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HEAT FLOW IN A PERIODICALLY FORCED, THERMOSTATED CHAIN II

TOMASZ KOMOROWSKI, JOEL L. LEBOWITZ, AND STEFANO OLLA

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 local temperature given by the expected value of the local energy and current. Scaling space and time diffusively yields, in the $n \rightarrow +\infty$ 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 is the work done by the periodic force which is computed explicitly for each n .

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 system: 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 [17]. 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 mechanism in real systems and produces a finite conductivity (cf. [5], [1]).

In a previous paper [14] we studied this system in the limit $t \rightarrow \infty$. We showed that in this limit the probability distribution of the phase configurations is periodic with the period of the external force. 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, which approaches, as $t \rightarrow \infty$, the periodic profile of [14].

The periodic forcing generates a Neumann type of 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 (2.27) below). On the left side the boundary condition is given by the assigned value T_- - the temperature of the heat bath.

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 [4, 2, 3, 13, 16]. But complete mathematical results, describing the time evolution of the macroscopic temperature profile, have been obtained only for unpinned chains [4, 13]. For infinite harmonic chains, without boundary conditions, rigorous results can be found in [9]. 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 2.5). Investigation about energy transport in anharmonic chain under periodic forcing can be found in [11], [10], and very recently in [18].

1.1. Structure of the article. In section 2 we give the precise dynamics and a statement of the two main theorems: Theorem 2.1 about the limit current generated at the boundary by a periodic force, and Theorem 2.4 about the convergence of the energy profile to the solution of the heat equation with mixed boundary conditions.

In section 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 2.4. 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 2.4, see section 5. The proof of the local equilibrium is postponed till section 7, after the analysis of the time evolution of the matrix for the time integrated covariances of positions and momenta. The latter is contained in section 6. Both in section 6 and section 7 we use results proven in [14], when possible.

Finally, section 8 contains the proof of Theorem 2.1, that involves only the dynamics of the averages of the configurations.

2. DESCRIPTION OF THE MODEL

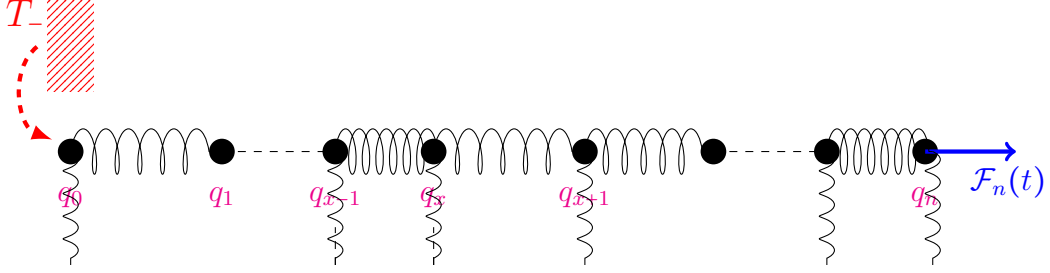
We consider a pinned chain of n -harmonic oscillators in contact on the left with a Langevin heat bath at temperature T_- , and with a periodic force acting on the last particle on the right. The configuration of particle positions and momenta are specified by

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

We should think of the positions q_x as relative displacement from a point, say x in a finite lattice $\{0, 1, \dots, n\}$. 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

$$\mathcal{E}_x(\mathbf{q}, \mathbf{p}) := \frac{p_x^2}{2} + \frac{1}{2}(q_x - q_{x-1})^2 + \frac{\omega_0^2 q_x^2}{2}, \quad x = 0, \dots, n, \quad (2.2)$$

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



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

$$\begin{aligned} \dot{q}_x(t) &= p_x(t), & x &\in \{0, \dots, n\}, \\ dp_x(t) &= (\Delta_N q_x - \omega_0^2 q_x) dt - 2p_x(t-) dN_x(\gamma t), & x &\in \{1, \dots, n-1\}, \end{aligned} \quad (2.3)$$

and at the boundaries by

$$\begin{aligned} dp_0(t) &= (q_1(t) - q_0(t) - \omega_0^2 q_0) dt - 2\gamma p_0(t) dt + \sqrt{4\gamma T_-} d\tilde{w}_-(t) \\ dp_n(t) &= (q_{n-1}(t) - q_n(t) - \omega_0^2 q_n(t)) dt + \mathcal{F}_n(t) dt - 2p_n(t-) dN_n(\gamma t). \end{aligned} \quad (2.4)$$

Here Δ_N is the Neumann discrete laplacian, corresponding to the choice $q_{n+1} := q_n$ and $q_{-1} = q_0$. Processes $\{N_x(t), x = 1, \dots, n\}$ are independent Poisson of intensity 1, while $\tilde{w}_-(t)$ 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 chosen 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

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

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

$$\int_0^1 \mathcal{F}(t) dt = 0, \quad \int_0^1 \mathcal{F}(t)^2 dt > 0. \quad (2.6)$$

The generator of the dynamics is given by

$$\mathcal{G}_t = \mathcal{A}_t + \gamma S_{\text{flip}} + 2\gamma S_-, \quad (2.7)$$

where

$$\mathcal{A}_t = \sum_{x=0}^n p_x \partial_{q_x} + \sum_{x=0}^n (\Delta_N q_x - \omega_0^2 q_x) \partial_{p_x} + \mathcal{F}_n(t) \partial_{p_n}, \quad (2.8)$$

and

$$S_{\text{flip}} F(\mathbf{p}, \mathbf{q}) = \sum_{x=1}^n \left(F(\mathbf{p}^x, \mathbf{q}) - F(\mathbf{p}, \mathbf{q}) \right), \quad (2.9)$$

where $F : \mathbb{R}^{2(n+1)} \rightarrow \mathbb{R}$ 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,

$$S_- = T_- \partial_{p_0}^2 - p_0 \partial_{p_0}. \quad (2.10)$$

The energy currents are given by

$$\mathcal{G}_t \mathcal{E}_x = j_{x-1,x} - j_{x,x+1}, \quad (2.11)$$

with

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

and at the boundaries

$$j_{-1,0} := 2\gamma (T_- - p_0^2(t)), \quad j_{n,n+1}(t) := -\mathcal{F}_n(t) p_n. \quad (2.12)$$

2.1. Statements of the main results.

2.1.1. *Macroscopic energy current due to work.* The first results concerns the work done by the forcing in a diffusive limit, i.e.

$$J_n(t, \mu) = \frac{1}{n} \int_0^{n^2 t} \mathbb{E}_\mu (j_{n,n+1}(s, \mathbf{q}(s), \mathbf{p}(s))) ds = -\frac{1}{n} \int_0^{n^2 t} \mathcal{F}_n(s) \mathbb{E}_\mu (p_n(s)) ds, \quad (2.13)$$

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.

Denote

$$\widehat{\mathcal{F}}(\ell) = \int_0^1 e^{-2\pi i \ell t} \mathcal{F}(t) dt. \quad (2.14)$$

Note that by (2.6) we have $\widehat{\mathcal{F}}(0) = 0$. We suppose that

$$\sum_{\ell} |\widehat{\mathcal{F}}(\ell)| < \infty. \quad (2.15)$$

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 $n \geq 1$

$$\mathcal{H}_n(\bar{\mathbf{q}}_n, \bar{\mathbf{p}}_n) \leq Cn^\delta. \quad (2.16)$$

Here $(\bar{\mathbf{q}}_n, \bar{\mathbf{p}}_n)$ the vector of the averages of the configuration with respect to μ_n . In Section 8.3 we prove the following.

