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THERMAL CONDUCTIVITY FOR A MOMENTUM CONSERVING MODEL

GIADA BASILE, CÉDRIC BERNARDIN, AND STEFANO OLLA

ABSTRACT. We present here complete mathematical proofs of the results announced in cond-mat/0509688. 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 harmonic oscillators perturbed by a stochastic dynamics conserving momentum and energy. We compute the finite-size thermal conductivity via Green-Kubo formula. In the limit as the size N of the system goes to infinity, conductivity diverges like N in dimension 1 and like $\ln N$ in dimension 2. Conductivity remains finite if $d \geq 3$ or if a pinning (on site potential) is present.

1. INTRODUCTION

We consider a system of harmonic (linear) coupled oscillators where the Hamiltonian dynamics are perturbed by a random exchange of momentum between nearest neighbors atoms. The random exchange of momentum conserves the total momentum and the total energy. We construct this noise with a diffusion on the surface of constant kinetic energy and momentum. Because of the conservation laws, this noise introduces a certain non-linearity in the model.

We compute explicitly the conductivity κ_N of the finite closed system of linear size N , by using Green-Kubo formula for the dynamics in the microcanonical ensemble. We find that it has a finite explicit limit as $N \rightarrow \infty$ in $d \geq 3$ or in the pinned cases, while it diverges like N in the unpinned 1-dimensional case, and like $\log N$ in the unpinned 2-dimensional case.

We compute also the thermal conductivity of the open system in contact with thermal reservoirs at different temperatures and we show that it coincides with the Green-Kubo definition.

The main difficulty in the calculation is in the use of certain equivalence of ensembles estimates that we prove separately in section 4.

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Key words and phrases. Thermal conductivity, Green-Kubo formula, anomalous heat transport, Fourier's law, non-equilibrium systems.

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2. THE DYNAMICS OF THE CLOSED SYSTEM

We consider the dynamics of the closed system of length N with periodic boundary conditions. The Hamiltonian is given by

$$\mathcal{H}_N = \frac{1}{2} \sum_{\mathbf{x}} [\mathbf{p}_{\mathbf{x}}^2 + \mathbf{q}_{\mathbf{x}} \cdot (\nu I - \alpha \Delta) \mathbf{q}_{\mathbf{x}}] .$$

The atoms are labeled by $\mathbf{x} \in \mathbb{T}_N^d$, the d -dimensional discrete torus of length N . We identify $\mathbb{T}_N^d = (\mathbb{Z}/N\mathbb{Z})^d$, i.e. $\mathbf{x} = \mathbf{x} + kN\mathbf{e}_j$ for any $j = 1, \dots, d$ and $k \in \mathbb{Z}$. We denote with ∇ , ∇^* and $\Delta = \nabla^* \cdot \nabla$ respectively the discrete gradient, its adjoint and the discrete Laplacian on \mathbb{T}_N^d . These are defined as

$$\nabla_{\mathbf{e}_j} f(\mathbf{x}) = f(\mathbf{x} + \mathbf{e}_j) - f(\mathbf{x}) \quad (1)$$

and

$$\nabla_{\mathbf{e}_j}^* f(\mathbf{x}) = f(\mathbf{x}) - f(\mathbf{x} - \mathbf{e}_j) \quad (2)$$

$\{\mathbf{q}_{\mathbf{x}}\}$ are the displacements of the atoms from their equilibrium positions. The parameter $\alpha > 0$ is the strength of the interparticles springs, and $\nu \geq 0$ is the strength of the pinning (on-site potential).

We consider the stochastic dynamics corresponding to the Fokker-Planck equation

$$\frac{\partial P}{\partial t} = (-A + \gamma S)P = LP . \quad (3)$$

where A is the usual Hamiltonian vector field

$$A = \sum_{\mathbf{x}} \{ \mathbf{p}_{\mathbf{x}} \cdot \partial_{\mathbf{q}_{\mathbf{x}}} + [(\alpha \Delta - \nu I) \mathbf{q}_{\mathbf{x}}] \cdot \partial_{\mathbf{p}_{\mathbf{x}}} \}$$

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 $\{\mathbf{p}_{\mathbf{x}}\}$ and generates a diffusion on the surface of constant kinetic energy and constant momentum. This is defined as follows. For every nearest neighbor atoms \mathbf{x} and \mathbf{z} , consider the $d - 1$ dimensional surface of constant kinetic energy and momentum

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

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

$$X_{\mathbf{x},\mathbf{z}}^{i,j} = (p_{\mathbf{z}}^j - p_{\mathbf{x}}^j)(\partial_{p_{\mathbf{z}}^i} - \partial_{p_{\mathbf{x}}^i}) - (p_{\mathbf{z}}^i - p_{\mathbf{x}}^i)(\partial_{p_{\mathbf{z}}^j} - \partial_{p_{\mathbf{x}}^j}) .$$

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

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

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

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

$$S \sum_{\mathbf{x}} \mathbf{p}_{\mathbf{x}} = 0, \quad S \mathcal{H}_N = 0$$

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, and we define

$$S = \frac{1}{6} \sum_{x \in \mathbb{T}_N^1} (Y_x)^2$$

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 Fokker-Planck equation (3) gives the time evolution of the probability distribution $P(\mathbf{q}, \mathbf{p}, t)$, given an initial distribution $P(\mathbf{q}, \mathbf{p}, 0)$. It correspond to the law at time t of the solution of the following stochastic differential equations:

$$\begin{aligned} d\mathbf{q}_{\mathbf{x}} &= \mathbf{p}_{\mathbf{x}} dt \\ d\mathbf{p}_{\mathbf{x}} &= -(\nu I - \alpha \Delta)\mathbf{q}_{\mathbf{x}} dt + 2\gamma \Delta \mathbf{p}_{\mathbf{x}} dt \\ &\quad + \frac{\sqrt{\gamma}}{2\sqrt{d-1}} \sum_{\mathbf{z}: \|\mathbf{z}-\mathbf{x}\|=1} \sum_{i,j=1}^d (X_{\mathbf{x},\mathbf{z}}^{i,j} \mathbf{p}_{\mathbf{x}}) dw_{\mathbf{x},\mathbf{z}}^{i,j}(t) \end{aligned} \quad (4)$$

where $\{w_{\mathbf{x},\mathbf{y}}^{i,j} = w_{\mathbf{y},\mathbf{x}}^{i,j}; \mathbf{x}, \mathbf{y} \in \mathbb{T}_N^d; i, j = 1, \dots, d; \|\mathbf{y} - \mathbf{x}\| = 1\}$ are independent standard Wiener processes. In $d = 1$ the sde are:

$$\begin{aligned} dp_x &= -(\nu I - \alpha \Delta)q_x dt + \frac{\gamma}{6} \Delta(4p_x + p_{x-1} + p_{x+1})dt \\ &\quad + \sqrt{\frac{\gamma}{3}} \sum_{k=-1,0,1} (Y_{x+k} p_x) dw_{x+k}(t) \end{aligned} \quad (5)$$

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

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

$$e_{\mathbf{x}} = \frac{1}{2} \mathbf{p}_{\mathbf{x}}^2 + \frac{\alpha}{4} \sum_{\mathbf{y}: |\mathbf{y}-\mathbf{x}|=1} (\mathbf{q}_{\mathbf{y}} - \mathbf{q}_{\mathbf{x}})^2 + \frac{\nu}{2} \mathbf{q}_{\mathbf{x}}^2,$$

the energy conservation law can be read locally as

$$e_{\mathbf{x}}(t) - e_{\mathbf{x}}(0) = \sum_{k=1}^d (J_{\mathbf{x}-\mathbf{e}_k, \mathbf{x}}(t) - J_{\mathbf{x}, \mathbf{x}+\mathbf{e}_k}(t))$$

