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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 annouced 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 current-current time correlation function and the thermal conductivity via Green-Kubo formula. We prove that the current-current time correlation function decay like $t^{-d/2}$ in the unpinned case and like $t^{-d/2-1}$ if a on-site harmonic potential is present.

1. The dynamics

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

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

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 $j = 1, \ldots, d$ 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

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

and

$$\nabla_{\mathbf{e}_{i}}^{*} f(\mathbf{x}) = f(\mathbf{x}) - f(\mathbf{x} - \mathbf{e}_{j})$$
⁽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 $\nu \ge 0$ is the strength of the pinning (on-site potential).

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

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

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where A is the usual Hamiltonian vector field

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

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 $\{\mathbf{p}_{\mathbf{x}}\}$ 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

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

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

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

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

Observe that this noise conserves the total momentum $\sum_{\mathbf{x}} \mathbf{p}_{\mathbf{x}}$ 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:

$$d\mathbf{q}_{\mathbf{x}} = \mathbf{p}_{\mathbf{x}} dt$$

$$d\mathbf{p}_{\mathbf{x}} = -(\nu I - \alpha \Delta)\mathbf{q}_{\mathbf{x}} dt + 2\gamma \Delta \mathbf{p}_{\mathbf{x}} dt$$

$$+ \frac{\sqrt{\gamma}}{2\sqrt{d-1}} \sum_{\mathbf{z}: \|\mathbf{z}-\mathbf{x}\|=1} \sum_{i,j=1}^{d} \left(X_{\mathbf{x},\mathbf{z}}^{i,j} \mathbf{p}_{\mathbf{x}} \right) dw_{\mathbf{x},\mathbf{z}}^{i,j}(t)$$
(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:

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

where here $\{w_x(t), x = 1, ..., N\}$ 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

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

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

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

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

$$M_{\mathbf{x},\mathbf{x}+\mathbf{e}_{k}}(t) = \sqrt{\frac{\gamma}{(d-1)}} \sum_{i,j} \int_{0}^{t} \left(X_{\mathbf{x},\mathbf{x}+\mathbf{e}_{k}}^{i,j} e_{\mathbf{x}} \right)(s) \, dw_{\mathbf{x},\mathbf{x}+\mathbf{e}_{k}}^{i,j}(s) \tag{7}$$

In d = 1 these martingales write explicitly as

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

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

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

and it can be written as

$$j_{\mathbf{x},\mathbf{x}+\mathbf{e}_k} = j^a_{\mathbf{x},\mathbf{x}+\mathbf{e}_k} + \gamma j^s_{\mathbf{x},\mathbf{x}+\mathbf{e}_k} \quad . \tag{9}$$

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

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

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

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

and in d = 1 is

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

2. Decay of the correlation function of the energy current

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 $(\sum_x \mathbf{p_x})^2 + \nu (\sum_\mathbf{x} \mathbf{q_x})^2$. Notice that the dynamics is invariant under the change of coordinates $\mathbf{p'_x} = \mathbf{p_x} - \sum_\mathbf{y} \mathbf{p_y}$ and $\mathbf{q'_x} = \mathbf{q_x} - \sum_\mathbf{y} \mathbf{q_y}$. Consequently, without any lost of generality, we can fix $\sum_\mathbf{x} \mathbf{p_x} = 0$ and $\sum_\mathbf{x} \mathbf{q_x} = 0$. So in the following we define as microcanonical measure the uniform probability measure on the $(N^{2d} - 2d - 1)$ -dimensional sphere

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

This is the unique invariant measure for the dynamics on this surface. We denote by $\langle \cdot \rangle_N$ (sometimes, we will omit the subscript N) the expectation with respect to the microcanonical measure .

Let us define $\mathfrak{J}_{\mathbf{e}_1} = \sum_{\mathbf{x}} j_{\mathbf{x},\mathbf{x}+\mathbf{e}_1}$. Because of the periodic boundary conditions, and being $j_{\mathbf{x},\mathbf{x}+\mathbf{e}_1}^s$ a spatial gradient (cf. (11)), we have that $\mathfrak{J}_{\mathbf{e}_1} = \sum_{\mathbf{x}} j_{\mathbf{x},\mathbf{x}+\mathbf{e}_1}^a$. We are interested in the decay of the correlation function:

$$C_{1,1}(t) = \lim_{N \to \infty} \frac{1}{N^d} \mathbb{E}(\mathfrak{J}_{\mathbf{e}_1}(t)\mathfrak{J}_{\mathbf{e}_1}(0)) = \lim_{N \to \infty} \sum_{\mathbf{x}} \mathbb{E}(j_{0,\mathbf{e}_1}^a(0)j_{\mathbf{x},\mathbf{x}+\mathbf{e}_1}^a(t)) \quad (12)$$

where \mathbb{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 5. Then we can write the Laplace transform of $C_{1,1}(t)$ as

$$\int_0^\infty e^{-\lambda t} C_{1,1}(t) \, dt = -\lim_{N \to \infty} \left\langle j_{0,\mathbf{e}_1}^a u_{\lambda,N} \right\rangle_N \tag{13}$$

