac{1}{\sqrt{n}} \mathcal{F}\left(\frac{t}{\theta}\right). \tag{2.5}$$

where $\mathcal{F}(t)$ is a 1-periodic function such that

$$\int_0^1 \mathcal{F}(t) dt = 0, \qquad \int_0^1 \mathcal{F}(t)^2 dt > 0 \quad \text{and} \quad \sum_{\ell \in \mathbb{Z}} |\widehat{\mathcal{F}}(\ell)| < +\infty.$$
 (2.6)

Here

$$\widehat{\mathcal{F}}(\ell) = \int_0^1 e^{-2\pi i \ell t} \mathcal{F}(t) dt, \quad \ell \in \mathbb{Z}, \tag{2.7}$$

are the Fourier coefficients of the force. Note that by (2.6) we have $\widehat{\mathcal{F}}(0)=0$.

For a given function $f: \{0, \dots, n\} \to \mathbb{R}$ define the Neumann laplacian

$$\Delta f_x := f_{x+1} + f_{x-1} - 2f_x, \ x = 0, \dots, n, \tag{2.8}$$

with the convention $f_{-1} := f_0$ and $f_{n+1} := f_n$. The generator of the dynamics can be then written as

$$G_t = A_t + \gamma S_{\text{flip}} + 2\gamma S_-, \tag{2.9}$$

where

$$\mathcal{A}_t = \sum_{x=0}^n p_x \partial_{q_x} + \sum_{x=0}^n (\Delta q_x - \omega_0^2 q_x) \partial_{p_x} + \mathcal{F}_n(t) \partial_{p_n}$$
 (2.10)

and

$$S_{\text{flip}}F(\mathbf{q}, \mathbf{p}) = \sum_{x=1}^{n} \Big(F(\mathbf{q}, \mathbf{p}^{x}) - F(\mathbf{q}, \mathbf{p}) \Big), \tag{2.11}$$

Here $F: \mathbb{R}^{2(n+1)} \to \mathbb{R}$ is a bounded and measurable function, \mathbf{p}^x is the velocity configuration with sign flipped at the x component, i.e. $\mathbf{p}^x = (p_0^x, \dots, p_n^x)$, with $p_y^x = p_y$, $y \neq x$ and $p_x^x = -p_x$. Furthermore,

$$S_{-} = T_{-} \partial_{p_0}^2 - p_0 \partial_{p_0}. \tag{2.12}$$



The microscopic energy currents are given by

$$G_t \mathcal{E}_x(t) = j_{x-1,x}(t) - j_{x,x+1}(t),$$
 (2.13)

with $\mathcal{E}_x(t) := \mathcal{E}_x(\mathbf{q}(t), \mathbf{p}(t))$ and

$$j_{x,x+1}(t) := -p_x(t)(q_{x+1}(t) - q_x(t)), \quad \text{if} \quad x \in \{0, \dots, n-1\}$$

and at the boundaries

$$j_{-1,0}(t) := 2\gamma \left(T_{-} - p_0^2(t)\right), \quad j_{n,n+1}(t) := -\mathcal{F}_n(t)p_n(t).$$
 (2.14)

2.1 Summary of Results Concerning Periodic Stationary State

The present section is devoted to presentation of the results of [14] (some additional facts are contained in [15]). They concern the case when the chain is in its (periodic) stationary state. More precisely, we say that the family of probability measures $\{\mu_t^P, t \in [0, +\infty)\}$ constitutes a *periodic stationary state* for the chain described by (2.3) and (2.4) if it is a solution of the forward equation: for any function F in the domain of G_t :

$$\partial_t \int F(\mathbf{q}, \mathbf{p}) \mu_t^P(\mathrm{d}\mathbf{q}, \mathrm{d}\mathbf{p}) = \int (\mathcal{G}_t F(\mathbf{q}, \mathbf{p})) \mu_t^P(\mathrm{d}\mathbf{q}, \mathrm{d}\mathbf{p}), \tag{2.15}$$

such that $\mu_{t+\theta}^P = \mu_t^P$.

Given a measurable function $F: \mathbb{R}^{2(n+1)} \to \mathbb{R}$ we denote

$$\langle \langle F \rangle \rangle := \frac{1}{\theta} \int_0^\theta dt \int_{\mathbb{R}^{2(n+1)}} F(\mathbf{q}, \mathbf{p}) \mu_t^P(d\mathbf{q}, d\mathbf{p}), \tag{2.16}$$

provided that $|F(\mathbf{q}, \mathbf{p})|$ is integrable w.r.t. the respective product measure.

It has been shown, see [14, Theorem 1.1, Proposition A.1] and also [15, Theorem A.2], that there exists a unique periodic, stationary state.

Theorem 2.1 For a fixed $n \ge 1$ there exists a unique periodic stationary state $\{\mu_s^P, s \in [0, +\infty)\}$ for the system (2.3)–(2.4). The measures μ_s^P are absolutely continuous with respect to the Lebesgue measure $d\mathbf{q}d\mathbf{p}$ and the respective densities $\mu_s^P(d\mathbf{q}, d\mathbf{p}) = f_s^P(\mathbf{q}, \mathbf{p})d\mathbf{q}d\mathbf{p}$ are strictly positive. The time averages of all the second moments $\langle\langle p_x p_y \rangle\rangle$, $\langle\langle p_x q_y \rangle\rangle$ and $\langle\langle q_x q_y \rangle\rangle$ are finite and $\min_x \langle\langle p_x^2 \rangle\rangle \ge T_-$. Furthermore, given an arbitrary initial probability distribution μ on $\mathbb{R}^{2(n+1)}$ and (μ_t) the solution of (2.15) such that $\mu_0 = \mu$, we have

$$\lim_{t \to +\infty} \|\mu_t - \mu_t^P\|_{\text{TV}} = 0. \tag{2.17}$$

Here $\|\cdot\|_{TV}$ *denotes the total variation norm.*

In the periodic stationary state the time averaged energy current $J_n = \langle \langle j_{x,x+1} \rangle \rangle$ is constant for x = -1, ..., n. In particular

$$J_n = -\frac{1}{\sqrt{n\theta}} \int_0^\theta \mathcal{F}\left(\frac{s}{\theta}\right) \overline{p}_n(s) ds, \qquad (2.18)$$

where $\overline{p}_x(s) := \int_{\mathbb{R}^{2(n+1)}} p_x \mu_s^P(d\mathbf{q}, d\mathbf{p})$. It turns out that the stationary current is of size O(1/n) as can be seen from the following.



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Theorem 2.2 (see Theorem 3.1 of [14]) Suppose that $\mathcal{F}(\cdot)$ satisfies (2.6) and, in addition, we also have $\sum_{\ell \in \mathbb{Z}} \ell^2 |\widehat{\mathcal{F}}(\ell)|^2 < +\infty$. Then,

$$\lim_{n \to +\infty} n J_n = J := -\left(\frac{2\pi}{\theta}\right)^2 \sum_{\ell \in \mathbb{Z}} \ell^2 \mathcal{Q}(\ell), \tag{2.19}$$

with $Q(\ell)$ given by,

$$\mathcal{Q}(\ell) = 4\gamma |\widehat{\mathcal{F}}(\ell)|^2 \int_0^1 \cos^2\left(\frac{\pi z}{2}\right) \left\{ \left[4\sin^2\left(\frac{\pi z}{2}\right) + \omega_0^2 - \left(\frac{2\pi\ell}{\theta}\right)^2 \right]^2 + \left(\frac{4\gamma\pi\ell}{\theta}\right)^2 \right\}^{-1} dz.$$
(2.20)

In the more general case when the forcing $\mathcal{F}_n(t)$ is θ_n -periodic, with the period $\theta_n = n^b \hat{\theta}$ and the amplitude n^a , i.e. $\mathcal{F}_n(t) = n^a \mathcal{F}\left(\frac{t}{\theta_n}\right)$, and

$$b - a = \frac{1}{2}, \quad a \le 0 \quad and \quad b > 0$$
 (2.21)

the convergence in (2.19) still holds. However, then

$$\mathcal{Q}(\ell) = 4\gamma |\widehat{\mathcal{F}}(\ell)|^2 \int_0^1 \cos^2\left(\frac{\pi z}{2}\right) \left[4\sin^2\left(\frac{\pi z}{2}\right) + \omega_0^2\right]^{-2} dz, \quad when \ b > 0. \tag{2.22}$$

Concerning the convergence of the energy profile we have shown the following, see [14, Theorem 3.4].

Theorem 2.3 *Under the assumptions of Theorem 2.2 we have*

$$\lim_{n \to \infty} \frac{1}{n} \sum_{x=0}^{n} \varphi\left(\frac{x}{n+1}\right) \langle \langle p_{x}^{2} \rangle \rangle = \lim_{n \to \infty} \frac{1}{n} \sum_{x=0}^{n} \varphi\left(\frac{x}{n+1}\right) \langle \langle \mathcal{E}_{x} \rangle \rangle = \int_{0}^{1} \varphi(u) T(u) du,$$
(2.23)

with

$$T(u) = T_{-} - \frac{4\gamma Ju}{D}, \quad u \in [0, 1],$$
 (2.24)

for any $\varphi \in C[0, 1]$. Here J is given by (2.19) and

$$D = 1 - \omega_0^2 \left(G_{\omega_0}(0) + G_{\omega_0}(1) \right) = \frac{2}{2 + \omega_0^2 + \omega_0 \sqrt{\omega_0^2 + 4}},$$
 (2.25)

where $G_{\omega_0}(\ell)$ is the Green function defined in (A.2).

Concerning the time variance of the average kinetic energy we have shown the following.

Theorem 2.4 (Theorem 9.1, [14]) Suppose that the forcing $\mathcal{F}_n(\cdot)$ is given by (2.5), where $\mathcal{F}(\cdot)$ satisfies the hypotheses made in Theorem 2.2. Then, there exists a constant C > 0 such that

$$\sum_{r=0}^{n} \frac{1}{\theta} \int_{0}^{\theta} \left(\overline{p_{x}^{2}}(t) - \langle \langle p_{x}^{2} \rangle \rangle \right)^{2} dt \leqslant \frac{C}{n^{2}}, \quad n = 1, 2, \dots$$
 (2.26)

Here $\overline{p_x^2}(t) := \int_{\mathbb{R}^{2(n+1)}} p_x^2 \mu_t^P (d\mathbf{q}, d\mathbf{p}).$



2.2 Statements of the Main Results

2.2.1 Macroscopic Energy Current Due to Work

The first results concerns the work done by the forcing in a diffusive limit, i.e.

$$J_{n}(t,\mu) = \frac{1}{n} \int_{0}^{n^{2}t} \mathbb{E}_{\mu} \left(j_{n,n+1}(s,\mathbf{q}(s),\mathbf{p}(s)) \right) ds = -\frac{1}{n} \int_{0}^{n^{2}t} \mathcal{F}_{n}(s) \mathbb{E}_{\mu} \left(p_{n}(s) \right) ds,$$
(2.27)

where \mathbb{E}_{μ} denotes the expectation of the process with the initial configuration (\mathbf{q}, \mathbf{p}) distributed according to a probability measure μ . We shall write $J_n(t, \mathbf{q}, \mathbf{p})$ if for a deterministic initial configuration (\mathbf{q}, \mathbf{p}) , i.e. $\mu = \delta_{\mathbf{q}, \mathbf{p}}$, the δ -measure that gives probability 1 to such configuration.

Assume furthermore that (μ_n) is a sequence of initial distributions, with each μ_n probability measure on $\mathbb{R}^{n+1} \times \mathbb{R}^{n+1}$. We suppose that there exist C > 0 and $\delta \in [0, 2)$ for which for any integer $n \ge 1$

$$\mathcal{H}_n(\overline{\mathbf{q}}_n, \overline{\mathbf{p}}_n) \leqslant C n^{\delta}. \tag{2.28}$$

Here $(\overline{\mathbf{q}}_n, \overline{\mathbf{p}}_n)$ is the vector of the averages of the configuration with respect to μ_n . We are interested essentially in the case $\delta = 1$, but Theorem 2.5 is valid also for any $\delta < 2$. In Proposition B.1 we prove that, in the diffusive time scaling, the energy due to the averages (2.28) becomes negligible at any time t > 0.

In Section B.2 of the Appendix we prove the following.

Theorem 2.5 *Under the assumptions listed above, we have*

$$\lim_{n \to +\infty} \sup_{t \ge 0} \left| J_n(t, \mu_n) - Jt \right| = 0, \tag{2.29}$$

where J is given by (2.19).

Remark 2.6 The asymptotic current J is the same as in the stationary state (cf. [14]) and it does not depend on the initial configuration.

Remark 2.7 Analogously to the stationary case, rescaling the period θ with n and the strength of the force in such a way that

$$\mathcal{F}_n(t) = n^a \mathcal{F}\left(\frac{t}{n^b \theta}\right), \quad b - a = \frac{1}{2}, \quad a \leqslant 0 \quad \text{and} \quad b > 0,$$
 (2.30)

Theorem 2.5 still holds, but with a different value of the current. Namely, J is given by (2.19) with $Q(\ell)$ defined by (2.22). Formula (2.22) corresponds to (2.20) with the value $\theta = \infty$. If $b - a \neq 1/2$ the macrosopic current nJ_n is not of order O(1), which leads to an anomalous behavior of the heat conductivity of the chain (it vanishes, if b - a > 1/2, becomes unbounded, if b - a < 1/2. The assumption $a \leq 0$ guarantees that the force acting on the system does not become infinite, as $n \to +\infty$.