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

$$J_{\mathbf{x}, \mathbf{x}+\mathbf{e}_k}(t) = \int_0^t j_{\mathbf{x}, \mathbf{x}+\mathbf{e}_k}(s) ds + M_{\mathbf{x}, \mathbf{x}+\mathbf{e}_k}(t). \quad (6)$$

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

$$M_{\mathbf{x}, \mathbf{x}+\mathbf{e}_k}(t) = \sqrt{\frac{\gamma}{(d-1)}} \sum_{i,j} \int_0^t \left(X_{\mathbf{x}, \mathbf{x}+\mathbf{e}_k}^{i,j} e_{\mathbf{x}} \right) (s) dw_{\mathbf{x}, \mathbf{x}+\mathbf{e}_k}^{i,j}(s) \quad (7)$$

In $d = 1$ these martingales write explicitly as

$$M_{x, x+1} = \sqrt{\frac{\gamma}{3}} \int_0^t \sum_{k=-1,0,1} (Y_{x+k} e_x) dw_{x+k}(t) \quad (8)$$

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

$$L e_{\mathbf{x}} = \sum_{k=1}^d (j_{\mathbf{x}-\mathbf{e}_k, \mathbf{x}} - j_{\mathbf{x}, \mathbf{x}+\mathbf{e}_k})$$

and it can be written as

$$j_{\mathbf{x}, \mathbf{x}+\mathbf{e}_k} = j_{\mathbf{x}, \mathbf{x}+\mathbf{e}_k}^a + \gamma j_{\mathbf{x}, \mathbf{x}+\mathbf{e}_k}^s. \quad (9)$$

The first term in (9) is the Hamiltonian contribution to the energy current

$$j_{\mathbf{x}, \mathbf{x}+\mathbf{e}_k}^a = -\frac{\alpha}{2} (\mathbf{q}_{\mathbf{x}+\mathbf{e}_k} - \mathbf{q}_{\mathbf{x}}) \cdot (\mathbf{p}_{\mathbf{x}+\mathbf{e}_k} + \mathbf{p}_{\mathbf{x}}) \quad (10)$$

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

$$\gamma j_{\mathbf{x}, \mathbf{x}+\mathbf{e}_k}^s = -\gamma \nabla_{\mathbf{e}_k} \mathbf{p}_{\mathbf{x}}^2 \quad (11)$$

and in $d = 1$ is

$$\begin{aligned} \gamma j_{x, x+1}^s &= -\gamma \nabla \varphi(p_{x-1}, p_x, p_{x+1}) \\ \varphi(p_{x-1}, p_x, p_{x+1}) &= \frac{1}{6} [p_{x+1}^2 + 4p_x^2 + p_{x-1}^2 + p_{x+1}p_{x-1} - 2p_{x+1}p_x - 2p_xp_{x-1}] \end{aligned}$$

3. GREEN-KUBO FORMULA

We define conductivity using the microcanonical version of the Green-Kubo formula.

The microcanonical measure is usually defined as the uniform measure on the energy surface defined by $\mathcal{H}_N = N^d e$. Our dynamics conserve also $(\sum_{\mathbf{x}} \mathbf{p}_{\mathbf{x}})^2 + \nu (\sum_{\mathbf{x}} \mathbf{q}_{\mathbf{x}})^2$. Notice that the dynamics is invariant under the change of coordinates $\mathbf{p}'_{\mathbf{x}} = \mathbf{p}_{\mathbf{x}} - \sum_{\mathbf{y}} \mathbf{p}_{\mathbf{y}}$ and $\mathbf{q}'_{\mathbf{x}} = \mathbf{q}_{\mathbf{x}} - \sum_{\mathbf{y}} \mathbf{q}_{\mathbf{y}}$. Consequently, without any loss of generality, we can fix $\sum_{\mathbf{x}} \mathbf{p}_{\mathbf{x}} = 0$ and $\sum_{\mathbf{x}} \mathbf{q}_{\mathbf{x}} = 0$. So in

the following we define as microcanonical measure the uniform probability measure on the $(N^{2d} - 2d - 1)$ -dimensional sphere

$$\left\{ \mathcal{H}_N = N^d e; \sum_{\mathbf{x}} \mathbf{p}_{\mathbf{x}} = 0; \sum_{\mathbf{x}} \mathbf{q}_{\mathbf{x}} = 0 \right\}$$

We denote by $\langle \cdot \rangle_N$ the expectation with respect to the microcanonical measure. The conductivity of the finite system in the direction \mathbf{e}_1 is defined as

$$\begin{aligned} \kappa_N^{1,1} &= \lim_{t \rightarrow \infty} \frac{d}{2e^2 t} \sum_{\mathbf{x}} \mathbb{E} (J_{\mathbf{x}, \mathbf{x} + \mathbf{e}_1}(t) J_{0, \mathbf{e}_1}(t)) \\ &= \lim_{t \rightarrow \infty} \frac{d}{2e^2 t} \frac{1}{N^d} \mathbb{E} \left(\left[\sum_{\mathbf{x}} J_{\mathbf{x}, \mathbf{x} + \mathbf{e}_1}(t) \right]^2 \right) \end{aligned} \quad (12)$$

where \mathbb{E} is the expectation starting with the microcanonical distribution defined above. We have used in (12) the translation invariance property of the microcanonical measure of the dynamics. Notice that the prefactor $\frac{d}{2e^2 t}$ is justified because the compressibility

$$\chi_N = \sum_{\mathbf{x}} (\langle e_{\mathbf{x}} e_0 \rangle_N - e^2) \underset{N \rightarrow \infty}{\sim} \frac{e^2}{d} \quad (13)$$

Theorem 1. *If $\nu = 0$, $\kappa_N^{1,1}$ diverges like N in dimension 1 and like $\log N$ in dimension 2. In all other cases $\kappa_N^{1,1}$ converges to a finite limit $\kappa^{1,1}$ given by*

$$\kappa^{1,1} = \gamma + \frac{\alpha^2}{2\gamma} \sum_{\mathbf{z}} (g(\mathbf{z} - \mathbf{e}_1) - g(\mathbf{z} + \mathbf{e}_1)) \Gamma(0, \mathbf{z})$$

where Γ is the kernel of the operator $(\nu I - \alpha \Delta)^{-1}$ on \mathbb{Z}^d and g is the solution of (39) on \mathbb{Z}^d if $d \geq 2$ or of (40) if $d = 1$.

The rest of this section is devoted to the proof of this theorem. The more technical computations are postponed to the appendix (section 5). We begin by the following lemma where we compute (to the main order in N) the conductivity of the finite system. Let u_N be the solution of the Poisson equation

$$Lu_N = \sum_{\mathbf{x}} j_{\mathbf{x}, \mathbf{x} + \mathbf{e}_1}^a$$

given explicitly in lemma 5.

Lemma 1.

$$\kappa_N^{1,1} = \gamma - \frac{d}{e^2} \langle j_{0, \mathbf{e}_1}^a u_N \rangle_N + \frac{O_N}{N^d} \quad (14)$$

where O_N is bounded in N .