Substituting in (13) the explicit form of $u_{\lambda,N}$ given in lemma 5, we have:

$$-\left\langle j_{0,\mathbf{e}_{1}}^{a}u_{\lambda,N}\right\rangle_{N} = \frac{\alpha^{2}}{2\gamma}\sum_{\mathbf{x},\mathbf{y}}g_{\lambda,N}(\mathbf{x}-\mathbf{y})\left\langle (\mathbf{q}_{\mathbf{e}_{1}}-\mathbf{q}_{0})\cdot(\mathbf{p}_{\mathbf{e}_{1}}+\mathbf{p}_{0})(\mathbf{p}_{\mathbf{x}}\cdot\mathbf{q}_{\mathbf{y}})\right\rangle_{N}$$
$$= \frac{\alpha^{2}}{2\gamma}\sum_{\mathbf{x},\mathbf{y}}g_{\lambda,N}(\mathbf{x}-\mathbf{y})\left\langle (\mathbf{q}_{\mathbf{e}_{1}}\cdot\mathbf{p}_{0}-\mathbf{q}_{0}\cdot\mathbf{p}_{\mathbf{e}_{1}})(\mathbf{p}_{\mathbf{x}}\cdot\mathbf{q}_{\mathbf{y}})\right\rangle_{N}$$
$$+ \frac{\alpha^{2}}{2\gamma}\sum_{\mathbf{x},\mathbf{y}}g_{\lambda,N}(\mathbf{x}-\mathbf{y})\left\langle (\mathbf{q}_{\mathbf{e}_{1}}\cdot\mathbf{p}_{\mathbf{e}_{1}}-\mathbf{q}_{0}\cdot\mathbf{p}_{0})(\mathbf{p}_{\mathbf{x}}\cdot\mathbf{q}_{\mathbf{y}})\right\rangle_{N}$$
(14)

Observe that the last term of the RHS of (14) is null by the translation invariance symmetry. So we have (using again the translation invariance and the antisymmetry of $g_{\lambda,N}$)

$$-\left\langle j_{0,\mathbf{e}_{1}}^{a}u_{\lambda,N}\right\rangle_{N}=\frac{\alpha^{2}}{2\gamma}\sum_{\mathbf{x},\mathbf{y}}g_{\lambda,N}(\mathbf{x}-\mathbf{y})\left\langle (\mathbf{q}_{\mathbf{e}_{1}}-\mathbf{q}_{-\mathbf{e}_{1}})\cdot\mathbf{p}_{0}\right)(\mathbf{p}_{\mathbf{x}}\cdot\mathbf{q}_{\mathbf{y}})\right\rangle_{N}$$

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 $\mu_{\mathbf{q}} = \mu_{\sqrt{2K_N(\mathbf{q})}}^{N^d}$ (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 $\mathbf{x} \neq 0$,

$$\langle ((\mathbf{q}_{\mathbf{e}_{1}} - \mathbf{q}_{\mathbf{e}_{1}}) \cdot \mathbf{p}_{0})(\mathbf{p}_{\mathbf{x}} \cdot \mathbf{q}_{\mathbf{y}}) \rangle_{N} = \sum_{i,j} \langle \mu_{\mathbf{q}} \left(\mathbf{p}_{0}^{i} \mathbf{p}_{\mathbf{x}}^{j} \right) (\mathbf{q}_{\mathbf{e}_{1}}^{i} - \mathbf{q}_{-\mathbf{e}_{1}}^{i}) \mathbf{q}_{\mathbf{y}}^{j} \rangle_{N}$$

$$= \sum_{i} \langle \mu_{\mathbf{q}} \left(\mathbf{p}_{0}^{i} \mathbf{p}_{\mathbf{x}}^{i} \right) (\mathbf{q}_{\mathbf{e}_{1}}^{i} - \mathbf{q}_{-\mathbf{e}_{1}}^{i}) \mathbf{q}_{\mathbf{y}}^{i} \rangle_{N}$$

$$= -\sum_{i=1}^{d} \left\langle \frac{2K_{N}(\mathbf{q})}{dN^{d}(N^{d} - 1)} (\mathbf{q}_{\mathbf{e}_{1}}^{i} - \mathbf{q}_{-\mathbf{e}_{1}}^{i}) \mathbf{q}_{\mathbf{y}}^{i} \right\rangle_{N}$$

$$= -\frac{1}{N^{d} - 1} \sum_{i=1}^{d} \left\langle (\mathbf{p}_{0}^{i})^{2} (\mathbf{q}_{\mathbf{e}_{1}}^{i} - \mathbf{q}_{-\mathbf{e}_{1}}^{i}) \mathbf{q}_{\mathbf{y}}^{i} \right\rangle_{N}$$