Remark 2.8 Using contour integration it is possible to calculate the quantities appearing in (2.20) and (2.22), see [15, Appendix D]. In the case of (2.20) we obtain

$$\mathcal{Q}(\ell) = \frac{\theta |\widehat{\mathcal{F}}(\ell)|^2}{2\pi \ell} \text{Im}\left(\left\{\frac{2}{\lambda(\omega_0,\,\ell)\sqrt{1+4/\lambda(\omega_0,\,\ell)}} + \frac{1}{2}\right\}\right)$$



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$$\left\{1+\frac{\lambda(\omega_0,\ell)}{2}\left(1+\sqrt{1+\frac{4}{\lambda(\omega_0,\ell)}}\right)\right\}^{-1}\right),\,$$

with

$$\lambda(\omega_0, \ell) := \omega_0^2 - \left(\frac{2\pi \ell}{\theta}\right)^2 + i\left(\frac{4\gamma \pi \ell}{\theta}\right).$$

Furthermore, in the case of (2.22) we have

$$Q(\ell) = \frac{2\gamma |\widehat{\mathcal{F}}(\ell)|^2 (4 + \omega_0^2)}{(\omega_0^4 + 4\omega_0^2 + 8)^{3/2}}.$$

2.2.2 Macroscopic Energy Profile

Let $v_{T-}(d\mathbf{q}, d\mathbf{p})$ be defined as the product Gaussian measure on Ω_n (see (2.1)) of zero average and variance $T_- > 0$ given by

$$\nu_{T_{-}}(\mathbf{d}\mathbf{q}, \mathbf{d}\mathbf{p}) := \frac{1}{Z} \prod_{r=0}^{n} \exp\left\{-\mathcal{E}_{x}(\mathbf{q}, \mathbf{p})/T_{-}\right\} \mathbf{d}\mathbf{q}\mathbf{d}\mathbf{p}, \tag{2.31}$$

where Z is the normalizing constant. Let $f(\mathbf{q}, \mathbf{p})$ be a probability density with respect to ν_{T_-} . We denote the relative entropy

$$\mathbf{H}_{n}(f) := \int_{\Omega_{n}} f(\mathbf{q}, \mathbf{p}) \log f(\mathbf{q}, \mathbf{p}) d\nu_{T_{-}}(\mathbf{q}, \mathbf{p}). \tag{2.32}$$

We assume now that the initial distribution μ_n has density $f_n(0, \mathbf{q}, \mathbf{p})$, with respect to ν_{T_-} , such that there exists a constant C > 0 for which

$$\mathbf{H}_n(f_n(0)) \leqslant Cn, \quad n = 1, 2, \dots$$
 (2.33)

For example, it can be verified that local Gibbs measures of the form

$$f_n(\mathbf{q}, \mathbf{p}) d\nu_{T_-}(\mathbf{q}, \mathbf{p}) = \prod_{x=0}^n \exp\left\{-\frac{\mathcal{E}_x(\mathbf{q}, \mathbf{p})}{T_{x,n}}\right\} d\mathbf{q} d\mathbf{p},$$
(2.34)

with $\inf_{x,n} T_{x,n} > 0$ satisfy (2.33). At this point we only remark that, due to the entropy inequality (see the proof of Corollary 3.2 below), assumption (2.33) implies

$$\sup_{n\geqslant 1} \mathbb{E}_{\mu_n} \left[\frac{1}{n+1} \sum_{x=0}^n \mathcal{E}_x(0) \right] < +\infty.$$

Furthermore, since the Hamiltonian $\mathcal{H}(\cdot,\cdot)$ is a convex function, by the Jensen inequality

$$\sup_{n\geqslant 1}\frac{1}{n+1}\mathcal{H}_n(\overline{\mathbf{q}}_n,\overline{\mathbf{p}}_n)\leqslant \sup_{n\geqslant 1}\mathbb{E}_{\mu_n}\left[\frac{1}{n+1}\sum_{x=0}^n\mathcal{H}_n(\mathbf{q},\mathbf{p})\right]<+\infty,$$

so (2.28) is satisfied with $\delta = 1$.

Denote by $\mathcal{M}_{fin}([0, 1])$, resp $\mathcal{M}_{+}([0, 1])$ the space of bounded variation, Borel, resp. positive, measures on the interval [0, 1] endowed with the weak topology. Before formulating



the main result we introduce the notion of a measured valued solution of the following initialboundary value problem

$$\partial_t T = \frac{D}{4\gamma} \partial_u^2 T, \quad u \in (0, 1),$$

$$T(t, 0) = T_-, \quad \partial_u T(t, 1) = -\frac{4\gamma J}{D}, \quad T(0, du) = T_0(du).$$
(2.35)

Here J and D are defined by (2.19) and (2.25), respectively and $T_0 \in \mathcal{M}_{fin}([0, 1])$.

Definition 2.9 We say that a function $T:[0,+\infty)\to\mathcal{M}_{\mathrm{fin}}([0,1])$ is a weak (measured valued) solution of (2.35) if: it belongs to $C([0,+\infty);\mathcal{M}_{\mathrm{fin}}([0,1]))$ and for any $\varphi\in C^2[0,1]$ such that $\varphi(0)=\varphi'(1)=0$ we have

$$\int_{0}^{1} \varphi(u)T(t, du) - \int_{0}^{1} \varphi(u)T_{0}(du) = \frac{D}{4\gamma} \int_{0}^{t} ds \int_{0}^{1} \varphi''(u)T(s, du) + \frac{DT_{-}t}{4\gamma} \varphi'(0) - Jt\varphi(1).$$
(2.36)

The proof of the uniqueness of the solution of (2.36) is quite routine. For completeness sake we present it in Appendix E.

Theorem 2.10 Suppose that the initial configurations (μ_n) satisfy (2.33). Assume furthermore that there exists $T_0 \in \mathcal{M}_+([0,1])$ such that

$$\lim_{n \to \infty} \mathbb{E}_{\mu_n} \left[\frac{1}{n+1} \sum_{x=0}^n \varphi\left(\frac{x}{n+1}\right) \mathcal{E}_x(0) \right] = \int_0^1 \varphi(u) T_0(\mathrm{d}u), \tag{2.37}$$

for any function $\varphi \in C[0, 1]$ - the space of continuous functions on [0, 1]. Here $\mathcal{E}_x(t) = \mathcal{E}_x(\mathbf{q}(t), \mathbf{p}(t))$. Then,

$$\lim_{n \to \infty} \frac{1}{n+1} \sum_{x=0}^{n} \varphi\left(\frac{x}{n+1}\right) \mathbb{E}_{\mu_n}\left(\mathcal{E}_x(n^2 t)\right) = \int_0^1 \varphi(u) T(t, du). \tag{2.38}$$

Here T(t, du) is the unique weak solution of (2.35), with the initial data given by measure T_0 in (2.37).

Remark 2.11 The initial energy $\mathcal{E}_x(0)$ can be represented as the sum $\mathcal{E}_x^{\text{th}} + \mathcal{E}_x^{\text{mech}}$ of the *thermal energy*

$$\mathcal{E}_x^{\text{th}} := \frac{1}{2} \left[(p_x')^2 + (q_x' - q_{x-1}')^2 + \omega_0^2 (q_x')^2 \right]$$

and the mechanical energy

$$\mathcal{E}_{x}^{\text{mech}} := \frac{1}{2} \left[\overline{p}_{x}^{2} + (\overline{q}_{x} - \overline{q}_{x-1})^{2} + \omega_{0}^{2} \overline{q}_{x}^{2} \right].$$

Here $q'_x = q_x - \overline{q}_x$ and $p'_x = p_x - \overline{p}_x$, with $\overline{p}_x := \int_{\Omega_n} p_x \mu_n(\mathrm{d}\mathbf{q}, \mathrm{d}\mathbf{p})$ and $\overline{q}_x := \int_{\Omega_n} q_x \mu_n(\mathrm{d}\mathbf{q}, \mathrm{d}\mathbf{p})$.

If $\mathcal{E}_{x}^{\text{mech}} \neq 0$ and satisfies (2.28), with $\delta = 1$, then the initial measure $T_0(du)$ is the macroscopic distribution of the total energy and not of the *temperature*, where the latter is understood as the thermal energy. Nevertheless, as a consequence of Proposition B.1, at any macroscopic positive time the entire mechanical energy is transformed immediately into



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the thermal energy, so that T(t, du) for t > 0 can be seen as the macroscopic temperature distribution. The situation is different for the unpinned dynamics ($\omega_0 = 0$) where the transfer of mechanical energy to thermal energy happens slowly at macroscopic times (see [13]).

Remark 2.12 Concerning Theorem 2.10, a similar proof will work in the case where two Langevin heat baths at two temperatures, T_- and T_+ are placed at the boundaries, in the absence of the periodic forcing. In this case the macroscopic equation will be the same but with boundary conditions $T(t, 0) = T_-$ and $T(t, 1) = T_+$.

Also, in the absence of any heat bath, we could apply two periodic forces $\mathcal{F}_n^{(0)}(t)$ and $\mathcal{F}_n^{(1)}(t)$ respectively at the left and right boundary. They will generate two incoming energy current, $J^{(0)} > 0$ on the left and $J^{(1)} < 0$ on the right, given by the corresponding formula (2.19), and we will have the same equation but with boundary conditions $\partial_u T(t,0) = -\frac{4\gamma J^{(0)}}{D}$ and $\partial_u T(t,1) = -\frac{4\gamma J^{(1)}}{D}$. Of course in this case the total energy increases in time and periodic stationary states do not exist.

In the case where both a heat bath and a periodic force are present on the same side, say on the right endpoint, then the macroscopic boundary condition arising is $T(t, 1) = T_+$, i.e. the periodic forcing is ineffective on the macroscopic level, and all the energy generated by its work will flow into the heat bath. It would be interesting to investigate what happens when the amplitude of the forcing is larger than considered here $(-1/2 < a \le 0 \text{ in } (2.30))$. However, it is not yet clear to us what occurs in this case.

Remark 2.13 If the initial data T_0 is C^1 smooth and satisfies the boundary condition in (2.35), then the initial-boundary value problem (2.35) has a unique strong solution T(t, u) that belongs to the intersection of the spaces $C([0, +\infty) \times [0, 1])$ and $C^{1,2}((0, +\infty) \times (0, 1))$ - the space of functions continuously differentiable once in the first and twice in the second variable, see e.g. [8, Corollary 5.3.2, p.147]. This solution coincides then with the unique weak solution in the sense of Definition 2.9.

Remark 2.14 In the proof of Theorem 2.10 we need to show a result about the equipartition of energy (cf. Proposition 4.1). As a consequence the limit profile of the energy equals the limit profile of the temperature, i.e. we have

$$\lim_{n \to \infty} \frac{1}{n+1} \sum_{x=0}^{n} \int_{0}^{+\infty} \varphi\left(t, \frac{x}{n+1}\right) \mathbb{E}_{\mu_n}\left(p_x^2(n^2t)\right) dt = \int_{0}^{+\infty} dt \int_{0}^{1} \varphi(t, u) T(t, du),$$
(2.39)

for any compactly supported test function.

3 Entropy, Energy and Currents Bounds

We first prove that the initial entropy bound (2.33) holds for all times.

Proposition 3.1 Suppose that the law of the initial configuration admits the density $f_n(0, \mathbf{q}, \mathbf{p})$ w.r.t. the Gibbs measure v_{T-} that satisfies (2.33). Then, for any t > 0 there exists $f_n(t, \mathbf{q}, \mathbf{p})$ - the density of the law of the configuration $(\mathbf{q}(t), \mathbf{p}(t))$. In addition, for any t there exists a constant C independent of n such that

$$\sup_{s \in [0, t]} \mathbf{H}_n(f_n(n^2s)) \leqslant Cn, \tag{3.1}$$



Proof For simplicity sake, we present here a proof under an additional assumption that $f_n(t, \mathbf{q}, \mathbf{p})$ is a smooth function such that $\mu_t(\mathbf{dq}, \mathbf{dp}) = f_n(t, \mathbf{q}, \mathbf{p})\mathbf{dqdp}$ is the solution of the forward equation (2.15). The general case is treated in Appendix F. Using (2.9) for the generator \mathcal{G}_t we conclude that

$$\mathbf{H}_n(f_n(n^2t)) - \mathbf{H}_n(f_n(0)) = \int_0^{n^2t} \mathrm{d}s \int_{\Omega_n} f_n(s) \mathcal{G}_s \log f_n(s) \mathrm{d}\nu_{T-} = \mathbf{I}_n + \mathbf{I}\mathbf{I}_n,$$

with

$$I_n := \gamma \int_0^{n^2 t} ds \int_{\Omega_n} f_n(s) \left(\mathcal{S}_{flip} + 2\mathcal{S}_- \right) \log f_n(s) d\nu_{T-},$$

$$II_n := \int_0^{n^2 t} ds \int_{\Omega_n} f_n(s) \mathcal{A}_s \log f_n(s) d\nu_{T-}.$$

We have that $I_n \leq 0$ because S_{flip} and S_- are symmetric negative operators with respect to the measure v_{T-} .

The only positive contribution comes from the second term where the boundary work defined by (2.27) appears:

$$II_n = \int_0^{n^2 t} \mathrm{d}s \mathcal{F}_n(s) \int_{\Omega_n} \frac{p_n}{T_-} f_n(s) \mathrm{d}\nu_{T_-} = -\frac{n}{T_-} J_n(t, \mu_0),$$

where $d\mu_0 := f_n(0)d\nu_{T-}$. Therefore

$$\mathbf{H}_n(f_n(n^2t)) \leqslant \mathbf{H}_n(f_n(0)) - \frac{n}{T_-} J_n(t, \mu_0).$$

The conclusion of the proposition then follows from a direct application of (2.33) and Theorem 2.5.

To abbreviate the notation we shall omit the index by the expectation sign, indicating the initial condition.

Corollary 3.2 (Energy bound) For any $t_* \ge 0$ we have

$$\sup_{t \in [0, t_*]} \sup_{n \ge 1} \mathbb{E} \left[\frac{1}{n+1} \sum_{x=0}^{n} \mathcal{E}_x(n^2 t) \right] = E(t_*) < +\infty.$$
 (3.2)

Proof It follows from the entropy inequality, see e.g. [9, p. 338], that for $\alpha > 0$ small enough we can find $C_{\alpha} > 0$ such that

$$\mathbb{E}\left[\sum_{x=0}^{n} \mathcal{E}_{x}(n^{2}t)\right] \leqslant \frac{1}{\alpha} \left(C_{\alpha}n + \mathbf{H}_{n}(t)\right), \quad t \geqslant 0.$$
(3.3)

From Theorem 2.5 and Corollary 3.2 we immediately conclude the following.

