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Thermal Conductivity for a Momentum Conservative Model

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Abstract: We introduce a model whose thermal conductivity diverges in dimension 1 and 2, while it remains finite in dimension 3. We consider a system of oscillators perturbed by a stochastic dynamics conserving momentum and energy. We compute thermal conductivity via Green-Kubo formula. In the harmonic case we compute the current-current time correlation function, that decay like $t^{-d/2}$ in the unpinned case and like $t^{-d/2-1}$ if an on-site harmonic potential is present. This implies a finite conductivity in $d \geq 3$ or in pinned cases, and we compute it explicitly. For general anharmonic strictly convex interactions we prove some upper bounds for the conductivity that behave qualitatively as in the harmonic cases.

1. Introduction

The mathematical deduction of Fourier's law and heat equation for the diffusion of energy from a microscopic Hamiltonian deterministic dynamics is one of the major open problems in non-equilibrium statistical mechanics [6]. Even the existence of the thermal conductivity defined by the Green-Kubo formula, is a challenging mathematical problem and it may be infinite in some low dimensional cases [13]. Let us consider the problem in a generic lattice system where dynamics conserves energy (between other quantities like momentum, etc.). For $\mathbf{x} \in \mathbb{Z}^d$, denote by $\mathcal{E}_{\mathbf{x}}(t)$ the energy of *atom* $\mathbf{x}$. To simplify notations let us consider the 1-dimensional case. Since the dynamics conserves the total energy, there exist *energy currents* $j_{x,x+1}$ (local functions of the coordinates of the system), such that

$$\frac{d}{dt}\mathcal{E}_x(t) = j_{x-1,x}(t) - j_{x,x+1}(t). \tag{1}$$

Another consequence of the conservation of energy is that there exists a family of stationary equilibrium measures parametrized by temperature value T (between other possible parameters). Let us denote by $< \cdot > = < \cdot >_T$ the expectation of the system starting from this equilibrium measure, and assume that parameters are set so that $< j_{x,y} > = 0$ (for example if total momentum is fixed to be null). Typically these measures are Gibbs measure with sufficiently fast decay of space correlations so that energy has static fluctuation that are Gaussian distributed if properly rescaled in space. Let us define the space-time correlations of the energy as

$$S(x,t) = < \mathcal{E}_x(t)\mathcal{E}_0(0) > - < \mathcal{E}_0 >^2 .$$

If thermal conductivity is finite, $S(x,t)$ should be solution of the diffusion equation (in a proper large space-time scale) and thermal conductivity (TC) can be defined as

$$\kappa(T) = \lim_{t\to\infty} \frac{1}{2tT^2} \sum_{x\in\mathbb{Z}} x^2 S(x,t). \tag{2}$$

By using the energy conservation law (1), time and space invariance (see Sect. 3), one can rewrite

$$\begin{aligned}\kappa(T) &= \lim_{t\to\infty} \frac{1}{2tT^2} \sum_{x\in\mathbb{Z}} \left\langle \left(\int_0^t j_{x,x+1}(s)ds \right) \left(\int_0^t j_{0,1}(s')ds' \right) \right\rangle \\ &= \frac{1}{T^2} \sum_{x\in\mathbb{Z}} \int_0^\infty \left\langle j_{x,x+1}(t)\, j_{0,1}(0) \right\rangle dt, \end{aligned} \tag{3}$$

which is the celebrated Green-Kubo formula for the thermal conductivity (cf. [17]).

One can see from (3) why the problem is so difficult for deterministic dynamics: one needs some control of time decay of the current-current correlations, a difficult problem even for finite dimensional dynamical systems. Furthermore in some one–dimensional systems, like the Fermi-Pasta-Ulam chain of unpinned oscillators, if total momentum is conserved by the dynamics, thermal conductivity is expected to be infinite (cf. [13] for a review of numerical results on this topic). Very few mathematically rigorous results exist for deterministic systems ([8,15]).

In this paper we consider stochastic perturbations of a deterministic Hamiltonian dynamics on a multidimensional lattice and we study the corresponding thermal conductivity as defined by (3). The stochastic perturbations are such that they exchange momentum between particles with a local random mechanism that conserves total energy and total momentum.

Thermal conductivity of Hamiltonian systems with stochastic dynamical perturbations have been studied for harmonic chains. In [5,7] the stochastic perturbation does not conserve energy, and in [3] only energy is conserved. The novelty of our work is that our stochastic perturbations conserve also momentum, with dramatic consequences in low dimensional systems. In fact we prove that for unpinned systems (where also the Hamiltonian dynamics conserve momentum, see the next section for a precise definition) with harmonic interactions, thermal conductivity is infinite in 1 and 2 dimensions, while it is finite for $d \geq 3$ or for pinned systems. Notice that for stochastic perturbations of harmonic systems that do not conserve momentum, thermal conductivity is always finite [3,7].

This divergence of TC in dimension 1 and 2 is expected generically for a deterministic Hamiltonian non-linear system when unpinned. So TC in our model behaves qualitatively like in a deterministic non-linear system, i.e. these stochastic interactions reproduce some of the features of the non-linear deterministic hamiltonian interactions. Also notice that because of the conservation laws, the noise that we introduce is of multiplicative type, i.e. intrinsically non-linear (cf. (6) and (7)). On the other hand, purely deterministic harmonic chains (pinned or unpinned and in any dimension) have always infinite conductivity [15]. In fact in these linear systems energy fluctuations are transported ballistically by waves that do not interact with each other. Consequently, in the harmonic case, our noise is entirely responsible for the finiteness of the TC in dimension 3 and for pinned systems. Also in dimension 1 and 2, the divergence of TC for unpinned harmonic systems is due to a superdiffusion of the energy fluctuations, not to ballistic transport (see [2,12] where this behavior is explained with a kinetic argument).

For anharmonic systems, even with the stochastic noise we are not able to prove the existence of thermal conductivity (finite or infinite). If the dimension d is greater than 3 and the system is pinned, we get a uniform bound on the finite size system conductivity. For low dimensional pinned systems ($d = 1, 2$), we can show the conductivity is finite if the interaction potential is quadratic and the pinning is generic. For the unpinned system we have to assume that the interaction between nearest-neighbor particles is strictly convex and quadratically bounded at infinity. This is because we need some information on the spatial decay of correlations in the stationary equilibrium measure, that decay slow in the unpinned system [9]. In this case, we prove the conductivity is finite in dimension $d \geq 3$ and we obtain upper bounds in the size N of the system of the form $\sqrt{N}$ in $d = 1$ and $(\log N)^2$ in $d = 2$ (see Theorem 3 for precise statements).

The paper is organized as follows. Section 2 is devoted to the precise description of the dynamics. In Sects. 3, we present our results. The proofs of the harmonic case are in Sect. 4 and 5 while the proofs of the anharmonic case are stated in Sect. 6. The final section contains technical lemmas related to equivalence of ensembles.

Notations. The canonical basis of $\mathbb{R}^d$ is noted $(\mathbf{e}_1, \mathbf{e}_2, \ldots, \mathbf{e}_d)$ and the coordinates of a vector $\mathbf{u} \in \mathbb{R}^d$ are noted $(\mathbf{u}^1, \ldots, \mathbf{u}^d)$. Its Euclidean norm $|\mathbf{u}|$ is given by $|\mathbf{u}| = \sqrt{(\mathbf{u}^1)^2 + \ldots + (\mathbf{u}^d)^2}$ and the scalar product of $\mathbf{u}$ and $\mathbf{v}$ is $\mathbf{u} \cdot \mathbf{v}$.

If N is a positive integer, $\mathbb{Z}_N^d$ denotes the d-dimensional discrete torus of length N and we identify $\mathbf{x} = \mathbf{x} + kN\mathbf{e}_j$ for any $j = 1, \ldots, d$ and $k \in \mathbb{Z}$.

If F is a function from $\mathbb{Z}^d$ (or $\mathbb{Z}_N^d$) into $\mathbb{R}$ then the (discrete) gradient of F in the direction $\mathbf{e}_j$ is defined by $(\nabla_{\mathbf{e}_j} F)(\mathbf{x}) = F(\mathbf{x} + \mathbf{e}_j) - F(\mathbf{x})$ and the Laplacian of F is given by $(\Delta F)(\mathbf{x}) = \sum_{j=1}^d \left\{F(\mathbf{x} + \mathbf{e}_j) + F(\mathbf{x} - \mathbf{e}_j) - 2F(\mathbf{x})\right\}$.

2. The Dynamics

In order to avoid difficulties with definitions of the dynamics and its stationary Gibbs measures, we start with a finite system and we will define thermal conductivity through an infinite volume limit procedure (see sect. 3).

We consider the dynamics of the system of length N with periodic boundary conditions. The atoms are labeled by $\mathbf{x} \in \mathbb{Z}_N^d$. Momentum of atom $\mathbf{x}$ is $\mathbf{p}_\mathbf{x} \in \mathbb{R}^d$ and its displacement from its equilibrium position is $\mathbf{q}_x \in \mathbb{R}^d$. The Hamiltonian is given by

$$\mathcal{H}_N = \sum_{\mathbf{x} \in \mathbb{Z}_N^d} \left[\frac{|\mathbf{p}_\mathbf{x}|^2}{2} + W(\mathbf{q}_\mathbf{x}) + \frac{1}{2} \sum_{|\mathbf{y}-\mathbf{x}|=1} V(\mathbf{q}_\mathbf{x} - \mathbf{q}_\mathbf{y}) \right].$$

We assume that V and W have the following form:

$$V(\mathbf{q_x} - \mathbf{q_y}) = \sum_{j=1}^{d} V_j(q^j_{\mathbf{x}} - q^j_{\mathbf{y}}), \qquad W(\mathbf{q_x}) = \sum_{j=1}^{d} W_j(q^j_{\mathbf{x}}),$$

and that V_j, W_j are smooth and even. We call V the interaction potential, and W the pinning potential. The case where $W = 0$ will be called unpinned.

We consider the stochastic dynamics generated by the operator

$$L \;=\; A + \gamma S\,. \tag{4}$$

The operator A is the usual Hamiltonian vector field

$$A = \sum_{\mathbf{x}} \left\{ \mathbf{p_x} \cdot \partial_{\mathbf{q_x}} - \partial_{\mathbf{q_x}} \mathcal{H}_N \cdot \partial_{\mathbf{p_x}} \right\},$$

while S is the generator of the stochastic perturbation and $\gamma > 0$ is a positive parameter that regulates its strength. The operator S acts only on the momentums $\{\mathbf{p_x}\}$ and generates a diffusion on the surface of constant kinetic energy and constant momentum. This is defined as follows. If $d \geq 2$, for every nearest neighbor atoms $\mathbf{x}$ and $\mathbf{z}$, consider the $d-1$ dimensional surface of constant kinetic energy and momentum

$$\mathbb{S}_{e,\mathbf{p}} \;=\; \left\{ (\mathbf{p_x}, \mathbf{p_z}) \in \mathbb{R}^{2d} : \frac{1}{2}\left(|\mathbf{p_x}|^2 + |\mathbf{p_z}|^2 \right) = e\,;\; \mathbf{p_x} + \mathbf{p_z} = \mathbf{p} \right\}.$$

The following vector fields are tangent to $\mathbb{S}_{e,\mathbf{p}}$:

$$X^{i,j}_{\mathbf{x},\mathbf{z}} = (p^j_{\mathbf{z}} - p^j_{\mathbf{x}})(\partial_{p^i_{\mathbf{z}}} - \partial_{p^i_{\mathbf{x}}}) - (p^i_{\mathbf{z}} - p^i_{\mathbf{x}})(\partial_{p^j_{\mathbf{z}}} - \partial_{p^j_{\mathbf{x}}}),$$

so $\sum_{i,j=1}^{d} (X^{i,j}_{\mathbf{x},\mathbf{z}})^2$ generates a diffusion on $\mathbb{S}_{e,\mathbf{p}}$ (see [11]). In $d \geq 2$ we define

$$\begin{aligned} S &= \frac{1}{2(d-1)} \sum_{\mathbf{x}} \sum_{i,j,k}^{d} \left(X^{i,j}_{\mathbf{x},\mathbf{x}+\mathbf{e}_k} \right)^2 \\ &= \frac{1}{4(d-1)} \sum_{\substack{\mathbf{x},\mathbf{z} \in \mathbb{Z}^d_N \\ |\mathbf{x}-\mathbf{z}|=1}} \sum_{i,j} \left(X^{i,j}_{\mathbf{x},\mathbf{z}} \right)^2, \end{aligned}$$

where $\mathbf{e}_1, \ldots, \mathbf{e}_d$ is canonical basis of $\mathbb{Z}^d$.

Observe that this noise conserves the total momentum $\sum_{\mathbf{x}} \mathbf{p_x}$ and energy $\mathcal{H}_N$, i.e.

$$S \sum_{\mathbf{x}} \mathbf{p_x} = 0\,, \quad S\,\mathcal{H}_N = 0.$$

In dimension 1, in order to conserve total momentum and total kinetic energy, we have to consider a random exchange of momentum between three consecutive atoms (because if $d = 1$, $\mathbb{S}_{e,\mathbf{p}}$ has dimension 0), and we define

$$S = \frac{1}{6} \sum_{x \in \mathbb{Z}^d_N} (Y_x)^2,$$

where

$$Y_x = (p_x - p_{x+1})\partial_{p_{x-1}} + (p_{x+1} - p_{x-1})\partial_{p_x} + (p_{x-1} - p_x)\partial_{p_{x+1}}$$

which is vector field tangent to the surface of constant energy and momentum of the three particles involved.

The corresponding Fokker-Planck equation for the time evolution of the probability distribution $P(\mathbf{q}, \mathbf{p}, t)$, given an initial distribution $P(\mathbf{q}, \mathbf{p}, 0)$ is given by

$$\frac{\partial P}{\partial t} = (-A + \gamma S)P = L^* P, \tag{5}$$

where L^* is the adjoint of L with respect to the Lebesgue measure.

Let $\{w^{i,j}_{\mathbf{x},\mathbf{y}};\ \mathbf{x}, \mathbf{y} \in \mathbb{Z}^d_N;\ i, j = 1, \dots, d;\ |\mathbf{y} - \mathbf{x}| = 1\}$ be independent standard Wiener processes, such that $w^{i,j}_{\mathbf{x},\mathbf{y}} = w^{i,j}_{\mathbf{y},\mathbf{x}}$. Equation (5) corresponds to the law at time t of the solution of the following stochastic differential equations:

$$\begin{aligned} d\mathbf{q}_\mathbf{x} &= \mathbf{p}_\mathbf{x}\, dt, \\ d\mathbf{p}_\mathbf{x} &= -\partial_{\mathbf{q}_\mathbf{x}} \mathcal{H}_N\, dt + 2\gamma \Delta \mathbf{p}_\mathbf{x}\, dt \\ &\quad + \frac{\sqrt{\gamma}}{2\sqrt{d-1}} \sum_{\mathbf{z}:|\mathbf{z}-\mathbf{x}|=1} \sum_{i,j=1}^{d} \left(X^{i,j}_{\mathbf{x},\mathbf{z}} \mathbf{p}_\mathbf{x} \right) dw^{i,j}_{\mathbf{x},\mathbf{z}}(t). \end{aligned} \tag{6}$$

In $d = 1$ these are:

$$\begin{aligned} dp_x &= -\partial_{q_x} H_N\, dt + \frac{\gamma}{6} \Delta(4p_x + p_{x-1} + p_{x+1}) dt \\ &\quad + \sqrt{\frac{\gamma}{3}} \sum_{k=-1,0,1} (Y_{x+k}\, p_x)\, dw_{x+k}(t), \end{aligned} \tag{7}$$

where here $\{w_x(t), x = 1, \dots, N\}$ are independent standard Wiener processes.