Theorem 2.1. *Under the assumptions listed above, we have*

$$\lim_{n \rightarrow +\infty} \sup_{t \geq 0} |J_n(t, \mu_n) - Jt| = 0, \quad (2.17)$$

where

$$J := - \left(\frac{2\pi}{\theta} \right)^2 \sum_{\ell \in \mathbb{Z}} \ell^2 \mathcal{Q}(\ell), \quad (2.18)$$

with $\mathcal{Q}(\ell)$ given by

$$\mathcal{Q}(\ell) = 4\gamma |\widehat{\mathcal{F}}(\ell)|^2 \int_0^1 \cos^2 \left(\frac{\pi z}{2} \right) \left\{ \left[4 \sin^2 \left(\frac{\pi z}{2} \right) + \omega_0^2 - \left(\frac{2\pi\ell}{\theta} \right)^2 \right]^2 + \left(\frac{2\gamma\pi\ell}{\theta} \right)^2 \right\}^{-1} dz \quad (2.19)$$

Remark 2.2. *The asymptotic current J is the same as in the stationary state (cf. [14]) and it does not depend on the initial configuration.*

Remark 2.3. *Rescaling the period θ with n and the strenght of the force is such way that*

$$\mathcal{F}_n(t) = n^a \mathcal{F} \left(\frac{t}{n^b \theta} \right), \quad b - a = \frac{1}{2}, \quad a \leq 0 \quad \text{and} \quad b \geq 0, \quad (2.20)$$

Theorem 2.1 still holds but with a different value of the current if $b > 0$ that has been calculated in [14]:

$$\mathcal{Q}(\ell) = 4\gamma |\widehat{\mathcal{F}}(\ell)|^2 \int_0^1 \cos^2 \left(\frac{\pi z}{2} \right) \left[4 \sin^2 \left(\frac{\pi z}{2} \right) + \omega_0^2 \right]^{-2} dz. \quad (2.21)$$

Formula (2.21) corresponds to (2.19) with the value $\theta = \infty$.

2.1.2. *Macroscopic energy profile.* Let $\nu_{T_-}(\mathrm{d}\mathbf{q}, \mathrm{d}\mathbf{p})$ be defined as the product Gaussian measure on Ω_n of zero average and variance $T_- > 0$ given by

$$\nu_{T_-}(\mathrm{d}\mathbf{q}, \mathrm{d}\mathbf{p}) := \frac{1}{Z} \prod_{x=0}^n \exp \{ -\mathcal{E}_x(\mathbf{q}, \mathbf{p})/T_- \} \mathrm{d}\mathbf{q} \mathrm{d}\mathbf{p}, \quad (2.22)$$

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

$$\mathbf{H}_n(f) := \int_{\Omega_n} f(\mathbf{q}, \mathbf{p}) \log f(\mathbf{q}, \mathbf{p}) \mathrm{d}\nu_{T_-}(\mathbf{q}, \mathbf{p}). \quad (2.23)$$

We assume now that the initial distribution μ has density $f_n(0, \mathbf{q}, \mathbf{p})$, with respect to ν_{T_-} , such that for all $n \geq 1$,

$$\mathbf{H}_n(f_n(0)) \leq Cn. \quad (2.24)$$

We also assume that there exists a continuous function $T_0 : [0, 1] \rightarrow (0, +\infty)$ such that

$$\lim_{n \rightarrow \infty} \mathbb{E}_\mu \left[\frac{1}{n+1} \sum_x \varphi \left(\frac{x}{n} \right) \mathcal{E}_x(0) \right] = \int_0^1 \varphi(u) T_0(u) \mathrm{d}u, \quad (2.25)$$

for any function $\varphi \in C[0, 1]$ - the space of continuous functions on $[0, 1]$. Recall that \mathbb{E}_μ denotes the expectation of the process $(\mathbf{q}(t), \mathbf{p}(t))$ with the initial configuration (\mathbf{q}, \mathbf{p}) distributed according to a probability measure μ . Here and in the following we denote $\mathcal{E}_x(t) = \mathcal{E}_x(\mathbf{q}(t), \mathbf{p}(t))$.

Theorem 2.4. *Under the assumptions made above for any $\varphi \in C[0, 1]$ and $t \geq 0$ we have*

$$\lim_{n \rightarrow \infty} \frac{1}{n+1} \sum_x \varphi \left(\frac{x}{n} \right) \mathbb{E}_\mu (\mathcal{E}_x(n^2 t)) = \int_0^1 \varphi(u) T(t, u) \mathrm{d}u, \quad (2.26)$$

where

$$\begin{aligned} \partial_t T &= \frac{D}{4\gamma} \partial_u^2 T, \quad u \in (0, 1), \\ T(t, 0) &= T_-, \quad \partial_u T(t, 1) = -\frac{4\gamma J}{D}, \quad T(0, u) = T_0(u). \end{aligned} \quad (2.27)$$

Here J is given by (2.18) and D is defined by

$$D = 1 - \omega_0^2 (G_{\omega_0}(0) + G_{\omega_0}(1)) = \frac{2}{2 + \omega_0^2 + \omega_0 \sqrt{\omega_0^2 + 4}}, \quad (2.28)$$

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

Remark 2.5. The derivation of (2.27) does not depend on the boundary conditions. The same 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 (2.18), 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.

Remark 2.6. If the initial data T_0 is C^1 smooth satisfies the boundary condition in (2.27), then equation (2.29) 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.

In the proof we will use the weak formulation of the boundary value problem (2.27) that reads as follows: for any $\varphi \in C^2[0, 1]$ such that $\varphi(0) = \varphi'(1) = 0$ we have

$$\begin{aligned} \int_0^1 T(t, u) \varphi(u) du - \int_0^1 T_0(u) \varphi(u) du &= \frac{D}{4\gamma} \int_0^t ds \int_0^1 T(s, u) \varphi''(u) du \\ &+ \frac{t D T_-}{4\gamma} \varphi'(0) - t J \varphi(1). \end{aligned} \quad (2.29)$$

Remark 2.7. In the proof of Theorem 2.4 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

$$\lim_{n \rightarrow \infty} \frac{1}{n+1} \sum_x \varphi\left(\frac{x}{n}\right) \mathbb{E}(p_x^2(n^2 t)) = \int_0^1 \varphi(u) T(t, u) du. \quad (2.30)$$

3. ENTROPY, ENERGY AND CURRENTS BOUNDS

Let $f_n(t, \mathbf{q}, \mathbf{p})$ be the density of the configuration $(\mathbf{q}(t), \mathbf{p}(t))$ w.r.t. the Gibbs measure ν_{T-} . Let us assume that the initial density $f_n(0, \mathbf{q}, \mathbf{p})$ is C^1 . The results presented in this section can be extended to a more general initial density satisfying only (2.24) by using the argument of section 3.2 in [5]. Under such regularity condition $f_n(t)$ is solution of the Fokker-Planck equation

$$\partial_t f_n(t) = \mathcal{G}_t^* f_n(t), \quad (3.1)$$

where \mathcal{G}_t^* is the adjoint of the generator \mathcal{G}_t w.r.t. the Gibbs measure ν_{T-} .

We first prove that the initial entropy bound (2.24) holds for all times.