Proof. Using the periodic conditions, we can write

$$\begin{aligned} \sum_{\mathbf{x}} J_{\mathbf{x}, \mathbf{x}+\mathbf{e}_1}(t) &= \int_0^t \sum_{\mathbf{x}} j_{\mathbf{x}, \mathbf{x}+\mathbf{e}_1}^a(s) ds + \sum_{\mathbf{x}} M_{\mathbf{x}, \mathbf{x}+\mathbf{e}_1}(t) \\ &= \int_0^t (Lu_N)(s) ds + \sum_{\mathbf{x}} M_{\mathbf{x}, \mathbf{x}+\mathbf{e}_1}(t) \\ &= u_N(t) - u_N(0) + \sum_{\mathbf{x}} \sum_k N_{\mathbf{x}, \mathbf{x}+\mathbf{e}_k}(t) + \sum_{\mathbf{x}} M_{\mathbf{x}, \mathbf{x}+\mathbf{e}_1}(t) \end{aligned} \quad (15)$$

where the martingales $N_{\mathbf{x}, \mathbf{x}+\mathbf{e}_k}$ are given by the stochastic integrals

$$N_{\mathbf{x}, \mathbf{x}+\mathbf{e}_k} = -\sqrt{\frac{\gamma}{(d-1)}} \sum_{\mathbf{x}} \sum_{i,j} \int_0^t \left(X_{\mathbf{x}, \mathbf{x}+\mathbf{e}_k}^{i,j} u_N \right) (s) dw_{\mathbf{x}, \mathbf{x}+\mathbf{e}_k}^{i,j}(s) \quad (16)$$

and in dimension 1 by

$$N_{x, x+1} = -\sqrt{\frac{\gamma}{3}} \sum_x \sum_{j=-1}^1 (Y_{x+j} u_N)(s) dw_{x+j}(s)$$

The first term of the RHS of (15) clearly goes to zero with t going to infinity since it is bounded by

$$2t^{-1} (\mathbb{E}(u_N^2(t)) + \mathbb{E}(u_N^2(0))) = 4t^{-1} \langle u_N^2 \rangle_N = O(t^{-1}) \quad (17)$$

Hence, we can forget the term $u_N(t) - u_N(0)$ of the last formula. In order to compute the expectation of the square of what is left, observe that

$$\begin{aligned} &\frac{d-1}{\gamma} \mathbb{E} \left(\left[\sum_{\mathbf{x}, k} N_{\mathbf{x}, \mathbf{x}+\mathbf{e}_k}(t) \right] \left[\sum_{\mathbf{x}} M_{\mathbf{x}, \mathbf{x}+\mathbf{e}_1}(t) \right] \right) \\ &= -\mathbb{E} \left(\left[\sum_{\mathbf{x}} \sum_{k, i, j} \int_0^t \left(X_{\mathbf{x}, \mathbf{x}+\mathbf{e}_k}^{i,j} u_N \right) (s) dw_{\mathbf{x}, \mathbf{x}+\mathbf{e}_k}^{i,j}(s) \right] \left[\sum_{\mathbf{y}} \sum_{l, r} \int_0^t \left(X_{\mathbf{y}, \mathbf{y}+\mathbf{e}_1}^{l,r} e_{\mathbf{y}} \right) (s) dw_{\mathbf{y}, \mathbf{y}+\mathbf{e}_1}^{l,r}(s) \right] \right) \\ &= -t \sum_{\mathbf{x}} \sum_{i, j} \left\langle \left(X_{\mathbf{x}, \mathbf{x}+\mathbf{e}_1}^{i,j} u_N \right) \left(X_{\mathbf{x}, \mathbf{x}+\mathbf{e}_1}^{i,j} e_{\mathbf{x}} \right) \right\rangle_N = t \sum_{\mathbf{x}} \sum_{i, j} \left\langle u_N \left(X_{\mathbf{x}, \mathbf{x}+\mathbf{e}_1}^{i,j} \right)^2 e_{\mathbf{x}} \right\rangle_N \\ &= 2t \sum_{\mathbf{x}} \langle u_N \nabla_{\mathbf{e}_1} \mathbf{p}_{\mathbf{x}}^2 \rangle_N = 0 \end{aligned}$$

and a similar calculation is true in $d = 1$.

In particular, we have

$$\lim_{t \rightarrow \infty} \mathbb{E} \left(\left[\int_0^t \sum_{\mathbf{x}} j_{\mathbf{x}, \mathbf{x}+\mathbf{e}_1}^a(s) ds \right] \left[\sum_{\mathbf{x}} M_{\mathbf{x}, \mathbf{x}+\mathbf{e}_1}(t) \right] \right) = 0 \quad (18)$$

Furthermore

$$\begin{aligned} &\frac{1}{t} \mathbb{E} \left(\left[\sum_{\mathbf{x}} M_{\mathbf{x}, \mathbf{x}+\mathbf{e}_1}(t) \right]^2 \right) = \frac{\gamma}{(d-1)} \sum_{\mathbf{x}} \sum_{i, j} \left\langle \left(X_{\mathbf{x}, \mathbf{x}+\mathbf{e}_1}^{i,j} (\mathbf{p}_{\mathbf{x}}^2/2) \right)^2 \right\rangle_N \\ &= \frac{\gamma}{(d-1)} \sum_{\mathbf{x}} \sum_{i \neq j} \left\langle \left(p_{\mathbf{x}}^j p_{\mathbf{x}+\mathbf{e}_1}^i - p_{\mathbf{x}}^i p_{\mathbf{x}+\mathbf{e}_1}^j \right)^2 \right\rangle_N \\ &= \frac{2\gamma}{(d-1)} \sum_{\mathbf{x}} \sum_{i \neq j} \langle (p_{\mathbf{x}}^j p_{\mathbf{x}+\mathbf{e}_1}^i)^2 \rangle_N - \frac{2\gamma}{(d-1)} \sum_{\mathbf{x}} \sum_{i \neq j} \langle (\mathbf{p}_{\mathbf{x}}^i \mathbf{p}_{\mathbf{x}+\mathbf{e}_1}^i \mathbf{p}_{\mathbf{x}}^j \mathbf{p}_{\mathbf{x}+\mathbf{e}_1}^j) \rangle_N \end{aligned}$$

Thanks to the equivalence of ensembles (cf. lemma 4), this last quantity is equal to

$$2\gamma N^d \frac{e^2}{d} + O_N \quad (19)$$

where O_N remains bounded as $N \rightarrow \infty$. The calculation in $d = 1$ is similar. Consequently the contribution to the conductivity given by the martingales $M_{\mathbf{x}, \mathbf{x} + \mathbf{e}_1}$ is γ .