Defining the energy of the atom $\mathbf{x}$ as

$$\mathcal{E}_\mathbf{x} = \frac{1}{2}\mathbf{p}_\mathbf{x}^2 + W(\mathbf{q}_\mathbf{x}) + \frac{1}{2} \sum_{\mathbf{y}:|\mathbf{y}-\mathbf{x}|=1} V(\mathbf{q}_\mathbf{y} - \mathbf{q}_\mathbf{x}),$$

the energy conservation law can be read locally as

$$\mathcal{E}_\mathbf{x}(t) - \mathcal{E}_\mathbf{x}(0) = \sum_{k=1}^{d} \left(J_{\mathbf{x}-\mathbf{e}_k,\mathbf{x}}([0, t]) - J_{\mathbf{x},\mathbf{x}+\mathbf{e}_k}([0, t]) \right),$$

where $J_{\mathbf{x},\mathbf{x}+\mathbf{e}_k}([0, t])$ is the total energy current between $\mathbf{x}$ and $\mathbf{x} + \mathbf{e}_k$ up to time t. This can be written as

$$J_{\mathbf{x},\mathbf{x}+\mathbf{e}_k}([0, t]) = \int_0^t j_{\mathbf{x},\mathbf{x}+\mathbf{e}_k}(s)\, ds + M_{\mathbf{x},\mathbf{x}+\mathbf{e}_k}(t). \tag{8}$$

In the above $M_{\mathbf{x},\mathbf{x}+\mathbf{e}_k}(t)$ are martingales that can be written explicitly as Itô stochastic integrals

$$M_{\mathbf{x},\mathbf{x}+\mathbf{e}_k}(t) = \sqrt{\frac{\gamma}{(d-1)}} \sum_{i,j} \int_0^t \left(X^{i,j}_{\mathbf{x},\mathbf{x}+\mathbf{e}_k} \mathcal{E}_{\mathbf{x}} \right)(s)\, dw^{i,j}_{\mathbf{x},\mathbf{x}+\mathbf{e}_k}(s). \tag{9}$$

In $d = 1$ these martingales are written explicitly as

$$M_{x,x+1}(t) = \sqrt{\frac{\gamma}{3}} \int_0^t \sum_{k=-1,0,1} (Y_{x+k}\mathcal{E}_x)\, dw_{x+k}(t). \tag{10}$$

The instantaneous energy currents $j_{\mathbf{x},\mathbf{x}+\mathbf{e}_k}$ satisfy the equation

$$L\mathcal{E}_{\mathbf{x}} = \sum_{k=1}^{d} \left(j_{\mathbf{x}-\mathbf{e}_k,\mathbf{x}} - j_{\mathbf{x},\mathbf{x}+\mathbf{e}_k} \right),$$

and it can be written as

$$j_{\mathbf{x},\mathbf{x}+\mathbf{e}_k} = j^a_{\mathbf{x},\mathbf{x}+\mathbf{e}_k} + \gamma j^s_{\mathbf{x},\mathbf{x}+\mathbf{e}_k} \quad . \tag{11}$$

The first term in (11) is the Hamiltonian contribution to the energy current

$$\begin{aligned} j^a_{\mathbf{x},\mathbf{x}+\mathbf{e}_k} &= -\frac{1}{2}(\nabla V)(\mathbf{q}_{\mathbf{x}+\mathbf{e}_k} - \mathbf{q}_{\mathbf{x}}) \cdot (\mathbf{p}_{\mathbf{x}+\mathbf{e}_k} + \mathbf{p}_{\mathbf{x}}) \\ &= -\frac{1}{2} \sum_{j=1}^{d} V'_j(q^j_{\mathbf{x}+\mathbf{e}_k} - q^j_{\mathbf{x}})(p^j_{\mathbf{x}+\mathbf{e}_k} + p^j_{\mathbf{x}}) \end{aligned} \tag{12}$$

while the noise contribution in $d \geq 2$ is

$$\gamma j^s_{\mathbf{x},\mathbf{x}+\mathbf{e}_k} = -\gamma(\nabla_{\mathbf{e}_k} \mathbf{p}^2)_{\mathbf{x}} \tag{13}$$

and in $d = 1$ is

$$\begin{aligned} \gamma j^s_{x,x+1} &= -\gamma \nabla \varphi(p_{x-1}, p_x, p_{x+1}), \\ \varphi(p_{x-1}, p_x, p_{x+1}) &= \frac{1}{6}[p^2_{x+1} + 4p^2_x + p^2_{x-1} + p_{x+1}p_{x-1} - 2p_{x+1}p_x - 2p_x p_{x-1}]. \end{aligned}$$

In the unpinned case ($W = 0$), given any values of $\mathcal{E} > 0$, the uniform probability measure on the constant energy-momentum shell

$$\Sigma_{N,\mathcal{E}} = \left\{ (\mathbf{p}, \mathbf{q}) : \mathcal{H}_N = N\mathcal{E},\ \sum_{\mathbf{x} \in \mathbb{Z}^d_N} \mathbf{p}_x = 0,\ \sum_{\mathbf{x} \in \mathbb{Z}^d_N} \mathbf{q}_{\mathbf{x}} = 0 \right\}$$

is stationary for the dynamics, and A and S are respectively antisymmetric and symmetric with respect to this measure. For the stochastic dynamics, we believe that these measures are also ergodic, i.e. total energy, total momentum and center of mass are the only conserved quantities. Notice that because of the periodic boundary conditions, no other conserved quantities associated to the distortion of the lattice exist. For example in $d = 1$ the total length of the chain $\sum_x (q_{x+1} - q_x)$ is automatically null.

In the pinned case, total momentum is not conserved, and the ergodic stationary measures are given by the uniform probability measures on the energy shells

$$\Sigma_{N,\mathcal{E}} = \{(\mathbf{p}, \mathbf{q}) : \mathcal{H}_N = N\mathcal{E}\}.$$

In both cases we refer to these measures as *microcanonical* Gibbs measures. We denote by $< \cdot >_{N,\mathcal{E}}$ the expectation with respect to these microcanonical measures.

We will also consider the dynamics starting from the canonical Gibbs measure $< \cdot >_{N,T}$ with temperature $T > 0$ defined on the phase space $(\mathbb{R}^{2d})^{\mathbb{Z}_N^d}$ by

$$< \cdot >_{N,T} = \frac{e^{-\mathcal{H}_N/T}}{Z_{N,T}} d\mathbf{q}\, d\mathbf{p}.$$

To avoid confusion between these measures we restrict the use of the subscript $\mathcal{E}$ for the microcanonical measure and the subscript T for the canonical measure.

3. Green-Kubo Formula and Statement of the Results

In the physical literature several variations of the Green-Kubo formula (3) can be found ([13,7]). As in (3), one can start with the infinite system and sum over all $\mathbf{x} \in \mathbb{Z}^d$. One can also start working with the finite system with periodic boundary conditions and sum over $\mathbf{x} \in \Lambda_N^d$, where Λ_N^d is a finite box of size N and take the thermodynamic limit $N \to \infty$ (before sending the time to infinity). In the finite case there is a choice of the equilibrium measure. If $< \cdot >$ is the canonical measure at temperature T, one refers to the derivation *à la* Kubo. If $< \cdot >$ is the microcanonical measure at energy $\mathcal{E}N^d$, one refers to the derivation *à la* Green. Because of the equivalence of ensembles one expects that these different definitions give all the same value of the conductivity, provided that temperature T and energy $\mathcal{E}$ are suitably related by the corresponding thermodynamis relation. Nevertheless a rigorous justification is absent in the literature.

In the sequel we will consider the microcanonical Green-Kubo formula (noted κ) and the canonical Green-Kubo formula (noted $\tilde{\kappa}$) starting from our finite system.

In the harmonic case we work out the microcanonical Green-Kubo version that we compute explicitly. Similar computations are valid (with less work) for the canonical version of the Green-Kubo formula and will give the same result. In the anharmonic case equivalence of ensembles is less developed and we deal only with the canonical version of the Green-Kubo formula.

The microcanonical Green-Kubo formula for the conductivity in the direction $\mathbf{e}_1$ is defined as the limit (when it exists)

$$\kappa^{1,1}(T) = \lim_{t\to\infty} \lim_{N\to\infty} \frac{1}{2T^2 t} \sum_{\mathbf{x}\in\mathbb{Z}_N^d} \mathbb{E}_{N,\mathcal{E}} \left[J_{\mathbf{x},\mathbf{x}+\mathbf{e}_1}([0,t])\, J_{0,\mathbf{e}_1}([0,t]) \right], \tag{14}$$

where $\mathbb{E}_{N,\mathcal{E}}$ is the expectation starting with the microcanonical distribution $< \cdot >_{N,\mathcal{E}}$, and the energy $\mathcal{E} = \mathcal{E}(T)$ is chosen such that it corresponds to the thermodynamic energy at temperature T (i.e. the average of the kinetic energy in the canonical measure). In the harmonic case $T = \mathcal{E}$.

Similarly the canonical version of the Green-Kubo formula is given by

$$\tilde{\kappa}^{1,1}(T) = \lim_{t\to\infty} \lim_{N\to\infty} \frac{1}{2T^2 t} \sum_{\mathbf{x}\in\mathbb{Z}_N^d} \mathbb{E}_{N,T}\left[J_{\mathbf{x},\mathbf{x}+\mathbf{e}_1}([0,t]) J_{0,\mathbf{e}_1}([0,t]) \right] \tag{15}$$

when this limit exists. Here $\mathbb{E}_{N,T}$ indicates the expectation with respect to the equilibrium dynamics starting with the canonical measure $<\cdot>_{N,T}$ at temperature T. These definitions are consistent with (2)–(3) as we show at the end of this section.

Our first results concern the (α, ν)*-harmonic case*:

$$V_j(r) = \alpha r^2, \quad W_j(q) = \nu q^2, \quad \alpha > 0, \quad \nu \geq 0. \tag{16}$$

Theorem 1. *In the* (α, ν)*-harmonic case (16), the limits defining* $\kappa^{1,1}$ *and* $\tilde{\kappa}^{1,1}$ *exist. They are finite if* $d \geq 3$ *or if the on-site harmonic potential is present* ($\nu > 0$)*, and are infinite in the other cases. When finite,* $\kappa(T)$ *and* $\tilde{\kappa}(T)$ *are independent of* T*, coincide and the following formula holds:*

$$\tilde{\kappa}^{1,1}(T) = \kappa^{1,1}(T) = \frac{1}{8\pi^2 d\gamma} \int_{[0,1]^d} \frac{(\partial_{\mathbf{k}^1}\omega)^2(\mathbf{k})}{\psi(\mathbf{k})} d\mathbf{k} + \frac{\gamma}{d}, \tag{17}$$

where $\omega(\mathbf{k})$ *is the dispertion relation*

$$\omega(\mathbf{k}) = \left(\nu + 4\alpha \sum_{j=1}^{d} \sin^2(\pi \mathbf{k}^j) \right)^{1/2} \tag{18}$$

and

$$\psi(\mathbf{k}) = \begin{cases} 8\sum_{j=1}^d \sin^2(\pi\mathbf{k}^j), & \text{if} \quad d \geq 2 \\ 4/3 \ \sin^2(\pi\mathbf{k})(1 + 2\cos^2(\pi\mathbf{k})), & \text{if} \quad d = 1. \end{cases} \tag{19}$$

Consequently in the unpinned harmonic cases in dimension $d = 1$ and 2, the conductivity of our model diverges. In order to understand the nature of this divergence we define the (microcanonical) conductivity of the finite system of size N as

$$\kappa_N^{1,1}(T) = \frac{1}{2T^2 t_N} \frac{1}{N^d} \mathbb{E}_{N,\mathcal{E}} \left(\left[\sum_{\mathbf{x}\in\mathbb{Z}_N^d} J_{\mathbf{x},\mathbf{x}+\mathbf{e}_1}([0,t_N]) \right]^2 \right), \tag{20}$$

where $t_N = N/v_s$ with $v_s = \lim_{\mathbf{k}\to 0} |\partial_{k_1}\omega(\mathbf{k})| = 2\alpha^{1/2}$ the sound velocity. This definition of the conductivity of the finite system is motivated by the following consideration: $\nabla_k \omega(\mathbf{k})$ is the group velocity of the $\mathbf{k}$-mode waves, and typically v_s is an upper bound for these velocities. Consequently t_N is the typical time a low $\mathbf{k}$ (acoustic) mode takes to cross around the system once. One defines similarly $\tilde{\kappa}_N^{1,1}(T)$ by

$$\tilde{\kappa}_N^{1,1}(T) = \frac{1}{2T^2 t_N} \frac{1}{N^d} \mathbb{E}_{N,T} \left(\left[\sum_{\mathbf{x}\in\mathbb{Z}_N^d} J_{\mathbf{x},\mathbf{x}+\mathbf{e}_1}([0,t_N]) \right]^2 \right). \tag{21}$$

We conjecture that κ_N (resp. $\tilde{\kappa}_N$) has the same asymptotic behavior as the conductivity defined in the non-equilibrium stationary state on the open system with thermostats at the boundary at different temperature, as defined in eg. [3,6,15].

With these definitions we have the following theorem:

Theorem 2. *In the harmonic case, if $W = 0$:*

(1) $\kappa_N \sim N^{1/2}$ *if* $d = 1$,
(2) $\kappa_N \sim \log N$ *if* $d = 2$.

In all other cases κ_N is bounded in N and converges to κ. Same results are valid for $\tilde{\kappa}_N$.

In fact we show that, in the harmonic case, we have

$$\lim_{N\to\infty} \frac{\tilde{\kappa}_N^{1,1}(T)}{\kappa_N^{1,1}(T)} = 1. \tag{22}$$

This is a consequence of Eq. (51) that one can easily check is also valid if the microcanonical measure is replaced by the canonical measure.

In the anharmonic case we cannot prove the existence of either $\tilde{\kappa}^{1,1}(T)$ or $\kappa^{1,1}(T)$, but we can establish upper bounds for the canonical version of the finite size Green-Kubo formula (21). Extra assumptions on the potentials V and W assuring a uniform control on the canonical static correlations (see (86–89)) have to be done. In the unpinned case $W = 0$, (89) is valid as soon as V is strictly convex. In the pinned case $W > 0$, (86) is "morally" valid as soon as the infinite volume Gibbs measure is unique. Exact assumptions are given in [4], Theorem 3.1 and Theorem 3.2. In the sequel, "the general anharmonic case" will refer to potentials V and W such that (86) (or (89)) is valid.