Proposition 3.1. *For any t there exists a constant C independent of n such that*

$$\sup_{s \in [0, t]} \mathbf{H}_n(f_n(n^2 s)) \leq Cn, \quad (3.2)$$

Proof. Using (2.23) for the generator \mathcal{G}_t we conclude that

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

with

$$\begin{aligned} \mathbf{I}_n &:= \gamma \int_0^{n^2 t} ds \int_{\Omega_n} f_n(s) (\mathcal{S}_{\text{flip}} + \mathcal{S}_-) \log f_n(s) d\nu_{T-}, \\ \mathbf{II}_n &:= \int_0^{n^2 t} ds \int_{\Omega_n} f_n(s) \mathcal{A}_s \log f_n(s) d\nu_{T-}. \end{aligned}$$

We have that $\mathbf{I}_n \leq 0$ because $\mathcal{S}_{\text{flip}}$ and \mathcal{S}_- are symmetric negative operators with respect to the measure ν_{T-} . The only positive contribution comes from the second term where the boundary work defined by (2.13) appears:

$$\mathbf{II}_n = \int_0^{n^2 t} ds \mathcal{F}_n(s) \int \frac{p_n}{T_-} f_n(s) d\nu_{T-} = -\frac{n}{T_-} J_n(t, f_n(0) d\nu_{T-}).$$

therefore

$$\mathbf{H}_n(f_n(n^2 t)) \leq \mathbf{H}_n(f_n(0)) - \frac{n}{T_-} J_n(t, f_n(0) d\nu_{T-}).$$

The conclusion of the proposition then follows from a direct application of (2.24) and Theorem 2.1. \square

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

$$\sup_{t \in [0, t_*]} \sup_{n \geq 1} \mathbb{E} \left[\frac{1}{n+1} \sum_{x=0}^n \mathcal{E}_x^{(n)}(n^2 t) \right] = E(t_*) < +\infty. \quad (3.3)$$

Proof. It follows from the entropy inequality, see e.g. [8, p. 338], that for $\alpha > 0$ small enough we can find $C_\alpha > 0$ such that

$$\mathbb{E} \left[\sum_x \mathcal{E}_x^{(n)}(n^2 t) \right] \leq \frac{1}{\alpha} (C_\alpha n + \mathbf{H}_n(t)), \quad t \geq 0, \quad (3.4)$$

□

From Theorems 2.1 and Corollary 3.2 we immediately conclude the following.

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

$$\sup_{x, t \in [0, t_*]} \left| \int_0^t \mathbb{E} [j_{x-1, x}(n^2 s)] ds \right| \leq \frac{C}{n}, \quad x = 0, \dots, n+1. \quad (3.5)$$

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

$$\left| \int_0^t \left\{ \mathbb{E} [p_0^2(n^2 s)] - T_- \right\} ds \right| \leq \frac{C}{n}, \quad (3.6)$$

Proof. By the local conservation of energy

$$n^{-2} \frac{d}{dt} \mathbb{E} [\mathcal{E}_x^{(n)}(n^2 t)] = \mathbb{E} [j_{x-1, x}^{(n)}(n^2 t) - j_{x, x+1}^{(n)}(n^2 t)]. \quad (3.7)$$

Therefore

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

and bound (3.5) follows directly from estimates (2.17) and (3.3). Estimate (3.6) is a consequence of the definition of $j_{-1, 0}$ (see (2.12)) and (3.5). □

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 $\varphi \in C[0, 1]$ is such that $\text{supp } \varphi \subset (0, 1)$. Then,*

$$\lim_{n \rightarrow +\infty} \frac{1}{n+1} \sum_{x=0}^n \varphi \left(\frac{x}{n+1} \right) \int_0^t \mathbb{E} \left[p_x^2(n^2 s) - (q_x(n^2 s) - q_{x-1}(n^2 s))^2 - \omega_0^2 q_x^2(n^2 s) \right] ds = 0. \quad (4.1)$$

Proof. After a simple calculation we obtain for $x = 1, \dots, n-1$,

$$p_x^2 - \omega_0^2 q_x^2 - (q_x - q_x)^2 = \nabla [q_x(q_{x+1} - q_x)] + \mathcal{G}_t(q_x p_x + 2\gamma q_x^2). \quad (4.2)$$

Therefore,

$$\begin{aligned} & \int_0^t \mathbb{E} \left[p_x^2(n^2 s) - \omega_0^2 q_x^2(n^2 s) - (q_x(n^2 s) - q_x(n^2 s))^2 \right] ds \\ &= \nabla \int_0^t \mathbb{E} [q_x(n^2 s)(q_{x+1}(n^2 s) - q_x(n^2 s))] ds \\ &+ n^{-2} \mathbb{E} [q_x(n^2 t) p_x(n^2 t) + 2\gamma q_x^2(n^2 t)] - n^{-2} \mathbb{E} [q_x(0) p_x(0) + 2\gamma q_x^2(0)]. \end{aligned} \quad (4.3)$$

After summing up against the test function φ (that has compact support strictly contained in $(0, 1)$) and using the energy bound (3.3) we conclude (4.1). \square

4.2. Fluctuation-dissipation relation. In analogy to [14, Section 5.1] define

$$\begin{aligned} \mathfrak{f}_x &:= \frac{1}{4\gamma} (q_{x+1} - q_x) (p_x + p_{x+1}) + \frac{1}{4} (q_{x+1} - q_x)^2, \quad x = 0, \dots, n-1, \\ \mathfrak{F}_x &:= p_x^2 + (q_{x+1} - q_x) (q_x - q_{x-1}) - \omega_0^2 q_x^2, \quad x = 0, \dots, n, \end{aligned} \quad (4.4)$$

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

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

5. LOCAL EQUILIBRIUM AND THE PROOF OF THEOREM 2.4

The fundamental ingredients in the proof of Theorem 2.4 are the identification of the work done at the boundary given by Theorem 2.1, the equipartition and the fluctuation-dissipation relation contained in section 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 $\text{supp } \varphi \subset (0, 1)$. Then*

$$\lim_{n \rightarrow +\infty} \frac{1}{n+1} \sum_{x=0}^n \varphi \left(\frac{x}{n+1} \right) \int_0^t \mathbb{E} [q_x(n^2 s) q_{x+\ell}(n^2 s) - G_{\omega_0}(\ell) p_x^2(n^2 s)] ds = 0, \quad (5.1)$$

for $\ell = 0, 1, 2$. Here $G_{\omega_0}(\ell)$ is given by (A.2).

At the boundaries the situation is a bit different and we have

Proposition 5.2.

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

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 section 7. As a consequence, recalling definition (4.4) and the bound (3.6), we have the following corollary

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

$$\lim_{n \rightarrow +\infty} \frac{1}{n+1} \sum_{x=0}^n \varphi\left(\frac{x}{n+1}\right) \int_0^t \mathbb{E}[\mathfrak{F}_x(n^2 s) - Dp_x^2(n^2 s)] ds = 0, \quad (5.3)$$

and

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

We apply Corollary 5.3 in order to prove Theorem 2.4. Let $\mathcal{M}_+([0, 1])$ be the space of the positive, Borel measures on the interval $[0, 1]$ endowed with the weak topology. The subset $\mathcal{M}_{+, E_*}([0, 1])$, consisting of measures with total mass less or equal to E_* , is compact in this topology and the topology is metrizable when restricted to this set. Define $\xi_n \in C([0, t_*], \mathcal{M}_+([0, 1]))$ as

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

We endow $C([0, t_*], \mathcal{M}_{+, E_*}([0, 1]))$ with the corresponding uniform topology. As a consequence of Corollary 3.2 for any $t_* > 0$ the total energy is bounded by $E_* = E(t_*)$ (see (3.3)) and we have that $\xi_n \in C([0, t_*], \mathcal{M}_{+, E_*}([0, 1]))$.