The last term is

$$\begin{aligned} \frac{1}{t} \mathbb{E} \left(\left[\sum_{\mathbf{x}, k} N_{\mathbf{x}, \mathbf{x} + \mathbf{e}_k}(t) \right]^2 \right) &= \frac{\gamma}{(d-1)} \sum_{\mathbf{x}} \sum_{i, j, k} \left\langle \left(X_{\mathbf{x}, \mathbf{x} + \mathbf{e}_k}^{i, j}(u_N) \right)^2 \right\rangle_N \\ &= 2\gamma \langle (-S)u_N, u_N \rangle_N = 2 \langle (-L)u_N, u_N \rangle_N \\ &= -2 \left\langle \sum_{\mathbf{x}} j_{\mathbf{x}, \mathbf{x} + \mathbf{e}_1}^a, u_N \right\rangle = -2N^d \langle j_{0, \mathbf{e}_1}^a, u_N \rangle_N \end{aligned}$$

So we have proved that

$$\kappa_N^{1,1} = \lim_{t \rightarrow \infty} \frac{d}{2e^2 t} \sum_{\mathbf{x}} \mathbb{E} (J_{\mathbf{x}, \mathbf{x} + \mathbf{e}_1}(t) J_{0, \mathbf{e}_1}(t)) = \gamma - \frac{d}{e^2} \langle j_{0, \mathbf{e}_1}^a, u_N \rangle_N + \frac{O_N}{N^d} \quad (20)$$

□

Substituting in (20) the explicit form of u_N given in lemma 5, we have:

$$\begin{aligned} -\frac{d}{e^2} \langle j_{0, \mathbf{e}_1}^a, u_N \rangle_N &= \frac{\alpha^2 d}{2\gamma e^2} \sum_{\mathbf{x}, \mathbf{y}} g_N(\mathbf{x} - \mathbf{y}) \langle (\mathbf{q}_{\mathbf{e}_1} - \mathbf{q}_0) \cdot (\mathbf{p}_{\mathbf{e}_1} + \mathbf{p}_0) (\mathbf{p}_{\mathbf{x}} \cdot \mathbf{q}_{\mathbf{y}}) \rangle_N \\ &= \frac{\alpha^2 d}{2\gamma e^2} \sum_{\mathbf{x}, \mathbf{y}} g_N(\mathbf{x} - \mathbf{y}) \langle (\mathbf{q}_{\mathbf{e}_1} \cdot \mathbf{p}_0 - \mathbf{q}_0 \cdot \mathbf{p}_{\mathbf{e}_1}) (\mathbf{p}_{\mathbf{x}} \cdot \mathbf{q}_{\mathbf{y}}) \rangle_N \\ &\quad + \frac{\alpha^2 d}{2\gamma e^2} \sum_{\mathbf{x}, \mathbf{y}} g_N(\mathbf{x} - \mathbf{y}) \langle (\mathbf{q}_{\mathbf{e}_1} \cdot \mathbf{p}_{\mathbf{e}_1} - \mathbf{q}_0 \cdot \mathbf{p}_0) (\mathbf{p}_{\mathbf{x}} \cdot \mathbf{q}_{\mathbf{y}}) \rangle_N \end{aligned} \quad (21)$$

Observe that the last term of the RHS of (21) is null by the translation invariance symmetry. So we have (using again the translation invariance and the antisymmetry of g_N)

$$-\frac{d}{e^2} \langle j_{0, \mathbf{e}_1}^a, u_N \rangle_N = \frac{\alpha^2 d}{2\gamma e^2} \sum_{\mathbf{x}, \mathbf{y}} g_N(\mathbf{x} - \mathbf{y}) \langle (\mathbf{q}_{\mathbf{e}_1} - \mathbf{q}_{-\mathbf{e}_1}) \cdot \mathbf{p}_0 (\mathbf{p}_{\mathbf{x}} \cdot \mathbf{q}_{\mathbf{y}}) \rangle_N$$

Define

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

and remark that conditionally to the positions configuration \mathbf{q} , the law of \mathbf{p} is $\mu_{\mathbf{q}} = \mu^{\frac{N^d}{\sqrt{2K_N(\mathbf{q})}}}$ (defined in lemma 3), meaning the uniform measure on

the surface

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

By using properties (i),(ii) and (iii) of lemma 3, one has for $\mathbf{x} \neq 0$,

$$\begin{aligned} \langle ((\mathbf{q}_{\mathbf{e}_1} - \mathbf{q}_{-\mathbf{e}_1}) \cdot \mathbf{p}_0)(\mathbf{p}_\mathbf{x} \cdot \mathbf{q}_\mathbf{y}) \rangle_N &= \sum_{i,j} \langle \mu_{\mathbf{q}} (p_0^i p_\mathbf{x}^j) (q_{\mathbf{e}_1}^i - q_{-\mathbf{e}_1}^i) q_\mathbf{y}^j \rangle_N \\ &= \sum_i \langle \mu_{\mathbf{q}} (p_0^i p_\mathbf{x}^i) (q_{\mathbf{e}_1}^i - q_{-\mathbf{e}_1}^i) q_\mathbf{y}^i \rangle_N \\ &= - \sum_{i=1}^d \left\langle \frac{2K_N(\mathbf{q})}{dN^d(N^d - 1)} (q_{\mathbf{e}_1}^i - q_{-\mathbf{e}_1}^i) q_\mathbf{y}^i \right\rangle_N \\ &= - \frac{1}{N^d - 1} \sum_{i=1}^d \langle (p_0^i)^2 (q_{\mathbf{e}_1}^i - q_{-\mathbf{e}_1}^i) q_\mathbf{y}^i \rangle_N \end{aligned} \quad (22)$$

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

$$\begin{aligned} \langle ((\mathbf{q}_{\mathbf{e}_1} - \mathbf{q}_{-\mathbf{e}_1}) \cdot \mathbf{p}_0)(\mathbf{p}_0 \cdot \mathbf{q}_\mathbf{y}) \rangle_N &= \sum_{i,j} \langle \mu_{\mathbf{q}} (p_0^i p_0^j) (q_{\mathbf{e}_1}^i - q_{-\mathbf{e}_1}^i) q_\mathbf{y}^j \rangle_N \\ &= \sum_{i=1}^d \langle \mu_{\mathbf{q}} (p_0^i p_0^i) (q_{\mathbf{e}_1}^i - q_{-\mathbf{e}_1}^i) q_\mathbf{y}^i \rangle_N \\ &= \sum_{i=1}^d \langle (p_0^i)^2 (q_{\mathbf{e}_1}^i - q_{-\mathbf{e}_1}^i) q_\mathbf{y}^i \rangle_N \end{aligned} \quad (23)$$

Since g_N is antisymmetric (see (39-40) and such that $\sum_{\mathbf{z}} g_N(\mathbf{z}) = 0$, one obtains easily

$$\begin{aligned} - \frac{d}{e^2} \langle j_{0,\mathbf{e}_1}^a u_N \rangle_N &= - \frac{\alpha^2 d}{2\gamma e^2} \sum_{\mathbf{y}} g_N(\mathbf{y}) \sum_i \langle (p_0^i)^2 (q_{\mathbf{e}_1}^i - q_{-\mathbf{e}_1}^i) q_\mathbf{y}^i \rangle_N \\ + \frac{\alpha^2 d}{2\gamma e^2} \frac{1}{N^d - 1} \sum_{\mathbf{x} \neq 0, \mathbf{y}} g_N(\mathbf{y} - \mathbf{x}) \sum_i \langle (p_0^i)^2 (q_{\mathbf{e}_1}^i - q_{-\mathbf{e}_1}^i) q_\mathbf{y}^i \rangle_N \\ &= - \left(1 + \frac{1}{N^d - 1} \right) \frac{\alpha^2 d}{2\gamma e^2} \sum_{\mathbf{y}} g_N(\mathbf{y}) \sum_i \langle (p_0^i)^2 (q_{\mathbf{e}_1}^i - q_{-\mathbf{e}_1}^i) q_\mathbf{y}^i \rangle_N \end{aligned} \quad (24)$$

We first prove that in the case $d = 1$ and $\nu = 0$ this last quantity grows like N .