$$(15)$$

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

$$\langle ((\mathbf{q}_{\mathbf{e}_{1}} - \mathbf{q}_{\mathbf{e}_{1}}) \cdot \mathbf{p}_{0})(\mathbf{p}_{0} \cdot \mathbf{q}_{\mathbf{y}}) \rangle_{N} = \sum_{i,j} \left\langle \mu_{\mathbf{q}} \left(\mathbf{p}_{0}^{i} \mathbf{p}_{0}^{j} \right) (\mathbf{q}_{\mathbf{e}_{1}}^{i} - \mathbf{q}_{-\mathbf{e}_{1}}^{i}) \mathbf{q}_{\mathbf{y}}^{j} \right\rangle_{N}$$
$$= \sum_{i=1}^{d} \left\langle \mu_{\mathbf{q}} \left(\mathbf{p}_{0}^{i} \mathbf{p}_{0}^{i} \right) (\mathbf{q}_{\mathbf{e}_{1}}^{i} - \mathbf{q}_{-\mathbf{e}_{1}}^{i}) \mathbf{q}_{\mathbf{y}}^{i} \right\rangle_{N} \quad (16)$$
$$= \sum_{i=1}^{d} \left\langle \left(\mathbf{p}_{0}^{i} \right)^{2} (\mathbf{q}_{\mathbf{e}_{1}}^{i} - \mathbf{q}_{-\mathbf{e}_{1}}^{i}) \mathbf{q}_{\mathbf{y}}^{i} \right\rangle_{N}$$

Since $g_{\lambda,N}$ is antisymmetric (see (56-57) and such that $\sum_{\mathbf{z}} g_{\lambda,N}(\mathbf{z}) = 0$, one obtains easily

$$-\left\langle j_{0,\mathbf{e}_{1}}^{a}u_{\lambda,N}\right\rangle_{N} = -\frac{\alpha^{2}}{2\gamma}\sum_{\mathbf{y}}g_{\lambda,N}(\mathbf{y})\sum_{i}\left\langle \left(p_{0}^{i}\right)^{2}\left(q_{\mathbf{e}_{1}}^{i}-q_{-\mathbf{e}_{1}}^{i}\right)q_{\mathbf{y}}^{i}\right\rangle_{N}$$
$$+\frac{\alpha^{2}}{2\gamma}\frac{1}{N^{d}-1}\sum_{\mathbf{x}\neq0,\mathbf{y}}g_{\lambda,N}(\mathbf{y}-\mathbf{x})\sum_{i}\left\langle \left(p_{0}^{i}\right)^{2}\left(q_{\mathbf{e}_{1}}^{i}-q_{-\mathbf{e}_{1}}^{i}\right)q_{\mathbf{y}}^{i}\right\rangle_{N}$$
$$=-\left(1+\frac{1}{N^{d}-1}\right)\frac{\alpha^{2}}{2\gamma}\sum_{\mathbf{y}}g_{\lambda,N}(\mathbf{y})\sum_{i}\left\langle \left(p_{0}^{i}\right)^{2}\left(q_{\mathbf{e}_{1}}^{i}-q_{-\mathbf{e}_{1}}^{i}\right)q_{\mathbf{y}}^{i}\right\rangle_{N}$$
$$(17)$$

We work out first the case $d \ge 2$ or $\nu > 0$. Let

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

By (iii) of lemma 4 and (66), we have

$$\left| - \left\langle j_{0,\mathbf{e}_{1}}^{a} u_{\lambda,N} \right\rangle_{N} - \frac{\alpha^{2} e^{2}}{2\gamma d} \sum_{\mathbf{y}} g_{\lambda,N}(\mathbf{y}) \left(\Gamma_{N}(\mathbf{y} + \mathbf{e}_{1}) - \Gamma_{N}(\mathbf{y} - \mathbf{e}_{1}) \right) \right|$$

$$\leq \frac{C\Gamma_{N}(0)}{N^{d}} \sum_{\mathbf{y}} |g_{\lambda,N}(\mathbf{y})| \leq \frac{C\Gamma_{N}(0)}{N^{d/2}} \left(\sum_{\mathbf{x}} (g_{\lambda,N}(\mathbf{x}))^{2} \right)^{1/2} \leq \frac{C'\Gamma_{N}(0)}{\lambda N^{d/2}}$$
(18)

It is well known (cf. (68)) that $\Gamma_N(0) \sim \log N$ if d = 2 and $\nu = 0$, while it stays bounded in the cases $d \geq 3$ or $\nu > 0$. If $d = 1, \nu = 0, \Gamma_N(0)$ is of order N. This is the reason we need to consider this case separately. Hence, if $d \geq 2$ or $\nu > 0$, the last term of (18) goes to 0.