Theorem 3. *Consider the general anharmonic case. There exists a constant C (depending on the temperature T) such that*

- *For $d \geq 3$,*
  (1) *either $W > 0$ is general*
  (2) *or if $W = 0$ and $0 < c_- \leq V_j'' \leq C_+ < \infty$ for any j, then*

$$\tilde{\kappa}_N^{1,1}(T) \leq C.$$

- *For $d = 2$, if $W = 0$ and $0 < c_- \leq V_j'' \leq C_+ < \infty$ for any j, then*

$$\tilde{\kappa}_N^{1,1}(T) \leq C(\log N)^2.$$

- *For $d = 1$, if $W = 0$ and $0 < c_- \leq V'' \leq C_+ < \infty$, then*

$$\tilde{\kappa}_N^{1,1}(T) \leq C\sqrt{N}.$$

- *Moreover, in any dimension, if V_j are quadratic and $W > 0$ is general then $\tilde{\kappa}_N^{1,1}(T) \leq C$.*

The proof of this statement is in Sect. 6.

We now relate the definition of the Green-Kubo (14) and (15) to the variance of the energy-energy correlations function (2).

Consider the infinite volume dynamics on $\mathbb{Z}^d$ under the infinite volume canonical Gibbs measure with temperature $T > 0$. The expectation is denoted by $\mathbb{E}_T$. Fix $t > 0$ and assume that the following sum makes sense:

$$D_T^{i,j}(t) = \sum_{\mathbf{x}\in\mathbb{Z}^d} \mathbf{x}^i \mathbf{x}^j \mathbb{E}_T\left[\,(\mathcal{E}_{\mathbf{x}}(t) - T)(\mathcal{E}_0(0) - T)\,\right] = \sum_{\mathbf{x}\in\mathbb{Z}^d} \mathbf{x}^i \mathbf{x}^j S(\mathbf{x}, t). \tag{23}$$

If $\mathbf{x} \neq 0$, by space and time invariance of the dynamics, we have

$$\mathbb{E}_T\left[(\mathcal{E}_{\mathbf{x}}(t) - T)(\mathcal{E}_0(0) - T)\right] = -\frac{1}{2}\mathbb{E}_T\left[\,(\mathcal{E}_{\mathbf{x}}(t) - \mathcal{E}_{\mathbf{x}}(0))\,(\mathcal{E}_0(t) - \mathcal{E}_0(0))\,\right]. \tag{24}$$

By definition of the current, we have for any $\mathbf{y} \in \mathbb{Z}^d$:

$$\mathcal{E}_{\mathbf{y}}(t) - \mathcal{E}_{\mathbf{y}}(0) = \sum_{k=1}^{d} \left(J_{\mathbf{y}-\mathbf{e}_k,\mathbf{y}}([0,t]) - J_{\mathbf{y},\mathbf{y}+\mathbf{e}_k}([0,t])\right). \tag{25}$$

By two discrete integration by parts one obtains

$$D_T^{i,j}(t) = \sum_{\mathbf{x}\in\mathbb{Z}^d} \mathbb{E}_T\left[J_{\mathbf{x},\mathbf{x}+\mathbf{e}_i}([0,t])\, J_{0,\mathbf{e}_j}([0,t])\right] \tag{26}$$

so that the thermal conductivity is equal to the space-time correlations of the total current

$$\kappa^{i,j}(T) = \delta_0(i-j) \lim_{t\to\infty} \frac{1}{2T^2 t} \sum_{\mathbf{x}\in\mathbb{Z}^d} \mathbb{E}_T\left[J_{\mathbf{x},\mathbf{x}+\mathbf{e}_i}([0,t])\, J_{0,\mathbf{e}_j}([0,t])\right]. \tag{27}$$

Of course this derivation is only formal even for fixed time $t > 0$. The problem is to define the infinite volume dynamics and to show $S(\mathbf{x}, t)$ has a sufficiently fast decay in $\mathbf{x}$. For the purely Hamiltonian dynamics, it is a challenging problem. For the stochastic dynamics it seems less difficult but remains technical. To avoid these difficulties we adopt a finite volume limit procedure starting from (3). This explains the definitions (14) and (15).

Consider now the closed dynamics on $\mathbb{Z}_N^d$ starting from the microcanonical state. The rest of the section is devoted to the proof of the following formula:

$$\begin{aligned}\frac{1}{2T^2 t}\frac{1}{N^d}\mathbb{E}_{N,\mathcal{E}}&\left(\left[\sum_{\mathbf{x}\in\mathbb{Z}_N^d} J_{\mathbf{x},\mathbf{x}+\mathbf{e}_1}([0,t])\right]^2\right)\\ &= (2T^2 t N^d)^{-1}\mathbb{E}_{N,\mathcal{E}}\left(\left[\sum_{\mathbf{x}\in\mathbb{Z}_N^d}\int_0^t j^a_{\mathbf{x},\mathbf{x}+\mathbf{e}_1}(s)ds\right]^2\right) + \frac{\gamma}{d} + \frac{O_N}{N^d},\end{aligned} \tag{28}$$

and an identical formula in the canonical case (with $\mathbb{E}_{N,\mathcal{E}}$ substituted by $\mathbb{E}_{N,T}$).

The term γ/d in (28) is the direct contribution of the stochastic dynamics to the thermal conductivity. In the microcaconical case we actually prove that is equal to

γ/d only for the harmonic case. A complete proof of (28) for anharmonic interaction demands an extension of the equivalence of ensembles estimates proven in Sect. 7. In the grancanonical case this problem does not appear.

Starting in the microcanonical case, remark that the first term on the RHS of (28) can be written as

$$(2T^2tN^d)^{-1}\mathbb{E}_{N,\mathcal{E}}\left(\left[\sum_{\mathbf{x}\in\mathbb{Z}_N^d}\int_0^t j^a_{\mathbf{x},\mathbf{x}+\mathbf{e}_1}(s)ds\right]^2\right)$$

$$=\frac{1}{T^2}\int_0^\infty\left(1-\frac{s}{t}\right)^+\sum_{\mathbf{x}\in\mathbb{Z}_N^d}\mathbb{E}_{N,\mathcal{E}}\left(j^a_{\mathbf{x},\mathbf{x}+\mathbf{e}_1}(s)j^a_{0,\mathbf{e}_1}(0)\right)ds. \tag{29}$$

If $\gamma = 0$, which corresponds to the purely Hamiltonian system, as N and then t goes to infinity, and if one can prove that the current-current correlation function has a sufficiently fast decay, then one recovers the usual Green-Kubo formula (3).

To prove (29) one uses space and time translation invariance of the dynamics

$$(2T^2tN^d)^{-1}\mathbb{E}_{N,\mathcal{E}}\left(\left[\sum_{\mathbf{x}}\int_0^t j^a_{\mathbf{x},\mathbf{x}+\mathbf{e}_1}(s)ds\right]^2\right)$$

$$=(2T^2tN^d)^{-1}\sum_{\mathbf{x},\mathbf{y}}\int_0^t ds\int_0^t du\ \mathbb{E}_{N,\mathcal{E}}\left(j^a_{\mathbf{x},\mathbf{x}+\mathbf{e}_1}(s)\ j^a_{\mathbf{y},\mathbf{y}+\mathbf{e}_1}(u)\right)$$

$$=(T^2tN^d)^{-1}\sum_{\mathbf{x},\mathbf{y}}\int_0^t ds\int_0^s du\ \mathbb{E}_{N,\mathcal{E}}\left(j^a_{\mathbf{x},\mathbf{x}+\mathbf{e}_1}(s)\ j^a_{\mathbf{y},\mathbf{y}+\mathbf{e}_1}(u)\right)$$

$$=(T^2tN^d)^{-1}\sum_{\mathbf{x},\mathbf{y}}\int_0^t ds\int_0^s du\ \mathbb{E}_{N,\mathcal{E}}\left(j^a_{\mathbf{x}-\mathbf{y},\mathbf{x}-\mathbf{y}+\mathbf{e}_1}(s-u)\ j^a_{0,\mathbf{e}_1}(0)\right)$$

$$=\frac{1}{T^2}\int_0^\infty\left(1-\frac{s}{t}\right)^+\sum_{x}\mathbb{E}_{N,\mathcal{E}}\left(j^a_{\mathbf{x},\mathbf{x}+\mathbf{e}_1}(s)j^a_{0,\mathbf{e}_1}(0)\right)ds.$$

We now give the proof of (28). Because of the periodic boundary conditions, since j^s if a *gradient* (cf. (13)), the corresponding terms cancel, and we can write

$$\sum_{\mathbf{x}}J_{\mathbf{x},\mathbf{x}+\mathbf{e}_1}([0,t])=\int_0^t\sum_{\mathbf{x}}j^a_{\mathbf{x},\mathbf{x}+\mathbf{e}_1}(s)\ ds+\sum_{\mathbf{x}}M_{\mathbf{x},\mathbf{x}+\mathbf{e}_1}(t)$$

$$=\int_0^t\mathfrak{J}_{\mathbf{e}_1}(s)\ ds+\mathfrak{M}_{\mathbf{e}_1}(t) \tag{30}$$

so that

$$
\begin{aligned}
&(tN^d)^{-1}\mathbb{E}_{N,\mathcal{E}}\left(\left[\sum_{\mathbf{x}} J_{\mathbf{x},\mathbf{x}+\mathbf{e}_1}([0,t])\right]^2\right)\\
&\quad = (tN^d)^{-1}\mathbb{E}_{N,\mathcal{E}}\left(\left[\int_0^t \mathfrak{J}_{\mathbf{e}_1}(s)ds\right]^2\right) + (tN^d)^{-1}\mathbb{E}_{N,\mathcal{E}}\left(\mathfrak{M}^2_{\mathbf{e}_1}(t)\right)\\
&\quad\quad +2(tN^d)^{-1}\mathbb{E}_{N,\mathcal{E}}\left(\left[\int_0^t \mathfrak{J}_{\mathbf{e}_1}(s)\, ds\right]\mathfrak{M}_{\mathbf{e}_1}(t)\right).
\end{aligned}
\tag{31}
$$

The third term on the RHS of (31) is shown to be zero by a time reversal argument and the second term on the RHS of (31) gives in the limit a contribution equal to γ/d.

To see the first claim let us denote by $\{\omega(s)\}_{0\le s\le t}$ the process $\{(\mathbf{p}_{\mathbf{x}}(s), \mathbf{q}_{\mathbf{x}}(s));\ \mathbf{x} \in \mathbb{Z}_N^d,\ 0 \le s \le t\}$ arising in (6) or in (7) for the one-dimensional case. The reversed process $\{\omega^*_s\}_{0\le s\le t}$ is defined as $\omega^*_s = \omega_{t-s}$. Under the microcanonical measure, the time reversed process is still Markov with generator $-A+\gamma S$. The total current $J_t(\omega_\cdot) = \sum_{\mathbf{x}} J_{\mathbf{x},\mathbf{x}+\mathbf{e}_1}([0,t])$ is a functional of $\{\omega_s\}_{0\le s\le t}$. By (6–7), we have in fact that $J_t(\cdot)$ is an anti-symmetric functional of $\{\omega_s\}_{0\le s\le t}$, meaning

$$
J_t(\{\omega^*_s\}_{0\le s\le t}) = -J_t(\{\omega_s\}_{0\le s\le t}).
\tag{32}
$$

In fact, similarly to (8), we have

$$
J_s(\omega^*_\cdot) = \int_0^s (\mathfrak{J}_{\mathbf{e}_1})^*(\omega^*(v))dv + \mathfrak{M}^*_{\mathbf{e}_1}(s), \quad 0 \le s \le t,
\tag{33}
$$

where $(\mathfrak{M}^*_{\mathbf{e}_1}(s))_{0\le s\le t}$ is a martingale with respect to the natural filtration of $(\omega^*_s)_{0\le s\le t}$ and $(\mathfrak{J}_{\mathbf{e}_1})^* = \sum_{\mathbf{x}} (j^a)^*_{\mathbf{x},\mathbf{x}+\mathbf{e}_1}$ is equal to $-\mathfrak{J}_{\mathbf{e}_1} = -\sum_{\mathbf{x}} j^a_{\mathbf{x},\mathbf{x}+\mathbf{e}_1}$.

We have then by time reversal

$$
\begin{aligned}
\mathbb{E}_{N,\mathcal{E}}[J_t(\omega_\cdot)\mathfrak{J}_{\mathbf{e}_1}(\omega(t))] &= -\mathbb{E}_{N,\mathcal{E}}[J_t(\omega^*_\cdot)\mathfrak{J}_{\mathbf{e}_1}(\omega^*(0))]\\
&= -\mathbb{E}_{N,\mathcal{E}}\left[\left(\int_0^t (\mathfrak{J}_{\mathbf{e}_1})^*(\omega^*(s))ds + \mathfrak{M}^*(t)\right)\mathfrak{J}_{\mathbf{e}_1}(\omega^*(0))\right]\\
&= -\mathbb{E}_{N,\mathcal{E}}\left[\left(\int_0^t {\mathfrak{J}_{\mathbf{e}_1}}^*(\omega^*(s))ds\right)\mathfrak{J}_{\mathbf{e}_1}(\omega^*(0))\right],
\end{aligned}
\tag{34}
$$

where the last equality follows from the martingale property of $\mathfrak{M}^*$. Recall now that $(\mathfrak{J}_{\mathbf{e}_1})^* = -\mathfrak{J}_{\mathbf{e}_1}$. By variables change $s \to t-s$ in the time integral, we get

$$
\mathbb{E}_{N,\mathcal{E}}[J_t(\omega_\cdot)\mathfrak{J}_{\mathbf{e}_1}(\omega(t))] = \mathbb{E}_{N,\mathcal{E}}\left[\left(\int_0^t \mathfrak{J}_{\mathbf{e}_1}(\omega(s))ds\right)\mathfrak{J}_{\mathbf{e}_1}(\omega(t))\right].
\tag{35}
$$

It follows that

$$\mathbb{E}_{N,\mathcal{E}}\left[\left(\int_0^t \mathfrak{J}_{\mathbf{e}_1}(\omega(s))ds\right)\mathfrak{M}_{\mathbf{e}_1}(t)\right] = \mathbb{E}_{N,\mathcal{E}}\left[\int_0^t \mathfrak{J}_{\mathbf{e}_1}(\omega(s))\mathfrak{M}_{\mathbf{e}_1}(s)ds\right]$$
$$= \int_0^t ds\ \mathbb{E}_{N,\mathcal{E}}\left[\mathfrak{J}_{\mathbf{e}_1}(\omega(s))\left(J_s(\omega.) - \int_0^s \mathfrak{J}_{\mathbf{e}_1}(\omega(v))dv\right)\right]. = 0 \tag{36}$$

For the second term on the RHS of (31) we have

$$(tN^d)^{-1}\mathbb{E}_{N,\mathcal{E}}\left(\mathfrak{M}^2_{\mathbf{e}_1}(t)\right) = \frac{\gamma}{(d-1)N^d}\sum_{\mathbf{x}}\sum_{i,j}\left\langle\left(X^{i,j}_{\mathbf{x},\mathbf{x}+\mathbf{e}_1}(\mathbf{p}^2_{\mathbf{x}}/2)\right)^2\right\rangle_{N,\mathcal{E}}$$
$$= \frac{\gamma}{(d-1)N^d}\sum_{\mathbf{x}}\sum_{i\neq j}\left\langle\left(p^j_{\mathbf{x}}p^i_{\mathbf{x}+\mathbf{e}_1} - p^i_{\mathbf{x}}p^j_{\mathbf{x}+\mathbf{e}_1}\right)^2\right\rangle_{N,\mathcal{E}}$$
$$= \frac{2\gamma}{(d-1)N^d}\sum_{\mathbf{x}}\sum_{i\neq j}\left\langle(p^j_{\mathbf{x}}p^i_{\mathbf{x}+\mathbf{e}_1})^2\right\rangle_{N,\mathcal{E}}$$
$$-\frac{2\gamma}{(d-1)N^d}\sum_{\mathbf{x}}\sum_{i\neq j}\left\langle(p^i_{\mathbf{x}}p^i_{\mathbf{x}+\mathbf{e}_1}p^j_{\mathbf{x}}p^j_{\mathbf{x}+\mathbf{e}_1})\right\rangle_{N,\mathcal{E}}.$$

Thanks to the equivalence of ensembles (cf. Lemma 7), this last quantity is equal to

$$2\gamma\frac{T^2}{d} + N^{-d}O_N, \tag{37}$$

where O_N remains bounded as $N \to \infty$. The calculation in $d = 1$ is similar. The contribution of the martingale term for the conductivity is hence γ/d and we have shown (28). Notice this is the only point where we have used the equivalence of ensembles results of Sect. 7 that we have proven only in the harmonic case. We conjecture these are true also for the anharmonic cases.