Let $G_N(z)$ the function on \mathbb{T}_N solution of the equation

$$\Delta (4G_N(z) + G_N(z+1) + G_N(z-1)) = -\delta(z) + N^{-1} \quad (25)$$

and normalized such that $\sum_z G_N(z) = 0$. We shows in appendix 5 that G_N behaves basically as the Green function of $(-\Delta)$ on \mathbb{T}_N as $N \rightarrow \infty$ and that

$g_N(z) = 3(G_N(z+1) - G_N(z-1))$. We use the notation $r_x = q_{x+1} - q_x$. Translation invariance and symmetry properties of G_N give

$$\begin{aligned} & - \sum_y g_N(y) \langle p_0^2(q_1 - q_{-1}) q_y \rangle_N \\ &= -3 \sum_y G_N(y) \langle p_0^2(q_1 - q_{-1})(q_{y-1} - q_{y+1}) \rangle_N \\ &= 3 \sum_y G_N(y) \langle p_0^2(r_0 + r_{-1})(r_y + r_{y-1}) \rangle_N \end{aligned} \quad (26)$$

Remark that in the microcanonical state, conditionally to the momentums configuration \mathbf{p} , \mathbf{r} is distributed according to the uniform measure on the surface

$$\left\{ (r_x)_{x \in \mathbb{T}_N}; \quad \alpha \sum_x r_x^2 = 2Ne - \sum_x p_x^2; \quad \sum_x r_x = 0 \right\}$$

It is easy to prove that $|\langle p_0^2 r_0^2 \rangle_N - \frac{e^2}{\alpha}| \leq C/N$ (the proof is similar to lemma 4 (i)). Consequently, by a similar argument as used for equation (24), we obtain

$$\begin{aligned} & 3 \sum_y G_N(y) \langle p_0^2(r_1 + r_0)(r_y + r_{y-1}) \rangle_N \\ &= 3 \sum_y (G_N(y+1) + 2G_N(y) + G_N(y-1)) \langle p_0^2 r_y r_0 \rangle_N \\ &= 3 \left(1 + \frac{1}{N-1}\right) (G_N(1) + 2G_N(0) + G_N(-1)) \langle p_0^2 r_0^2 \rangle_N \end{aligned}$$

It is easy to prove that $|\langle p_0^2 r_0^2 \rangle_N - \frac{e^2}{\alpha}| \leq C/N$ (the proof is similar to lemma 4 (i)). Since $G_N(0)$ and $G_N(1)$ have order N , we have obtained

$$\kappa_N = \gamma + \frac{3\alpha}{\gamma} (G_N(0) + G_N(1)) + O_N(1) \quad (27)$$

where $O_N(1)$ remains finite as $N \rightarrow \infty$.

We now deal with the cases $d \geq 2$ or $\nu > 0$. Let

$$\Gamma_N(\mathbf{x}) = (\nu I - \alpha \Delta)^{-1}(\mathbf{x})$$

By (iii) of lemma 4 and by lemma 6, we have

$$\begin{aligned}
& \left| -\frac{d}{e^2} \langle j_{0,\mathbf{e}_1}^a u_N \rangle_N - \frac{\alpha^2}{2\gamma} \sum_{\mathbf{x}} (g_N(\mathbf{x} - \mathbf{e}_1) - g_N(\mathbf{x} + \mathbf{e}_1)) \Gamma_N(\mathbf{x}) \right| \\
& \leq \frac{C\Gamma_N(0)}{N^d} \sum_{\mathbf{x}} |g_N(\mathbf{x} - \mathbf{e}_1) - g_N(\mathbf{x} + \mathbf{e}_1)| \leq \frac{C\Gamma_N(0)}{N^{d/2}} \left(\sum_{\mathbf{x}} (\nabla_{\mathbf{e}_1} g_N(\mathbf{x}))^2 \right)^{1/2} \\
& \leq \frac{C'\Gamma_N(0)}{N^{d/2}} \tag{28}
\end{aligned}$$

In lemma 7, we prove that $\Gamma_N(0) \sim \log N$ if $d = 2$ and $\nu = 0$, while it stay bounded in the cases $d \geq 3$ or $\nu > 0$. If $d = 1, \nu = 0$, this result is still valid but of minor interest since $\Gamma_N(0)$ is of order N . It explains why we considered this case separately. Hence, if $d \geq 2$ or $\nu > 0$, the last term of (28) goes to 0. And finally we have the equation

$$\kappa_N^{1,1} = \gamma + \frac{\alpha^2}{2\gamma} \sum_{\mathbf{x}} (g_N(\mathbf{x} - \mathbf{e}_1) - g_N(\mathbf{x} + \mathbf{e}_1)) \Gamma_N(\mathbf{x}) + o_N(1) \tag{29}$$

A simple Fourier analysis (see lemma 8 below) shows that, if $\nu = 0$ (i.e. the unpinned case), (29) diverges like like $\log N$ in dimension 2. In all other cases $\kappa_N^{1,1}$ converge to a finite limit $\kappa^{1,1}$ given by

$$\begin{aligned}
\kappa^{1,1} &= \gamma + \frac{\alpha^2}{2\gamma} \sum_{\mathbf{z}} (g_N(\mathbf{z} - \mathbf{e}_1) - g_N(\mathbf{z} + \mathbf{e}_1)) \Gamma(0, \mathbf{z}) \\
&= \gamma + \frac{\alpha^2}{2\gamma} \sum_{\mathbf{z}} g(\mathbf{z}) (\Gamma(0, \mathbf{z} + \mathbf{e}_1) - \Gamma(0, \mathbf{z} - \mathbf{e}_1)) \tag{30}
\end{aligned}$$

Observe that this expression diverges for $\gamma \rightarrow 0$, as expected since deterministic harmonic oscillators have infinite conductivity [4].

4. EQUIVALENCE OF ENSEMBLES

In this part, we establish a result of equivalence of ensembles for the microcanonical measure $\langle \cdot \rangle_N$ 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 ensemble for the uniform measure on the sphere. This last result proved in [3] 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}^∞) with an error of order k^{-1} . We recall first the following well known properties of the uniform measure on the sphere.

Lemma 2. (*Symmetry properties of the uniform measure on the sphere*)

Let λ_r^k be the uniform measure on the sphere

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

of radius r and dimension $dk - 1$.

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

ii) Conditionally to $\{\mathbf{x}_1, \dots, \mathbf{x}_k\} \setminus \{\mathbf{x}_i\}$, 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 3. Let μ_r^k be the uniform measure on the surface defined by

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

We have the following properties:

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

ii) If $i \neq j \in \{1, \dots, k\}$ then for every $h, \ell \in \{1, \dots, k\}$ (distincts or not), $\mu_r^k(x_h^i x_\ell^j) = 0$.