5.1. Compactness. Since $\mathcal{M}_{+, E_*}([0, 1])$ is compact, 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]. For any $0 \leq s < t \leq t_*$ we have

$$\begin{aligned} \xi_n(t, \varphi) - \xi_n(s, \varphi) &= \frac{n^2}{n+1} \int_s^t \sum_{x=0}^n \varphi_x \mathbb{E}[(j_{x-1, x} - j_{x, x+1})(n^2 \tau)] d\tau \\ &= \frac{n^2}{n+1} \sum_{x=0}^{n-1} (\varphi_{x+1} - \varphi_x) \int_s^t \mathbb{E}[j_{x, x+1}(n^2 \tau)] d\tau \\ &\quad + \frac{n^2}{n+1} \int_s^t (\varphi_0 \mathbb{E}[j_{-1, 0}(n^2 \tau)] - \varphi_n \mathbb{E}[j_{n, n+1}(n^2 \tau)]) d\tau, \end{aligned} \quad (5.6)$$

and by using a slight modification of Corollary 3.3 we have for any $\varphi \in C^1([0, 1])$

$$|\xi_n(t, \varphi) - \xi_n(s, \varphi)| \leq C(t - s). \quad (5.7)$$

This is enough to establish compactness in $C([0, t_*], \mathcal{M}_+([0, 1]))$.

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

$$\varphi(0) = \varphi'(1) = 0. \quad (5.8)$$

In what follows we show that

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

The symbol $o_n(t)$ stands for a quantity that satisfies

$$\lim_{n \rightarrow +\infty} \sup_{s \in [0, t]} |o_n(s)| = 0 \quad \text{for any } t > 0. \quad (5.10)$$

Thus any limiting point of (ξ^n) has to be the unique weak solution of (2.29) and this obviously proves the conclusion of Theorem 2.4.

By an approximation argument we can restrict ourselves to the case when $\text{supp } \varphi'' \subset (0, 1)$. Then as in (5.6) we have

$$\begin{aligned} \xi_n(t, \varphi) - \xi_n(0, \varphi) &= \frac{n^2}{n+1} \sum_{x=0}^{n-1} (\varphi_{x+1} - \varphi_x) \int_0^t \mathbb{E}[j_{x,x+1}(n^2\tau)] d\tau \\ &\quad - \frac{n^2}{n+1} \varphi_n \int_0^t \mathbb{E}[j_{n,n+1}(n^2\tau)] d\tau, \end{aligned} \quad (5.11)$$

By Theorem 2.1 the last term converges to $-\varphi(1)Jt$. On the other hand from (4.5) we have

$$\frac{n^2}{n+1} \sum_{x=0}^{n-1} (\varphi_{x+1} - \varphi_x) \int_0^t \mathbb{E}[j_{x,x+1}(n^2\tau)] d\tau = \sum_{j=1}^3 I_{n,j}, \quad (5.12)$$

where

$$\begin{aligned} I_{n,1} &:= -\frac{1}{4\gamma} \left(\frac{n}{n+1} \right)^2 \sum_{x=0}^{n-1} \nabla_n \varphi_x \int_0^t \mathbb{E}[\nabla \mathfrak{F}_x(n^2s)] ds, \\ I_{n,2} &:= \left(\frac{1}{n+1} \right)^2 \sum_{x=0}^{n-1} \nabla_n \varphi_x \mathbb{E}[\mathfrak{f}_x(n^2t) - \mathfrak{f}_x(0)] ds \\ I_{n,3} &:= -\frac{1}{4\gamma} \left(\frac{n}{n+1} \right)^2 \nabla_n \varphi_{n-1} \int_0^t \mathcal{F}_n(n^2s) \mathbb{E}[q_n(n^2s) - q_{n-1}(n^2s)] ds. \end{aligned}$$

It is easy to see from Theorem 3.2 that $I_{n,2} = o_n(t)$. Using the fact that $\varphi'(1) = 0$ and the estimate (8.14) respectively we conclude also that $I_{n,3} = o_n(t)$. Thanks to Theorem 3.2 and (5.8) we have

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

By Corollary 5.3 and the equipartition property (Proposition 4.1) we have

$$\begin{aligned} I_{n,1}^{(1)} &= \frac{D}{4\gamma(n+1)} \sum_{x=0}^n \varphi''\left(\frac{x}{n+1}\right) \int_0^t \mathbb{E}[p_x^2(n^2s)] ds + o_n(1) \\ &= \frac{D}{4\gamma(n+1)} \sum_{x=0}^n \varphi''\left(\frac{x}{n+1}\right) \int_0^t \mathbb{E}[\mathcal{E}_x(n^2s)] ds + o_n(1) \end{aligned}$$

and

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

Thus (5.9) follows. \square

6. THE EVOLUTION OF THE COVARIANCE MATRIX

6.1. Dynamics of fluctuations. Denote

$$q'_x(t) := q_x(n^2t) - \bar{q}_x(n^2t) \quad \text{and} \quad p'_x(t) := p_x(n^2t) - \bar{p}_x(n^2t) \quad (6.1)$$

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

$$\begin{aligned} \dot{q}'_x(t) &= n^2 p'_x(t), & x &\in \{0, \dots, n\}, \\ dp'_x(t) &= n^2 (\Delta q'_x - \omega_0^2 q'_x) dt - 2\gamma n^2 p'_x(t) dt - 2p_x(t-) d\tilde{N}_x(\gamma n^2 t), & x &\in \{1, \dots, n\}, \end{aligned} \quad (6.2)$$

and at the left boundary

$$dp'_0(t) = n^2 (\Delta q'_0 - \omega_0^2 q'_0) dt - 2\gamma n^2 p'_0(t) dt + \sqrt{4\gamma T_-} n d\tilde{w}_-(t). \quad (6.3)$$

Here $\tilde{N}_x(t) := N_x(t) - t$. 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

$$S_n(t) = \mathbb{E}_{\mu_n}[\mathbf{X}'(t) \otimes \mathbf{X}'(t)] = \begin{bmatrix} S_n^{(q)}(t) & S_n^{(q,p)}(t) \\ S_n^{(p,q)}(t) & S_n^{(p)}(t) \end{bmatrix}, \quad (6.4)$$

where

$$S_n^{(q)}(t) = \left[\mathbb{E}_{\mu_n}[q'_x(t)q'_y(t)] \right]_{x,y=0,\dots,n}, \quad S_n^{(q,p)}(t) = \left[\mathbb{E}_{\mu_n}[q'_x(t)p'_y(t)] \right]_{x,y=0,\dots,n}, \quad (6.5)$$

$$S_n^{(p)}(t) = \left[\mathbb{E}_{\mu_n}[p'_x(t)p'_y(t)] \right]_{x,y=0,\dots,n} \quad \text{and} \quad S_n^{(p,q)}(t) = \left[S_n^{(q,p)}(t) \right]^T.$$

6.2. Structure of the covariance matrix. Given a vector $\mathbf{y} = (y_0, y_1, \dots, y_n)$, define also the matrix valued function

$$D_2(\mathbf{y}) = 4\gamma \begin{bmatrix} T_- & 0 & 0 & \dots & 0 \\ 0 & y_1 & 0 & \dots & 0 \\ 0 & 0 & y_2 & \dots & 0 \\ \vdots & \vdots & \vdots & \ddots & \vdots \\ 0 & 0 & 0 & \dots & y_n \end{bmatrix}. \quad (6.6)$$

Let $\Sigma_2(\mathbf{y})$ be the 2×2 block matrix

$$\Sigma_2(\mathbf{y}) = \begin{bmatrix} 0_{n+1} & 0_{n+1} \\ 0_{n+1} & D_2(\mathbf{y}) \end{bmatrix}. \quad (6.7)$$