Observe that all the arguments above between (30) and (37) apply directly also to the canonical definition of the Green-Kubo but without the small error in N (because for the canonical measure momentums $\mathbf{p_x}$ are independently distributed and the equivalence of ensembles approximations are in fact equalities). Therefore we have the similar formula to (28):

$$\frac{1}{2T^2t}\sum_{\mathbf{x}}\mathbb{E}_{N,T}\left(J_{\mathbf{x},\mathbf{x}+\mathbf{e}_1}([0,t])J_{0,\mathbf{e}_1}([0,t])\right)$$
$$= (2T^2N^dt)^{-1}\mathbb{E}_{N,T}\left(\left[\sum_{\mathbf{x}}\int_0^t j^a_{\mathbf{x},\mathbf{x}+\mathbf{e}_1}(s)ds\right]^2\right) + \frac{\gamma}{d}. \tag{38}$$

In the next sections we will consider the (α, ν)-harmonic case and we will compute explicitly the limit (as $N \to \infty$ and then $t \to \infty$) of the two first term on the RHS of (31).

4. Correlation Function of the Energy Current in the Harmonic Case

We consider the (α, ν)-harmonic case (16). We recall that $\mathfrak{J}_{\mathbf{e}_1} = \sum_{\mathbf{x}} j_{\mathbf{x},\mathbf{x}+\mathbf{e}_1}$. Because of the periodic boundary conditions, and being $j^s_{\mathbf{x},\mathbf{x}+\mathbf{e}_1}$ a spatial gradient (cf. (13)), we have that $\mathfrak{J}_{\mathbf{e}_1} = \sum_{\mathbf{x}} j^a_{\mathbf{x},\mathbf{x}+\mathbf{e}_1}$. We are interested in the decay of the correlation function:

$$C_{1,1}(t) = \lim_{N\to\infty} \frac{1}{N^d} \mathbb{E}_{N,\mathcal{E}}(\mathfrak{J}_{\mathbf{e}_1}(t)\mathfrak{J}_{\mathbf{e}_1}(0)) = \lim_{N\to\infty} \sum_{\mathbf{x}} \mathbb{E}_{N,\mathcal{E}}(j^a_{0,\mathbf{e}_1}(0) j^a_{\mathbf{x},\mathbf{x}+\mathbf{e}_1}(t)), \quad (39)$$

where $\mathbb{E}_{N,\mathcal{E}}$ is the expectation starting with the microcanonical distribution defined above.

For $\lambda > 0$, let $u_{\lambda,N}$ be the solution of the Poisson equation

$$\lambda u_{\lambda,N} - L u_{\lambda,N} = -\sum_{\mathbf{x}} j^a_{\mathbf{x},\mathbf{x}+\mathbf{e}_1}$$

given explicitly in Lemma 2 of Sect. 5. By Lemma 1, we can write the Laplace transform of $C_{1,1}(t)$ as

$$\int_0^\infty dt e^{-\lambda t} C_{1,1}(t)\, dt = \lim_{N\to\infty} \left\langle j^a_{0,\mathbf{e}_1} u_{\lambda,N} \right\rangle_{N,\mathcal{E}}. \quad (40)$$

Substituting in (40) the explicit form of $u_{\lambda,N}$ given in Lemma 2, we have:

$$\begin{aligned} -\left\langle j^a_{0,\mathbf{e}_1} u_{\lambda,N} \right\rangle_{N,\mathcal{E}} &= \frac{\alpha^2}{2\gamma} \sum_{\mathbf{x},\mathbf{y}} g_{\lambda,N}(\mathbf{x}-\mathbf{y}) \left\langle (\mathbf{q}_{\mathbf{e}_1} - \mathbf{q}_0)\cdot(\mathbf{p}_{\mathbf{e}_1} + \mathbf{p}_0)(\mathbf{p}_{\mathbf{x}}\cdot\mathbf{q}_{\mathbf{y}}) \right\rangle_{N,\mathcal{E}} \\ &= \frac{\alpha^2}{2\gamma} \sum_{\mathbf{x},\mathbf{y}} g_{\lambda,N}(\mathbf{x}-\mathbf{y}) \left\langle (\mathbf{q}_{\mathbf{e}_1}\cdot\mathbf{p}_0 - \mathbf{q}_0\cdot\mathbf{p}_{\mathbf{e}_1})(\mathbf{p}_{\mathbf{x}}\cdot\mathbf{q}_{\mathbf{y}}) \right\rangle_{N,\mathcal{E}} \\ &\quad + \frac{\alpha^2}{2\gamma} \sum_{\mathbf{x},\mathbf{y}} g_{\lambda,N}(\mathbf{x}-\mathbf{y}) \left\langle (\mathbf{q}_{\mathbf{e}_1}\cdot\mathbf{p}_{\mathbf{e}_1} - \mathbf{q}_0\cdot\mathbf{p}_0)(\mathbf{p}_{\mathbf{x}}\cdot\mathbf{q}_{\mathbf{y}}) \right\rangle_{N,\mathcal{E}}. \end{aligned} \quad (41)$$

Observe that the last term on the RHS of (41) is null by the translation invariance property. So we have (using again the translation invariance and the antisymmetry of $g_{\lambda,N}$)

$$-\left\langle j^a_{0,\mathbf{e}_1} u_{\lambda,N} \right\rangle_{N,e} = \frac{\alpha^2}{2\gamma} \sum_{\mathbf{x},\mathbf{y}} g_{\lambda,N}(\mathbf{x}-\mathbf{y}) \left\langle (\mathbf{q}_{\mathbf{e}_1} - \mathbf{q}_{-\mathbf{e}_1})\cdot\mathbf{p}_0)(\mathbf{p}_{\mathbf{x}}\cdot\mathbf{q}_{\mathbf{y}}) \right\rangle_{N,e}.$$

Define

$$K_N(\mathbf{q}) = N^d \mathcal{E} - \frac{1}{2} \sum_{\mathbf{x}} \mathbf{q}_{\mathbf{x}} \cdot (\nu I - \alpha\Delta)\mathbf{q}_{\mathbf{x}}.$$

In the unpinned case $\nu = 0$, conditionally to the positions configuration $\mathbf{q}$, the law of $\mathbf{p}$ is $\mu_{\mathbf{q}} = \mu^{N^d}_{\sqrt{2K_N(\mathbf{q})}}$ (defined in Lemma 6), meaning the uniform measure on the surface

$$\left\{ (\mathbf{p}_{\mathbf{x}})_{\mathbf{x}\in\mathbb{Z}^d_N};\quad \frac{1}{2}\sum_{\mathbf{x}} \mathbf{p}^2_{\mathbf{x}} = K_N(\mathbf{q});\quad \sum_{\mathbf{x}} \mathbf{p}_{\mathbf{x}} = 0 \right\}.$$

By using properties (i),(ii) and (iii) of Lemma 6, one has for $\mathbf{x} \neq 0$,

$$\begin{aligned}\left\langle ((\mathbf{q}_{\mathbf{e}_1} - \mathbf{q}_{\mathbf{e}_1}) \cdot \mathbf{p}_0)(\mathbf{p}_{\mathbf{x}} \cdot \mathbf{q}_{\mathbf{y}}) \right\rangle_{N,\mathcal{E}} &= \sum_{i,j} \left\langle \mu_{\mathbf{q}} \left(p_0^i p_{\mathbf{x}}^j \right) (q_{\mathbf{e}_1}^i - q_{-\mathbf{e}_1}^i) q_{\mathbf{y}}^j \right\rangle_{N,\mathcal{E}} \\ &= \sum_{i} \left\langle \mu_{\mathbf{q}} \left(p_0^i p_{\mathbf{x}}^i \right) (q_{\mathbf{e}_1}^i - q_{-\mathbf{e}_1}^i) q_{\mathbf{y}}^i \right\rangle_{N,\mathcal{E}} \\ &= -\sum_{i=1}^{d} \left\langle \frac{2K_N(\mathbf{q})}{dN^d(N^d-1)} (q_{\mathbf{e}_1}^i - q_{-\mathbf{e}_1}^i) q_{\mathbf{y}}^i \right\rangle_{N,\mathcal{E}} \\ &= -\frac{1}{N^d-1} \sum_{i=1}^{d} \left\langle (p_0^i)^2 (q_{\mathbf{e}_1}^i - q_{-\mathbf{e}_1}^i) q_{\mathbf{y}}^i \right\rangle_{N,\mathcal{E}}. \end{aligned} \tag{42}$$

For $\mathbf{x} = 0$, one gets

$$\begin{aligned}\left\langle ((\mathbf{q}_{\mathbf{e}_1} - \mathbf{q}_{\mathbf{e}_1}) \cdot \mathbf{p}_0)(\mathbf{p}_0 \cdot \mathbf{q}_{\mathbf{y}}) \right\rangle_{N,\mathcal{E}} &= \sum_{i,j} \left\langle \mu_{\mathbf{q}} \left(p_0^i p_0^j \right) (q_{\mathbf{e}_1}^i - q_{-\mathbf{e}_1}^i) q_{\mathbf{y}}^j \right\rangle_{N,\mathcal{E}} \\ &= \sum_{i=1}^{d} \left\langle \mu_{\mathbf{q}} \left(p_0^i p_0^i \right) (q_{\mathbf{e}_1}^i - q_{-\mathbf{e}_1}^i) q_{\mathbf{y}}^i \right\rangle_{N,\mathcal{E}} \\ &= \sum_{i=1}^{d} \left\langle \left(p_0^i \right)^2 (q_{\mathbf{e}_1}^i - q_{-\mathbf{e}_1}^i) q_{\mathbf{y}}^i \right\rangle_{N,\mathcal{E}}. \end{aligned} \tag{43}$$

In the pinned case $\nu > 0$, conditionally to the positions configuration $\mathbf{q}$, the law of $\mathbf{p}$ is $\lambda_{\mathbf{q}} = \lambda^{N^d}_{\sqrt{2K_N(\mathbf{q})}}$ (defined in Lemma 5), meaning the uniform measure on the surface

$$\left\{ (\mathbf{p}_{\mathbf{x}})_{\mathbf{x} \in \mathbb{Z}_N^d}; \quad \frac{1}{2} \sum_{\mathbf{x}} \mathbf{p}_{\mathbf{x}}^2 = K_N(\mathbf{q}) \right\}.$$

We proceed in a similar way and we observe that if $\mathbf{x} \neq 0$, $\lambda_{\mathbf{q}}(p_0^i p_{\mathbf{x}}^i) = 0$ (cf. ii) of Lemma 5)

Since $g_{\lambda,N}$ is antisymmetric (see (64–65)) and such that $\sum_{\mathbf{z}} g_{\lambda,N}(\mathbf{z}) = 0$, one obtains easily in both cases (pinned and unpinned)

$$\begin{aligned} -\left\langle j_{0,\mathbf{e}_1}^a u_{\lambda,N} \right\rangle_{N,e} &= -\frac{\alpha^2}{2\gamma} \sum_{\mathbf{y}} g_{\lambda,N}(\mathbf{y}) \sum_i \left\langle \left(p_0^i \right)^2 (q_{\mathbf{e}_1}^i - q_{-\mathbf{e}_1}^i) q_{\mathbf{y}}^i \right\rangle_{N,\mathcal{E}} \\ &\quad + \frac{\alpha^2}{2\gamma} \frac{\mathbf{1}_{\nu=\mathbf{0}}}{N^d-1} \sum_{\mathbf{x} \neq 0, \mathbf{y}} g_{\lambda,N}(\mathbf{y}-\mathbf{x}) \sum_i \left\langle \left(p_0^i \right)^2 (q_{\mathbf{e}_1}^i - q_{-\mathbf{e}_1}^i) q_{\mathbf{y}}^i \right\rangle_{N,\mathcal{E}} \\ &= -\left(1 + \frac{\mathbf{1}_{\nu=0}}{N^d-1} \right) \frac{\alpha^2}{2\gamma} \sum_{\mathbf{y}} g_{\lambda,N}(\mathbf{y}) \sum_i \left\langle \left(p_0^i \right)^2 (q_{\mathbf{e}_1}^i - q_{-\mathbf{e}_1}^i) q_{\mathbf{y}}^i \right\rangle_{N,\mathcal{E}}. \end{aligned} \tag{44}$$

Let $\Gamma_N(\mathbf{x})$, $\mathbf{x} \in \mathbb{Z}_N^d$, be the unique solution of

$$(\nu I - \alpha \Delta) \Gamma_N = \delta_{\mathbf{e}_1} - \delta_{-\mathbf{e}_1} \tag{45}$$

such that $\sum_{\mathbf{x} \in \mathbb{Z}_N^d} \Gamma_N(\mathbf{x}) = 0$.

By (iii) of Lemma 7 and (77), we have

$$\left| -\left\langle j^a_{0,\mathbf{e}_1} u_{\lambda,N} \right\rangle_{N,\mathcal{E}} - \left(1 + \frac{\mathbf{1}_{\nu=0}}{N^d - 1}\right) \frac{\alpha^2 \mathcal{E}^2}{2\gamma d} \sum_{\mathbf{y}} g_{\lambda,N}(\mathbf{y}) \Gamma_N(\mathbf{y}) \right|$$
$$\leq \frac{C \log N}{N^d} \sum_{\mathbf{y}} \left| g_{\lambda,N}(\mathbf{y}) \right| \leq \frac{C \log N}{N^{d/2}} \left(\sum_{\mathbf{x}} (g_{\lambda,N}(\mathbf{x}))^2 \right)^{1/2} \leq \frac{C' \log N}{\lambda N^{d/2}}. \quad (46)$$

Hence the last term of (46) goes to 0.

Taking the limit as $N \to \infty$ we obtain (see (80))

$$\int_0^\infty e^{-\lambda t} C_{1,1}(t)\, dt = \frac{\alpha^2 \mathcal{E}^2}{2d\gamma} \sum_{\mathbf{z}} g_\lambda(\mathbf{z}) \Gamma(z), \quad (47)$$

where g_λ are solutions of the same equations as $g_{\lambda,N}$ but on $\mathbb{Z}^d$ and Γ is the solution of the same equation as Γ_N but on $\mathbb{Z}^d$.