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

$$\mu_r^k(x_h^i x_\ell^i) = -\frac{r^2}{dk(k-1)} = -\frac{\mu_r^k((x_h^i)^2)}{k-1} = -\frac{\mu_r^k((x_\ell^i)^2)}{k-1} \quad (31)$$

Lemma 4. (*Equivalence of ensembles*)

There exists a positive constant $C = C(d, e)$ such that:

i) If $i \neq j$, $\left| \left\langle \left(\mathbf{p}_0^j \mathbf{p}_{\mathbf{e}_1}^i \right)^2 \right\rangle - \frac{e^2}{d^2} \right| \leq \frac{C}{N^d}$

ii) If $i \neq j$, $\left| \left\langle \left(\mathbf{p}_0^i \mathbf{p}_{\mathbf{e}_1}^i \mathbf{p}_0^j \mathbf{p}_{\mathbf{e}_1}^j \right) \right\rangle_N \right| \leq \frac{C}{N^d}$

iii) For any i and any $\mathbf{x} \in \mathbb{T}_N^d$, $\left| \left\langle \mathbf{q}_\mathbf{x}^i \mathbf{q}_0^i (\mathbf{p}_0^i)^2 \right\rangle_N - \left(\frac{e}{d} \right)^2 \Gamma_N(\mathbf{x}) \right| \leq \frac{C \Gamma_N(0)}{N^d}$

Proof. We take the Fourier transform of the positions and of the momentums (defined by (47)) and we define

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

where $\omega(\xi) = N^{-d/2} \sqrt{\nu + 4\alpha \sum_{k=1}^d \sin^2(\pi \xi^k / N)}$ is the dispersion relation. The factor $1 - \delta$ in the definition above is due to the condition $\sum_{\mathbf{x}} \mathbf{p}_\mathbf{x} = \sum_{\mathbf{x}} \mathbf{q}_\mathbf{x} = 0$ assumed in the microcanonical state. Then the energy can be written as

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

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:

$$\begin{aligned}\Re e(\tilde{\mathbf{p}})(\xi) &= \Re e(\tilde{\mathbf{p}})(-\xi), & \Re e(\tilde{\mathbf{q}})(\xi) &= \Re e(\tilde{\mathbf{q}})(-\xi) \\ \Im m(\tilde{\mathbf{p}})(\xi) &= -\Im m(\tilde{\mathbf{p}})(-\xi), & \Im m(\tilde{\mathbf{q}})(\xi) &= -\Im m(\tilde{\mathbf{q}})(-\xi)\end{aligned}\quad (32)$$

On $\mathbb{T}_N^d \setminus \{0\}$, 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 (32), we have

$$\mathcal{H}_N = \sum_{\xi \in \mathbb{U}_N^d} \{ \Re e^2(\tilde{\mathbf{p}}(\xi)) + \Im m^2(\tilde{\mathbf{p}}(\xi)) + \Re e^2(\tilde{\mathbf{q}}(\xi)) + \Im m^2(\tilde{\mathbf{q}}(\xi)) \} \quad (33)$$

It follows that in the microcanonical state, the random variables

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

are distributed according to the uniform measure on the sphere of radius $\sqrt{N^d e}$ (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 ([3]) can be applied for these random variables.

i) By using inverse Fourier transform and (32), we have

$$\left\langle \left(\mathbf{p}_0^j \mathbf{p}_{\mathbf{e}_1}^i \right)^2 \right\rangle_N = \frac{1}{N^{2d}} \sum_{\xi, \xi', \eta, \eta' \neq 0} \langle \tilde{\mathbf{p}}^j(\xi) \tilde{\mathbf{p}}^j(\xi') \tilde{\mathbf{p}}^i(\eta) \tilde{\mathbf{p}}^i(\eta') \rangle_N e^{-\frac{2i\pi \mathbf{e}_1 \cdot (\eta + \eta')}{N}} \quad (34)$$

It is easy to check by using (ii) of lemma 2 that the only terms in this sum which are nonzero are only for $\xi' = -\xi$ and $\eta = -\eta'$. One gets hence

$$\left\langle \left(\mathbf{p}_0^j \mathbf{p}_{\mathbf{e}_1}^i \right)^2 \right\rangle_N = \frac{1}{N^{2d}} \sum_{\xi, \eta \neq 0} \langle |\tilde{\mathbf{p}}^j(\xi)|^2 |\tilde{\mathbf{p}}^i(\eta)|^2 \rangle_N \quad (35)$$

Classical equivalence of ensembles estimates of [3] show that this last sum is equal to $(e/d)^2 + O(N^{-d})$.

ii) Similary, one has

$$\begin{aligned}\left\langle \left(\mathbf{p}_0^i \mathbf{p}_{\mathbf{e}_1}^i \mathbf{p}_0^j \mathbf{p}_{\mathbf{e}_1}^j \right) \right\rangle_N \\ = \frac{1}{N^{2d}} \sum_{\xi, \eta, \eta' \neq 0} \langle \tilde{\mathbf{p}}^i(\xi) \tilde{\mathbf{p}}^i(\xi') \tilde{\mathbf{p}}^j(\eta) \tilde{\mathbf{p}}^j(\eta') \rangle_N \exp\left(-\frac{2i\pi \mathbf{e}_1 \cdot (\xi' + \eta')}{N}\right)\end{aligned}\quad (36)$$

It is easy to check by using (ii) of lemma 2 that the only terms in this sum which are nonzero are only for $\xi' = -\xi$ and $\eta' = -\eta$. One gets hence

$$\left\langle \left(\mathbf{p}_0^i \mathbf{p}_{\mathbf{e}_1}^i \mathbf{p}_0^j \mathbf{p}_{\mathbf{e}_1}^j \right) \right\rangle_N = \frac{1}{N^{2d}} \sum_{\xi, \eta \neq 0} \langle |\tilde{\mathbf{p}}^i(\xi)|^2 |\tilde{\mathbf{p}}^j(\eta)|^2 \rangle_N \exp\left(\frac{2i\pi \mathbf{e}_1 \cdot (\xi + \eta)}{N}\right) \quad (37)$$

Using classical equivalence of ensembles estimates ([3]), one obtains

$$\left\langle (\mathbf{p}_0^i \mathbf{p}_{\mathbf{e}_1}^i \mathbf{p}_0^j \mathbf{p}_{\mathbf{e}_1}^j) \right\rangle_N = \frac{e^2}{d^2} \left(\frac{1}{N^d} \sum_{\xi \neq 0} e^{\frac{2i\pi \mathbf{e}_1 \cdot \xi}{N}} \right)^2 + O(N^{-d}) = O(N^{-d}) \quad (38)$$

iii) By using the symmetry properties of the measure ($\langle \tilde{q}(\xi)^i \tilde{q}(\xi')^i \tilde{\mathbf{p}}^i(\eta) \tilde{\mathbf{p}}^i(\eta') \rangle_N = 0$ for $\xi \neq -\xi'$ or $\eta \neq -\eta'$), one has

$$\begin{aligned} & \left\langle q_{\mathbf{x}}^i q_0^i (p_0^i)^2 \right\rangle_N \\ &= \frac{1}{N^{3d}} \sum_{\xi, \xi', \eta, \eta' \neq 0} \left\langle \tilde{q}(\xi)^i \tilde{q}(\xi')^i \tilde{\mathbf{p}}^i(\eta) \tilde{\mathbf{p}}^i(\eta') \right\rangle_N \frac{\exp(-2i\pi \xi \cdot \mathbf{x}/N)}{\omega(\xi) \omega(\xi')} \\ &= \frac{1}{N^{3d}} \sum_{\xi, \eta} \left\langle |\tilde{q}(\xi)^j \tilde{\mathbf{p}}^i(\eta)|^2 \right\rangle_N \frac{\exp(-2i\pi \xi \cdot \mathbf{x}/N)}{\omega(\xi)^2} \\ &= \frac{1}{N^{2d}} \sum_{\xi} \left\langle |\tilde{q}(\xi)^j \tilde{\mathbf{p}}^i(\mathbf{e}_1)|^2 \right\rangle_N \frac{\exp(-2i\pi \xi \cdot \mathbf{x}/N)}{\omega(\xi)^2} \end{aligned}$$

Estimates of [3] give

$$\left| \left\langle (\tilde{q}(\xi)^i)^2 (\tilde{\mathbf{p}}_0^i)^2 \right\rangle_N - \left(\frac{e}{d} \right)^2 \right| \leq \frac{C}{N^d}$$

and one obtains easily (iii). \square

5. APPENDIX

Lemma 5. (*Poisson equation*)

$$u_N = L^{-1} \left(\sum_{\mathbf{x}} j_{\mathbf{x}, \mathbf{x} + \mathbf{e}_1}^a \right) = \frac{\alpha}{\gamma} \sum_{\mathbf{x}, \mathbf{y}} g_N(\mathbf{x} - \mathbf{y}) \mathbf{p}_{\mathbf{x}} \cdot \mathbf{q}_{\mathbf{y}}$$

where $g_N(\mathbf{z})$ is the solution (such that $\sum_{\mathbf{z}} g_N(\mathbf{z}) = 0$) of the equation

$$4\Delta g_N(\mathbf{z}) = (\delta(\mathbf{z} - \mathbf{e}_1) - \delta(\mathbf{z} + \mathbf{e}_1)) \quad (39)$$

for $d \geq 2$, or

$$\frac{1}{3}\Delta [4g_N(z) + g_N(z+1) + g_N(z-1)] = (\delta(z-1) - \delta(z+1)) \quad (40)$$

for $d = 1$.