Here 0_{n+1} is $(n+1) \times (n+1)$ null matrix. We have

$$S_n(t) = \mathbb{E}_{\mu_n} \left[e^{-An^2t} \mathbf{X}'(0) \otimes \mathbf{X}'(0) e^{-A^T n^2t} \right] + n^2 \int_0^t e^{-An^2(t-s)} \Sigma_2(\overline{\mathbf{p}^2}(n^2s)) e^{-A^T n^2(t-s)} ds$$

where A is given by (8.2) and $\overline{\mathbf{p}^2}(s) = [\mathbb{E}_{\mu_n} p_1^2(s), \dots, \mathbb{E}_{\mu_n} p_n^2(s)]$. Consequently

$$\frac{1}{n^2} \frac{d}{dt} S_n(t) = -AS_n(t) - S_n(t)A^T + \Sigma_2(\overline{\mathbf{p}^2}(n^2t)). \quad (6.8)$$

Denoting

$$\langle \langle S_n \rangle \rangle_t = \int_0^t S_n(s) ds, \quad \langle \langle \mathbf{p}^2 \rangle \rangle_t = \int_0^t \overline{\mathbf{p}^2}(n^2s) ds, \quad (6.9)$$

we have by integrating in (6.8)

$$A \langle \langle S_n \rangle \rangle_t + \langle \langle S_n \rangle \rangle_t A^T - \Sigma_2(\langle \langle \mathbf{p}^2 \rangle \rangle_t) = R_n, \quad (6.10)$$

where, both here and in the following, R_n denotes a generic matrix with entries of order n^{-2} as $n \rightarrow \infty$.

In the following $\{\psi_i(x), \mu_j, j = 0, \dots, n\}$ are the eigenfunctions and eigenvalues of $\omega_0^2 - \Delta_N$, defined by (A.3) in Appendix A.

Given a matrix $[B_{x,x'}]_{x,x'=0,\dots,n}$ we let

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

Then we have the inverse relations

$$B_{x,x'} = \sum_{j,j'=0}^n \tilde{B}_{j,j'} \psi_j(x) \psi_{j'}(x'). \quad (6.11)$$

Following the same algebraic calculation as in [14], section 6.3, we obtain

$$\langle \langle \tilde{S}_{j,j'}^{(q)} \rangle \rangle_t = \frac{2\Theta(\mu_j, \mu_{j'})}{\mu_j + \mu_{j'}} \tilde{F}_{j,j'}(t) + R_n, \quad (6.12)$$

where

$$\tilde{F}_{j,j'}(t) := \sum_{y=0}^n \psi_j(y) \psi_{j'}(y) \langle \langle p_y^2 \rangle \rangle_t + (T_- t - \langle \langle p_0^2 \rangle \rangle_t) \psi_j(0) \psi_{j'}(0), \quad (6.13)$$

and

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

We also have

$$\tilde{S}_{j,j'}^{(p)}(t) = \Theta(\mu_j, \mu_{j'}) \tilde{F}_{j,j'}(t) + R_n \quad (6.14)$$

Finally,

$$\tilde{S}_{j,j'}^{(q,p)}(t) = \frac{\Theta(\mu_j, \mu_{j'})}{2\gamma(\mu_j + \mu_{j'})} (\mu_j - \mu_{j'}) \tilde{F}_{j,j'}(t) + R_n \quad (6.15)$$

6.3. Some bounds on the kinetic energy. From (6.14) we have

$$\langle \langle S_{x,x}^{(p)} \rangle \rangle_t = \sum_y M_{x,y} \langle \langle p_y^2 \rangle \rangle_t + (T_- t - \langle \langle p_0^2 \rangle \rangle_t) M_{x,0} + R_n \quad (6.16)$$

where

$$M_{x,y} := \sum_{j,j'=0}^n \Theta(\mu_j, \mu_{j'}) \psi_j(x) \psi_{j'}(x) \psi_j(y) \psi_{j'}(y). \quad (6.17)$$

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

$$\sum_{y'=0}^n M_{x,y'} = \sum_{y'=0}^n M_{y',x} \equiv 1 \quad \text{and} \quad M_{x,y} > 0 \quad \text{for all } x, y = 0, \dots, n. \quad (6.18)$$

Using energy estimates (3.3), bounds on the momenta averages (8.14), together with (3.6) and (6.18), we conclude that

$$\langle \langle p_x^2 \rangle \rangle_t = \sum_y M_{x,y} \langle \langle p_y^2 \rangle \rangle_t + \rho_{x,n}(t), \quad (6.19)$$

where the symbol $\rho_{x,n}(t)$ satisfies

$$\sup_{s \in [0,t]} \sum_{x=0}^n |\rho_{x,n}(s)| = O\left(\frac{1}{n}\right), \quad (6.20)$$

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

Proposition 6.1. *There exists $c_* > 0$ such that*

$$\sum_{x,y=0}^n (\delta_{x,y} - M_{x,y}) f_y f_x \geq c_* \sum_{x=0}^{n-1} (\nabla f_x)^2, \quad \text{for any } (f_x) \in \mathbb{R}^{n+1}, n = 1, 2, \dots \quad (6.21)$$

Multiplying both sides of (6.19) by $\langle \langle p_x^2 \rangle \rangle_t$, summing over x and using Proposition 6.1 we immediately conclude the following.

Corollary 6.2. *There exists $C > 0$ such that*

$$\sum_{x=0}^{n-1} [\langle \langle p_x^2 \rangle \rangle_t - \langle \langle p_{x+1}^2 \rangle \rangle_t]^2 \leq \frac{C}{n+1} \sum_{x=0}^n \langle \langle p_x^2 \rangle \rangle_t, \quad n = 1, 2, \dots \quad (6.22)$$

Proposition 6.3. *For any $t > 0$ there exists $C > 0$ such that*

$$\begin{aligned} \sum_{x=0}^{n-1} [\langle \langle p_x^2 \rangle \rangle_t - \langle \langle p_{x+1}^2 \rangle \rangle_t]^2 &\leq \frac{C}{n+1}, \quad n = 1, 2, \dots, \\ \sup_{x=0, \dots, n} \langle \langle p_x^2 \rangle \rangle_t &\leq C. \end{aligned} \quad (6.23)$$

Proof. As a direct consequence of (3.3) and Corollary 6.2 we have: for any $t > 0$ there exists $C > 0$ such that

$$\sum_{x=0}^{n-1} [\langle \langle p_x^2 \rangle \rangle_t - \langle \langle p_{x+1}^2 \rangle \rangle_t]^2 \leq C \quad (6.24)$$

and

$$\sup_{x=0,\dots,n} \langle \langle p_x^2 \rangle \rangle_t \leq Cn^{1/2}, \quad n = 1, 2, \dots \quad (6.25)$$

Indeed, estimate (6.24) is obvious in light of (6.22). To prove (6.25) note that by the Cauchy-Schwarz inequality

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

and (6.25) follows, thanks to (3.6).