Using Parseval relation and the explicit form of the Fourier transform of g_λ (cf. (74)) and Γ, one gets the following formula for the Laplace transform of $C_{1,1}(t)$ for $d \geq 2$:

$$\frac{\alpha^2 \mathcal{E}^2}{d} \int_{[0,1]^d} d\mathbf{k} \left(\frac{\sin^2(2\pi \mathbf{k}^1)}{\nu + 4\alpha \sum_{j=1}^d \sin^2(\pi \mathbf{k}^j)} \right) \frac{1}{\lambda + 8\gamma \sum_{j=1}^d \sin^2(\pi \mathbf{k}^j)}. \quad (48)$$

By injectivity of Laplace tranform, $C_{1,1}(t)$ is given by:

$$C_{1,1}(t) = \frac{\alpha^2 \mathcal{E}^2}{d} \int_{[0,1]^d} d\mathbf{k} \left(\frac{\sin^2(2\pi \mathbf{k}^1)}{\nu + 4\alpha \sum_{j=1}^d \sin^2(\pi \mathbf{k}^j)} \right)$$
$$\exp\left\{ -8\gamma t \sum_{j=1}^d \sin^2(\pi \mathbf{k}^j) \right\}. \quad (49)$$

For the one dimensional case, the equation for $g_{\lambda,N}$ (resp. g_λ) is different (see (75)) and we get the following integral representation of the correlation function of the energy current:

$$C_{1,1}(t) = \alpha \mathcal{E}^2 \int_0^1 dk \cos^2(\pi k) \exp\left\{ -\frac{4\gamma t}{3} \sin^2(\pi k)(1 + 2\cos^2(\pi k)) \right\}. \quad (50)$$

In any dimension, we have the following unified formula for $C_{1,1}(t)$

$$C_{1,1}(t) = \frac{\mathcal{E}^2}{4\pi^2 d} \int_{[0,1]^d} (\partial_{\mathbf{k}^1} \omega(\mathbf{k}))^2 e^{-t\gamma\psi(\mathbf{k})} d\mathbf{k}, \quad (51)$$

where $\omega(\mathbf{k})$ is defined by (18) and $\psi(\mathbf{k})$ by (19). Observe that the same formula holds if we replace $\mathbb{E}_{N,\mathcal{E}}$ by $\mathbb{E}_{N,T}$. In this last case, the situation is simpler since we do not need equivalence of ensembles.

Standard analysis shows the behavior of $C_{1,1}(t)$ as t goes to infinity is governed by the behavior of the function $(\partial_{\mathbf{k}^1}\omega(\mathbf{k}))^2$ and $\psi(\mathbf{k})$ around the minimal value of ψ which is 0. In fact, $\psi(\mathbf{k}) = 0$ if and only if $\mathbf{k} = 0$ or $\mathbf{k} = (1, \dots, 1)$. By symmetry, we can treat only the case $\mathbf{k} = 0$. Around $\mathbf{k} = 0$, $\psi(\mathbf{k}) \sim a|\mathbf{k}|^2$ and $(\partial_{\kappa^1}\omega(\mathbf{k}))^2 \sim b(\nu + |\mathbf{k}|^2)^{-1}(\mathbf{k}^1)^2$, where a and b are positive constants depending on ν and α. Essentially, $C_{1,1}(t)$ has the same behavior as

$$\int_{\mathbf{k}\in[0,1]^d} d\mathbf{k} \frac{(k^1)^2 e^{-a\gamma t|\mathbf{k}|^2}}{\nu + |\mathbf{k}|^2} = \frac{1}{t^{d/2+1}} \int_{[0,\sqrt{t}]^d} d\mathbf{k} \frac{(\mathbf{k}^1)^2 e^{-a\gamma|\mathbf{k}|^2}}{\nu + t^{-1}|\mathbf{k}|^2}. \tag{52}$$

Hence, we have proved the following theorem:

Theorem 4. *In the (α, ν)-harmonic case, the current-current time correlation function $C_{1,1}(t)$ decays like*

- $C_{1,1}(t) \sim t^{-d/2}$ *in the unpinned case ($\nu = 0$)*
- $C_{1,1}(t) \sim t^{-d/2-1}$ *in the pinned case ($\nu > 0$)*

5. Conductivity in the Harmonic Case

Lemma 1. *Consider the (α, ν)-harmonic case. For any time t, the following limit exists:*

$$C_{1,1}(t) = \lim_{N\to\infty} \frac{1}{N^d} \mathbb{E}_{N,\mathcal{E}}(\mathfrak{J}_{\mathbf{e}_1}(t)\mathfrak{J}_{\mathbf{e}_1}(0)). \tag{53}$$

and

$$\int_0^\infty dt e^{-\lambda t} C_{1,1}(t)\, dt = \lim_{N\to\infty} \left\langle j^a_{0,\mathbf{e}_1} u_{\lambda,N} \right\rangle_{N,\mathcal{E}}. \tag{54}$$

The same result holds with $\mathbb{E}_{N,\mathcal{E}}$ replaced by $\mathbb{E}_{N,T}$.

Proof. We only prove this lemma in the microcanonical setting. Let us define

$$f_N(t) = \frac{1}{N^d} \mathbb{E}_{N,\mathcal{E}}(\mathfrak{J}_{\mathbf{e}_1}(t)\mathfrak{J}_{\mathbf{e}_1}(0)). \tag{55}$$

We first prove the sequence $(f_N)_N$ is uniformly bounded. By Cauchy-Schwarz and stationarity, we have

$$\begin{aligned} |f_N(t)| &\le \frac{1}{N^d} \sqrt{\left\langle \mathfrak{J}^2_{\mathbf{e}_1}(t) \right\rangle_{N,\mathcal{E}}} \sqrt{\left\langle \mathfrak{J}^2_{\mathbf{e}_1}(0) \right\rangle_{N,\mathcal{E}}} \\ &= \frac{1}{N^d} \left\langle \mathfrak{J}^2_{\mathbf{e}_1} \right\rangle_{N,\mathcal{E}}. \end{aligned} \tag{56}$$

We now use symmetry properties of the microcanonical ensemble to show this last term is bounded above by a constant independent of N,

$$N^{-d} < \mathfrak{J}_{\mathbf{e}_1}^2 >_{N,\mathcal{E}} = \sum_{\mathbf{x}} < j_{0,\mathbf{e}_1}^a j_{\mathbf{x},\mathbf{x}+\mathbf{e}_1}^a >_{N,\mathcal{E}}$$

$$= \frac{\alpha^2}{4} \sum_{\mathbf{x}} \sum_{i,j=1}^{d} \left\langle (q_{\mathbf{e}_1}^i - q_0^i)(q_{\mathbf{x}+\mathbf{e}_1}^j - q_{\mathbf{x}}^j)(p_{\mathbf{e}_1}^i + p_0^i)(p_{\mathbf{x}+\mathbf{e}_1}^j + p_{\mathbf{x}}^j) \right\rangle_{N,\mathcal{E}}.$$

In the unpinned case $\nu = 0$, conditionally to the positions configuration $\mathbf{q}$, the law of $\mathbf{p}$ is $\mu_{\mathbf{q}} = \mu^{N^d}_{\sqrt{2K_N(\mathbf{q})}}$ (defined in Lemma 6).

By using properties (i), (ii) and (iii) of Lemma 6, one has

$$N^{-d} < \mathfrak{J}_{\mathbf{e}_1}^2 >_{N,\mathcal{E}} = \frac{\alpha^2}{4} \sum_{i=1}^{d} \left\langle (q_{\mathbf{e}_1}^i - q_0^i)(q_{2\mathbf{e}_1}^i - q_{-\mathbf{e}_1}^i - 3q_{\mathbf{e}_1}^i + 3q_0^i)(p_0^i)^2 \right\rangle_{N,\mathcal{E}}. \tag{57}$$

By Cauchy-Schwarz inequality, the modulus of this last quantity is bounded above by

$$\alpha[8 < \mathcal{E}_0^2 >_{N,\mathcal{E}} + \frac{1}{2} < \mathcal{E}_{\mathbf{e}_1}^2 >_{N,\mathcal{E}}] = \frac{17}{2} < \mathcal{E}_0^2 >_{N,\mathcal{E}}, \tag{58}$$

where the last equality is a consequence of the invariance by translation of $< \cdot >_{N,\mathcal{E}}$. Let $(X_1, \ldots, X_{N^d})$ be a random vector with law $\lambda^{N^d}_{\sqrt{N^d \mathcal{E}}}$, meaning the uniform measure on the N^d-dimensional sphere of radius $\sqrt{N^d \mathcal{E}}$. The vector of energies $(\mathcal{E}_{\mathbf{x}}, \mathbf{x} \in \mathbb{Z}_N^d)$ has the same law as $(X_1^2, \ldots, X_{N^d}^2)$. By Lemma 4, $\mathbb{E}(X_1^4) = < \mathcal{E}_0^2 >_{N,\mathcal{E}}$ is bounded above by a constant independent of N. Hence there exists a positive constant C such that

$$|f_N(t)| \leq C. \tag{59}$$

Similarly, inequality (59) can be proved in the pinned case $\nu > 0$. Let $f(t)$ be any limit point of the sequence $(f_N(t))_{N \geq 1}$ and choose a subsequence $(N_k)_{k \geq 0}$ such that (f_{N_k}) converges to f (for the pointwise convergence topology). By Lebesgue's theorem, we have

$$\lim_{k \to \infty} \int_0^\infty e^{-\lambda t} f_{N_k}(t) dt = \int_0^\infty e^{-\lambda t} f(t) dt. \tag{60}$$

But we have that

$$\int_0^\infty e^{-\lambda t} f_N(t) dt = - < j_{0,\mathbf{e}_1}, u_{\lambda,N} >_{N,\mathcal{E}} \tag{61}$$

and we have seen in Sect. 4 this last quantity converges as N goes to infinity to

$$\int_0^\infty e^{-\lambda t} f_\infty(t) dt, \tag{62}$$

where f_∞ is given by (see (18–19) for the notations)

$$f_\infty(t) = \frac{\mathcal{E}^2}{4\pi^2 d} \int_{[0,1]^d} (\partial_{\mathbf{k}^1}\omega(\mathbf{k}))^2 e^{-t\gamma\psi(\mathbf{k})} d\mathbf{k}. \tag{63}$$

By injectivity of the Laplace transform, we get $f(t) = f_\infty(t)$. Uniqueness of limit points implies $(f_N(t))_{N\geq 1}$ converges to $f_\infty(t)$ for any t. It follows also we can inverse time integral and infinite volume limit in the left hand side of (54) and the lemma is proved. □

Lemma 2 *(Resolvent equation).*

$$u_{\lambda,N} = (\lambda - L)^{-1}\left(-\sum_{\mathbf{x}} j^a_{\mathbf{x},\mathbf{x}+\mathbf{e}_1}\right) = \frac{\alpha}{\gamma}\sum_{\mathbf{x},\mathbf{y}} g_{\lambda,N}(\mathbf{x}-\mathbf{y})\mathbf{p}_{\mathbf{x}}\cdot\mathbf{q}_{\mathbf{y}},$$

where $g_{\lambda,N}(\mathbf{z})$ is the solution (such that $\sum_{\mathbf{z}} g_{\lambda,N}(\mathbf{z}) = 0$) of the equation

$$\frac{2\lambda}{\gamma} g_{\lambda,N}(\mathbf{z}) - 4\Delta g_{\lambda,N}(\mathbf{z}) = (\delta(\mathbf{z}+\mathbf{e}_1) - \delta(\mathbf{z}-\mathbf{e}_1)) \tag{64}$$

for $d \geq 2$, or

$$\frac{2\lambda}{\gamma} g_{\lambda,N}(z) - \frac{1}{3}\Delta\left[4g_{\lambda,N}(z) + g_{\lambda,N}(z+1) + g_{\lambda,N}(z-1)\right] = (\delta(z+1) - \delta(z-1)) \tag{65}$$

for $d = 1$. Moreover, $Au_{\lambda,N} = 0$ and $Lu_{\lambda,N} = \gamma S u_{\lambda,N}$.

Proof. We only give the proof for the dimension $d \geq 2$ since the proof for the one dimensional case is similar. Let $u_{\lambda,N} = \frac{\alpha}{\gamma}\sum_{\mathbf{x},\mathbf{y}} g_{\lambda,N}(\mathbf{x}-\mathbf{y})\mathbf{p}_{\mathbf{x}}\cdot\mathbf{q}_{\mathbf{y}}$. The generator L is equal to the sum of the Liouville operator A and of the noise operator γS. The action of A on $u_{\lambda,N}$ is null. Indeed, we have:

$$Au_{\lambda,N} = \frac{\alpha}{\gamma}\sum_{\mathbf{x}}[(\alpha\Delta - \nu I)\mathbf{q}_{\mathbf{x}}]\cdot\left(\sum_{\mathbf{y}} g_{\lambda,N}(\mathbf{x}-\mathbf{y})\mathbf{q}_{\mathbf{y}}\right) + \frac{\alpha}{\gamma}\sum_{\mathbf{y},\mathbf{x}} g_{\lambda,N}(\mathbf{x}-\mathbf{y})\mathbf{p}_{\mathbf{x}}\cdot\mathbf{p}_{\mathbf{y}}. \tag{66}$$

Here, and in the sequel of the proof, sums indexed by $\mathbf{x}$, $\mathbf{y}$, $\mathbf{z}$ are indexed by $\mathbb{Z}_N$ and sums indexed by i, j, k, ℓ are indexed by $\{1,\ldots,d\}$. Summation by parts can be performed (without outcoming boundary terms since we are on the torus) and we get

$$Au_{\lambda,N} = \frac{\alpha}{\gamma}\sum_{\mathbf{x}}[(\alpha\Delta - \nu I)g_{\lambda,N}](\mathbf{x}-\mathbf{y})\mathbf{q}_x\mathbf{q}_{\mathbf{y}} + \frac{\alpha}{\gamma}\sum_{\mathbf{y},\mathbf{x}} g_{\lambda,N}(\mathbf{x}-\mathbf{y})\mathbf{p}_{\mathbf{x}}\cdot\mathbf{p}_{\mathbf{y}}. \tag{67}$$

Remark now that the function $\delta(\cdot - \mathbf{e}_1) - \delta(\cdot + \mathbf{e}_1)$ is antisymmetric. Hence $g_{\lambda,N}$, and consequently $\Delta g_{\lambda,N}$, is still antisymmetric. We have therefore $Au_{\lambda,N}$ which is of the form:

$$Au_{\lambda,N} = \sum_{\mathbf{x},\mathbf{y}}\{a_1(\mathbf{x}-\mathbf{y})\mathbf{p}_{\mathbf{x}}\cdot\mathbf{p}_{\mathbf{y}} + a_2(\mathbf{x}-\mathbf{y})\mathbf{q}_{\mathbf{x}}\cdot\mathbf{q}_{\mathbf{y}}\} \tag{68}$$

with a_1, a_2 antisymmetric. Using the antisymmetricity of a_1 and a_2, it is easy to show that the last two sums are zero and hence $Au_{\lambda,N} = 0$.