Taking the limit as $N \to \infty$ we obtain

$$\int_0^\infty e^{-\lambda t} C_{1,1}(t) \, dt = \frac{\alpha^2 e^2}{2d\gamma} \sum_{\mathbf{z}} g_\lambda(\mathbf{z}) \left(\Gamma(0, \mathbf{z} + \mathbf{e}_1) \right) - \Gamma(0, \mathbf{z} - \mathbf{e}_1) \tag{19}$$

where g_{λ} are solutions of the same equations but in \mathbb{Z}^d . Using Parseval relation and the explicit form of the Fourier transform of g_{λ} (cf. (71)), one

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gets the following formula for the Laplace transform of $C_{1,1}(t)$:

$$\frac{\alpha^2 e^2}{d} \int_{[0,1]^d} d\mathbf{k} \left(\frac{\sin^2(2\pi \mathbf{k}^1)}{\nu + 4\alpha \sum_{j=1}^d \sin^2(\pi \mathbf{k}^j)} \right) \frac{1}{\lambda + 8\gamma \sum_{j=1}^d \sin^2(\pi \mathbf{k}^j)}$$
(20)

By injectivity of Laplace transform, we have the following explicit formula for $C_{1,1}(t)$:

$$C_{1,1}(t) = \frac{\alpha^2 e^2}{d} \int_{[0,1]^d} d\mathbf{k} \left(\frac{\sin^2(2\pi \mathbf{k}^1)}{\nu + 4\alpha \sum_{j=1}^d \sin^2(\pi \mathbf{k}^j)} \right) \exp\left\{ -8\gamma t \sum_{j=1}^d \sin^2(\pi \mathbf{k}^j) \right\}$$
(21)

In the 1-dimensional case, if $\nu = 0$ we have to proceed a bit differently. Let $G_{\lambda,N}(z)$ the function on \mathbb{T}_N solution of the equation (65) for d = 1 case.

We shows in appendix 5 that $G_{\lambda,N}$ behaves basically as the Green function of $(-\Delta)$ on \mathbb{T}_N as $N \to \infty$ and that $g_{\lambda,N}(z) = (G_{\lambda,N}(z+1) - G_{\lambda,N}(z-1))$. We use the notation $r_x = q_{x+1} - q_x$. Translation invariance and symmetry properties of $G_{\lambda,N}$ give

$$-\sum_{y} g_{\lambda,N}(y) \left\langle p_{0}^{2}(q_{1}-q_{-1}) q_{y} \right\rangle_{N}$$

$$= -\sum_{y} G_{\lambda,N}(y) \left\langle p_{0}^{2}(q_{1}-q_{-1})(q_{y-1}-q_{y+1}) \right\rangle_{N}$$

$$= \sum_{y} G_{\lambda,N}(y) \left\langle p_{0}^{2}(r_{0}+r_{-1})(r_{y}+r_{y-1}) \right\rangle_{N}$$
(22)

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 (17), we obtain

$$\sum_{y} G_{\lambda,N}(y) \left\langle p_{0}^{2}(r_{1}+r_{0})(r_{y}+r_{y-1}) \right\rangle_{N}$$

= $\sum_{y} \left(G_{\lambda,N}(y+1) + 2G_{\lambda,N}(y) + G_{\lambda,N}(y-1) \right) \left\langle p_{0}^{2}r_{y}r_{0} \right\rangle_{N}$
= $\left(1 + \frac{1}{N-1} \right) \left(G_{\lambda,N}(1) + 2G_{\lambda,N}(0) + G_{\lambda,N}(-1) \right) \left\langle p_{0}^{2}r_{0}^{2} \right\rangle_{N}$

It is easy to prove that $| < p_0^2 r_0^2 >_N - \frac{e^2}{\alpha} | \le C/N$ (the proof is similar to lemma 4 (i)).

Again by taking the limit as $N \to \infty$ we obtain

$$\int_0^\infty e^{-\lambda t} C_{1,1}(t) \, dt = \frac{\alpha e^2}{\gamma} \left(G_\lambda(0) + G_\lambda(1) \right) \tag{23}$$

In appendix 5, we compute explicitly this last quantity. Elementary trigonometric manipulations then show that for $d = 1, \nu = 0$, the formula giving the Laplace transform of the current-current correlations of the energy $C_{1,1}(t)$ is still given by formula (23) (cf. (69) and (70)).