From (6.19) and (6.20) we conclude that for any $t > 0$ we can find $C > 0$ such that

$$\begin{aligned} \sum_{x=0}^{n-1} \left(\langle \langle p_x^2 \rangle \rangle_t - \langle \langle p_{x+1}^2 \rangle \rangle_t \right)^2 &\leq \sum_{x=0}^n |\rho_{x,n}(t)| \langle \langle p_x^2 \rangle \rangle_t \\ &\leq \sup_x \langle \langle p_x^2 \rangle \rangle_t \sum_{x=0}^n |\rho_{x,n}(t)| \leq \frac{C}{n+1} \sup_x \langle \langle p_x^2 \rangle \rangle_t \end{aligned} \quad (6.26)$$

Using the Cauchy-Schwarz inequality we conclude

$$\begin{aligned} \sup_x \langle \langle p_x^2 \rangle \rangle_t &\leq \langle \langle p_0^2 \rangle \rangle_t + \sum_{x=0}^{n-1} \left| \langle \langle p_x^2 \rangle \rangle_t - \langle \langle p_{x+1}^2 \rangle \rangle_t \right| \\ &\leq \langle \langle p_0^2 \rangle \rangle_t + \sqrt{n} \left\{ \sum_{x=0}^{n-1} \left(\langle \langle p_x^2 \rangle \rangle_t - \langle \langle p_{x+1}^2 \rangle \rangle_t \right)^2 \right\}^{1/2} \end{aligned} \quad (6.27)$$

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

$$\begin{aligned} D_n &\leq \frac{C}{n+1} \sup_x \langle \langle p_x^2 \rangle \rangle_t, \\ \sup_x \langle \langle p_x^2 \rangle \rangle_t &\leq \langle \langle p_0^2 \rangle \rangle_t + \sqrt{n+1} D_n^{1/2} \leq \langle \langle p_0^2 \rangle \rangle_t + C + C \sup_x \langle \langle p_x^2 \rangle \rangle_t^{1/2}, \end{aligned} \quad (6.28)$$

for all $n = 1, 2, \dots$. Thus the second estimate of (6.23) follows, which in turn implies the first estimate of (6.23) as well.

7. PROOF OF LOCAL EQUILIBRIUM

We prove here Proposition 5.1 and 5.2.

7.1. Proof of Proposition 5.1. Let

$$\Phi(\mu_j, \mu_{j'}) = \frac{2\Theta(\mu_j, \mu_{j'})}{\mu_j + \mu_{j'}}. \quad (7.1)$$

For a fixed integer ℓ define

$$\overline{K}^{(n,\ell)}(x) := \frac{1}{4(n+1)^2} \sum_{j,j'=-n-1}^n \Phi(\mu_j, \mu_{j'}) \cos\left(\frac{\pi j x}{n+1}\right) \cos\left(\frac{\pi j'(x-\ell)}{n+1}\right). \quad (7.2)$$

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

$$|\overline{K}_1^{(n,\ell)}(x)| \leq \frac{C}{1+x^2}, \quad x = 0, \dots, n \quad (7.3)$$

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

$$\left| \sum_{y=0}^n \overline{K}^{(n,\ell)}(x-y) - G_{\omega_0}(\ell) \right| \leq \frac{C}{n^2}, \quad \delta n \leq x \leq (1-\delta)n. \quad (7.4)$$

for $n = 1, 2, \dots$.

By virtue of (8.14) we have

$$\lim_{n \rightarrow +\infty} \frac{1}{n+1} \sum_{x=0}^n \varphi\left(\frac{x}{n+1}\right) \int_0^t \mathbb{E}[q_x(n^2 s)] \mathbb{E}[q_{x+\ell}(n^2 s)] ds = 0. \quad (7.5)$$

It suffices therefore to prove that

$$\lim_{n \rightarrow +\infty} \frac{1}{n+1} \sum_{x=0}^n \varphi\left(\frac{x}{n+1}\right) \left\{ \langle \langle S_{x,x+\ell}^{(q)} \rangle \rangle_t - G_{\omega_0}(\ell) \langle \langle p_x^2 \rangle \rangle_t \right\} = 0. \quad (7.6)$$

We prove (7.6) for $\ell = 0$, the argument for other values of ℓ are similar. By (6.12) we have

$$\langle \langle S_{x,x}^{(q)} \rangle \rangle_t = \sum_{y=0}^n H_{x,y}^{(n)} \langle \langle p_y^2 \rangle \rangle_t + B_n(t, x) + o_n, \quad (7.7)$$

with

$$\begin{aligned}
H_{x,y}^{(n)} &= \sum_{y=0}^n \sum_{j,j'} \Phi(\mu_j, \mu_{j'}) \psi_j(y) \psi_{j'}(y) \psi_j(x) \psi_{j'}(x), \\
B_n(t, x) &= \sum_{j,j'} \psi_j(x) \psi_{j'}(x) \Phi(\mu_j, \mu_{j'}) \left(T_- t - \langle p_0^2 \rangle_t \right) \psi_j(0) \psi_{j'}(0).
\end{aligned} \tag{7.8}$$

Using (3.3) and (3.6) we conclude that $\lim_{n \rightarrow +\infty} \sup_x |B_n(t, x)| = 0$. Furthermore, if $\delta n \leq x \leq (1 - \delta)n$,

$$\sum_y H_{x,y}^{(n)} = G_{\omega^2}(0) + o(n) \tag{7.9}$$

Then we have that

$$\begin{aligned}
& \frac{1}{n+1} \sum_{x=0}^n \varphi\left(\frac{x}{n+1}\right) \left\{ \langle S_{x,x+\ell}^{(q)} \rangle_t - G_{\omega_0}(\ell) \langle p_x^2 \rangle_t \right\} \\
&= \frac{1}{n+1} \sum_{x=0}^n \varphi\left(\frac{x}{n+1}\right) \sum_{y=0}^n H_{x,y}^{(n)} \left[\langle p_y^2 \rangle_t - \langle p_x^2 \rangle_t \right] + o_n.
\end{aligned} \tag{7.10}$$

Using Schwarz inequality and (6.23) we obtain the bound

$$\begin{aligned}
\sum_{y=0}^n H_{x,y}^{(n)} \left[\langle p_y^2 \rangle_t - \langle p_x^2 \rangle_t \right] &\leq \sum_{y=0}^n |H_{x,y}^{(n)}| \sum_{z=x}^{y-1} |\langle p_{z+1}^2 \rangle_t - \langle p_z^2 \rangle_t| \leq \sum_{z=0}^n \sum_{y=0}^z |H_{x,y}^{(n)}| |\langle p_{z+1}^2 \rangle_t - \langle p_z^2 \rangle_t| \\
&\leq \left[\sum_{z=0}^n \left(\sum_{y=0}^z |H_{x,y}^{(n)}| \right)^2 \right]^{1/2} \left[\sum_{z=0}^n |\langle p_{z+1}^2 \rangle_t - \langle p_z^2 \rangle_t|^2 \right]^{1/2} \leq \left[\sum_{z=0}^n \left(\sum_{y=0}^z |H_{x,y}^{(n)}| \right)^2 \right]^{1/2} \frac{C}{\sqrt{n}}.
\end{aligned} \tag{7.11}$$

It follows from results in Section 8.1 of [14] that $\sum_{z=0}^n \left(\sum_{y=0}^z |H_{x,y}^{(n)}| \right)^2 \leq C$, and Proposition 5.1 follows for $\ell = 0$.

□

7.2. Proof of Proposition 5.2. From Propositions 8.1 we have

$$\lim_{n \rightarrow +\infty} \int_0^t \bar{q}_0^2(s) ds = 0.$$

It suffices therefore to calculate $\int_0^t \mathbb{E}(q_0'(s)^2) ds = \langle S_{0,0}^{(q)} \rangle_t$.