Corollary 3.3 (Current size) For any $t_* \ge 0$ there exists C > 0 such that

$$\sup_{x=0,\dots,n+1,\ t\in[0,t_*]} \left| \int_0^t \mathbb{E}\left[j_{x-1,x}(n^2s)\right] ds \right| \leqslant \frac{C}{n}, \quad n=1,2,\dots$$
 (3.4)



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In particular, for any t > 0 there exists C > 0 such that

$$\left| \int_0^t \left\{ \mathbb{E} \left[p_0^2(n^2 s) \right] - T_- \right\} \mathrm{d}s \right| \leqslant \frac{C}{n}, \tag{3.5}$$

Proof By the local conservation of energy

$$n^{-2} \frac{\mathrm{d}}{\mathrm{d}t} \mathbb{E}[\mathcal{E}_x(n^2 t)] = \mathbb{E}\Big[j_{x-1,x}(n^2 t) - j_{x,x+1}(n^2 t)\Big]. \tag{3.6}$$

Therefore

$$\int_0^t \mathbb{E} j_{x-1,x}(n^2 s) ds = \int_0^t \mathbb{E} j_{n,n+1}(n^2 s) ds + n^{-2} \sum_{y=x}^n \left(\mathbb{E} [\mathcal{E}_y(n^2 t)] - \mathbb{E} [\mathcal{E}_y(0)] \right), \quad (3.7)$$

and bound (3.4) follows directly from estimates (2.29) and (3.2). Estimate (3.5) is a consequence of the definition of $j_{-1,0}$ (see (2.14)) and (3.4).

4 Equipartition of Energy and Fluctuation-Dissipation Relations

4.1 Equipartition of the Energy

In the present section we show the equipartition property of the energy.

Proposition 4.1 *Suppose that* $\varphi \in C^1[0, 1]$ *is such that* supp $\varphi \subset (0, 1)$. *Then,*

$$\lim_{n \to +\infty} \frac{1}{n+1} \sum_{x=0}^{n} \varphi\left(\frac{x}{n+1}\right) \int_{0}^{t} \mathbb{E}\left[p_{x}^{2}(n^{2}s) - \left(q_{x}(n^{2}s) - q_{x-1}(n^{2}s)\right)^{2} - \omega_{0}^{2}q_{x}^{2}(n^{2}s)\right] ds = 0. \tag{4.1}$$

Proof After a simple calculation we obtain the following fluctuation-dissipation relation: for x = 1, ..., n - 1,

$$p_x^2 - \omega_0^2 q_x^2 - (q_x - q_{x-1})^2 = \nabla^* \left[q_x (q_{x+1} - q_x) \right] + \mathcal{G}_t \left(q_x p_x + \gamma q_x^2 \right), \tag{4.2}$$

where the discrete gradient ∇ and its adjoint ∇^* are defined in (A.1) below. Therefore,

$$\int_{0}^{t} \mathbb{E} \Big[p_{x}^{2}(n^{2}s) - \omega_{0}^{2} q_{x}^{2}(n^{2}s) - (q_{x}(n^{2}s) - q_{x}(n^{2}s))^{2} \Big] ds$$

$$= \nabla \int_{0}^{t} \mathbb{E} \Big[q_{x}(n^{2}s)(q_{x+1}(n^{2}s) - q_{x}(n^{2}s)) \Big] ds$$

$$+ n^{-2} \mathbb{E} \Big[q_{x}(n^{2}t) p_{x}(n^{2}t) + 2\gamma q_{x}^{2}(n^{2}t) \Big] - n^{-2} \mathbb{E} \Big[q_{x}(0) p_{x}(0) + 2\gamma q_{x}^{2}(0) \Big]. \tag{4.3}$$

After summing up against the test function φ (that has compact support strictly contained in (0, 1)) and using the energy bound (3.2) we conclude (4.1).



4.2 Fluctuation-Dissipation Relation

In analogy to [14, Section 5.1] define

$$f_x := \frac{1}{4\gamma} (q_{x+1} - q_x) (p_x + p_{x+1}) + \frac{1}{4} (q_{x+1} - q_x)^2, \qquad x = 0, \dots, n - 1,$$

$$\mathfrak{F}_x := p_x^2 + (q_{x+1} - q_x) (q_x - q_{x-1}) - \omega_0^2 q_x^2, \qquad x = 0, \dots, n,$$

$$(4.4)$$

with the convention that $q_{-1} = q_0$, $q_n = q_{n+1}$. Then

$$j_{x,x+1} = -\frac{1}{4\nu} \nabla \mathfrak{F}_x + \mathcal{G}_t \mathfrak{f}_x - \frac{\delta_{x,n-1}}{4\nu} \mathcal{F}_n(t) (q_n - q_{n-1}), \quad x = 0, \dots, n-1.$$
 (4.5)

5 Local Equilibrium and the Proof of Theorem 2.10

The fundamental ingredients in the proof of Theorem 2.10 are the identification of the work done at the boundary given by Theorem 2.5, the equipartition and the fluctuation-dissipation relation contained in Theorem 4, and the following *local equilibrium* results. In the bulk we have the following:

Proposition 5.1 *Suppose that* $\varphi \in C[0, 1]$ *is such that* supp $\varphi \subset (0, 1)$. *Then*

$$\lim_{n \to +\infty} \frac{1}{n+1} \sum_{x=0}^{n} \varphi\left(\frac{x}{n+1}\right) \int_{0}^{t} \mathbb{E}\left[q_{x}(n^{2}s)q_{x+\ell}(n^{2}s) - G_{\omega_{0}}(\ell)p_{x}^{2}(n^{2}s)\right] ds = 0, \quad (5.1)$$

for $\ell = 0, 1, 2$. Here $G_{\omega_0}(\ell)$ is the Green's function of $-\Delta_{\mathbb{Z}} + \omega_0^2$, where $\Delta_{\mathbb{Z}}$ is the lattice laplacian, see (A.2).

At the left boundary the situation is a bit different, due to the fact that $q_0 = q_{-1}$, and we have

Proposition 5.2 We have

$$\lim_{n \to +\infty} \int_0^t \mathbb{E} \left[q_0^2(n^2 s) - \left(G_{\omega_0}(1) + G_{\omega_0}(0) \right) p_0^2(n^2 s) \right] ds = 0.$$
 (5.2)

The proofs of Propositions 5.1 and 5.2 require the analysis of the evolution of the covariance matrix of the position and momenta vector and will be done in Appendix D. As a consequence, recalling definition (4.4), the bound (3.5) and the identity $2G_{\omega_0}(1) - G_{\omega_0}(0) - G_{\omega_0}(2) = -\omega_0^2 G_{\omega_0}(1)$ we have the following corollary

Corollary 5.3 For any t > 0 and $\varphi \in C[0, 1]$ such that supp $\varphi \subset (0, 1)$ we have

$$\lim_{n \to +\infty} \frac{1}{n+1} \sum_{s=0}^{n} \varphi\left(\frac{x}{n+1}\right) \int_{0}^{t} \mathbb{E}\left[\mathfrak{F}_{x}(n^{2}s) - Dp_{x}^{2}(n^{2}s)\right] \mathrm{d}s = 0$$
 (5.3)

and

$$\lim_{n \to +\infty} \int_0^t \left\{ \mathbb{E} \left[\mathfrak{F}_0(n^2 s) \right] - DT_- \right\} \mathrm{d}s = 0. \tag{5.4}$$

Here D is defined in (2.25).



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5.1 Proof of Theorem 2.10

Consider the subset $\mathcal{M}_{+,E_*}([0,1])$ of $\mathcal{M}_{+}([0,1])$ (the space of all positive, finite Borel measures on [0,1]) consisting of measures with total mass less than or equal to E_* . It is compact in the topology of weak convergence of measures. In addition, the topology is metrizable when restricted to this set.

For any $t \in [0, t_*]$ and $\varphi \in C[0, 1]$ define

$$\xi_n(t,\varphi) = \frac{1}{n+1} \sum_{x=0}^n \varphi_x \mathbb{E} \left[\mathcal{E}_x(n^2 t) \right], \qquad \varphi_x := \varphi\left(\frac{x}{n+1}\right)$$
 (5.5)

for any $\varphi \in C[0, 1]$. Since flips of the momenta do not affect the energies \mathcal{E}_x , we have $\xi_n \in C([0, t_*], \mathcal{M}_+([0, 1]))$. Here $C([0, t_*], \mathcal{M}_{+, E_*}([0, 1]))$ is endowed with the topology of the uniform convergence. As a consequence of Corollary 3.2 for any $t_* > 0$ the total energy is bounded by $E_* = E(t_*)$ (see (3.2)) and we have that $\xi_n \in C([0, t_*], \mathcal{M}_{+, E_*}([0, 1]))$.

5.2 Compactness

Since $\mathcal{M}_{+,E_*}([0,1])$ is compact, in order to show that (ξ_n) is compact, we only need to control modulus of continuity in time of $\xi_n(t,\varphi)$ for any $\varphi \in C^1[0,1]$, see e.g. [12, p. 234]. This will be consequence of the following Proposition.

Proposition 5.4

$$\lim_{\delta \downarrow 0} \limsup_{n \to \infty} \sup_{0 \leqslant s, t \leqslant t_k, |t-s| < \delta} |\xi_n(t, \varphi) - \xi_n(s, \varphi)| = 0$$
 (5.6)

The proof of Proposition 5.4 is postponed untill Sect. 5.4, we first use it to proceed with the limit identification argument.

5.3 Limit Identification

Consider a smooth test function $\varphi \in C^2[0, 1]$ such that

$$\varphi(0) = \varphi'(1) = 0. \tag{5.7}$$

In what follows we use the following notation. For a given function $\varphi : [0, 1] \to \mathbb{R}$ and $n = 1, 2, \ldots$ we define discrete approximations of the function itself and of its gradient, respectively by

$$\varphi_x := \varphi(\frac{x}{n+1}), \quad (\nabla_n \varphi)_x := (n+1) \left(\varphi(\frac{x+1}{n+1}) - \varphi(\frac{x}{n+1}) \right), \text{ for } x \in \{0, \dots, n\}.$$
 (5.8)

We use the convention $\varphi(-\frac{1}{n+1}) = \varphi(0)$. Let $0 < t_* < +\infty$ be fixed. In what follows we show that, for any $t \in [0, t_*]$

$$\xi_n(t,\varphi) - \xi_n(0,\varphi) = \frac{\varphi'(0)DT_-t}{4\gamma} - Jt\varphi(1) + \frac{D}{4\gamma} \int_0^t \xi_n(s,\varphi'') ds + o_n.$$
 (5.9)

Here, and in what follows o_n denotes a quantity satisfying $\lim_{n\to+\infty} o_n = 0$. Thus any limiting point of $(\xi_n(t))$ has to be the unique weak solution of (2.36) and this obviously proves the conclusion of Theorem 2.10.



By an approximation argument we can restrict ourselves to the case when supp $\varphi'' \subset (0, 1)$. Then as in (5.14) we have

$$\xi_{n}(t,\varphi) - \xi_{n}(0,\varphi) = \frac{n^{2}}{n+1} \sum_{x=0}^{n-1} (\varphi_{x+1} - \varphi_{x}) \int_{0}^{t} \mathbb{E}\left[j_{x,x+1}(n^{2}\tau)\right] d\tau - \frac{n^{2}}{n+1} \varphi_{n} \int_{0}^{t} \mathbb{E}\left[j_{n,n+1}(n^{2}\tau)\right] d\tau,$$
(5.10)

By Theorem 2.5 the last term converges to $-\varphi(1)Jt$. On the other hand from (4.5) we have

$$\frac{n^2}{n+1} \sum_{x=0}^{n-1} (\varphi_{x+1} - \varphi_x) \int_0^t \mathbb{E}\left[j_{x,x+1}(n^2\tau)\right] d\tau = \sum_{j=1}^3 I_{n,j},$$
 (5.11)

where

$$I_{n,1} := -\frac{1}{4\gamma} \left(\frac{n}{n+1} \right)^2 \sum_{x=0}^{n-1} \nabla_n \varphi_x \int_0^t \mathbb{E} \left[\nabla \mathfrak{F}_x(n^2 s) \right] ds,$$

$$I_{n,2} := \left(\frac{1}{n+1} \right)^2 \sum_{x=0}^{n-1} \nabla_n \varphi_x \mathbb{E} \left[f_x(n^2 t) - f_x(0) \right],$$

$$I_{n,3} := -\frac{1}{4\gamma} \left(\frac{n}{n+1} \right)^2 \nabla_n \varphi_{n-1} \int_0^t \mathcal{F}_n(n^2 s) \mathbb{E} \left[q_n(n^2 s) - q_{n-1}(n^2 s) \right] ds.$$

It is easy to see from Corollary 3.2 that $I_{n,2} = \overline{o}_n(t)$. Here the symbol $\overline{o}_n(t)$ stands for a quantity that satisfies

$$\lim_{n \to +\infty} \sup_{s \in [0, t_*]} |\overline{o}_n(s)| = 0. \tag{5.12}$$

Using the fact that $\varphi'(1) = 0$ and the estimate (B.15) respectively we conclude also that $I_{n,3} = \overline{o}_n(t)$. Thanks to Corollary 3.2 and (5.7) we have

$$\begin{split} & I_{n,1} = \sum_{j=1}^{3} I_{n,1}^{(j)} + \overline{o}_n(t), \quad \text{where} \\ & I_{n,1}^{(1)} := \frac{1}{4\gamma(n+1)} \sum_{x=0}^{n} \varphi'' \left(\frac{x}{n+1} \right) \int_0^t \mathbb{E} \left[\mathfrak{F}_x(n^2 s) \right] \mathrm{d}s, \\ & I_{n,1}^{(2)} := -\frac{1}{4\gamma} \left(\frac{n}{n+1} \right)^2 \varphi' \left(\frac{n-1}{n+1} \right) \int_0^t \mathbb{E} \left[\mathfrak{F}_n(n^2 s) \right] \mathrm{d}s = \overline{o}_n(t), \\ & I_{n,1}^{(3)} := \frac{1}{4\gamma} \varphi'(0) \int_0^t \mathbb{E} \left[\mathfrak{F}_0(n^2 s) \right] \mathrm{d}s. \end{split}$$

Since supp $\varphi'' \subset (0, 1)$, by Corollary 5.3 and the equipartition property (Proposition 4.1) for a fixed $t \in [0, t_*]$ we have

$$I_{n,1}^{(1)} = \frac{D}{4\gamma(n+1)} \sum_{x=0}^{n} \varphi''\left(\frac{x}{n+1}\right) \int_{0}^{t} \mathbb{E}\left[p_{x}^{2}(n^{2}s)\right] ds + \overline{o}_{n}(t)$$

$$= \frac{D}{4\gamma(n+1)} \sum_{x=0}^{n} \varphi''\left(\frac{x}{n+1}\right) \int_{0}^{t} \mathbb{E}\left[\mathcal{E}_{x}(n^{2}s)\right] ds + o_{n}. \tag{5.13}$$



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Concluding, we have obtained

$$\lim_{n \to +\infty} \mathbf{I}_{n,1}^{(3)} = \frac{\varphi'(0)DT_{-}t}{4\gamma}.$$

Thus (5.9) follows.