As before we have the following integral representation of the correlation function of the energy current:

$$C_{1,1}(t) = \alpha e^2 \int_0^1 dk \cos^2(\pi k) \exp\left\{-\frac{4\gamma t}{3}\sin^2(\pi k)(1+2\cos^2(\pi k))\right\}$$
(24)

In the two cases $(d \ge 2 \text{ and } d = 1)$, we obtain that $C_{1,1}(t)$ is of the form

$$C_{1,1}(t) = \frac{e^2}{4\pi^2 d} \int_{[0,1]^d} (\partial_{\mathbf{k}^1} \omega(\mathbf{k}))^2 e^{-t\gamma\psi(\mathbf{k})} d\mathbf{k}$$
(25)

where

$$\omega(\mathbf{k}) = (\nu + 4\alpha \sum_{j=1}^{d} \sin^2(\pi \mathbf{k}^j))^{1/2}$$
(26)

is the dispertion relation of the system, and

$$\psi(\mathbf{k}) = \begin{cases} 8 \sum_{j=1}^{d} \sin^2(\pi \mathbf{k}^j), & \text{if } d \ge 2\\ 4/3 \sin^2(\pi \mathbf{k})(1 + 2\cos^2(\pi \mathbf{k})), & \text{if } d = 1 \end{cases}$$
(27)

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

$$\int_{\mathbf{k}\in[0,1]^d} d\mathbf{k} \frac{(\mathbf{k}^1)^2 e^{-a\gamma t \|\mathbf{k}\|^2}}{\nu + \|\mathbf{k}\|^2} = \frac{1}{t^{d/2+1}} \int_{[0,\sqrt{t}]^d} d\mathbf{k} \frac{(\mathbf{k}^1)^2 e^{-a\gamma \|\mathbf{k}\|^2}}{\nu + t^{-1} \|\mathbf{k}\|^2}$$
(28)

Hence, we have proved the following theorem

Theorem 1. The current-current time correlation function $C_{1,1}(t)$ decays like $t^{-d/2}$ in the unpinned case ($\nu = 0$) and like $t^{-d/2-1}$ if a on-site harmonic potential is present ($\nu > 0$).

THERMAL CONDUCTIVITY

3. Green-Kubo formula

The conductivity in the direction \mathbf{e}_1 is defined by Green-Kubo formula as

$$\kappa^{1,1} = \lim_{t \to \infty} \lim_{N \to \infty} \frac{1}{2e^2 t} \sum_{\mathbf{x}} \mathbb{E} \left(J_{\mathbf{x},\mathbf{x}+\mathbf{e}_1}(t) J_{0,\mathbf{e}_1}(t) \right)$$
$$= \lim_{t \to \infty} \lim_{N \to \infty} \frac{1}{2e^2 t} \frac{1}{N^d} \mathbb{E} \left(\left[\sum_{\mathbf{x}} J_{\mathbf{x},\mathbf{x}+\mathbf{e}_1}(t) \right]^2 \right)$$
(29)

where \mathbb{E} is the expectation starting with the microcanonical distribution defined above. We have used in (29) the translation invariance property of the microcanonical measure of the dynamics.

Using the periodic boundary conditions, we can write

$$\sum_{\mathbf{x}} J_{\mathbf{x},\mathbf{x}+\mathbf{e}_1}(t) = \int_0^t \sum_{\mathbf{x}} j^a_{\mathbf{x},\mathbf{x}+\mathbf{e}_1}(s) \, ds + \sum_{\mathbf{x}} M_{\mathbf{x},\mathbf{x}+\mathbf{e}_1}(t) \tag{30}$$

so that

$$(tN^d)^{-1}E\left(\left[\sum_{\mathbf{x}} J_{\mathbf{x},\mathbf{x}+\mathbf{e}_1}(t)\right]^2\right)$$
$$=(tN^d)^{-1}E\left(\left[\sum_{\mathbf{x}} \int_0^t j_{\mathbf{x},\mathbf{x}+\mathbf{e}_1}^a(s)ds\right]^2\right) + (tN^d)^{-1}E\left(\left[\sum_{\mathbf{x}} M_{\mathbf{x},\mathbf{x}+\mathbf{e}_1}(t)\right]^2\right)$$
$$+2(tN^d)^{-1}\mathbb{E}\left(\left[\int_0^t \sum_{\mathbf{x}} j_{\mathbf{x},\mathbf{x}+\mathbf{e}_1}^a(s)\,ds\right]\left[\sum_{\mathbf{x}} M_{\mathbf{x},\mathbf{x}+\mathbf{e}_1}(t)\right]\right)$$
(31)

The limit (as $N \to \infty$ and then $t \to \infty$) of the first term of the RHS of (31) is

$$\lim_{\eta \to 0} \int_0^\infty e^{-\eta t} C_{1,1}(t) dt$$
 (32)

In the appendix, we compute this last quantity ((70), (71)). Remark that if $\nu = 0$ and d = 1, 2, this quantity is infinite. Since we prove in the sequel that the martingale term gives a finite contribution to the conductivity in any case, it follows that $\kappa^{1,1} = +\infty$ if $\nu = 0$ and d = 1 or d = 2. Concerning the second term of the RHS of (31), we have

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

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

$$2\gamma t N^d \frac{e^2}{d} + O_N \tag{33}$$

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 .