We have, see (6.12) and (7.1),

$$\langle \langle S_{0,0}^{(q)} \rangle \rangle_t = \sum_{y=0}^n \sum_{j,j'=0}^n \Phi(\mu_j, \mu_{j'}) \psi_j(0) \psi_{j'}(0) \psi_j(y) \psi_{j'}(y) \langle \langle p_y^2 \rangle \rangle_t \quad (7.12)$$

$$\begin{aligned} &+ \sum_{j,j'=0}^n \Phi(\mu_j, \mu_{j'}) \psi_j(0)^2 \psi_{j'}(0)^2 (T_- t - \langle \langle p_0^2 \rangle \rangle_t) + o_n(t) \\ &= \sum_{y=0}^n H_y^{(n)} \langle \langle p_y^2 \rangle \rangle_t + o_n(t). \end{aligned} \quad (7.13)$$

Here

$$H_y^{(n)} := \sum_{j,j'=0}^n \Phi(\mu_j, \mu_{j'}) \psi_j(0) \psi_{j'}(0) \psi_j(y) \psi_{j'}(y) \quad (7.14)$$

That has the property

$$\begin{aligned} \sum_{y=0}^n H_y^{(n)} &= \sum_{j=0}^n \Phi(\mu_j, \mu_j) \psi_j(0)^2 = \sum_{j=0}^n \frac{1}{\mu_j} \psi_j(0)^2 \\ &= \frac{1}{n+1} \sum_{j=0}^n \frac{\cos^2\left(\frac{\pi j}{2(n+1)}\right)}{\omega_0^2 + 4 \sin^2\left(\frac{\pi j}{2(n+1)}\right)} \xrightarrow{n \rightarrow \infty} G_{\omega_0^2}(0) + G_{\omega_0^2}(1). \end{aligned} \quad (7.15)$$

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

$$|H_y^{(n)}| \leq \frac{C}{(1+y^2)}, \quad y = 0, \dots, n, \quad n \geq 1. \quad (7.16)$$

Then, proceeding as in (7.11) using the Cauchy-Schwarz inequality and the first estimate of (6.23) we conclude that we obtain

$$\sum_{y=0}^n |H_y^{(n)}| \left| \langle \langle p_y^2 \rangle \rangle_t - \langle \langle p_0^2 \rangle \rangle_t \right| \leq \frac{C}{\sqrt{n}}$$

Hence

$$\langle \langle S_{0,0}^{(q)} \rangle \rangle_t = \left(\sum_{y=0}^n H_{y,0}^{(n)} \right) \langle \langle p_0^2 \rangle \rangle_t + o_n(t) = G_{\omega_0^2}(0) + G_{\omega_0^2}(1) + o_n. \quad (7.17)$$

□

8. THE DYNAMICS OF MEANS AND THE PROOF OF THEOREM 2.1

8.1. The dynamics of means. Let μ be a Borel probability measure on $\mathbb{R}^{2(n+1)}$ and let $(\bar{\mathbf{q}}, \bar{\mathbf{p}})$ be the vector of the μ -averages of initial data. In the following we denote by $\begin{pmatrix} \bar{\mathbf{q}}(t) \\ \bar{\mathbf{p}}(t) \end{pmatrix}$ the vector means of positions and momenta by $\bar{q}_x(t) = \mathbb{E}_{\mathbf{q}, \mathbf{p}}(q_x(t))$ and $\bar{p}_x(t) = \mathbb{E}_{\mathbf{q}, \mathbf{p}}(p_x(t))$. Let $\mathbf{e}_{2(n+1)}$ the $2(n+1)$ vector defined by $e_{2(n+1),j} = \delta_{2(n+1),j}$. Then the evolution equation is given by

$$\begin{pmatrix} \bar{\mathbf{q}}(t) \\ \bar{\mathbf{p}}(t) \end{pmatrix} = e^{-At} \begin{pmatrix} \bar{\mathbf{q}} \\ \bar{\mathbf{p}} \end{pmatrix} + \int_0^t \mathcal{F}_n(s) e^{-A(t-s)} \mathbf{e}_{2(n+1)} ds. \quad (8.1)$$

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

$$A = \begin{pmatrix} 0 & -\text{Id}_{n+1} \\ -\Delta_N + \omega_0^2 & 2\gamma \text{Id}_{n+1} \end{pmatrix} \quad (8.2)$$

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

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

and defining

$$\begin{pmatrix} \bar{\mathbf{y}}(t) \\ \bar{\mathbf{z}}(t) \end{pmatrix} := e^{-At} \mathbf{e}_{2(n+1)}, \quad (8.3)$$

we can write

$$\begin{pmatrix} \bar{\mathbf{q}}(t) \\ \bar{\mathbf{p}}(t) \end{pmatrix} = e^{-At} \begin{pmatrix} \bar{\mathbf{q}} \\ \bar{\mathbf{p}} \end{pmatrix} + \sum_{\ell} \frac{\widehat{\mathcal{F}}(\ell)}{\sqrt{n}} \int_0^t e^{2\pi i \ell s / \theta} \begin{pmatrix} \bar{\mathbf{y}}(t-s) \\ \bar{\mathbf{z}}(t-s) \end{pmatrix} ds. \quad (8.4)$$

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

Let

$$\lambda_{j,\pm} := \gamma \pm \sqrt{\gamma^2 - \mu_j} \quad (8.5)$$

be the two solutions of the equation $\lambda^2 - 2\gamma\lambda + \mu_j = 0$. Note that $\lambda_{j,+}\lambda_{j,-} = \mu_j$. Then,

$$\tilde{u}_j(t) = \frac{\exp\{-\lambda_{j,-}t\}}{2\sqrt{\gamma^2 - \mu_j}} \left[\lambda_{j,+}\tilde{q}_j + \tilde{p}_j - (\lambda_{j,-}\tilde{q}_j + \tilde{p}_j) \exp\{-2t\sqrt{\gamma^2 - \mu_j}\} \right] \quad (8.6)$$

and

$$\tilde{v}_j(t) = \frac{\exp\{-\lambda_{j,-}t\}}{2\sqrt{\gamma^2 - \mu_j}} \left[(\mu_j\tilde{q}_j + \lambda_{j,+}\tilde{p}_j) \exp\{-2t\sqrt{\gamma^2 - \mu_j}\} - \mu_j\tilde{q}_j - \lambda_{j,-}\tilde{p}_j \right] \quad (8.7)$$

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

$$\tilde{u}_j(t) = \left[(1 + \gamma t)\tilde{q}_j + \tilde{p}_j t \right] e^{-\gamma t}, \quad \tilde{v}_j(t) = \left[\mu_j t \tilde{q}_j + (1 - \gamma t)\tilde{p}_j \right] e^{-\gamma t}.$$

Then, by (8.6) and (8.7), we conclude that the components of $e^{-At}\mathbf{e}_{2(n+1)}$ equal

$$\begin{aligned} \tilde{y}_j(t) &= -\psi_j(n) \frac{\exp\{-\lambda_{j,-}t\} \left[1 - \exp\{-2t\sqrt{\gamma^2 - \mu_j}\} \right]}{2\sqrt{\gamma^2 - \mu_j}}, \\ \tilde{z}_j(t) &= \psi_j(n) \frac{\exp\{-\lambda_{j,-}t\} \left[\lambda_{j,+} - \lambda_{j,-} \exp\{-2t\sqrt{\gamma^2 - \mu_j}\} \right]}{2\sqrt{\gamma^2 - \mu_j}}, \end{aligned} \quad (8.8)$$

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

Elementary calculations lead to the following bounds

$$\operatorname{Re}\lambda_{j,\pm} \geq \gamma_* := \min\left\{\gamma, \frac{\omega_0^2}{2\gamma}\right\}, \quad |\lambda_{j,\pm}| \leq \gamma + |\gamma^2 - \omega_0^2 - 4|^{1/2}, \quad j = 0, \dots, n. \quad (8.9)$$