5.4 Proof of Proposition 5.4

From the calculation made in (5.10)–(5.13) we conclude that for any function $\varphi \in C^2[0, 1]$ satisfying (5.7) we have

$$\xi_n(t,\varphi) - \xi_n(s,\varphi) = \frac{\varphi'(0)DT_-}{4\gamma}(t-s) - J\varphi(1)(t-s) + \frac{D}{4\gamma(n+1)} \sum_{x=0}^n \varphi''\left(\frac{x}{n+1}\right) \int_s^t \mathbb{E}\left[p_x^2(n^2\tau)\right] d\tau + \overline{o}_n(t) + \overline{o}_n(s)$$

$$(5.14)$$

for any $0 \le s < t \le t_*$ and (5.6) follows immediately. A density argument completes the proof.

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Declarations

Conflict of interest In addition, the authors have no conflicts of interest to declare that are relevant to the content of this article.

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Appendix A: The Discrete Laplacian

A.1: Discrete Gradient and Laplacian

Recall that the lattice gradient, its adjoint and laplacian of any $f: \mathbb{Z} \to \mathbb{R}$ are defined as

$$\nabla f_x = f_{x+1} - f_x, \quad \nabla^* f_x = f_{x-1} - f_x$$
 (A.1)

and $\Delta_{\mathbb{Z}} f_x = -\nabla^* \nabla f_x = f_{x+1} + f_{x-1} - 2f_x, x \in \mathbb{Z}$, respectively.



Suppose that $\omega_0 > 0$. Consider the Green's function of $-\Delta_{\mathbb{Z}} + \omega_0^2$, where $\Delta_{\mathbb{Z}}$ is the laplacian on the integer lattice \mathbb{Z} . It is given by, see e.g. [17, (27)],

$$G_{\omega_0}(x) = \left(-\Delta_{\mathbb{Z}} + \omega_0^2\right)^{-1}(x) = \int_0^1 \left\{4\sin^2(\pi u) + \omega_0^2\right\}^{-1} \cos(2\pi u x) du$$
$$= \frac{1}{\omega_0 \sqrt{\omega_0^2 + 4}} \left\{1 + \frac{\omega_0^2}{2} + \omega_0 \sqrt{1 + \frac{\omega_0^2}{4}}\right\}^{-|x|}, \quad x \in \mathbb{Z}. \tag{A.2}$$

A.2: Discrete Neumann Laplacian $-\Delta$

Let λ_j and ψ_j , j = 0, ..., n be the respective eigenvalues and eigenfunctions for the discrete Neumann laplacian $-\Delta$ defined in (2.8). They are given by

$$\lambda_j = 4\sin^2\left(\frac{\pi j}{2(n+1)}\right), \quad \psi_j(x) = \left(\frac{2-\delta_{0,j}}{n+1}\right)^{1/2}\cos\left(\frac{\pi j(2x+1)}{2(n+1)}\right), \quad x, j = 0, \dots, n.$$
(A.3)

The eigenvalues of $\omega_0^2 - \Delta$ are given by

$$\mu_j = \omega_0^2 + \lambda_j = \omega_0^2 + 4\sin^2\left(\frac{\pi j}{2(n+1)}\right), \quad j = 0, \dots, n.$$
 (A.4)

Appendix B: The Dynamics of the Means

Let μ be a Borel probability measure on $\mathbb{R}^{2(n+1)}$ and let $(\overline{\mathbf{q}}, \overline{\mathbf{p}})$ be the vector of the μ -averages of initial data. In the following we denote by $\left(\frac{\overline{\mathbf{q}}(t)}{\overline{\mathbf{p}}(t)}\right)$ the vector means of positions and momenta by $\overline{q}_x(t) = \mathbb{E}_{\mathbf{q},\mathbf{p}}(q_x(t))$ and $\overline{p}_x(t) = \mathbb{E}_{\mathbf{q},\mathbf{p}}(p_x(t))$. Let $\mathbf{e}_{2(n+1)}$ be the 2(n+1) vector defined by $\mathbf{e}_{2(n+1),j} = \delta_{2(n+1),j}$. Then, performing the averages in (2.3) and (2.4), we conclude the evolution equation for the averages. Its solution is given by

$$\left(\frac{\overline{\mathbf{q}}(t)}{\overline{\mathbf{p}}(t)}\right) = e^{-At} \left(\frac{\overline{\mathbf{q}}}{\overline{\mathbf{p}}}\right) + \int_0^t \mathcal{F}_n(s) e^{-A(t-s)} \mathbf{e}_{2(n+1)} ds.$$
 (B.1)

Here A is a 2 \times 2 block matrix made of $(n + 1) \times (n + 1)$ matrices of the form

$$A = \begin{pmatrix} 0 & -\mathrm{Id}_{n+1} \\ -\Delta + \omega_0^2 \mathrm{Id}_{n+1} & 2\gamma \mathrm{Id}_{n+1} \end{pmatrix}, \tag{B.2}$$

where Id_{n+1} is the $(n+1)\times(n+1)$ identity matrix.

Using the expansion

$$\mathcal{F}(t) = \sum_{\ell \in \mathbb{Z}} \widehat{\mathcal{F}}(\ell) e^{2\pi i \ell t}$$

and defining

$$\left(\frac{\overline{\mathbf{y}}(t)}{\overline{\mathbf{z}}(t)}\right) := e^{-At}\mathbf{e}_{2(n+1)},\tag{B.3}$$



we can write

$$\left(\frac{\overline{\mathbf{q}}(t)}{\overline{\mathbf{p}}(t)}\right) = e^{-At} \left(\frac{\overline{\mathbf{q}}}{\overline{\mathbf{p}}}\right) + \sum_{\ell \in \mathbb{Z}} \frac{\widehat{\mathcal{F}}(\ell)}{\sqrt{n}} \int_0^t e^{2\pi i \ell s/\theta} \left(\frac{\overline{\mathbf{y}}(t-s)}{\overline{\mathbf{z}}(t-s)}\right) \mathrm{d}s.$$
(B.4)

To find the formulas for the components of $\overline{v}_x(t)$, $\overline{u}_x(t)$, $x=0,\ldots,n$ of the vector $\left(\frac{\overline{\mathbf{u}}(t)}{\overline{\mathbf{v}}(t)}\right):=e^{-At}\left(\frac{\overline{\mathbf{q}}}{\overline{\mathbf{p}}}\right)$ it is convenient to use the Fourier coordinates in the base ψ_j of the eigenvectors for the Neumann laplacian Δ , see (A.3). Let $\widetilde{u}_j(t)=\sum_{x=0}^n\overline{u}_x(t)\psi_j(x)$ and $\widetilde{v}_j(t)=\sum_{x=0}^n\overline{v}_x(t)\psi_j(x)$ be the Fourier coordinates of the vector $(\overline{\mathbf{u}}(t),\overline{\mathbf{v}}(t))$. Likewise, we let $\widetilde{q}_j=\sum_{x=0}^n\overline{q}_x\psi_j(x)$ and $\widetilde{p}_j=\sum_{x=0}^n\overline{p}_x\psi_j(x)$, with \overline{q}_x , \overline{p}_x , $x=0,\ldots,n$ the components of $(\overline{\mathbf{q}},\overline{\mathbf{p}})$.

Let

$$\lambda_{j,\pm} := \gamma \pm \sqrt{\gamma^2 - \mu_j} \tag{B.5}$$

be the two solutions of the equation

$$\lambda^2 - 2\gamma\lambda + \mu_i = 0. \tag{B.6}$$

Note that $\lambda_{i,+}\lambda_{i,-} = \mu_{i}$. Then,

$$\widetilde{u}_{j}(t) = \frac{1}{2\sqrt{\gamma^{2} - \mu_{j}}} \left[-(\lambda_{j, -}\widetilde{q}_{j} + \widetilde{p}_{j}) \exp\left\{-\lambda_{j, +}t\right\} + (\lambda_{j, +}\widetilde{q}_{j} + \widetilde{p}_{j}) \exp\left\{-\lambda_{j, -}t\right\} \right]. \tag{B.7}$$

and

$$\widetilde{v}_{j}(t) = \frac{1}{2\sqrt{\gamma^{2} - \mu_{j}}} \Big[(\mu_{j}\widetilde{q}_{j} + \lambda_{j,+}\widetilde{p}_{j}) \exp\left\{-\lambda_{j,+}t\right\} - (\mu_{j}\widetilde{q}_{j} + \lambda_{j,-}\widetilde{p}_{j}) \exp\left\{-\lambda_{j,-}t\right\} \Big],$$
(B.8)

in the case when $\mu_i \neq \gamma^2$. When $\gamma^2 = \mu_i$ (then $\lambda_{i,\pm} = \gamma$) we have

$$\widetilde{u}_j(t) = \left[(1 + \gamma t) \widetilde{q}_j + \widetilde{p}_j t \right] e^{-\gamma t}, \qquad \widetilde{v}_j(t) = \left[\gamma^2 t \widetilde{q}_j + (1 - \gamma t) \widetilde{p}_j \right] e^{-\gamma t},$$

Then, by (B.7) and (B.8), we conclude that the components of $e^{-At}\mathbf{e}_{2(n+1)}$ equal

$$\widetilde{y}_{j}(t) = \frac{\psi_{j}(n)}{2\sqrt{\gamma^{2} - \mu_{j}}} \left(-\exp\left\{-\lambda_{j,+}t\right\} + \exp\left\{-\lambda_{j,-}t\right\} \right),
\widetilde{z}_{j}(t) = \frac{\psi_{j}(n)}{2\sqrt{\gamma^{2} - \mu_{j}}} \left(\lambda_{j,+}\exp\left\{-\lambda_{j,+}t\right\} - \lambda_{j,-}\exp\left\{-\lambda_{j,-}t\right\} \right).$$
(B.9)

in the case when $\mu_j \neq \gamma^2$. In the case that $\gamma^2 = \mu_j$ (then $\lambda_{j,\pm} = \gamma$) we have $\widetilde{y}_j(t) = \psi_j(n)te^{-\gamma t}$ and $\widetilde{z}_j(t) = \psi_j(n)(1-\gamma t)e^{-\gamma t}$.

Elementary calculations lead to the following bounds

$$\operatorname{Re}\lambda_{j,\pm} \geqslant \gamma_* := \min \left\{ \gamma, \frac{\omega_0^2}{2\gamma} \right\}, \quad |\lambda_{j,\pm}| \leqslant \gamma + |\gamma^2 - \omega_0^2 - 4|^{1/2}, \quad j = 0, \dots, n.$$
 (B.10)

Hence, there exists C > 0 such that

$$|\widetilde{y}_j(t)| + |\widetilde{z}_j(t)| \leqslant C(t+1)e^{-\gamma_* t} |\psi_j(n)| \tag{B.11}$$



for all $t \ge 0$, j = 0, ..., n, n = 1, 2, ... By the Plancherel identity, (B.7) and (B.8) we conclude also that there exist constants C, C' > 0 such that, for all $t \ge 0$ and $n \in \mathbb{N}$,

$$\sum_{x=0}^{n} \left[\overline{u}_{x}^{2}(t) + \overline{v}_{x}^{2}(t) \right] = \sum_{j=0}^{n} \left[\widetilde{u}_{j}^{2}(t) + \widetilde{v}_{j}^{2}(t) \right] \\
\leqslant C(t+1)e^{-\gamma_{*}t} \sum_{j=0}^{n} \left(\widetilde{q}_{j}^{2} + \widetilde{p}_{j}^{2} \right) \leqslant C'(t+1)e^{-\gamma_{*}t} \mathcal{H}_{n}\left(\overline{\mathbf{q}}, \overline{\mathbf{p}} \right). \tag{B.12}$$

B.1: L2 Norms of the Means

By (B.4), the triangle inequality and the Plancherel theorem

$$\begin{split} &\sum_{x=0}^{n} \int_{0}^{t} \left[\overline{q}_{x}^{2}(s) + \overline{p}_{x}^{2}(s) \right] \mathrm{d}s \leqslant C \sum_{x=0}^{n} \int_{0}^{t} \left[\overline{u}_{x}^{2}(s) + \overline{v}_{x}^{2}(s) \right] \mathrm{d}s \\ &+ \frac{C}{n} \sum_{j=0}^{n} \left[\left| \sum_{\ell \in \mathbb{Z}} \widehat{\mathcal{F}}(\ell) \int_{0}^{t} e^{2\pi i \ell s / \theta} \widetilde{y}_{j}(t-s) \mathrm{d}s \right|^{2} + \left| \sum_{\ell \in \mathbb{Z}} \widehat{\mathcal{F}}(\ell) \int_{0}^{t} e^{2\pi i \ell s / \theta} \widetilde{z}_{j}(t-s) \mathrm{d}s \right|^{2} \right]. \end{split}$$

$$(B.13)$$

The constant appearing here below do not depend on t and n. Using (2.6), (B.11) and (B.12) we conclude therefore that

$$\sum_{x=0}^{n} \int_{0}^{t} \left[\overline{q}_{x}^{2}(s) + \overline{p}_{x}^{2}(s) \right] ds \leqslant C \mathcal{H}_{n} \left(\overline{\mathbf{q}}, \overline{\mathbf{p}} \right) + \frac{C}{n} \left(\sum_{\ell \in \mathbb{Z}} |\widehat{\mathcal{F}}(\ell)| \right)^{2}. \tag{B.14}$$

From (B.14) we conclude therefore the following.