We now prove the third term is zero by a time reversal argument. Let us denote by $\{\omega(s)\}_{0\leq s\leq t}$ the process $\{(\mathbf{p}_{\mathbf{x}}(s), \mathbf{q}_{\mathbf{x}}(s); \mathbf{x} \in \mathbb{T}_N^d\}_{0\leq s\leq t}$ arising in (4) or in (5) for the one-dimensional case. The reversed process $\{\omega_s^*\}_{0\leq s\leq t}$ 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 $J_t(\omega) =$ $\sum_{\mathbf{x}} J_{\mathbf{x},\mathbf{x}+\mathbf{e}_1}(t)$ can be seen as a functional of $\{\omega_s\}_{0\leq s\leq t}$. By (4-5), we have in fact that $J_t(\cdot)$ is an anti-symmetric functional of $\{\omega_s\}_{0\leq s\leq t}$, meaning

$$J_t(\{\omega_s^*\}_{0 \le s \le t}) = -J_t(\{\omega_s\}_{0 \le s \le t})$$
(34)

In fact, similarly to (6), we have

$$J_s(\omega_{\cdot}^*) = \int_0^s (j^a)^* (\omega^*(v)) dv + M^*(s), \quad 0 \le s \le t$$
 (35)

where $(M^*(s))_{0 \le s \le t}$ is a martingale with respect to the natural filtration of $(\omega_s^*)_{0 \le s \le t}$ and $(j^a)^* = \sum_{\mathbf{x}} (j^a)^*_{\mathbf{x}, \mathbf{x} + \mathbf{e}_1}$ is equal to $-j^a = -\sum_{\mathbf{x}} j^a_{\mathbf{x}, \mathbf{x} + \mathbf{e}_1}$. We have then by time reversal

$$\mathbb{E}[J_t(\omega)j^a(\omega(t))] = -\mathbb{E}[J_t(\omega)j^a(\omega^*(0))]$$
$$= -\mathbb{E}\left[\left(\int_0^t (j^a)^*(\omega^*(s))ds + M^*(t)\right)j^a(\omega^*(0))\right]$$
$$= -\mathbb{E}\left[\left(\int_0^t (j^a)^*(\omega^*(s))ds\right)j^a(\omega^*(0))\right]$$
(36)

where the last equality follows from the martingale property of M^* . Recall now that $(j^a)^* = -j^a$. By variables change $s \to t - s$ in the time integral, we get

$$\mathbb{E}[J_t(\omega)j^a(\omega(t))] = \mathbb{E}\left[\left(\int_0^t j^a(\omega(s))ds\right)j^a(\omega(t))\right]$$
(37)

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Let
$$M(t) = \sum_{\mathbf{x}} M_{\mathbf{x}, \mathbf{x}+\mathbf{e}_1}(t)$$
. It follows

$$\mathbb{E}\left[\left(\int_0^t j^a(\omega(s))ds\right)M(t)\right] = \mathbb{E}\left[\int_0^t j^a(\omega(s))M(s)ds\right]$$

$$= \mathbb{E}\left(\int_0^t j^a((\omega(s))\left(J_s(\omega_{\cdot}) - \int_0^s j^a(\omega(v))dv\right)\right)\right)$$

$$= 0$$
(38)

We have obtained the following theorem

Theorem 2. The thermal conductivity $\kappa^{1,1}$ is finite if $d \ge 3$ or if a on-site harmonic potential is present and is infinite in the other cases. In the case where it is finite, we have the formula

$$\kappa^{1,1} = \frac{\gamma}{d} + \frac{1}{8\pi^2 d\gamma} \int_{[0,1]^d} \frac{(\partial_{\mathbf{k}^1} \omega)^2(\mathbf{k})}{\psi(\mathbf{k})} d\mathbf{k}$$
(39)

where ω and ψ are defined in (26) and (27).

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} . In fact, the equivalence of ensembles of Diaconis and Freedman is expressed in terms of a very precize estimate of variation distanc 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 [3].

Lemma 1. Let $\lambda_{rn^{1/2}}^n$ be the uniform measure on the sphere

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

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 a function on \mathbb{R}^k such that

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

$$(40)$$

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

$$\lim_{n \to \infty} \sup \left| \lambda_{rn^{1/2}}^n(\phi) - \lambda_r^\infty(\phi) \right| \le C' \tag{41}$$

Proof. This lemma is proved in [3] for ϕ positive bounded by 1. Without loss of generality, we can assume r = 1 and we simplify the notations by denoting $\lambda_{rn^{1/2}}^n$ 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] and has density (cf [3])

$$f(u) = \mathbf{1}_{\{0 \le u \le n\}} \cdot \frac{1}{n} \frac{\Gamma(n/2)}{\Gamma(k/2)\Gamma[(n-k)/2]} \left(\frac{u}{n}\right)^{(k/2)-1} \left(1 - \frac{u}{n}\right)^{((n-k)/2)-1}$$
(42)