A simple computation shows that if $\ell \in \{1, \dots, d\}$ then

$$\begin{aligned} S(p_{\mathbf{x}}^{\ell}) &= \frac{1}{2(d-1)} \sum_{\mathbf{y}} \sum_{i \neq j,k} (X_{\mathbf{y},\mathbf{y}+\mathbf{e}_k}^{i,j})^2 (p_{\mathbf{x}}^{\ell}) \\ &= \frac{2}{2(d-1)} \sum_{i \neq \ell,k} (X_{\mathbf{x},\mathbf{x}+\mathbf{e}_k}^{i,\ell})^2 (p_{\mathbf{x}}^{\ell}) + \frac{2}{2(d-1)} \sum_{i \neq \ell,k} (X_{\mathbf{x}-\mathbf{e}_k,\mathbf{x}}^{i \neq \ell,k})^2 (p_{\mathbf{x}}^{\ell}) \\ &= \frac{1}{d-1} \sum_{i \neq \ell,k} \left\{ (p_{\mathbf{x}+\mathbf{e}_k}^{\ell} - p_{\mathbf{x}}^{\ell}) - (p_{\mathbf{x}}^{\ell} - p_{\mathbf{x}-\mathbf{e}_k}^{\ell}) \right\} \\ &= 2\Delta(p_{\mathbf{x}}^{\ell}). \end{aligned}$$

Since the action of S is only on the $\mathbf{p}$'s, we have

$$\begin{aligned} \gamma S u_{\lambda,N} &= \alpha \sum_{\mathbf{x},\mathbf{y}} g_{\lambda,N}(\mathbf{x}-\mathbf{y}) S(\mathbf{p}_{\mathbf{x}}) \cdot \mathbf{q}_{\mathbf{y}} \\ &= 2\alpha \sum_{\mathbf{x},\mathbf{y}} g_{\lambda,N}(\mathbf{x}-\mathbf{y}) (\Delta \mathbf{p}_{\mathbf{x}}) \cdot \mathbf{q}_{\mathbf{y}} \\ &= 2\alpha \sum_{\mathbf{x},\mathbf{y}} (\Delta g_{\lambda,N})(\mathbf{x}-\mathbf{y}) \mathbf{p}_{\mathbf{x}} \cdot \mathbf{q}_{\mathbf{y}}, \end{aligned}$$

where in the last line, we performed a summation by parts. Since $g_{\lambda,N}$ is a solution of (64), we have

$$\lambda u_{\lambda,N} - \gamma S u_{\lambda,N} = \frac{\alpha}{2} \sum_{\mathbf{x}} \mathbf{p}_{\mathbf{x}} \cdot (\mathbf{q}_{\mathbf{x}+\mathbf{e}_1} - \mathbf{q}_{\mathbf{x}-\mathbf{e}_1}) = -\sum_{\mathbf{x}} j_{\mathbf{x},\mathbf{x}+\mathbf{e}_1}^{a}. \tag{69}$$

□

Let us define the Fourier transform $\hat{v}(\xi),\ \xi \in \mathbb{Z}_N^d$, of the function v on $\mathbb{Z}_N^d$ as

$$\hat{v}(\xi) = \sum_{\mathbf{z} \in \mathbb{Z}_N^d} v(\mathbf{z}) \exp(2i\pi \xi \cdot \mathbf{z}/N). \tag{70}$$

The inverse transform is given by

$$v(\mathbf{z}) = \frac{1}{N^d} \sum_{\xi \in \mathbb{Z}_N^d} \hat{v}(\xi) \exp(-2i\pi \xi \cdot \mathbf{z}/N) \tag{71}$$

On $\mathbb{Z}^d$ we define similarly:

$$\hat{v}(\mathbf{k}) = \sum_{\mathbf{z} \in \mathbb{Z}^d} v(\mathbf{z}) \exp(2i\pi \mathbf{k} \cdot \mathbf{z}), \quad \mathbf{k} \in [0,1]^d. \tag{72}$$

and its inverse by

$$v(\mathbf{z}) = \int_{[0,1]^d} \hat{v}(\mathbf{k}) \exp(-2i\pi \mathbf{k} \cdot \mathbf{z}).$$

For $\lambda > 0$, the function $g_\lambda : \mathbb{Z}^d \to \mathbb{R}$ is the solution on $\mathbb{Z}^d$ of the equation

$$\begin{aligned}
&\frac{2\lambda}{\gamma} g_\lambda(\mathbf{z}) - 4\Delta g_\lambda(\mathbf{z}) = \delta_0(\mathbf{z}+\mathbf{e}_1) - \delta_0(\mathbf{z}+\mathbf{e}_1), \quad d \geq 2,\\
&\frac{2\lambda}{\gamma} g_\lambda(z) - \frac{1}{3}\Delta\left(4g_\lambda(z) + g_\lambda(z+1) + g_\lambda(z-1)\right) = \delta_0(z+1) - \delta_0(z-1), \quad d = 1.
\end{aligned} \tag{73}$$

Then we have

$$\hat{g}_\lambda(\mathbf{k}) = \frac{-2i\pi \sin(2\pi \mathbf{k}^1)}{\dfrac{2\lambda}{\gamma} + 16\sum_{j=1}^d \sin^2(\pi \mathbf{k}^j)}, \quad \text{if } d \geq 2 \tag{74}$$

and

$$\hat{g}_\lambda(k) = \frac{-2i\pi \sin(2\pi k)}{\dfrac{2\lambda}{\gamma} + \dfrac{8}{3}\sin^2(\pi k)\left(1 + 2\cos^2(\pi k)\right)}, \quad \text{if } d = 1. \tag{75}$$

Since $g_{\lambda,N}$ is the solution of the same equation as g_λ but on $\mathbb{Z}_N^d$, we have the following formula for $\hat{g}_{\lambda,N}$:

$$\hat{g}_{\lambda,N}(\xi) = \hat{g}_\lambda(\xi/N). \tag{76}$$

The following bound follows easily from Parseval relation:

$$\sum_{\mathbf{x}\in\mathbb{Z}_N^d} (g_{\lambda,N}(\mathbf{x}))^2 \leq \frac{\gamma^2}{\lambda^2} \tag{77}$$

Similarly, the function Γ_N defined in (45) has Fourier transform given by

$$\hat{\Gamma}_N(\xi) = \hat{\Gamma}(\xi/N), \tag{78}$$

where

$$\hat{\Gamma}(\mathbf{k}) = \frac{-2i \sin(2\pi \mathbf{k}^1)}{\nu + 4\alpha \sum_{j=1}^d \sin^2(\pi \mathbf{k}^j)}. \tag{79}$$

Let us denote by z^* the conjugate of the complex number z and observe that the function $\mathbf{k} \in [0,1]^d \to \hat{g}_\lambda(\mathbf{k})\left[\hat{\Gamma}(\mathbf{k})\right]^* \in \mathbb{R}^+$ is continuous. Hence we have the following convergence of Riemann sums:

$$\begin{aligned}
\sum_{\mathbf{y}\in\mathbb{Z}_N^d} g_{\lambda,N}(\mathbf{y})\Gamma_N(\mathbf{y}) &= \frac{1}{N^d}\sum_{\xi\in\mathbb{Z}_N^d} \hat{g}_{\lambda,N}(\xi)[\hat{\Gamma}_N(\xi)]^*\\
&\xrightarrow[N\to\infty]{} \int_{[0,1]^d} d\mathbf{k}\,\hat{g}_\lambda(\mathbf{k})[\hat{\Gamma}(\mathbf{k})]^* = \sum_{\mathbf{y}\in\mathbb{Z}^d} g_\lambda(\mathbf{y}).\Gamma(\mathbf{y}).
\end{aligned} \tag{80}$$

The limits as $\lambda \to 0$ of the above expressions give the values for the conductivity (up to a multiplicative constant) when this is finite. If $\nu = 0$ it diverges if $d = 1$ or 2.

6. Anharmonic Case: Bounds on the Thermal Conductivity

We consider in this section the general anharmonic case and we prove Theorem 3. Recall (38), then all we need to estimate is

$$(2T^2N^{d+1})^{-1}\mathbb{E}_{N,T}\left(\left[\sum_{\mathbf{x}}\int_0^N j^a_{\mathbf{x},\mathbf{x}+\mathbf{e}_1}(s)ds\right]^2\right). \tag{81}$$

Let us define $\sum_{\mathbf{x}} j^a_{\mathbf{x},\mathbf{x}+\mathbf{e}_1} = \mathfrak{J}_{\mathbf{e}_1}$, then we have the general bound ([16], Lemma 3.9)

$$\begin{aligned}\mathbb{E}_{N,T}\left(\left[\int_0^N \mathfrak{J}_{\mathbf{e}_1}(s)ds\right]^2\right) &\leq 10N\left\langle \mathfrak{J}_{\mathbf{e}_1}, (N^{-1}-L)^{-1}\mathfrak{J}_{\mathbf{e}_1}\right\rangle_{N,T}\\ &\leq 10N\left\langle \mathfrak{J}_{\mathbf{e}_1}, (N^{-1}-\gamma S)^{-1}\mathfrak{J}_{\mathbf{e}_1}\right\rangle_{N,T}.\end{aligned} \tag{82}$$

Recall that $S(\mathbf{p_x}) = 2\Delta(\mathbf{p_x})$ if $d \geq 2$ and $S(p_x) = \frac{1}{6}\Delta(4p_x + p_{x+1} + p_{x-1})$ if $d = 1$,

$$(N^{-1}-\gamma S)^{-1}\mathfrak{J}_{\mathbf{e}_1} = \sum_{j=1}^{d}\sum_{\mathbf{y}} G_N(\mathbf{x}-\mathbf{y})p_x^j V_j'(q^j_{\mathbf{y}+\mathbf{e}_1} - q^j_{\mathbf{y}}), \tag{83}$$

where $G_N(\mathbf{z})$ is the solution of the resolvent equation

$$\begin{cases} N^{-1}G_N(\mathbf{z}) - 2\gamma(\Delta G_N)(\mathbf{z}) = -\frac{1}{2}\left[\delta_0(\mathbf{z}) + \delta_{\mathbf{e}_1}(\mathbf{z})\right], \quad d \geq 2\\ \quad N^{-1}G_N(\mathbf{z}) - \frac{\gamma}{6}[4(\Delta G_N)(\mathbf{z}) + (\Delta G_N)(\mathbf{z}+1) + (\Delta G_N)(\mathbf{z}-1)]\\ = -\frac{1}{2}[\delta_0(\mathbf{z}) + \delta_1(\mathbf{z})], \quad d = 1.\end{cases} \tag{84}$$

The left-hand side of (82) is equal to

$$-5TN^{d+1}\sum_{j=i}^{d}\sum_{\mathbf{x}}(G_N(\mathbf{x}) + G_N(\mathbf{x}+\mathbf{e}_1))\left\langle V_j'(q^j_{\mathbf{x}+\mathbf{e}_1} - q^j_{\mathbf{x}})V_j'(q^j_{\mathbf{e}_1} - q^j_0)\right\rangle_{N,T}. \tag{85}$$

- **Pinned case.**

  In the pinned case, the correlations $\left\langle V_j'(q^j_{\mathbf{x}+\mathbf{e}_1} - q^j_{\mathbf{x}})V_j'(q^j_{\mathbf{e}_1} - q^j_0)\right\rangle_{N,T}$ decay exponentially in $\mathbf{x}$,

$$\left|\left\langle V_j'(q^j_{\mathbf{x}+\mathbf{e}_1} - q^j_{\mathbf{x}})V_j'(q^j_{\mathbf{e}_1} - q^j_0)\right\rangle_{N,T}\right| \leq Ce^{-c|\mathbf{x}|}. \tag{86}$$

  It follows that the previous expression is bounded by

$$CT^2tN^d\sum_{\mathbf{x}}|G_N(\mathbf{x}) + G_N(\mathbf{x}+\mathbf{e}_1)|e^{-c|\mathbf{x}|}.$$

Since G_N is bounded in $d \geq 3$, it follows that (81) is uniformly bounded in N. In low dimensions, our estimates are too rough and we obtain only diverging upper-bounds. Nevertheless, if $V_j(r) = \alpha_j r^2$ are quadratics and W_j are general but strictly positive then

$$\begin{aligned} &\left\langle V_j'(q^j_{\mathbf{x}+\mathbf{e}_1} - q^j_{\mathbf{x}}) V_j'(q^j_{\mathbf{e}_1} - q^j_0) \right\rangle_{N,T} \\ &= \alpha_j \left\{ 2 < q^j_{\mathbf{x}} q^j_0 >_{N,T} - < q^j_{\mathbf{x}-\mathbf{e}_1} q^j_0 >_{N,T} - < q^j_{\mathbf{x}+\mathbf{e}_1} q^j_0 >_{N,T} \right\}. \end{aligned} \tag{87}$$

As a function of $\mathbf{x}$, this quantity is a Laplacian in the first direction and by integration by parts, the left-hand side of (81) is upper bounded by

$$C \sum_{\mathbf{x}} |(\Delta G_N)(\mathbf{x}) + (\Delta G_N)(\mathbf{x} + \mathbf{e}_1)| \, e^{-c|\mathbf{x}|}. \tag{88}$$

By Lemma 3, this quantity is uniformly bounded in N.

- **Unpinned case.**

In the unpinned case, we assume that $0 < c \leq V_j''(q) \leq C < +\infty$. We have (cf. [9], Theorem 6.2, that can be proved in finite volume uniformly)

$$\left| \left\langle V_j'(q^j_{\mathbf{x}+\mathbf{e}_1} - q^j_{\mathbf{x}}) V_j'(q^j_{\mathbf{e}_1} - q^j_0) \right\rangle_{N,T} \right| \leq C|\mathbf{x}|^{-d}. \tag{89}$$

In the one dimensional case, the random variables $r_x = q_{x+1} - q_x$ are i.i.d. and $< V'(r_x) >_{N,T} = 0$. Only the term corresponding to $x = 0$ remains in the sum of (85). By Lemma 3, we get the upper bound

$$(G_N(0) + G_N(1)) \left\langle V'(r_0^2) \right\rangle_{N,T} \leq C\sqrt{N}. \tag{90}$$

For the unpinned two dimensional case, we obtain the upper bound

$$\begin{aligned} C &\sum_{\mathbf{x} \in \mathbb{Z}_N^2} |G_N(\mathbf{x}) + G_N(\mathbf{x} + \mathbf{e}_1)| |\mathbf{x}|^{-d} \\ &\leq C \log N \sum_{\mathbf{x} \in \mathbb{Z}_N^2} |\mathbf{x}|^{-2} \\ &\sim C(\log N)^2. \end{aligned} \tag{91}$$

For the case $d \geq 3$, we use the first point of Lemma 3, (89) and the fact that

$$\sum_{\mathbf{x} \in \mathbb{Z}_N^d} |\mathbf{x}|^{-d} \sim \log N. \tag{92}$$

Lemma 3. *Let G_N be the solution of the discrete equation (84). There exists a constant $C > 0$ independent of N such that*

- $G_N(\mathbf{x}) \leq C(|\mathbf{x}|^{d-2} + N^{-1/2}), \quad d \geq 3$
- $G_N(\mathbf{x}) \leq C \log N, \quad d = 2$
- $G_N(\mathbf{x}) \leq C\sqrt{N}, \quad d = 1$
- $|G_N(\mathbf{x} + \mathbf{e}_1) + G_N(\mathbf{x} - \mathbf{e}_1) - 2G_N(\mathbf{x})| \leq C, \quad d \geq 1.$