Moreover, $Au_N = 0$ and $Lu_N = \gamma Su_N$.

Proof. We give the proof for the dimension $d \geq 2$ since the proof for the one dimensional case is similar. Let $u_N = \frac{\alpha}{\gamma} \sum_{\mathbf{x}, \mathbf{y}} g_N(\mathbf{x} - \mathbf{y}) \mathbf{p}_{\mathbf{x}} \cdot \mathbf{q}_{\mathbf{y}}$. 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_N is null. Indeed, we have:

$$Au_N = \frac{\alpha}{\gamma} \sum_{\mathbf{x}} [(\alpha\Delta - \nu I)\mathbf{q}_{\mathbf{x}}] \cdot \left(\sum_{\mathbf{y}} g_N(\mathbf{x} - \mathbf{y})\mathbf{q}_{\mathbf{y}} \right) + \frac{\alpha}{\gamma} \sum_{\mathbf{y}, \mathbf{x}} g_N(\mathbf{x} - \mathbf{y})\mathbf{p}_{\mathbf{x}} \cdot \mathbf{p}_{\mathbf{y}} \quad (41)$$

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

$$Au_N = \frac{\alpha}{\gamma} \sum_{\mathbf{x}} [(\alpha\Delta - \nu I)g_N](\mathbf{x} - \mathbf{y})\mathbf{q}_{\mathbf{x}}\mathbf{q}_{\mathbf{y}} + \frac{\alpha}{\gamma} \sum_{\mathbf{y}, \mathbf{x}} g_N(\mathbf{x} - \mathbf{y})\mathbf{p}_{\mathbf{x}} \cdot \mathbf{p}_{\mathbf{y}} \quad (42)$$

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

$$Au_N = \sum_{\mathbf{x}, \mathbf{y}} \{a_1(\mathbf{x} - \mathbf{y})\mathbf{p}_{\mathbf{x}} \cdot \mathbf{p}_{\mathbf{y}} + a_2(\mathbf{x} - \mathbf{y})\mathbf{q}_{\mathbf{x}} \cdot \mathbf{q}_{\mathbf{y}}\} \quad (43)$$

with a_1, a_2 antisymmetric. Using the antisymmetry of a_1 and a_2 , it is easy to show that the last two sums are zero and hence $Au_N = 0$.

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

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

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

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

where in the last line, we performed an integration by parts. Since g_N is solution of (39), we have

$$\gamma S u_N = -\frac{\alpha}{2} \sum_{\mathbf{x}} \mathbf{p}_{\mathbf{x}} \cdot (\mathbf{q}_{\mathbf{x}+\mathbf{e}_1} - \mathbf{q}_{\mathbf{x}-\mathbf{e}_1}) = \sum_{\mathbf{x}} j_{\mathbf{x}, \mathbf{x}+\mathbf{e}_1}^a \quad (44)$$

□

Lemma 6. *In any dimension d , we have the uniform bound in N :*

$$\sum_{\mathbf{x} \in \mathbb{T}_N^d} (\nabla_{\mathbf{e}_1}^* g_N)^2(\mathbf{x}) \leq C(d) \quad (45)$$

If $d = 1$ then $g_N = 3[G_N(\mathbf{x} + 1) - G_N(\mathbf{x} - 1)]$ where G_N is the solution of (25) and

$$\lim_{N \rightarrow \infty} N^{-1}[G_N(0) + G_N(1)] = \frac{1}{2\pi^2} \quad (46)$$

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

$$\hat{v}(\xi) = \sum_{\mathbf{z} \in \mathbb{T}_N^d} v(\mathbf{z}) \exp(2i\pi\xi \cdot \mathbf{z}/N) \quad (47)$$

The inverse transform is given by

$$v(\mathbf{z}) = \frac{1}{N^d} \sum_{\xi \in \mathbb{T}_N^d} \hat{v}(\xi) \exp(-2i\pi\xi \cdot \mathbf{z}/N) \quad (48)$$

A simple computation shows that the Fourier transform \hat{g}_N of the function g_N is given by

$$\hat{g}_N(\xi) = -\frac{i(1 - \delta_0(\xi)) \sin(2\pi\xi^1/N)}{8 \left[\sum_{k=1}^d \sin^2(\pi\xi^k/N) \right]}, \quad \text{if } d \geq 2 \quad (49)$$

and by

$$\hat{g}_N(\xi) = -\frac{3i}{4} \frac{(1 - \delta_0(\xi)) \sin(2\pi\xi/N)}{[2 + \cos(2\pi\xi/N)] \sin^2(\pi\xi/N)}, \quad \text{if } d = 1 \quad (50)$$

Using Parseval's relation and standard analysis, one obtains the first part of the lemma.

The Fourier transform \hat{G}_N of G_N is given by

$$\hat{G}_N(\xi) = \frac{1 - \delta(\xi)}{8 \sin^2\left(\frac{\pi\xi}{N}\right) \left(2 + \cos\left(\frac{2\pi\xi}{N}\right)\right)} \quad (51)$$

Using the inverse transform and elementary trigonometric properties, one gets

$$N^{-1} [G_N(0) + G_N(1)] = \frac{1}{4N^2} \sum_{\xi \neq 0} \frac{\cos^2\left(\frac{\pi\xi}{N}\right)}{\sin^2\left(\frac{\pi\xi}{N}\right) \left(1 + \cos^2\left(\frac{\pi\xi}{N}\right)\right)} \quad (52)$$

This last quantity converges with N and its limit is given by

$$\lim_{N \rightarrow \infty} N^{-1} \int_{N^{-1}}^{1/2} \frac{\cos^2(\pi u)}{\sin^2(\pi u) (1 + \cos^2(\pi u))} du = \frac{1}{2\pi^2} \quad (53)$$

□

Lemma 7. *Let Γ_N be the kernel of the operator $(\nu I - \alpha \Delta)^{-1}$ on \mathbb{T}_N^d . Then we have*

$$\begin{aligned} \Gamma_N(0) & \text{ is of order } N \text{ if } d = 1, \nu = 0. \\ \Gamma_N(0) & \text{ is of order } \log N \text{ if } d = 2, \nu = 0. \\ \Gamma_N(0) & \text{ is of order } 1 \text{ if } d \geq 3 \text{ or } \nu = 0. \end{aligned}$$

Proof. We have

$$\hat{\Gamma}_N(\xi) = (1 - \delta(\xi)) \left(\nu + 4\alpha \sum_{k=1}^d \sin^2(\pi \xi^k / N) \right)^{-1} \quad (54)$$

so that

$$\Gamma_N(0) = \frac{1}{N^d} \sum_{\xi \neq 0} \frac{1}{\nu + 4\alpha \sum_{k=1}^d \sin^2(\pi \xi^k / N)} \quad (55)$$

Standard analysis gives the result. □

Lemma 8. $\sum_{\mathbf{x}} [g_N(\mathbf{x} - \mathbf{e}_1) - g_N(\mathbf{x} + \mathbf{e}_1)] \Gamma_N(\mathbf{x})$ diverges like N if $d = 1, \nu = 0$, like $\log N$ if $d = 2, \nu = 0$ and converges in all other cases to a finite limit given by

$$\sum_{\mathbf{z}} (g(\mathbf{z} - \mathbf{e}_1) - g(\mathbf{z} + \mathbf{e}_1))(\mathbf{z}) \Gamma(\mathbf{z})$$

where g and Γ are defined just after (30).