On the other hand, the law of $(x_1 + \ldots + x_k)^2$ under λ^{∞} is χ_k^2 with density (cf [3])

$$g(u) = \frac{1}{2^{k/2} \Gamma(k/2)} e^{-u/2} u^{(k/2)-1}$$
(43)

With these notations, we have

$$|\lambda^{n}(\phi) - \lambda^{\infty}(\phi)| \le C \int_{0}^{\infty} u^{\theta} |f(u) - g(u)| du$$
(44)

The RHS of the inequality above is equal to

$$2C\int_0^\infty u^\theta \left(\frac{f(u)}{g(u)} - 1\right)^+ g(u)du + C\int_0^\infty u^\theta(g(u) - f(u))du \qquad (45)$$

In [3], it is proved $2\left(\frac{f(u)}{g(u)}-1\right)^{+} \leq 2(k+3)/(n-k-3)$ as soon as $k \in \{1,\ldots,n-4\}$. The second term of (45) can be computed explicitly and is equal to

$$\frac{\Gamma\left((2\theta+k)/2\right)}{\Gamma(k/2)} \left[2^{\theta} - \frac{n^{\theta}\Gamma(n/2)}{\Gamma(\theta+n/2)} \right]$$
(46)

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

We recall here 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) Conditionaly to $\{\mathbf{x}_1, \ldots, \mathbf{x}_k\} \setminus \{\mathbf{x}_i\}$, 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

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

We have the following properties:

i) μ_r^k is invariant by any permutation of the coordinates. ii) If $i \neq j \in \{1, ..., d\}$ then for every $h, \ell \in \{1, ..., k\}$ (distincts or not), $\mu_r^k(\mathbf{x}_h^i \mathbf{x}_\ell^j) = 0.$ iii) If $h \neq \ell \in \{1, ..., k\}$ and $i \in \{1, ..., d\}$,

$$\mu_r^k(\mathbf{x}_h^i \mathbf{x}_\ell^i) = -\frac{r^2}{dk(k-1)} = -\frac{\mu_r^k(\mathbf{x}_h^2)}{k-1} = -\frac{\mu_r^k(\mathbf{x}_\ell^2)}{k-1}$$
(47)

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

Proof. We take the Fourier transform of the positions and of the momentums (defined by (62)) and we define

$$\tilde{\mathbf{q}}(\xi) = (1 - \delta(\xi))\omega(\xi)\hat{\mathbf{q}}(\xi), \qquad \tilde{\mathbf{p}}(\xi) = N^{-d/2}(1 - \delta(\xi))\hat{\mathbf{p}}(\xi), \qquad \xi \in \mathbb{T}_d^N$$
(48)

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

$$\mathcal{H}_{N} = \frac{1}{2} \sum_{\xi \neq 0} \left\{ |\tilde{\mathbf{p}}(\xi)|^{2} + |\tilde{\mathbf{q}}(\xi)|^{2} \right\}$$
$$= \frac{1}{2} \sum_{\xi \neq 0} \left\{ \Re e^{2}(\tilde{\mathbf{p}}(\xi)) + \Im m^{2}(\tilde{\mathbf{p}}(\xi)) + \Re e^{2}(\tilde{\mathbf{q}}(\xi)) + \Im m^{2}(\tilde{\mathbf{q}}(\xi)) \right\}$$

Since $\mathbf{p}_{\mathbf{x}}, \mathbf{q}_{\mathbf{x}}$ 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:

$$\Re e(\tilde{\mathbf{p}})(\xi) = \Re e(\tilde{\mathbf{p}})(-\xi), \qquad \Re e(\tilde{\mathbf{q}})(\xi) = \Re e(\tilde{\mathbf{q}})(-\xi) \Im m(\tilde{\mathbf{p}})(\xi) = -\Im m(\tilde{\mathbf{p}})(-\xi), \qquad \Im m(\tilde{\mathbf{q}})(\xi) = -\Im m(\tilde{\mathbf{q}})(-\xi)$$
(49)

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 $\sim (\mathbb{U}_N^d \text{ is of cardinal } (N^d - 1)/2)$. With these notations and by using (49), we have

$$\mathcal{H}_{N} = \sum_{\xi \in \mathbb{U}_{N}^{d}} \left\{ \Re e^{2}(\tilde{\mathbf{p}}(\xi)) + \Im m^{2}(\tilde{\mathbf{p}}(\xi)) + \Re e^{2}(\tilde{\mathbf{q}}(\xi)) + \Im m^{2}(\tilde{\mathbf{q}}(\xi)) \right\}$$
(50)

It follows that in the microcanonical state, the random variables

$$((\mathfrak{R}e ilde{\mathbf{p}})(\xi),(\mathfrak{I}m ilde{\mathbf{p}})(\xi),(\mathfrak{R}e ilde{\mathbf{q}})(\xi),\mathfrak{I}m ilde{\mathbf{q}})(\xi))_{\xi\in\mathbb{U}_N^d}$$