Hence, there exists $C > 0$ such that

$$|\tilde{y}_j(t)| + |\tilde{z}_j(t)| \leq C(t+1)e^{-\gamma_* t}|\psi_j(n)| \quad (8.10)$$

for all $t \geq 0$, $j = 0, \dots, n$, $n = 1, 2, \dots$. By the Plancherel identity, (8.6) and (8.7) we conclude also that there exist constants $C, C' > 0$ such that, for all $t \geq 0$ and $n \in \mathbb{N}$,

$$\begin{aligned} \sum_{x=0}^n \left[\bar{u}_x^2(t) + \bar{v}_x^2(t) \right] &= \sum_{j=0}^n \left[\tilde{u}_j^2(t) + \tilde{v}_j^2(t) \right] \\ &\leq C(t+1)e^{-\gamma_* t} \sum_{j=0}^n \left(\tilde{q}_j^2 + \tilde{p}_j^2 \right) \leq C'(t+1)e^{-\gamma_* t} \mathcal{H}_n(\bar{\mathbf{q}}, \bar{\mathbf{p}}). \end{aligned} \quad (8.11)$$

8.2. L^2 norms of the means. By (8.4) and the Plancherel theorem

$$\begin{aligned} \sum_{x=0}^n \int_0^t [\bar{q}_x^2(s) + \bar{p}_x^2(s)] ds &\leq C \sum_{x=0}^n \int_0^t [\bar{u}_x^2(s) + \bar{v}_x^2(s)] ds \\ &+ \frac{C}{n} \sum_{j=0}^n \left[\left| \sum_{\ell} \widehat{\mathcal{F}}(\ell) \int_0^t e^{2\pi i \ell s / \theta} \widetilde{y}_j(t-s) ds \right|^2 + \left| \sum_{\ell} \widehat{\mathcal{F}}(\ell) \int_0^t e^{2\pi i \ell s / \theta} \widetilde{z}_j(t-s) ds \right|^2 \right]. \end{aligned} \quad (8.12)$$

The constant appearing here below do not depend on t and n . Using (8.10) and (8.11) we conclude therefore that

$$\sum_{x=0}^n \int_0^t [\bar{q}_x^2(s) + \bar{p}_x^2(s)] ds \leq C \mathcal{H}_n(\bar{\mathbf{q}}, \bar{\mathbf{p}}) + \frac{C}{n} \left(\sum_{\ell} |\widehat{\mathcal{F}}(\ell)| \right)^2. \quad (8.13)$$

From (8.13) we conclude therefore the following.

Proposition 8.1. *Assume that the hypotheses of Theorem 2.1 are in force. Then, there exists $C > 0$ such that*

$$\sum_{x=0}^n \int_0^t [\bar{q}_x^2(n^2 s) + \bar{p}_x^2(n^2 s)] ds \leq \frac{C}{n^{2-\delta}}, \quad (8.14)$$

for all $t \geq 0$, $n = 1, 2, \dots$. Here δ is as in (2.16).

8.3. **The proof of Theorem 2.1.** We show (2.17) and (2.18). Recall that the initial configuration (\mathbf{q}, \mathbf{p}) is distributed according to μ_n . For the work done we have

$$\begin{aligned} W_n(t) &:= \int_0^t \mathcal{F}_n(s) \bar{p}_n(s) ds \\ &= \sum_j \psi_j(n) \sum_{\ell} \frac{1}{\sqrt{n}} \widehat{\mathcal{F}}(\ell) \int_0^t e^{i2\pi \ell s / \theta} \widetilde{p}_j(s)^* ds. \end{aligned} \quad (8.15)$$

Using (8.1) the utmost right hand side can be rewritten in the form $W_{n,i}(t) + W_{n,f}(t)$ where

$$\begin{aligned} W_{n,i}(t) &:= \sum_j \psi_j(n) \sum_{\ell} \frac{1}{\sqrt{n}} \widehat{\mathcal{F}}(\ell) \int_0^t e^{i2\pi \ell s / \theta} \widetilde{v}_j(s)^* ds, \\ W_{n,f}(t) &:= \frac{1}{n} \sum_j \psi_j(n) \sum_{\ell, \ell'} \widehat{\mathcal{F}}(\ell) \widehat{\mathcal{F}}(\ell')^* \int_0^t ds e^{i2\pi(\ell - \ell')s / \theta} \int_0^s e^{i2\pi \ell' s' / \theta} \widetilde{z}_j(s')^* ds' \end{aligned} \quad (8.16)$$

Thanks to (2.15) and the Cauchy-Schwarz inequality we conclude from (8.11)

$$|W_{n,i}(t)| \leq \frac{C}{\sqrt{n}} \mathcal{H}_n^{1/2}(\bar{\mathbf{q}}_n, \bar{\mathbf{p}}_n) \int_0^t (s+1)^{1/2} e^{-\gamma_* s/2} ds.$$

Thanks to (2.16) $\lim_{n \rightarrow +\infty} |W_{n,i}(n^2 t)|/n = 0$. Using (8.8) we have

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

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

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

while $W_{n,f}^{(2)}(t)$ is exponentially small in time. After a direct calculation we obtain

$$W_{n,f}^{(1)}(t) = -\frac{2\gamma t}{n} \left(\frac{2\pi}{\theta} \right)^2 \sum_{j=0}^n \sum_{\ell} \frac{\psi_j^2(n) \ell^2 |\widehat{\mathcal{F}}(\ell)|^2}{\left\{ \left[\mu_j - (2\pi \ell/\theta)^2 \right]^2 + \left[2\gamma(2\pi \ell/\theta) \right]^2 \right\}} = -\frac{Jt}{n},$$

so that $\lim_{n \rightarrow \infty} J_n(t) = -\lim_{n \rightarrow \infty} W_n(n^2 t)/n = Jt$, and Theorem 2.1 follows. \square

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APPENDIX A. THE DISCRETE LAPLACIAN

A.1. Discrete gradient and laplacian. Recall that the lattice gradient and laplacian of any $f : \mathbb{Z} \rightarrow \mathbb{R}$ are defined as $\nabla f_x = f_{x+1} - f_x$ and $\Delta f_x = f_{x+1} + f_{x-1} - 2f_x$, $x \in \mathbb{Z}$, respectively.

For a given function $\varphi : [0, 1] \rightarrow \mathbb{R}$ and $n = 1, 2, \dots$ we define three discrete approximations: of the function itself, of its gradient and Laplacian, respectively by

$$\begin{aligned} \varphi_x &:= \varphi\left(\frac{x}{n+1}\right), & (\nabla_n \varphi)_x &:= (n+1)\left(\varphi\left(\frac{x+1}{n+1}\right) - \varphi\left(\frac{x}{n+1}\right)\right), \\ (\Delta_n \varphi)_x &:= (n+1)^2\left(\varphi\left(\frac{x+1}{n+1}\right) + \varphi\left(\frac{x-1}{n+1}\right) - 2\varphi\left(\frac{x}{n+1}\right)\right), & x &\in \{0, \dots, n\}. \end{aligned} \quad (\text{A.1})$$

We have used the convention $\varphi(-\frac{1}{n+1}) = \varphi(0)$.

Suppose that $\omega_0 > 0$. Consider the Green's function of $-\Delta + \omega_0^2$ on the integer lattice \mathbb{Z} . It is given by, see e.g. [15, (27)],

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

A.2. Discrete Neumann laplacian $-\Delta_N$. Let λ_j and ψ_j , $j = 0, \dots, n$ be the respective eigenvalues and eigenfunctions for the discrete Neumann laplacian $-\Delta_N$, i.e. $\psi_j(-1) = \psi_j(0)$ and $\psi_j(n) = \psi_j(n+1)$. They are given by

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

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

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

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