Proposition B.1 Assume that the hypotheses of Theorem 2.5 are in force. Then, there exists C > 0 such that

$$\sum_{x=0}^{n} \int_{0}^{t} \left[\overline{q}_{x}^{2}(n^{2}s) + \overline{p}_{x}^{2}(n^{2}s) \right] \mathrm{d}s \leqslant \frac{C}{n^{\kappa}}, \tag{B.15}$$

for all $t \ge 0$, n = 1, 2, ... Here $\kappa = \min\{2 - \delta, 1\}$ and δ is as in (2.28). If the hypotheses of Theorem 2.10 hold, then $\delta = 1$ and (B.15) is satisfied with $\kappa = 1$.

B.2: The Proof of Theorem 2.5

We show (2.29) and (2.19). Recall that the initial configuration (\mathbf{q} , \mathbf{p}) is distributed according to μ_n . For the work done we have

$$W_n(t) := \int_0^t \mathcal{F}_n(s) \overline{p}_n(s) ds$$

$$= \sum_i \psi_j(n) \sum_{\ell \in \mathbb{Z}} \frac{1}{\sqrt{n}} \widehat{\mathcal{F}}(\ell)^* \int_0^t e^{-i2\pi \ell s/\theta} \widetilde{p}_j(s) ds.$$
(B.16)

We have $J_n(t; \mu) = -W_n(n^2t)/n$, see (2.27).



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Using (B.1) the utmost right hand side can be rewritten in the form $W_{n,i}(t) + W_{n,f}(t)$ where

$$W_{n,i}(t) := \sum_{j=0}^{n} \psi_{j}(n) \sum_{\ell \in \mathbb{Z}} \frac{1}{\sqrt{n}} \widehat{\mathcal{F}}(\ell)^{*} \int_{0}^{t} e^{-i2\pi\ell s/\theta} \widetilde{v}_{j}(s) ds,$$

$$W_{n,f}(t) := \frac{1}{n} \sum_{j=0}^{n} \psi_{j}(n) \sum_{\ell,\ell' \in \mathbb{Z}} \widehat{\mathcal{F}}(\ell)^{*} \widehat{\mathcal{F}}(\ell') \int_{0}^{t} ds \ e^{i2\pi(\ell'-\ell)s/\theta} \int_{0}^{s} e^{-i2\pi\ell' s'/\theta} \widetilde{z}_{j}(s') ds',$$

$$(B.17)$$

with $\widetilde{v}_i(s)$ and $\widetilde{z}_i(s')$ defined in (B.8) and (B.9).

Thanks to the last estimate of (2.6) and the Cauchy-Schwarz inequality we conclude from (B.12)

$$|W_{n,i}(t)| \leqslant \frac{C}{\sqrt{n}} \mathcal{H}_n^{1/2} \left(\overline{\mathbf{q}}_n, \overline{\mathbf{p}}_n\right) \int_0^t (s+1)^{1/2} e^{-\gamma_* s/2} \mathrm{d}s.$$

Thanks to (2.28) $\lim_{n\to+\infty} |W_{n,i}(n^2t)|/n = 0$. Using (B.9) we have

$$\begin{split} &\int_0^s e^{-i2\pi\ell's'/\theta} \widetilde{z}_j(s') \mathrm{d}s' \\ &= \frac{\psi_j(n)}{\lambda_{j,+} - \lambda_{j,-}} \left[\frac{\lambda_{j,-} \left[e^{-s(\lambda_{j,-} + 2\pi i\ell'/\theta)} - 1 \right]}{2\pi i\ell'/\theta + \lambda_{j,-}} - \frac{\lambda_{j,+} \left[e^{-s(\lambda_{j,+} + 2\pi i\ell'/\theta)} - 1 \right]}{2\pi i\ell'/\theta + \lambda_{j,+}} \right], \end{split}$$

so that we can decompose the work done in $W_{n,f}(t) = W_{n,f}^{(1)}(t) + W_{n,f}^{(2)}(t)$, where

$$\begin{split} &\frac{1}{n}W_{n,f}^{(1)}(n^2t) := -\frac{1}{n^2}\sum_{j=0}^n \frac{\psi_j^2(n)}{\lambda_{j,+} - \lambda_{j,-}} \\ &\sum_{\ell,\ell' \in \mathbb{Z}} \widehat{\mathcal{F}}^*(\ell)\widehat{\mathcal{F}}(\ell') \Big(\frac{\lambda_{j,-}}{2\pi i \ell'/\theta + \lambda_{j,-}} - \frac{\lambda_{j,+}}{2\pi i \ell'/\theta + \lambda_{j,+}}\Big) \\ &\times \int_0^{n^2t} \exp\left\{2\pi i s(\ell'-\ell)/\theta\right\} \mathrm{d}s \\ &= -t\sum_{j=0}^n \frac{\psi_j^2(n)}{\lambda_{j,+} - \lambda_{j,-}} \sum_{\ell \in \mathbb{Z}} |\widehat{\mathcal{F}}(\ell)|^2 \Big(\frac{\lambda_{j,-}}{2\pi i \ell/\theta + \lambda_{j,-}} - \frac{\lambda_{j,+}}{2\pi i \ell/\theta + \lambda_{j,+}}\Big) \\ &+ O\left(\frac{1}{n^2}\right) \end{split}$$

and

$$\begin{split} &\frac{1}{n}W_{n,f}^{(2)}(n^2t) := \frac{1}{n^2}\sum_{j=0}^n \frac{\psi_j^2(n)}{\lambda_{j,+} - \lambda_{j,-}} \\ &\sum_{\ell,\ell' \in \mathbb{Z}} \widehat{\mathcal{F}}^{\star}(\ell)\widehat{\mathcal{F}}(\ell') \int_0^{n^2t} \left(\frac{\lambda_{j,+} \exp\left\{-(2\pi i \ell'/\theta + \lambda_{j,+})s\right\}}{2\pi i \ell'/\theta + \lambda_{j,+}}\right) \\ &- \frac{\lambda_{j,-} \exp\left\{-(2\pi i \ell'/\theta + \lambda_{j,-})s\right\}}{2\pi i \ell'/\theta + \lambda_{j,-}} \right) \mathrm{d}s. \end{split}$$



Using (B.6) and integrating over the s variable we conclude that

$$\begin{split} &\frac{1}{n}W_{n,f}^{(2)}(n^2t) = \frac{1}{n^2} \sum_{j=0}^n \psi_j^2(n) \sum_{\ell,\ell' \in \mathbb{Z}} \widehat{\mathcal{F}}^*(\ell) \widehat{\mathcal{F}}(\ell') \\ &\times \Big\{ \frac{1 - \exp\left\{ - (2\pi i \ell'/\theta + \lambda_{j,+}) n^2 t \right\}}{(2\pi i \ell'/\theta + \lambda_{j,+})} \cdot \frac{2\pi i \ell'/\theta}{\mu_j - (2\pi \ell'/\theta)^2 - 4\gamma \pi i \ell'/\theta} \\ &\quad + \frac{\lambda_{j,-}}{(2\pi i \ell'/\theta + \lambda_{j,-})} \Big[\exp\left\{ - (2\pi i \ell'/\theta + \lambda_{j,-}) n^2 t \right\} \frac{1 - \exp\left\{ - 2\sqrt{\gamma^2 - \mu_j} n^2 t \right\}}{2\sqrt{\gamma^2 - \mu_j} (2\pi i \ell'/\theta + \lambda_{j,-})} \\ &\quad + \frac{\exp\left\{ - (2\pi i \ell'/\theta + \lambda_{j,+}) n^2 t \right\}}{(2\pi i \ell'/\theta + \lambda_{j,+})} - \frac{1}{\mu_j - (2\pi \ell'/\theta)^2 - 4\gamma \pi i \ell'/\theta} \Big] \Big\}. \end{split}$$

Here we have used the fact that

$$\lambda_{j,+} - \lambda_{j,-} = 2\sqrt{\gamma^2 - \mu_j}.\tag{B.18}$$

Recalling (B.10) we obtain that $\frac{1}{n}W_{n,f}^{(2)}(n^2t) = O\left(\frac{1}{n^2}\right)$ for each t > 0.

Concerning $W_{n,f}^{(1)}(t)$, we use (B.6) and obtain

$$\frac{1}{n}W_{n,f}^{(1)}(n^2t) = -t\sum_{i=0}^{n}\sum_{\ell\in\mathbb{Z}}\frac{(2\pi i\ell/\theta)\psi_j^2(n)|\widehat{\mathcal{F}}(\ell)|^2}{\mu_j - (2\pi\ell/\theta)^2 - 2\gamma(2\pi i\ell/\theta)} + O\Big(\frac{1}{n^2}\Big)$$

After substituting for $\psi_i(n)$ and μ_i from (A.3) and (A.4) correspondingly, we obtain

$$\begin{split} \frac{1}{n}W_{n,f}^{(1)}(n^2t) &= \frac{4\gamma t}{n+1} \sum_{j=0}^{n} \sum_{\ell \in \mathbb{Z}} \frac{\cos^2\left(\frac{\pi j}{2(n+1)}\right) (2\pi\ell/\theta)^2 \, |\widehat{\mathcal{F}}(\ell)|^2}{\left[\omega_0^2 + 4\sin^2\left(\frac{j\pi}{2(n+1)}\right) - (2\pi\ell/\theta)^2\right]^2 + \left[(4\gamma\pi\ell/\theta)\right]^2} \\ &\quad + O\left(\frac{1}{n^2}\right) \\ &= -Jt + O\left(\frac{1}{n^2}\right), \end{split}$$

so that

$$\lim_{n \to \infty} J_n(t) = -\lim_{n \to \infty} W_n(n^2 t)/n = Jt$$

and Theorem 2.5 follows.

Appendix C: The Evolution of the Covariance Matrix

C.1: Dynamics of Fluctuations

Denote

$$q'_x(t) := q_x(n^2t) - \overline{q}_x(n^2t)$$
 and $p'_x(t) := p_x(n^2t) - \overline{p}_x(n^2t)$ (C.1)



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for x = 0, ..., n. From (2.3) and (2.4) we get

$$\dot{q}'_{x}(t) = n^{2} p'_{x}(t), \qquad x \in \{0, \dots, n\},$$

$$dp'_{x}(t) = n^{2} \left(\Delta q'_{x} - \omega_{0}^{2} q'_{x} \right) dt - 2\gamma n^{2} p'_{x}(t) dt - 2p_{x}(n^{2}t) d\widetilde{N}_{x}(\gamma n^{2}t), \quad x \in \{1, \dots, n\}$$
(C.2)

and at the left boundary

$$dp'_{0}(t) = n^{2} \left(\Delta q'_{0} - \omega_{0}^{2} q'_{0} \right) dt - 2\gamma n^{2} p'_{0}(t) dt + \sqrt{4\gamma T_{-}} n d\widetilde{w}_{-}(t).$$
 (C.3)

Here $\widetilde{N}_x(t) := N_x(t) - t$. Let $\mathbf{X}'(t) = [q_0'(t), \dots, q_n'(t), p_0'(t), \dots, p_n'(t)]$. Denote by $S_n(t)$ the the covariance matrix

$$S_n(t) = \mathbb{E}_{\mu_n} \left[\mathbf{X}'(t) \otimes \mathbf{X}'(t) \right] = \begin{bmatrix} S_n^{(q)}(t) & S_n^{(q,p)}(t) \\ S_n^{(p,q)}(t) & S_n^{(p)}(t) \end{bmatrix}, \tag{C.4}$$

where

$$S_{n}^{(q)}(t) = \left[\mathbb{E}_{\mu_{n}} [q_{x}'(t)q_{y}'(t)] \right]_{x,y=0,\dots,n}, \quad S_{n}^{(q,p)}(t) = \left[\mathbb{E}_{\mu_{n}} [q_{x}'(t)p_{y}'(t)] \right]_{x,y=0,\dots,n},$$

$$S_{n}^{(p)}(t) = \left[\mathbb{E}_{\mu_{n}} [p_{x}'(t)p_{y}'(t)] \right]_{x,y=0,\dots,n} \quad \text{and} \quad S_{n}^{(p,q)}(t) = \left[S_{n}^{(q,p)}(t) \right]^{T}. \quad (C.5)$$

C.2: Structure of the Covariance Matrix

Given a vector $\mathfrak{y} = (y_0, y_1, \dots, y_n)$, define also the matrix valued function

$$D(\mathfrak{y}) = 4\gamma \begin{bmatrix} T_{-} & 0 & 0 & \dots & 0 \\ 0 & y_{1} & 0 & \dots & 0 \\ 0 & 0 & y_{2} & \dots & 0 \\ \vdots & \vdots & \vdots & \vdots & \vdots \\ 0 & 0 & 0 & \dots & y_{r} \end{bmatrix}.$$
 (C.6)

Let $\Sigma(\mathfrak{y})$ be the 2 × 2 block matrix

$$\Sigma(\mathfrak{y}) = \begin{bmatrix} 0_{n+1} & 0_{n+1} \\ 0_{n+1} & D(\mathfrak{y}) \end{bmatrix}. \tag{C.7}$$

Here 0_{n+1} is $(n+1) \times (n+1)$ null matrix. From (C.2) and (C.3) we conclude

$$S_n(t) = \mathbb{E}_{\mu_n} \left[e^{-An^2t} \mathbf{X}'(0) \otimes \mathbf{X}'(0) e^{-A^T n^2 t} \right] + n^2 \int_0^t e^{-An^2(t-s)} \Sigma \left(\overline{\mathbf{p}^2}(n^2 s) \right) e^{-A^T n^2(t-s)} ds$$

where A is given by (B.2) and $\overline{\mathbf{p}^2}(s) = [\mathbb{E}_{\mu_n} p_1^2(s), \dots, \mathbb{E}_{\mu_n} p_n^2(s)]$. Consequently

$$\frac{1}{n^2} \frac{\mathrm{d}}{\mathrm{d}t} S_n(t) = -A S_n(t) - S_n(t) A^T + \Sigma \left(\overline{\mathbf{p}^2}(n^2 t) \right). \tag{C.8}$$

Denoting

$$\langle\langle S_n \rangle\rangle_t = \int_0^t S_n(s) ds, \qquad \langle\langle \mathbf{p}^2 \rangle\rangle_t = \int_0^t \overline{\mathbf{p}^2}(n^2 s) ds,$$
 (C.9)

we have, by integrating in (C.8),

$$A\langle\langle S_n \rangle\rangle_t + \langle\langle S_n \rangle\rangle_t A^T - \Sigma \Big(\langle\langle \mathbf{p}^2 \rangle\rangle_t\Big) = \frac{1}{n^2} \Big[S_n(0) - S_n(t)\Big]. \tag{C.10}$$



In the following $\{\psi_j(x), \mu_{j'}\}_{x,j,j'=0,...,n}$ are the eigenfunctions and eigenvalues of $\omega_0^2 - \Delta$, given in (A.3) in Appendix A.