Proof. In the proof, C is a constant independent of N but which can change from line to line. We first treat the case $d \geq 3$. We use Fourier's transform representation of G_N:

$$G_N(\mathbf{x}) = -\frac{1}{2N^d} \sum_{\mathbf{k}\in\mathbb{Z}_N^d} (1 + e^{2i\pi\mathbf{k}^1/N}) \frac{e^{-2i\pi\mathbf{k}\cdot\mathbf{x}/N}}{\theta_N(\mathbf{k}/N)}, \tag{93}$$

where $\theta_N(\mathbf{u}) = N^{-1} + 8\gamma \sum_{j=1}^d \sin^2(\pi\mathbf{u}^j)$. G_N can also be written in the following form:

$$G_N(\mathbf{x}) = -\frac{1}{2}\left[F_N(\mathbf{x}) + F_N(\mathbf{x} - \mathbf{e}_1)\right], \tag{94}$$

where

$$F_N(\mathbf{x}) = \frac{1}{N^d} \sum_{\mathbf{k}\in\mathbb{Z}_N^d} \frac{e^{-2i\pi\mathbf{k}\cdot\mathbf{x}/N}}{\theta_N(\mathbf{k}/N)}. \tag{95}$$

Let us introduce the continuous Fourier's transform representation of the Green function F_∞ on $\mathbb{Z}^d$ given by:

$$F_\infty(\mathbf{x}) = \int_{[0,1]^d} \frac{\exp(2i\pi\mathbf{x}\cdot\mathbf{u})}{\theta(\mathbf{u})} d\mathbf{u}, \tag{96}$$

where $\theta(\mathbf{u}) = 8\gamma \sum_{j=1}^d \sin^2(\pi\mathbf{u}^j)$. Remark that F_∞ is well defined because $d \geq 3$. We have to prove there exists a constant $C > 0$ independent of N such that

$$F_N(\mathbf{x}) \leq C(|\mathbf{x}|^{d-2} + N^{-1/2}). \tag{97}$$

Observe that by symmetries of F_N, we can restrict our study to the case $\mathbf{x} \in [0, N/2]^d$. We want to show that $F_N(\mathbf{x})$ is well approximated by $F_\infty(\mathbf{x})$. We have

$$F_N(\mathbf{x}) - F_\infty(\mathbf{x}) = F_N(\mathbf{x}) - F_\infty^N(\mathbf{x}) + F_\infty^N(\mathbf{x}) - F_\infty(\mathbf{x}), \tag{98}$$

where

$$F_\infty^N(\mathbf{x}) = \int_{[0,1]^d} \frac{\exp(2i\pi\mathbf{x}\cdot\mathbf{u})}{\theta_N(\mathbf{u})} d\mathbf{u}. \tag{99}$$

For each $\mathbf{k} \in \mathbb{Z}_N^d$, we introduce the hypercube $Q_\mathbf{k} = \prod_{j=1}^d [\mathbf{k}^j/N, (\mathbf{k}^j + 1)/N)$ and we divide $[0, 1]^d$ following the partition $\cup_{\mathbf{k}\in\mathbb{Z}_N^d} Q_\mathbf{k}$. By using this partition, we get

$$\begin{aligned} F_N(\mathbf{x}) - F_\infty^N(\mathbf{x}) = \sum_{\mathbf{k}\in\mathbb{Z}_N^d} \int_{Q_\mathbf{k}} d\mathbf{u} \frac{e^{2i\pi\mathbf{k}\cdot\mathbf{x}/N} - e^{2i\pi\mathbf{u}\cdot\mathbf{x}}}{\theta_N(\mathbf{k}/N)} \\ + \int_{Q_\mathbf{k}} d\mathbf{u} e^{2i\pi\mathbf{u}\cdot\mathbf{x}} \left(\frac{1}{\theta_N(\mathbf{k}/N)} - \frac{1}{\theta_N(\mathbf{u})} \right). \end{aligned} \tag{100}$$

Remark that

$$\int_{Q_{\mathbf{k}}} d\mathbf{u} e^{2i\pi \mathbf{u}\cdot\mathbf{x}} = \frac{e^{2i\pi \mathbf{k}\cdot\mathbf{x}/N}}{N^d}\varphi(\mathbf{x}/N), \tag{101}$$

where

$$\varphi(\mathbf{u}) = \prod_{j=1}^{d} e^{2i\pi \mathbf{u}^j} \prod_{j=1}^{d} \frac{\sin(\pi \mathbf{u}^j)}{(\pi \mathbf{u}^j)}. \tag{102}$$

It follows that the first term on the right-hand side of (100) is equal to

$$(1-\varphi(\mathbf{x}/N))F_N(\mathbf{x}) \tag{103}$$

so that

$$F_N(\mathbf{x}) = \frac{F_\infty^N(\mathbf{x})}{\varphi(\mathbf{x}/N)} + \frac{1}{\varphi(\mathbf{x}/N)} \sum_{\mathbf{k}\in\mathbb{Z}_N^d} \int_{Q_{\mathbf{k}}} d\mathbf{u} e^{2i\pi \mathbf{u}\cdot\mathbf{x}} \left(\frac{1}{\theta_N(\mathbf{k}/N)} - \frac{1}{\theta_N(\mathbf{u})} \right). \tag{104}$$

The next step consists to show that the second term on the right-hand side of (104) is small. In the sequel, C is a positive constant independent of N but which can change from line to line. For each $\mathbf{u} \in Q_{\mathbf{k}}$, we have

$$\sin^2(\pi \mathbf{u}^j) - \sin^2(\pi \mathbf{k}^j/N) = \pi \sin(2\pi c_j)(\mathbf{u}^j - \mathbf{k}^j/N). \tag{105}$$

for some $c_j \in [\mathbf{k}^j/N, (\mathbf{k}^j+1)/N)$. Consequently, we have

$$|\sin^2(\pi \mathbf{u}^j) - \sin^2(\pi \mathbf{k}^j/N)| \le \frac{C}{N} |\sin(\pi \mathbf{k}^j/N)|. \tag{106}$$

Moreover, there exists a positive constant C such that

$$\forall \mathbf{k} \in \mathbb{Z}_N^d, \forall \mathbf{u} \in Q_{\mathbf{k}}, \quad \theta_N(\mathbf{u}) \ge C\theta_N(\mathbf{k}/N). \tag{107}$$

It follows that the modulus of the second term on the right-hand side of (104) is bounded by

$$\frac{C}{|\varphi(\mathbf{x}/N)|} \sum_{j=1}^{d} \frac{1}{N^d} \sum_{\mathbf{k}\in\mathbb{Z}_N^d} \frac{N^{-1}|\sin(\pi \mathbf{k}^j/N)|}{\theta_N(\mathbf{k}/N)^2}. \tag{108}$$

Since the modulus of the function $\varphi(\mathbf{u})$ is bounded below by a positive constant on $[0, 1/2]^d$, this last term is of the same order as

$$N^{-1} \sum_{j=1}^{d} \int_{[0,1]^d} \frac{|\sin(\pi \mathbf{u}^j)|}{\theta_N(\mathbf{u})^2} d\mathbf{u}. \tag{109}$$

Elementary standard analysis shows that this term is of the same order as

$$N^{-1} \int_0^1 \frac{r^d}{(N^{-1}+r^2)^2} dr. \tag{110}$$

For $d \geq 4$, this term is clearly of order N^{-1}. For $d = 3$, the change of variables $r = N^{-1/2}v$ gives an integral of order $N^{-1}\log N$. In conclusion, we proved

$$F_N(\mathbf{x}) = \frac{F_\infty^N(\mathbf{x})}{\varphi(\mathbf{x}/N)} + O\left(\frac{\log N}{N}\right). \tag{111}$$

Moreover, it is not difficult to show that

$$|F_\infty(\mathbf{x}) - F_\infty^N(\mathbf{x})| \leq CN^{-1/2}. \tag{112}$$

Since we have (cf. [14], Theorem 4.5)

$$F_\infty(\mathbf{x}) \leq C|\mathbf{x}|^{2-d} \tag{113}$$

we obtained the first point of the lemma.

For the 1- and 2-dimensional estimates, we have that $|G_N(\mathbf{x})| \leq G_N(0)$ and by standard analysis, there exists a constant $C > 0$ independent of N such that

$$G_N(0) \leq C \int_{[0,1/2]^d} d\mathbf{k} \frac{1}{N^{-1} + \sum_{j=1}^d \sin^2(\pi \mathbf{k})}. \tag{114}$$

By using the inequality $\sin^2(\pi u) \geq 4u^2$, one gets $G_N(0)$ is of same order as

$$\int_{[0,1/2]^d} d\mathbf{k} \frac{1}{N^{-1} + |\mathbf{k}|^2}. \tag{115}$$

This last quantity is of order $\sqrt{N}$ if $d = 1$ and $\log N$ if $d = 2$.

Let us now prove the final statement. Assume $d \geq 2$ (the case $d = 1$ can be proved in a similar way). We have

$$\begin{aligned}
&|G_N(\mathbf{x} + \mathbf{e}_1) + G_N(\mathbf{x} - \mathbf{e}_1) - 2G_N(\mathbf{x})| \\
&= \left| \frac{2}{N^d} \sum_{\mathbf{k} \in \mathbb{Z}_N^d} (1 + e^{2i\pi \mathbf{k}^1/N}) \sin^2(\pi \mathbf{k}_1/N) \frac{e^{-2i\pi \mathbf{k}\cdot\mathbf{x}/N}}{\theta_N(\mathbf{k}/N)} \right| \\
&\leq \frac{4}{N^d} \sum_{\mathbf{k} \in \mathbb{Z}_N^d} \frac{\sin^2(\pi \mathbf{k}_1/N)}{\theta_N(\mathbf{k}/N)} \\
&\leq (2\gamma)^{-1}.
\end{aligned} \tag{116}$$

□

7. Appendix: Equivalence of Ensembles

In this part, we establish a result of equivalence of ensembles for the microcanonical measure $< \cdot >_{N,\mathcal{E}}$, since it does not seem to appear in the literature. The decomposition in normal modes permits to obtain easily the results we need from the classical equivalence of the ensemble for the uniform measure on the sphere. This last result proved in [10] says that the expectation of a local function in the microcanonical ensemble (the uniform measure on the sphere of radius $\sqrt{k}$ in this context) is equal to the expectation of the same function in the canonical ensemble (the standard gaussian measure on $\mathbb{R}^{\infty}$) with an error of order k^{-1}. In fact, the equivalence of ensembles of Diaconis and Freedman is expressed in terms of a very precise estimate of variation distance between the microcanonical ensemble and the canonical ensemble. In this paper, we need to consider equivalence of ensembles for unbounded functions and to be self-contained we prove in the following lemma a slight modification of estimates of [10].

Lemma 4. *Let $\lambda^n_{rn^{1/2}}$ be the uniform measure on the sphere*

$$S^n_{rn^{1/2}} = \left\{ (\mathbf{x}_1, \ldots, \mathbf{x}_n) \in \mathbb{R}^n; \quad \sum_{\ell=1}^{n} x_\ell^2 = nr^2 \right\}$$

of radius r and dimension $n-1$ and λ^∞_r the Gaussian product measure with mean 0 and variance r^2. Let $\theta > 0$ and ϕ be a function on $\mathbb{R}^k$ such that

$$|\phi(x_1, \ldots, x_k)| \leq C \left(\sum_{\ell=1}^{k} x_\ell^2 \right)^{\theta}, \quad C > 0. \tag{117}$$

There exists a constant C' (depending on C, θ, k, r) such that

$$\limsup_{n\to\infty} \quad n \left| \lambda^n_{rn^{1/2}}(\phi) - \lambda^\infty_r(\phi) \right| \leq C'. \tag{118}$$

Proof. This lemma is proved in [10] for ϕ positive bounded by 1. Without loss of generality, we can assume $r = 1$ and we simplify the notations by denoting $\lambda^n_{rn^{1/2}}$ with λ^n and λ^∞_r with λ^∞. The law of $(x_1 + \ldots + x_k)^2$ under λ^n is n times a $\beta[k/2, (n-k)/2]$ distribution and has density (cf. [10])

$$f(u) = \mathbf{1}_{\{0 \leq u \leq n\}} \cdot \frac{1}{n} \frac{\Gamma(n/2)}{\Gamma(k/2)\Gamma[(n-k)/2]} \left(\frac{u}{n}\right)^{(k/2)-1} \left(1 - \frac{u}{n}\right)^{((n-k)/2)-1}. \tag{119}$$

On the other hand, the law of $(x_1 + \ldots + x_k)^2$ under λ^∞ is χ^2_k with density (cf. [10])

$$g(u) = \frac{1}{2^{k/2}\Gamma(k/2)} e^{-u/2} u^{(k/2)-1}. \tag{120}$$

With these notations, we have

$$\left| \lambda^n(\phi) - \lambda^\infty(\phi) \right| \leq C \int_0^\infty u^\theta |f(u) - g(u)| du. \tag{121}$$

The RHS of the inequality above is equal to

$$2C\int_0^\infty u^\theta \left(\frac{f(u)}{g(u)}-1\right)^+ g(u)du + C\int_0^\infty u^\theta (g(u)-f(u))du. \tag{122}$$

In [10], it is proved $2\left(\frac{f(u)}{g(u)}-1\right)^+ \leq 2(k+3)/(n-k-3)$ as soon as $k\in\{1,\dots,n-4\}$. The second term of (122) can be computed explicitly and is equal to

$$\frac{\Gamma\left((2\theta+k)/2\right)}{\Gamma(k/2)}\left[2^\theta - \frac{n^\theta\Gamma(n/2)}{\Gamma(\theta+n/2)}\right]. \tag{123}$$

A Taylor expansion shows that this term is bounded by C'/n for n large enough. □

We recall here the following well known properties of the uniform measure on the sphere.

Lemma 5 *(Symmetry properties of the uniform measure on the sphere). Let λ_r^k be the uniform measure on the sphere*

$$S_r^k = \left\{(\mathbf{x}_1,\dots,\mathbf{x}_k)\in(\mathbb{R}^d)^k;\quad \sum_{\ell=1}^k \mathbf{x}_\ell^2 = r^2\right\}$$

of radius r and dimension $dk-1$.

i) *λ_r^k is invariant by any permutation of coordinates.*

ii) *Conditionally to $\{\mathbf{x}_1,\dots,\mathbf{x}_k\}\backslash\{\mathbf{x}_i\}$, the law of $\mathbf{x}_i$ has an even density w.r.t. the Lebesgue measure on $\mathbb{R}^d$.*

In the same spirit, we have the following lemma.