Proof. $\sum_{\mathbf{x}} [g_N(\mathbf{x} - \mathbf{e}_1) - g_N(\mathbf{x} + \mathbf{e}_1)] \Gamma_N(\mathbf{x})$ is equal to

$$\frac{1}{4N^d} \sum_{\xi \in \mathbb{T}_N^d \setminus \{0\}} \frac{\sin^2(2\pi \xi^1 / N)}{\left[\sum_{k=1}^d \sin^2(\pi \xi^k / N) \right] \left[\nu + 4\alpha \sum_{k=1}^d \sin^2(\pi \xi^k / N) \right]}, \quad \text{if } d \geq 2 \quad (56)$$

and to

$$\frac{6}{N} \sum_{\xi \in \mathbb{T}_N^1 \setminus \{0\}} \frac{\cos^2(\pi \xi / N)}{[2 + \cos(2\pi \xi / N)] [\nu + 4\alpha \sin^2(\pi \xi / N)]}, \quad \text{if } d = 1 \quad (57)$$

Trigonometric manipulations and standard analysis give the result by letting N going to infinity. □

6. OPEN SYSTEM

We consider now the open case where the finite system is in contact with 2 heat baths at different temperatures T_ℓ and T_r . We model these external thermal baths with Ornstein-Uhlenbeck processes at given temperatures. Let $\Xi_N = \{1, \dots, N\} \times \mathbb{T}_N^{d-1}$. Hence Ξ_N is a box of $(\mathbb{Z}^d)^N$ of length N with periodic boundary conditions in any direction different from the first direction. Atoms are now labeled by $\mathbf{x} \in \Xi_N$ and the dynamics is generated by the operator

$$L = A + \gamma S + B_\ell + B_r$$

where A and S are defined as before (with the laplacian Δ taken with Neumann boundary conditions), while B_ℓ and B_r are the contributions of the heat baths defined by

$$B_\ell = \frac{1}{2} \sum_{\mathbf{x} \in \Xi_N} \delta_1(x_1) (T_\ell \partial_{\mathbf{p}_x}^2 - \mathbf{p}_x \cdot \partial_{\mathbf{p}_x})$$

$$B_r = \frac{1}{2} \sum_{\mathbf{x} \in \Xi_N} \delta_N(x_1) (T_r \partial_{\mathbf{p}_x}^2 - \mathbf{p}_x \cdot \partial_{\mathbf{p}_x}).$$

If $T_\ell = T_r = T$ the centered gaussian product measure of variance T is the unique stationary state. When $T_\ell \neq T_r$, this system has still a unique stationary measure, but it cannot be computed explicitly. Let us denote the expectation with respect to this stationary measure with $\langle \cdot \rangle_{ss, N}$. The conductivity of this finite system can be defined as

$$\kappa_N^{ss} = \frac{N \langle j_{\mathbf{x}, \mathbf{x} + \mathbf{e}_1} \rangle_{ss, N}}{T_\ell - T_r}.$$

We prove that

$$\kappa_N^{ss} \underset{N \rightarrow \infty}{\sim} \kappa_N^{1,1}.$$

This is a consequence of a decomposition of the energy current in a space derivative plus a time derivative. In order to keep notations simple, let us consider the case $d = 1$. Define the functions

$$h_x = \frac{\alpha}{\gamma} \sum_z g(z) p_{x+z} q_x$$

and

$$\phi_x = \frac{\alpha}{2\gamma} \sum_{z \geq 1} g(z) \left[\sum_{y \geq 1}^z \psi_{x+y}^z + \alpha (q_{x-z-1} q_x - q_{x-z} q_{x-1}) \right]$$

$$+ \frac{\alpha}{2} (p_{x-1} + p_x) q_x + \gamma \varphi(p_{x-1}, p_x, p_{x+1})$$

where

$$\psi_x^z = p_{x-z} p_x + q_{x-z} (\alpha \Delta - \nu I) q_x.$$

Then by explicit calculation one can write

$$j_{x, x+1} = -\nabla \phi_x + L h_x \quad . \quad (58)$$

It follows that $\langle j_{x,x+1} \rangle_{ss,N} = -\nabla \langle \phi_x \rangle_{ss,N}$. By stationarity, this expected current is constant in x , so

$$\begin{aligned} N \langle j_{x,x+1} \rangle_{ss,N} &= \sum_x \langle j_{x,x+1} \rangle_{ss,N} \\ &= \langle \phi_1 \rangle_{ss,N} - \langle \phi_N \rangle_{ss,N} \quad . \end{aligned}$$

By the thermalization due to the heat baths, one can show that $\langle \phi_1 \rangle_{ss,N} \sim \langle \phi_1 \rangle_{N,T_\ell}$ (where $\langle \cdot \rangle_{N,T_\ell}$ (resp. $\langle \cdot \rangle_{N,T_r}$) is the grand-canonical measure at temperature T_ℓ (resp. T_r)) and $\langle \phi_N \rangle_{ss,N} \sim \langle \phi_N \rangle_{N,T_r}$. A simple checking shows that

$$\langle \phi_1 \rangle_{N,T_\ell} - \langle \phi_N \rangle_{N,T_r} \sim \kappa_N^{1,1} (T_\ell - T_r) \quad (59)$$

This argument can be made rigorous by a proper localization of the functions h and ϕ and an entropy production argument [2]. A decomposition similar to (58) is valid also in $d \geq 2$. One can use (58) directly in the Green-Kubo formula (12), obtaining the same result as above, by noticing that in the periodic case $\sum_x \nabla \phi_x = 0$ and that $\sum_x h_x = L^{-1} (\sum_{\mathbf{x}} j_{\mathbf{x},\mathbf{x}+\mathbf{e}_1}^a)$.

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7. FORMULAIRE

Some formulas we use:

$$S\mathbf{p}_{\mathbf{x}} = 2\Delta\mathbf{p}_{\mathbf{x}} \quad d \geq 2 \quad (60)$$

$$Sp_x = \frac{1}{6}\Delta(4p_x + p_{x+1} + p_{x-1}) \quad d = 1 \quad (61)$$

$$Se_{\mathbf{x}} = S\mathbf{p}_{\mathbf{x}}^2/2 = \Delta\mathbf{p}_{\mathbf{x}} \quad d \geq 2 \quad (62)$$

$$Se_x = Sp_x^2/2 = \frac{1}{6}\Delta(4p_x^2 + p_{x+1}^2 + p_{x-1}^2) \quad d = 1 \quad (63)$$

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