Given a matrix $[B_{x,x'}]_{x,x'=0,\dots,n}$ we define its Fourier transform

$$\widetilde{B}_{j,j'} = \sum_{x,x'=0}^{n} B_{x,x'} \psi_j(x) \psi_{j'}(x'), \quad j, j' = 0, \dots, n.$$

Then we have the inverse relations

$$B_{x,x'} = \sum_{j,j'=0}^{n} \widetilde{B}_{j,j'} \psi_j(x) \psi_{j'}(x'). \tag{C.11}$$

Following analogous algebraic calculation to those of [14, section 6.3], see also Section C.4 below for a detailed calculation, we obtain

$$\langle \langle \widetilde{S}_{j,j'}^{(p)} \rangle \rangle_t = \Theta(\mu_j, \mu_{j'}) \widetilde{F}_{j,j'}(t) + \frac{1}{n^2} \widetilde{R}_{j,j'}^{(p)}(t), \tag{C.12}$$

where

$$\widetilde{F}_{j,j'}(t) := \sum_{y=0}^{n} \psi_j(y) \psi_{j'}(y) \langle \langle p_y^2 \rangle \rangle_t + \left(T_- t - \langle \langle p_0^2 \rangle \rangle_t \right) \psi_j(0) \psi_{j'}(0) \tag{C.13}$$

and

$$\Theta(\mu_j, \mu_{j'}) = \left[1 + \frac{(\mu_j - \mu_{j'})^2}{8\gamma^2(\mu_j + \mu_{j'})} \right]^{-1}.$$
 (C.14)

Concerning $\widetilde{R}_{j,j'}^{(p)}(t)$, it is of the form

$$\widetilde{R}_{j,j'}^{(p)}(t) = \sum_{l \in \mathbb{Z}} \Xi_{l}^{(p)}(\mu_{j}, \mu_{j'}) \left[\widetilde{S}_{j,j'}^{(l)}(t) - \widetilde{S}_{j,j'}^{(l)}(0) \right], \tag{C.15}$$

where Z is a 3 element set consisting of indices p,q and pq and $\Xi_t^{(p)}$ are some C^{∞} smooth functions defined on $[\omega_0^2, 4+\omega_0^2] \times [\omega_0^2, 4+\omega_0^2]$.

We also have

$$\langle \langle \widetilde{S}_{j,j'}^{(q)} \rangle \rangle_t = \frac{2\Theta(\mu_j, \mu_{j'})}{\mu_j + \mu_{j'}} \widetilde{F}_{j,j'}(t) + \frac{1}{n^2} \widetilde{R}_{j,j'}^{(q)}(t), \tag{C.16}$$

and

$$\langle\langle \widetilde{S}_{j,j'}^{(q,p)}\rangle\rangle_t = \frac{\Theta(\mu_j,\mu_{j'})}{2\gamma(\mu_j+\mu_{j'})}(\mu_j-\mu_{j'})\widetilde{F}_{j,j'}(t) + \frac{1}{n^2}\widetilde{R}_{j,j'}^{(q,p)}(t), \tag{C.17}$$

where the matrices $\widetilde{R}_{j,j'}^{(q)}(t)$ and $\widetilde{R}_{j,j'}^{(q,p)}(t)$ are given by analogues of (C.15).

C.3: Some Bounds on the Kinetic Energy

From (C.12) we have

$$\langle\langle S_{x,x}^{(p)}\rangle\rangle_t = \sum_{y=0}^n M_{x,y} \langle\langle p_y^2\rangle\rangle_t + \left(T_- t - \langle\langle p_0^2\rangle\rangle_t\right) M_{x,0} + r_{n,x}^{(p)}(t), \tag{C.18}$$

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where $\langle \langle S_{x,x}^{(p)} \rangle \rangle_t = \int_0^t [p_x'(s)]^2 ds$,

$$M_{x,y} := \sum_{j,j'=0}^{n} \Theta(\mu_j, \mu_{j'}) \psi_j(x) \psi_{j'}(x) \psi_j(y) \psi_{j'}(y), \tag{C.19}$$

and

$$r_{n,x}^{(p)}(t) := \frac{1}{n^2} \sum_{j,j'=0}^{n} \widetilde{R}_{j,j'}^{(p)}(t) \psi_j(x) \psi_{j'}(x). \tag{C.20}$$

The latter satisfy the following estimates: for each t > 0 there exists C > 0 such that

$$\sup_{s \in [0,t]} \sum_{x=0}^{n} |r_{n,x}^{(p)}(s)| \leqslant \frac{C}{n+1}, \quad n = 1, 2, \dots$$
 (C.21)

The proof of (C.21) can be found in Section C.4.1 below.

It has been shown in [14, Appendix A] that

$$\sum_{y'=0}^{n} M_{x,y'} = \sum_{y'=0}^{n} M_{y',x} \equiv 1 \quad \text{and} \quad M_{x,y} > 0 \quad \text{for all } x, y = 0, \dots, n.$$
 (C.22)

Recall that $\langle \langle p_x^2 \rangle \rangle_t = \langle \langle S_{x,x}^{(p)} \rangle_t + \int_0^t \overline{p}_x^2 (n^2 s) ds$. Under the assumptions of Theorem 2.10 we may admit $\delta = 1$ in the conclusion of Proposition B.1. Thanks to (B.15) we conclude that for each t > 0 there exists C > 0 such that

$$\sum_{n=0}^{n} \int_{0}^{t} \overline{p}_{x}^{2}(n^{2}s) ds \leqslant \frac{C}{n}, \quad n = 1, 2, \dots$$
 (C.23)

From (C.23), (C.21), and (3.5) we infer therefore that

$$\langle \langle p_x^2 \rangle \rangle_t = \sum_{y=0}^n M_{x,y} \langle \langle p_y^2 \rangle \rangle_t + \rho_x(t), \tag{C.24}$$

where $\rho_x(t)$ satisfies: for any t > 0 there exists C > 0 such that

$$\sup_{s \in [0,t]} \sum_{x=0}^{n} |\rho_x(s)| \leqslant \frac{C}{n+1}, \quad n = 1, 2, \dots$$
 (C.25)

The following lower bound on the matrix $[M_{x,y}]$ comes from [14, Proposition 7.1] (see also [7]).

Proposition C.1 There exists $c_* > 0$ such that

$$\sum_{x,y=0}^{n} (\delta_{x,y} - M_{x,y}) f_y f_x \geqslant c_* \sum_{x=0}^{n-1} (\nabla f_x)^2, \quad \text{for any } (f_x) \in \mathbb{R}^{n+1}, \ n = 1, 2, \dots$$
 (C.26)

Multiplying both sides of (C.24) by $\langle \langle p_x^2 \rangle \rangle_t$, summing over x and using Proposition C.1 together with estimate (C.24) we immediately conclude the following.

Corollary C.2 For any t > 0 there exists C > 0 such that

$$\sum_{x=0}^{n-1} [\langle \langle p_x^2 \rangle \rangle_t - \langle \langle p_{x+1}^2 \rangle \rangle_t]^2 \leqslant \frac{C}{n+1} \sum_{x=0}^n \langle \langle p_x^2 \rangle \rangle_t, \quad n = 1, 2, \dots$$
 (C.27)



Proposition C.3 For any t > 0 there exists C > 0 such that

$$\sum_{x=0}^{n-1} [\langle \langle p_x^2 \rangle \rangle_t - \langle \langle p_{x+1}^2 \rangle \rangle_t]^2 \leqslant \frac{C}{n+1}, \quad n = 1, 2, \dots,$$

$$\sup_{x=0,\dots,n} \langle \langle p_x^2 \rangle \rangle_t \leqslant C.$$
(C.28)

Proof As a direct consequence of (3.2) and Corollary C.2 we have: for any t > 0 there exists C > 0 such that

$$\sum_{x=0}^{n-1} [\langle \langle p_x^2 \rangle \rangle_t - \langle \langle p_{x+1}^2 \rangle \rangle_t]^2 \leqslant C$$
 (C.29)

and

$$\sup_{x=0,\dots,n} \langle \langle p_x^2 \rangle \rangle_t \leqslant C n^{1/2}, \quad n = 1, 2, \dots$$
 (C.30)

Indeed, estimate (C.29) is obvious in light of (C.27). To prove (C.30) note that by the Cauchy-Schwarz inequality

$$\begin{split} &\langle\langle p_x^2\rangle\rangle_t\leqslant \sum_{y=1}^n|\langle\langle p_y^2\rangle\rangle_t-\langle\langle p_{y-1}^2\rangle\rangle_t|+\langle\langle p_0^2\rangle\rangle_t\\ &\leqslant \sqrt{n}\left\{\sum_{y=1}^n[\langle\langle p_y^2\rangle\rangle_t-\langle\langle p_{y-1}^2\rangle\rangle_t]^2\right\}^{1/2}+\langle\langle p_0^2\rangle\rangle_t\leqslant C\sqrt{n}+\langle\langle p_0^2\rangle\rangle_t \end{split}$$

and (C.30) follows, thanks to (3.5).

From (C.24) and (C.25) we conclude that for any t > 0 we can find C > 0 such that

$$\sum_{x=0}^{n-1} \left(\langle \langle p_x^2 \rangle \rangle_t - \langle \langle p_{x+1}^2 \rangle \rangle_t \right)^2 \leqslant \sum_{x=0}^n |\rho_x(t)| \langle \langle p_x^2 \rangle \rangle_t$$

$$\leqslant \sup_x \langle \langle p_x^2 \rangle \rangle_t \sum_{x=0}^n |\rho_x(t)| \leqslant \frac{C}{n+1} \sup_x \langle \langle p_x^2 \rangle \rangle_t$$
(C.31)

Using the Cauchy-Schwarz inequality we conclude

$$\sup_{x} \langle \langle p_{x}^{2} \rangle \rangle_{t} \leq \langle \langle p_{0}^{2} \rangle \rangle_{t} + \sum_{x=0}^{n-1} \left| \langle \langle p_{x}^{2} \rangle \rangle_{t} - \langle \langle p_{x+1}^{2} \rangle \rangle_{t} \right|$$

$$\leq \langle \langle p_{0}^{2} \rangle \rangle_{t} + \sqrt{n} \left\{ \sum_{x=0}^{n-1} \left(\langle \langle p_{x}^{2} \rangle \rangle_{t} - \langle \langle p_{x+1}^{2} \rangle \rangle_{t} \right)^{2} \right\}^{1/2}$$
(C.32)

Denote $D_n := \sum_{x=0}^{n-1} \left(\langle \langle p_x^2 \rangle \rangle_t - \langle \langle p_{x+1}^2 \rangle \rangle_t \right)^2$. We can summarize the inequalities obtained as follows: for any t > 0 there exists C > 0 such that

$$D_{n} \leqslant \frac{C}{n+1} \sup_{x} \langle \langle p_{x}^{2} \rangle \rangle_{t},$$

$$\sup_{x} \langle \langle p_{x}^{2} \rangle \rangle_{t} \leqslant \langle \langle p_{0}^{2} \rangle \rangle_{t} + \sqrt{n+1} D_{n}^{1/2} \leqslant \langle \langle p_{0}^{2} \rangle \rangle_{t} + C + C \sup_{x} \langle \langle p_{x}^{2} \rangle \rangle_{t}^{1/2},$$
 (C.33)

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for all n = 1, 2, ... Thus the second estimate of (C.28) follows, which in turn implies the first estimate of (C.28) as well.