Lemma 6. *Let μ_r^k be the uniform measure on the surface defined by*

$$M_r^k = \left\{(\mathbf{x}_1,\dots,\mathbf{x}_k)\in(\mathbb{R}^d)^k;\quad \sum_{\ell=1}^k \mathbf{x}_\ell^2 = r^2;\quad \sum_{\ell=1}^k \mathbf{x}_\ell = 0\right\}.$$

We have the following properties:

i) *μ_r^k is invariant by any permutation of the coordinates.*

ii) *If $i\neq j\in\{1,\dots,d\}$ then for every $h,\ell\in\{1,\dots,k\}$ (distinct or not), $\mu_r^k(\mathbf{x}_h^i\mathbf{x}_\ell^j)=0$.*

iii) *If $h\neq\ell\in\{1,\dots,k\}$ and $i\in\{1,\dots,d\}$,*

$$\mu_r^k(\mathbf{x}_h^i\mathbf{x}_\ell^i) = -\frac{r^2}{dk(k-1)} = -\frac{\mu_r^k(\mathbf{x}_h^2)}{k-1} = -\frac{\mu_r^k(\mathbf{x}_\ell^2)}{k-1}. \tag{124}$$

Lemma 7. *(Equivalence of ensembles.) Consider the (α,ν)-harmonic case. There exists a positive constant $C=C(d,\mathcal{E})$ such that:*

i) *If* $i \neq j$, $\left|\left\langle \left(p_0^j p_{\mathbf{e}_1}^i\right)^2 \right\rangle_{N,\mathcal{E}} - \frac{\mathcal{E}^2}{d^2}\right| \leq \frac{C}{N^d}$.

ii) *If* $i \neq j$, $\left|\left\langle (p_0^i p_{\mathbf{e}_1}^i p_0^j p_{\mathbf{e}_1}^j) \right\rangle_{N,\mathcal{E}}\right| \leq \frac{C}{N^d}$.

iii) *For any* i *and any* $\mathbf{y} \in \mathbb{Z}_N^d$, *we have*

$$\left|\left\langle q_{\mathbf{y}}^j (q_{-\mathbf{e}_1}^j - q_{\mathbf{e}_1}^j)(p_0^j)^2 \right\rangle_{N,\mathcal{E}} - \left(\frac{\mathcal{E}}{d}\right)^2 \Gamma_N(\mathbf{y})\right| \leq \frac{C \log N}{N^d}.$$

Proof. Let us treat only the unpinned case $\nu = 0$. The pinned case is similar. We take the Fourier transform of the positions and of the momentums (defined by (70)) and we define

$$\tilde{\mathbf{q}}(\xi) = (1 - \delta(\xi))\omega(\xi)\hat{\mathbf{q}}(\xi), \quad \tilde{\mathbf{p}}(\xi) = N^{-d/2}(1 - \delta(\xi))\hat{\mathbf{p}}(\xi), \quad \xi \in \mathbb{Z}_d^N, \tag{125}$$

where $\omega(\xi) = 2N^{-d/2}\sqrt{\alpha \sum_{k=1}^d \sin^2(\pi \xi^k / N)}$ is the normalized dispersion relation. The factor $1 - \delta$ in the definition above is due to the condition $\sum_{\mathbf{x}} \mathbf{p_x} = \sum_{\mathbf{x}} \mathbf{q_x} = 0$ assumed in the microcanonical state. Then the energy can be written as

$$\begin{aligned}
\mathcal{H}_N &= \frac{1}{2}\sum_{\xi \neq 0} \left\{ |\tilde{\mathbf{p}}(\xi)|^2 + |\tilde{\mathbf{q}}(\xi)|^2 \right\} \\
&= \frac{1}{2}\sum_{\xi \neq 0} \left\{ \Re e^2(\tilde{\mathbf{p}}(\xi)) + \Im m^2(\tilde{\mathbf{p}}(\xi)) + \Re e^2(\tilde{\mathbf{q}}(\xi)) + \Im m^2(\tilde{\mathbf{q}}(\xi)\right\}.
\end{aligned}$$

Since $\mathbf{p_x}, \mathbf{q_x}$ are real, $\Re e(\tilde{\mathbf{p}}), \Re e(\tilde{\mathbf{q}})$ are even and $\Im m(\tilde{\mathbf{p}}), \Im m(\tilde{\mathbf{q}})$ are odd:

$$\begin{aligned}
&\Re e(\tilde{\mathbf{p}})(\xi) = \Re e(\tilde{\mathbf{p}})(-\xi), \quad \Re e(\tilde{\mathbf{q}})(\xi) = \Re e(\tilde{\mathbf{q}})(-\xi), \\
&\Im m(\tilde{\mathbf{p}})(\xi) = -\Im m(\tilde{\mathbf{p}})(-\xi), \quad \Im m(\tilde{\mathbf{q}})(\xi) = -\Im m(\tilde{\mathbf{q}})(-\xi).
\end{aligned} \tag{126}$$

On $\mathbb{Z}_N^d \backslash \{0\}$, we define the relation $\xi \sim \xi'$ if and only if $\xi = -\xi'$. Let $\mathbb{U}_N^d$ be a class of representants for $\sim$ ($\mathbb{U}_N^d$ is of cardinal $(N^d - 1)/2$). With these notations and by using (126), we have

$$\mathcal{H}_N = \sum_{\xi \in \mathbb{U}_N^d} \left\{ \Re e^2(\tilde{\mathbf{p}}(\xi)) + \Im m^2(\tilde{\mathbf{p}}(\xi)) + \Re e^2(\tilde{\mathbf{q}}(\xi)) + \Im m^2(\tilde{\mathbf{q}}(\xi)\right\}. \tag{127}$$

It follows that in the microcanonical state, the random variables

$$((\Re e \tilde{\mathbf{p}})(\xi), \quad (\Im m \tilde{\mathbf{p}})(\xi), \quad (\Re e \tilde{\mathbf{q}})(\xi), \quad \Im m \tilde{\mathbf{q}})(\xi))_{\xi \in \mathbb{U}_N^d}$$

are distributed according to the uniform measure on the sphere of radius $\sqrt{N^d \mathcal{E}}$ (which is not true without the restriction on the set $\mathbb{U}_N^d$). The classical results of equivalence of ensembles for the uniform measure on the sphere ([10]) can be applied for these random variables.

i) By using inverse Fourier transform and (126), we have

$$\left\langle \left(p_0^j p_{\mathbf{e}_1}^i\right)^2 \right\rangle_{N,\mathcal{E}} = \frac{1}{N^{2d}} \sum_{\xi,\xi',\eta,\eta' \neq 0} \left\langle \tilde{p}^j(\xi)\tilde{p}^j(\xi')\tilde{p}^i(\eta)\tilde{p}^i(\eta') \right\rangle_{N,\mathcal{E}} e^{-\dfrac{2i\pi \mathbf{e}_1 \cdot (\eta+\eta')}{N}}. \tag{128}$$

It is easy to check by using (ii) of Lemma 5 that the only terms in this sum which are nonzero are only for $\xi' = -\xi$ and $\eta = -\eta'$. One gets hence

$$\left\langle \left(p_0^j p_{\mathbf{e}_1}^i\right)^2 \right\rangle_{N,\mathcal{E}} = \frac{1}{N^{2d}} \sum_{\xi,\eta \neq 0} \left\langle \left|\tilde{p}^j(\xi)\right|^2 \left|\tilde{p}^i(\eta)\right|^2 \right\rangle_{N,\mathcal{E}}. \tag{129}$$

Classical equivalence of ensembles estimates of [10] show that this last sum is equal to $(\mathcal{E}/d)^2 + O(N^{-d})$.

ii) Similarly, one has

$$\begin{aligned}\left\langle (p_0^i p_{\mathbf{e}_1}^i p_0^j p_{\mathbf{e}_1}^j) \right\rangle_{N,\mathcal{E}} &= \frac{1}{N^{2d}} \sum_{\xi,xi',\eta,\eta' \neq 0} \left\langle \tilde{p}^i(\xi)\tilde{p}^i(\xi')\tilde{p}^j(\eta)\tilde{p}^j(\eta') \right\rangle_{N,\mathcal{E}} \\ &\quad \times \exp\left(-\frac{2i\pi \mathbf{e}_1}{N} \cdot (\xi' + \eta')\right).\end{aligned} \tag{130}$$

It is easy to check by using (ii) of Lemma 5 that the only terms in this sum which are nonzero are for $\xi' = -\xi$ and $\eta' = -\eta$. One gets hence

$$\begin{aligned}\left\langle (p_0^i p_{\mathbf{e}_1}^i p_0^j p_{\mathbf{e}_1}^j) \right\rangle_{N,\mathcal{E}} &= \frac{1}{N^{2d}} \sum_{\xi,\eta \neq 0} \left\langle \left|\tilde{p}^i(\xi)\right|^2 \left|\tilde{p}^j(\eta)\right|^2 \right\rangle_{N,\mathcal{E}} \\ &\quad \times \exp\left(\frac{2i\pi \mathbf{e}_1}{N} \cdot (\xi + \eta)\right).\end{aligned} \tag{131}$$

Using classical equivalence of ensembles estimates ([10]), one obtains

$$\left\langle (p_0^i p_{\mathbf{e}_1}^i p_0^j p_{\mathbf{e}_1}^j) \right\rangle_{N,\mathcal{E}} = \frac{\mathcal{E}^2}{d^2} \left(\frac{1}{N^d} \sum_{\xi \neq 0} e^{\dfrac{2i\pi \mathbf{e}_1}{N} \cdot \xi} \right)^2 + O(N^{-d}) = O(N^{-d}). \tag{132}$$

iii) By using the symmetry properties, we have

$$\left\langle \tilde{q}^j(\xi)\tilde{q}^j(\xi')\tilde{p}^j(\eta)\tilde{p}^j(\eta') \right\rangle_{N,\mathcal{E}} = 0$$

for $\xi \neq -\xi'$ or $\eta \neq -\eta'$. Hence one has

$$\begin{aligned}
&\left\langle q_{\mathbf{x}}^j q_{\mathbf{z}}^j (p_0^j)^2 \right\rangle_{N,\mathcal{E}} \\
&\quad = \frac{1}{N^{3d}} \sum_{\xi,\xi',\eta,\eta'\neq 0} \left\langle \tilde{q}^j(\xi)\tilde{q}^j(\xi')\tilde{p}^j(\eta)\tilde{p}^j(\eta')\right\rangle_{N,\mathcal{E}} \frac{\exp\left(-2i\pi(\xi\cdot\mathbf{z}+\xi'\cdot\mathbf{y})/N\right)}{\omega(\xi)\omega(\xi')} \\
&\quad = \frac{1}{N^{3d}} \sum_{\xi,\eta\neq 0} \left\langle \left|\tilde{q}^j(\xi)\tilde{p}^i(\eta)\right|^2\right\rangle_{N,\mathcal{E}} \frac{\exp\left(-2i\pi\xi\cdot(\mathbf{z}-\mathbf{y})/N\right)}{\omega(\xi)^2} \\
&\quad = \frac{1}{N^{2d}} \sum_{\xi\neq 0} \left\langle \left|\tilde{q}^j(\xi)\tilde{p}^j(\mathbf{e}_1)\right|^2\right\rangle_{N,\mathcal{E}} \frac{\exp\left(-2i\pi\xi\cdot(\mathbf{z}-\mathbf{y})/N\right)}{\omega(\xi)^2},
\end{aligned}$$

Estimates of [10] give

$$\left|\left\langle (\tilde{q}^j(\xi))^2(\tilde{p}^j(\mathbf{e}_1))^2\right\rangle_{N,\mathcal{E}} - \left(\frac{\mathcal{E}}{d}\right)^2\right| \leq \frac{C}{N^d}.$$

It follows that

$$\left\langle q_{\mathbf{y}}^j (q_{-\mathbf{e}_1}^j - q_{\mathbf{e}_1}^j)(p_0^j)^2\right\rangle_{N,\mathcal{E}} = \frac{\mathcal{E}^2}{dN^{2d}} \sum_{\xi\neq 0} \frac{e^{-2i\pi\xi\cdot(-\mathbf{e}_1-\mathbf{y})/N} - e^{-2i\pi\xi\cdot(\mathbf{e}_1-\mathbf{y})/N}}{\omega(\xi)^2} + R_N,$$

where

$$|R_N| \leq CN^{-2d} \sum_{\xi\neq 0} \frac{|\sin(2\pi\xi^1/N)|}{4\alpha\sum_{k=1}^d \sin^2(\pi\xi^k/N)}.$$

To obtain iii) observe that

$$\frac{1}{N^{2d}} \sum_{\xi\neq 0} \frac{e^{-2i\pi\xi\cdot(-\mathbf{e}_1-\mathbf{y})/N} - e^{-2i\pi\xi\cdot(\mathbf{e}_1-\mathbf{y})/N}}{\omega(\xi)^2} = \Gamma_N(y)$$

and

$$N^{-2d} \sum_{\xi\neq 0} \frac{|\sin(2\pi\xi^1/N)|}{4\alpha\sum_{k=1}^d \sin^2(\pi\xi^k/N)} \sim \begin{cases} \log N/N, & d=1 \\ 1/N, & d=2 \\ 1/N^d, & d\geq 3. \end{cases}$$

□

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References

1. Basile, G., Bernardin, C., Olla, S.: A momentum conserving model with anomalous thermal conductivity in low dimension. Phys. Rev. Lett. **96**, 204303 (2006)
2. Basile, G., Olla, S., Spohn, H.: *Energy transport in stochastically perturbed lattice dynamics*. http://arxiv.org/abs/0805.3012, 2008
3. Bernardin, C., Olla, S.: Fourier's law for a microscopic model of heat conduction. J. Stat. Phys. **121**(3/4), 271–289 (2005)
4. Bodineau, T., Helffer, B.: Correlations, Spectral gap and Log-Sobolev inequalities for unbounded spins systems. In: *Differential equations and mathematical physics* (*Birmingham, AL, 1999*), AMS/IP Stud. Adv. Math., **16**, Providence, RI: Amer. Math. Soc., 2000, pp 51–66
5. Bolsterli, M., Rich, M., Visscher, W.M.: Simulation of nonharmonic interactions in a crystal by self-consistent reservoirs. Phys. Rev. A **4**, 1086–1088 (1970)
6. Bonetto, F., Lebowitz, J.L., Rey-Bellet, L.: Fourier's law: A challenge to theorists, In: *Mathematical Physics 2000*, Fokas, A. et al. (eds.), London, Imperial College Press, 2000, pp. 128–150
7. 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)
8. Bricmont, J., Kupianen, A.: Towards a Derivation of Fouriers Law for Coupled Anharmonic Oscillators. Comm. Math. Phys. **274**(3), 555–626 (2007)
9. Deuschel, J.D., Delmotte, T.: On estimating the derivative of symmetric diffusions in stationary random environment, with pplications to $\nabla\phi$ interface model. Prob. Theory Relat. Fields **133**, 358–390 (2005)
10. Diaconis, P., Freedman, D.: A dozen de Finetti style results in search of a theory. Ann. Inst. H. Poincaré (Probabilités Et Statistiques), **23**, 397–423 (1987)
11. Ikeda, N., Watanabe, S.: *Stochastic differential equations and diffusion processes*, North-Holland Mathematical Library, **24**. Amsterdam: North-Holland Publishing Co., 1989
12. Jara, M., Komorowski, T., Olla, S.: *Limit theorems for additive functionals of a Markov chain*. http://arxiv.org/abs/0809.0177, 2008
13. Lepri, S., Livi, R., Politi, A.: Thermal Conduction in classical low-dimensional lattices. Phys Rep. **377**, 1–80 (2003)
14. Mangad, M.: Asymptotic expansions of Fourier transforms and discrete polyharmonic Green's functions. Pacific J. Math. **20**, 85–98 (1967)
15. Lebowitz, J.L., Lieb, E., Rieder, Z.: Properties of harmonic crystal in a stationary non-equilibrium state. J. Math. Phys. **8**, 1073–1078 (1967)
16. Sethuraman, S.: Central limit theorems for additive functionals of the simple exclusion process. Ann. Probab. **28**(1), 277–302 (2000)
17. Spohn, H.: *Large Scale Dynamics of interacting Particles*. Berlin-Heidelberg-New York: Springer, 1991

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