C.4: Calculation of $\widetilde{R}^{(p)}(t)$, $\widetilde{R}^{(q)}(t)$ and $\widetilde{R}^{(q,p)}(t)$

Equation (C.10) leads to the following equations (see (B.2) and (C.6)):

$$\langle \langle \widetilde{S}_{j,j'}^{(q,p)} \rangle \rangle_{t} + \langle \langle \widetilde{S}_{j,j'}^{(p,q)} \rangle \rangle_{t} = \frac{1}{n^{2}} \left[\widetilde{S}_{j,j'}^{(q)}(0) - \widetilde{S}_{j,j'}^{(q)}(t) \right] \text{ and } \left(\langle \langle \widetilde{S}^{(p,q)} \rangle \rangle_{t} \right)^{T} = \langle \langle \widetilde{S}^{(q,p)} \rangle \rangle_{t},$$

$$\langle \langle \widetilde{S}_{j,j'}^{(q)} \rangle \rangle_{t} \mu_{j'} + 2\gamma \langle \langle \widetilde{S}_{j,j'}^{(q,p)} \rangle \rangle_{t} - \langle \langle \widetilde{S}_{j,j'}^{(p)} \rangle \rangle_{t} = \frac{1}{n^{2}} \left[\widetilde{S}_{j,j'}^{(q,p)}(0) - \widetilde{S}_{j,j'}^{(q,p)}(t) \right],$$

$$\mu_{j} \langle \langle \widetilde{S}_{j,j'}^{(q)} \rangle \rangle_{t} + 2\gamma \langle \langle \widetilde{S}_{j,j'}^{(p,q)} \rangle \rangle_{t} - \langle \langle \widetilde{S}_{j,j'}^{(p)} \rangle \rangle_{t} = \frac{1}{n^{2}} \left[\widetilde{S}_{j,j'}^{(p,q)}(0) - \widetilde{S}_{j,j'}^{(p,q)}(t) \right],$$

$$\mu_{j} \langle \langle \widetilde{S}_{j,j'}^{(q,p)} \rangle \rangle_{t} - \langle \langle \widetilde{S}_{j,j'}^{(q,p)} \rangle \rangle_{t} \mu_{j'} = \widetilde{D}_{j,j'} (\langle \langle \mathbf{p}^{2} \rangle \rangle_{t}) - 4\gamma \langle \langle \widetilde{S}_{j,j'}^{(p)} \rangle \rangle_{t} + \frac{1}{n^{2}} \left[\widetilde{S}_{j,j'}^{(p)}(0) - \widetilde{S}_{j,j'}^{(p)}(t) \right].$$

Adding and subtracting the second and the third equations sideways we can rewrite (C.34) as follows

$$\langle \langle \widetilde{S}_{j,j'}^{(q,p)} \rangle \rangle_{t} = -\langle \langle \widetilde{S}_{j,j'}^{(p,q)} \rangle \rangle_{t} + \frac{1}{n^{2}} \left[\widetilde{S}_{j,j'}^{(q)}(0) - \widetilde{S}_{j,j'}^{(q)}(t) \right],$$

$$\langle \langle \widetilde{S}_{j,j'}^{(p)} \rangle \rangle_{t} = \frac{1}{2} \left(\mu_{j} + \mu_{j'} \right) \langle \langle \widetilde{S}_{j,j'}^{(q)} \rangle \rangle_{t} + \frac{1}{n^{2}} \left[\widetilde{B}_{j,j'}^{(p)}(0) - \widetilde{B}_{j,j'}^{(p)}(t) \right],$$

$$4\gamma \langle \langle \widetilde{S}_{j,j'}^{(q,p)} \rangle \rangle_{t} = \langle \langle \widetilde{S}_{j,j'}^{(q)} \rangle \rangle_{t} (\mu_{j} - \mu_{j'}) + \frac{1}{n^{2}} \left[\widetilde{B}_{j,j'}^{(q,p)}(0) - \widetilde{B}_{j,j'}^{(q,p)}(t) \right],$$

$$(\mu_{j} - \mu_{j'}) \langle \langle \widetilde{S}_{j,j'}^{(q,p)} \rangle \rangle_{t} = 4\gamma \widetilde{F}_{j,j'}(t) - 4\gamma \langle \langle \widetilde{S}_{j,j'}^{(p)} \rangle \rangle_{t} + \frac{1}{n^{2}} \left[\widetilde{S}_{j,j'}^{(p)}(t) - \widetilde{S}_{j,j'}^{(p)}(0) \right], \quad (C.35)$$

where $\widetilde{F}_{j,j'}(t)$ is given by (C.13) and

$$\widetilde{B}_{j,j'}^{(p)}(t) := \frac{1}{2} \Big(2\gamma \widetilde{S}_{j,j'}^{(q)}(t) + \widetilde{S}_{j,j'}^{(q,p)}(t) + \widetilde{S}_{j,j'}^{(p,q)}(t) \Big),
\widetilde{B}_{j,j'}^{(q,p)}(t) := 2\gamma \widetilde{S}_{j,j'}^{(q)}(t) + \widetilde{S}_{j,j'}^{(q,p)}(t) - \widetilde{S}_{j,j'}^{(p,q)}(t).$$
(C.36)

Hence,

$$\langle \langle \widetilde{S}_{j,j'}^{(q)} \rangle \rangle_{t} = \frac{2\Theta(\mu_{j}, \mu_{j'})}{\mu_{j} + \mu_{j'}} \widetilde{F}_{j,j'}(t) + \frac{1}{n^{2}} \left[\widetilde{L}_{j,j'}^{(q)}(t) - \widetilde{L}_{j,j'}^{(q)}(0) \right],$$

$$\langle \langle \widetilde{S}_{j,j'}^{(p)} \rangle \rangle_{t} = \Theta(\mu_{j}, \mu_{j'}) \widetilde{F}_{j,j'}(t) + \frac{1}{n^{2}} \left[\widetilde{L}_{j,j'}^{(p)}(t) - \widetilde{L}_{j,j'}^{(p)}(0) \right],$$

$$\langle \langle \widetilde{S}_{j,j'}^{(q,p)} \rangle \rangle_{t} = \frac{\Theta(\mu_{j}, \mu_{j'})}{2\gamma(\mu_{j} + \mu_{j'})} (\mu_{j} - \mu_{j'}) \widetilde{F}_{j,j'}(t) + \frac{1}{n^{2}} \left[\widetilde{L}_{j,j'}^{(q,p)}(t) - \widetilde{L}_{j,j'}^{(q,p)}(0) \right],$$
(C.37)

with $\Theta(\cdot, \cdot)$ given by (C.14) and

$$\begin{split} \widetilde{L}_{j,j'}^{(q)}(t) &:= \frac{2\Theta(\mu_{j},\mu_{j'})}{\mu_{j} + \mu_{j'}} \Big(\widetilde{B}_{j,j'}^{(p)}(t) + \frac{\mu_{j} - \mu_{j'}}{(4\gamma)^{2}} \widetilde{B}_{j,j'}^{(q,p)}(t) + \frac{1}{4\gamma} \widetilde{S}_{j,j'}^{(p)}(t) \Big), \\ \widetilde{L}_{j,j'}^{(p)}(t) &:= \frac{1}{2} \Big(\mu_{j} + \mu_{j'} \Big) \widetilde{L}_{j,j'}^{(q)}(t) - \widetilde{B}_{j,j'}^{(p)}(t), \\ \widetilde{L}_{j,j'}^{(q,p)}(t) &:= -\frac{1}{4\gamma} \widetilde{B}_{j,j'}^{(q,p)}(t) + \frac{\mu_{j} - \mu_{j'}}{4\gamma} \widetilde{L}_{j,j'}^{(q)}(t). \end{split}$$



C.4.1: Proof of (C.21)

Using (C.41) and (C.15) we can write

$$r_{n,x}^{(p)}(t) := \sum_{\iota \in \mathbb{Z}} \left[g_{x,\iota}^{(p)}(t) - g_{x,\iota}^{(p)}(0) \right],$$

$$g_{x,\iota}^{(p)}(t) := \frac{1}{n^2} \sum_{j,j'=0}^{n} \Xi_{\iota}^{(p)}(\mu_j, \mu_{j'}) \psi_j(x) \psi_{j'}(x) \psi_j(y) \psi_{j'}(y') S_n^{(\iota)}(t). \tag{C.38}$$

Here Z is a set consisting of indices p, q and pq and $\Xi_t^{(p)}$ are some C^{∞} smooth functions. In what follows we show that for any t > 0 there exists C > 0 such that

$$\sup_{s \in [0,t]} \sum_{x=0}^{n} |g_{x,t}^{(p)}(s)| \leqslant \frac{C}{n+1}, \quad n = 1, 2, \dots$$
 (C.39)

This, in light of (D.12), clearly implies (C.21).

Consider only the case $\iota = p$, as the other cases can be argued in the same manner. Then,

$$g_{x,p}^{(p)}(t) = \frac{1}{n^2} \sum_{j,j'=0}^{n} \sum_{y,y'=0}^{n} \Xi_p^{(p)}(\mu_j, \mu_{j'}) \psi_j(x) \psi_{j'}(x) \psi_j(y) \psi_{j'}(y') \mathbb{E}_{\mu_n}[p_y'(t)p_{y'}'(t)].$$

Using (A.3) and elementary trigonometric identities we obtain

$$g_{x,p}^{(p)}(t) = \frac{1}{n^2} \sum_{y,y'=0}^{n} \mathbb{E}_{\mu_n} [p_y'(t) p_{y'}'(t)] K_n(x, y, y'), \text{ wher}$$

$$K_n(x, y, y') := \frac{1}{(n+1)^2} \sum_{j,j'=-n}^{n} \Xi_p^{(p)}(\mu_j, \mu_{j'})$$

$$\times \left[\cos \left(\frac{\pi j(x-y)}{n+1} \right) + \cos \left(\frac{\pi j(x+y+1)}{n+1} \right) \right]$$

$$\left[\cos \left(\frac{\pi j'(x-y')}{n+1} \right) + \cos \left(\frac{\pi j'(x+y'+1)}{n+1} \right) \right].$$

Using [14, Lemma B.1] we conclude that there exists C > 0 such that

$$|K_n(x, y, y')| \le Ck_n(x, y)k_n(x, y'), \quad x, y = 0, \dots, n, n = 1, 2, \dots, \text{ where}$$

$$k_n(x, y) := \frac{1}{1 + (x - y)^2} + \frac{1}{1 + (x + y - 2n)^2}.$$
(C.40)

We conclude therefore that

$$\sum_{x=0}^{n} |g_{x,p}^{(p)}(t)| \leq \frac{C}{n^2} \sum_{x=0}^{n} \mathbb{E}_{\mu_n} \left[\left(\sum_{y=0}^{n} p_y'(t) k_n(x,y) \right)^2 \right]$$

$$= \frac{C}{n^2} \mathbb{E}_{\mu_n} \left[\sup_{\|h\|_{\ell^2} = 1} \sum_{x=0}^{n} h_x \sum_{y=0}^{n} p_y'(t) k_n(x,y) \right]. \tag{C.41}$$

The supremum extends over all real valued sequences $h=(h_0,\ldots,h_n)$, with $\|h\|_{\ell^2}^2=\sum_{x=0}^n h_x^2=1$. Using an elementary inequality $h_x p_y'(t)\leqslant h_x^2/2+[p_y'(t)]^2/2$ we can estimate



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the right hand side of (C.41) by

$$\frac{C}{2n^2} \sup_{\|h\|_{\ell^2} = 1} \sum_{x=0}^n h_x^2 \sum_{y=0}^n k_n(x, y) + \frac{C}{2n^2} \mathbb{E}_{\mu_n} \left[\sum_{y=0}^n [p_y'(t)]^2 \sum_{x=0}^n k_n(x, y) \right] \\
\leqslant \frac{CK}{2n^2} \left(1 + \sum_{y=0}^n \mathbb{E}_{\mu_n} [p_y'(t)]^2 \right),$$

where $K = \sup_{x,n} \sum_{y=0}^{n} \left(k_n(x, y) + k_n(y, x) \right)$. Estimate (C.39) for $\iota = p$ is then a straightforward consequence of the energy bound (3.2).

Appendix D: Proof of Local Equilibrium

We prove here Propositions 5.1 and 5.2.

D.1: Proof of Proposition 5.1

Suppose that $\rho \in (0, 1/2)$ is such that supp $\varphi \subset (\rho, 1 - \rho)$. Let

$$\Phi\left(\mu_{j}, \mu_{j'}\right) = \frac{2\Theta(\mu_{j}, \mu_{j'})}{\mu_{j} + \mu_{j'}}.$$
(D.1)

For a fixed integer ℓ define

$$\overline{K}^{(n,\ell)}(x) := \frac{1}{4(n+1)^2} \sum_{j,j'=-n-1}^{n} \Phi\left(\mu_j, \mu_{j'}\right) \cos\left(\frac{\pi j x}{n+1}\right) \cos\left(\frac{\pi j'(x-\ell)}{n+1}\right). \quad (D.2)$$

By [14, Lemma B.1], for a given ℓ there exists C > 0 such that

$$|\overline{K}_1^{(n,\ell)}(x)| \le \frac{C}{1+x^2}, \quad x = 0, \dots, n$$
 (D.3)

for $n = 1, 2, \dots$ It has been shown in Section 8.1 of [14] that for any $\rho \in (0, 1/2)$ there exists C > 0 such that

$$\left| \sum_{y=0}^{n} \overline{K}^{(n,\ell)}(x-y) - G_{\omega_0}(\ell) \right| \leqslant \frac{C}{n^2}, \quad \rho n \leqslant x \leqslant (1-\rho)n. \tag{D.4}$$

for n = 1, 2, ...

By virtue of (B.15) we have

$$\lim_{n \to +\infty} \frac{1}{n+1} \sum_{r=0}^{n} \varphi\left(\frac{x}{n+1}\right) \int_{0}^{t} \mathbb{E}\left[q_{x}(n^{2}s)\right] \mathbb{E}\left[q_{x+\ell}(n^{2}s)\right] ds = 0.$$
 (D.5)

It suffices therefore to prove that

$$\lim_{n \to +\infty} \frac{1}{n+1} \sum_{x=0}^{n} \varphi\left(\frac{x}{n+1}\right) \left\{ \langle \langle S_{x,x+\ell}^{(q)} \rangle \rangle_{t} - G_{\omega_{0}}(\ell) \langle \langle p_{x}^{2} \rangle \rangle_{t} \right\} = 0.$$
 (D.6)



We prove (D.6) for $\ell = 0$, the argument for other values of ℓ are similar. By (C.16) we have

$$\langle\langle S_{x,x}^{(q)}\rangle\rangle_t = \sum_{y=0}^n H_{x,y}^{(n)} \langle\langle p_y^2\rangle\rangle_t + B_n(t,x) + r_{n,x}^{(q)}(t), \tag{D.7}$$

with (cf (C.16))

$$H_{x,y}^{(n)} := \sum_{j,j'=0}^{n} \Phi\left(\mu_{j}, \mu_{j'}\right) \psi_{j}(y) \psi_{j'}(y) \psi_{j}(x) \psi_{j'}(x),$$

$$B_{n}(t,x) := \sum_{j,j'=0}^{n} \psi_{j}(x) \psi_{j'}(x) \Phi\left(\mu_{j}, \mu_{j'}\right) \left(T_{-}t - \langle\langle p_{0}^{2} \rangle\rangle_{t}\right) \psi_{j}(0) \psi_{j'}(0) \qquad (D.8)$$

$$r_{n,x}^{(q)}(t) := \frac{1}{n^{2}} \sum_{j,j'=0}^{n} \psi_{j}(x) \psi_{j'}(x) \widetilde{R}_{j,j'}^{(q)}(t).$$

Using (3.2) and (3.5) we conclude that $\lim_{n\to+\infty} \sup_x \left| B_n(t,x) \right| = 0$. Likewise, by (C.16) and (C.37), we conclude that $\lim_{n\to+\infty} \sup_x \left| r_{n,x}^{(q)}(t) \right| = 0$.

Furthermore, by (D.4), if $\rho n \le x \le (1 - \rho)n$,

$$\sum_{y=0}^{n} H_{x,y}^{(n)} = G_{\omega_0}(0) + o_{n,x}(t), \tag{D.9}$$

where, for any fixed t>0 we have $\lim_{n\to+\infty}\sup_{\rho n\leqslant x\leqslant (1-\rho)n}\left|o_{n,x}(t)\right|=0$. Then we have that

$$\frac{1}{n+1} \sum_{x=0}^{n} \varphi\left(\frac{x}{n+1}\right) \left\{ \langle \langle S_{x,x}^{(q)} \rangle \rangle_{t} - G_{\omega_{0}}(0) \langle \langle p_{x}^{2} \rangle \rangle_{t} \right\}
= \frac{1}{n+1} \sum_{x=0}^{n} \varphi\left(\frac{x}{n+1}\right) \sum_{y=0}^{n} H_{x,y}^{(n)} \left[\langle \langle p_{y}^{2} \rangle \rangle_{t} - \langle \langle p_{x}^{2} \rangle \rangle_{t} \right] + o_{n}(t).$$
(D.10)

Here and below $\lim_{n\to+\infty} o_n(t) = 0$ for each t > 0. We have

$$\left| \sum_{y=0}^{n} H_{x,y}^{(n)} \left[\langle \langle p_{y}^{2} \rangle \rangle_{t} - \langle \langle p_{x}^{2} \rangle \rangle_{t} \right] \right| \leq \sum_{y=0}^{n} |H_{x,y}^{(n)}| \sum_{z=x}^{y-1} \left| \langle \langle p_{z+1}^{2} \rangle \rangle_{t} - \langle \langle p_{z}^{2} \rangle \rangle_{t} \right|. \tag{D.11}$$

It follows from [14, Lemma B.1] that there exists C > 0 such that

$$|H_{x,y}^{(n)}| \le \frac{C}{1 + (x - y)^2}, \quad \rho n \le x \le (1 - \rho)n, \ y = 0, \dots, n, \ n = 1, 2, \dots$$

Using Cauchy-Schwarz inequality and (C.28) we conclude that the right hand side of (D.11) is estimated by

$$\frac{C}{(n+1)^{1/2}} \sum_{y=0}^{n} |H_{x,y}^{(n)}||y-x|^{1/2} \leqslant \frac{C'}{(n+1)^{1/2}}, \quad n = 1, 2, \dots$$
 (D.12)

for some constant C' independent of x = 0, ..., n and n = 1, 2, ... and Proposition 5.1 follows for $\ell = 0$.



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D.2: Proof of Proposition 5.2

From Proposition B.1 we have

$$\lim_{n \to +\infty} \int_0^t \overline{q}_0^2(s) \mathrm{d}s = 0.$$

It suffices therefore to calculate $\int_0^t \mathbb{E}(q_0'(s)^2) ds = \langle \langle S_{0,0}^{(q)} \rangle \rangle_t$. We have, see (C.16) and (D.1),

$$\langle \langle S_{0,0}^{(q)} \rangle \rangle_{t} = \sum_{y=0}^{n} \sum_{j,j'=0}^{n} \Phi(\mu_{j}, \mu_{j'}) \psi_{j}(0) \psi_{j'}(0) \psi_{j}(y) \psi_{j'}(y) \langle \langle p_{y}^{2} \rangle \rangle_{t}$$

$$+ \sum_{j,j'=0}^{n} \Phi(\mu_{j}, \mu_{j'}) \psi_{j}(0)^{2} \psi_{j'}(0)^{2} \left(T_{-}t - \langle \langle p_{0}^{2} \rangle \rangle_{t} \right) + o_{n}(t)$$

$$= \sum_{y=0}^{n} H_{y}^{(n)} \langle \langle p_{y}^{2} \rangle \rangle_{t} + o_{n}(t). \tag{D.13}$$

and

$$H_{y}^{(n)} := \sum_{j,j'=0}^{n} \Phi(\mu_{j}, \mu_{j'}) \psi_{j}(0) \psi_{j'}(0) \psi_{j}(y) \psi_{j'}(y). \tag{D.14}$$

The coefficients $H_{v}^{(n)}$ have the property

$$\sum_{y=0}^{n} H_{y}^{(n)} = \sum_{j=0}^{n} \Phi(\mu_{j}, \mu_{j}) \psi_{j}(0)^{2} = \sum_{j=0}^{n} \frac{1}{\mu_{j}} \psi_{j}(0)^{2}$$

$$= \frac{1}{n+1} \sum_{j=0}^{n} \frac{\cos^{2}\left(\frac{\pi j}{2(n+1)}\right)}{\omega_{0}^{2} + 4\sin^{2}\left(\frac{\pi j}{2(n+1)}\right)} \xrightarrow{n \to \infty} G_{\omega_{0}}(0) + G_{\omega_{0}}(1).$$
(D.15)

Using [14, Lemma B.1] we conclude that there exists C > 0 such that

$$|H_y^{(n)}| \le \frac{C}{1+y^2}, \quad y = 0, \dots, n, \ n = 1, 2, \dots$$
 (D.16)

Then, proceeding as in (D.11)–(D.12), by using the Cauchy-Schwarz inequality, the first estimate of (C.28) and (D.16), we conclude that

$$\sum_{y=0}^{n} |H_{y}^{(n)}| \left| \langle \langle p_{y}^{2} \rangle \rangle_{t} - \langle \langle p_{0}^{2} \rangle \rangle_{t} \right| \leqslant \frac{C}{\sqrt{n}}.$$

Hence

$$\langle\langle S_{0,0}^{(q)} \rangle\rangle_t = \left(\sum_{y=0}^n H_{y,0}^{(n)}\right) \langle\langle p_0^2 \rangle\rangle_t + o_n(t) = G_{\omega_0}(0) + G_{\omega_0}(1) + o_n(t). \tag{D.17}$$



Appendix E: Uniqueness of Solutions to (2.35)

Theorem E.1 Suppose that $T_0 \in \mathcal{M}_{fin}([0,1])$. Then, the initial-boundary value problem (2.35) has a unique weak solution in the sense of Definition 2.9.

Proof Let $\overline{T}(s, du)$ be the signed measure given by the difference of two solutions with the same initial and boundary data. It satisfies the equation

$$\int_0^1 \varphi(u) \overline{T}(t, du) = \frac{D}{4\gamma} \int_0^t ds \int_0^1 \varphi''(u) \overline{T}(s, du)$$
 (E.1)

for any $\varphi \in C^2[0, 1]$ such that $\varphi(0) = \varphi'(1) = 0$.

The above implies that also

$$\int_{0}^{1} \varphi(t, u) \overline{T}(t, du) = \int_{0}^{t} ds \int_{0}^{1} \left(\partial_{s} \varphi(s, u) + \frac{D}{4\gamma} \partial_{uu}^{2} \varphi(s, u) \right) \overline{T}(s, du)$$
 (E.2)

for any $\varphi \in C^{1,2}([0, +\infty) \times [0, 1])$, such that $\varphi(t, 0) = \partial_u \varphi(t, 1) = 0$, $t \ge 0$. Suppose now that $\varphi_0 \in C^1[0, 1]$ satisfies

$$\varphi_0(0) = \varphi_0'(1) = 0 \tag{E.3}$$

and $\varphi(t, u)$ is the strong solution of

$$\partial_s \varphi(s, u) + \frac{D}{4\gamma} \partial_u^2 \varphi(s, u) = 0, \quad u \in (0, 1), \ s < t,$$

$$\varphi(s, 0) = \partial_u \varphi(s, 1) = 0, \quad s < t,$$

$$\varphi(t, u) = \varphi_0(u).$$
(E.4)

Such a solution exists and is unique, thanks to e.g. [8, Corollary 5.3.2, p.147]. It belongs to $C^{1,2}((-\infty, t] \times [0, 1])$. We conclude that

$$\int_{0}^{1} \varphi_0(u) \overline{T}(t, du) = 0 \tag{E.5}$$

for any $\varphi_0 \in C^1[0, 1]$ satisfying (E.3).

Consider now an arbitrary $\psi \in C[0, 1]$. Let $\varphi_0(u) := -u \int_u^1 \psi(u') du' - \int_0^u \psi(u') du'$. It satisfies (E.3) and $\varphi_0''(u) = \psi(u)$, thus

$$\int_0^t \mathrm{d}s \int_0^1 \psi(u) \overline{T}(s, \mathrm{d}u) = 0$$

which ends the proof of uniqueness.

Appendix F: Proof of Proposition 3.1

Proof of Proposition 3.1 in the General Case

Denote by $\mathcal{P}_{s,t}$, s < t, the evolution family corresponding to the transition probabilities of the Markov family generated by the dynamics (2.3) and (2.4). Let $\mu \mathcal{P}_{s,t}$ be the probability distribution obtained by transporting the distribution μ at time s by the random flow $\mathcal{S}_{s,t}$.



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Using the calculation performed in [5, pp. 1232] we conclude that the relative entropy satisfies the following inequality

$$\mathbf{H}_{n}(f_{n}(n^{2}t)) - \mathbf{H}_{n}(f_{n}(0)) \leqslant \inf_{\psi} \int_{0}^{n^{2}t} \mathrm{d}s \int_{\Omega_{n}} \frac{\left(\mathcal{G}_{s} + \mathcal{G}_{s}^{*}\right)\psi}{\psi} \mathrm{d}\left(\mu_{0}\mathcal{P}_{0,s}\right), \tag{F.1}$$

where $d\mu_0 = f_n(0)d\nu_{T_-}$, \mathcal{G}_t^* is the adjoint with respect to ν_{T_-} and the infimum is taken over all smooth densities ψ , w.r.t. the Gaussian measure ν_{T_-} , that are bounded away from 0. Arguing as in the proof of Proposition 3.1 in the smooth initial data case, we conclude that for any ψ under the infimum the right hand side of (F.1) is less than, or equal to

$$\frac{1}{T_{-}}\int_{0}^{n^{2}t}\mathrm{d}s\mathcal{F}_{n}(s)\int_{\Omega_{n}}p_{n}\mathrm{d}\left(\mu_{0}\mathcal{P}_{0,s}\right)=-\frac{n}{T_{-}}J_{n}(t,\mu_{0}).$$

From this point on the proof follows from an application of (2.33) and Theorem 2.5.

References

- 1. Basile, G., Bernardin, C., Jara, M., Komorowski, T., Olla, S.: Thermal conductivity in harmonic lattices with random collisions. In: Lepri, S. (ed.) Thermal Transport in Low Dimensions: From Statistical Physics to Nanoscale Heat Transfer. Lecture Notes in Physics, vol. 921. Springer, Berlin (2016)
- 2. Bernardin, C., Kannan, V., Lebowitz, J.L., Lukkarinen, J.: Non-equilibrium stationary states of harmonic chains with bulk noises. Eur. J. Phys. B 84, 685 (2011)
- Bernardin, C., Kannan, V., Lebowitz, J.L., Lukkarinen, J.: Harmonic systems with bulk noises. J. Stat. Phys. 146, 800 (2012)
- Bernardin, C., Olla, S.: Fourier law and fluctuations for a microscopic model of heat conduction. J. Stat. Phys. 118(3/4), 271–289 (2005). https://doi.org/10.1007/s10955-005-7578-9
- Bernardin, C., Olla, S.: Transport properties of a chain of anharmonic oscillators with random flip of velocities. J. Stat. Phys. 145, 1224–1255 (2011). https://doi.org/10.1007/s10955-011-0385-6
- Bonetto, F., Lebowitz, J.L., Rey-Bellet, L.: Fourier's law: A challenge to theorists. In: Fokas, A., Grigoryan, A., Kibble, T., Zegarlinski, B. (eds.) Mathematical Physics, pp. 128–150. Imperial College Press, London (2000)
- Bonetto, F., Lebowitz, J.L., Lukkarinen, J.: Fourier's law for a harmonic crystal with self-consistent stochastic reservoirs. J. Stat. Phys. 116, 783–813 (2004)
- Friedman, A.: Partial Differential Equations of Parabolic Type. Prentice-Hall Inc, Englewood Cliffs, NJ (1964)
- Kipnis, C., Landim, C.: Scaling Limits of Interacting Particle Systems, Grundlehren Math, Wiss, vol. 320. Springer, Berlin (1999)
- Johansson, M., Kopidakis, G., Lepri, S., Aubry, S.: Transmission thresholds in time-periodically driven non-linear disordered systems. EPL 86, 10009 (2009)
- Geniet, F., Leon, J.: Energy transmission in the forbidden band gap of a nonlinear chain. Phys. Rev. Lett. 89, 134102 (2002). https://doi.org/10.1103/PhysRevLett.89.134102
- 12. Kelley, J.L.: General topology. Springer-Verlag, ISBN 978-0-387-90125-1 (1991)
- Komorowski, T., Olla, S., Simon, M.: Hydrodynamic limit for a chain with thermal and mechanical boundary forces. Electron. J. Probab. 26, 1–49 (2021). https://doi.org/10.1214/21-EJP581
- Komorowski, T., Lebowitz, J.L., Olla, S.: Heat flow in a periodically forced, thermostatted chain. Commun. Math. Phys. (2023). https://doi.org/10.1007/s00220-023-04654-4
- Komorowski, T., Lebowitz, J.L., Olla, S.: Heat flow in a periodically forced, thermostatted chain with internet supplement. arXiv:2205.03839
- Komorowski, T., Lebowitz, J.L., Olla, S., Simon, M.: On the Conversion of Work into Heat: Microscopic Models and Macroscopic Equations (2022). https://doi.org/10.48550/arXiv.2212.00093
- 17. Ray, K.: Green's Function on Lattices. arXiv:1409.7806
- Lukkarinen, J.: Thermalization in harmonic particle chains with velocity flips. J. Stat. Phys. 155(6), 1143–1177 (2014)
- Rieder, Z., Lebowitz, J.L., Lieb, E.: Properties of harmonic crystal in a stationary non-equilibrium state. J. Math. Phys. 8, 1073–1078 (1967)



 Prem, A., Bulchandani, V B., Sondhi, S.L.: Dynamics and transport in the boundary–driven dissipative Klein-Gordon chain. arXiv:2209.03977v1 (2022)

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