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 (49), we have

$$\left\langle \left(\mathbf{p}_{0}^{j} \mathbf{p}_{\mathbf{e}_{1}}^{i} \right)^{2} \right\rangle_{N} = \frac{1}{N^{2d}} \sum_{\xi, \xi', \eta, \eta' \neq 0} \left\langle \tilde{\mathbf{p}}^{j}(\xi) \tilde{\mathbf{p}}^{j}(\xi') \tilde{\mathbf{p}}^{i}(\eta) \tilde{\mathbf{p}}^{i}(\eta') \right\rangle_{N} e^{-\frac{2i\pi \mathbf{e}_{1} \cdot (\eta + \eta')}{N}}$$
(51)

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

$$\left\langle \left(\mathbf{p}_{0}^{j} \mathbf{p}_{\mathbf{e}_{1}}^{i} \right)^{2} \right\rangle_{N} = \frac{1}{N^{2d}} \sum_{\xi, \eta \neq 0} \left\langle \left| \tilde{\mathbf{p}}^{j}(\xi) \right|^{2} \left| \tilde{\mathbf{p}}^{i}(\eta) \right|^{2} \right\rangle_{N}$$
(52)

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

$$\left\langle \left(\mathbf{p}_{0}^{i} \mathbf{p}_{\mathbf{e}_{1}}^{i} \mathbf{p}_{0}^{j} \mathbf{p}_{\mathbf{e}_{1}}^{j} \right) \right\rangle_{N}$$

$$= \frac{1}{N^{2d}} \sum_{\xi, xi', \eta, \eta' \neq 0} \left\langle \tilde{\mathbf{p}}^{i}(\xi) \tilde{\mathbf{p}}^{i}(\xi') \tilde{\mathbf{p}}^{j}(\eta) \tilde{\mathbf{p}}^{j}(\eta') \right\rangle_{N} \exp\left(-\frac{2i\pi \mathbf{e}_{1}}{N} \cdot (\xi' + \eta')\right)$$
⁽⁵³⁾

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

$$\left\langle \left(\mathbf{p}_{0}^{i}\mathbf{p}_{\mathbf{e}_{1}}^{i}\mathbf{p}_{0}^{j}\mathbf{p}_{\mathbf{e}_{1}}^{j}\right)\right\rangle_{N} = \frac{1}{N^{2d}}\sum_{\xi,\eta\neq0}\left\langle \left|\tilde{\mathbf{p}}^{i}(\xi)\right|^{2}\left|\tilde{\mathbf{p}}^{j}(\eta)\right|^{2}\right\rangle_{N}\exp\left(\frac{2i\pi\mathbf{e}_{1}}{N}\cdot\left(\xi+\eta\right)\right)$$
(54)

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

$$\left\langle \left(\mathbf{p}_{0}^{i}\mathbf{p}_{\mathbf{e}_{1}}^{i}\mathbf{p}_{0}^{j}\mathbf{p}_{\mathbf{e}_{1}}^{j}\right)\right\rangle_{N} = \frac{e^{2}}{d^{2}} \left(\frac{1}{N^{d}}\sum_{\xi\neq0}e^{\frac{2i\pi\mathbf{e}_{1}}{N}\cdot\xi}\right)^{2} + O(N^{-d}) = O(N^{-d}) \quad (55)$$

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

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

Estimates of [3] give

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

and one obtains easily (iii).

5. Appendix

Lemma 5. (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

$$\frac{2\lambda}{\gamma}g_{\lambda,N}(\mathbf{z}) - 4\Delta g_{\lambda,N}(\mathbf{z}) = \left(\delta(\mathbf{z} + \mathbf{e}_1) - \delta(\mathbf{z} - \mathbf{e}_1)\right)$$
(56)

for
$$d \ge 2$$
, or

$$\frac{2\lambda}{\gamma}g_{\lambda,N}(z) - \frac{1}{3}\Delta \left[4g_{\lambda,N}(z) + g_{\lambda,N}(z+1) + g_{\lambda,N}(z-1)\right] = \left(\delta(z+1) - \delta(z-1)\right)$$
(57)

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

Proof. We 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:

$$Au_{\lambda,N} = \frac{\alpha}{\gamma} \sum_{\mathbf{x}} [(\alpha \Delta - \nu I) \mathbf{q}_{\mathbf{x}}] \cdot \left(\sum_{\mathbf{y}} g_{\lambda,N} (\mathbf{x} - \mathbf{y}) \mathbf{q}_{\mathbf{y}} \right) + \frac{\alpha}{\gamma} \sum_{\mathbf{y},\mathbf{x}} g_{\lambda,N} (\mathbf{x} - \mathbf{y}) \mathbf{p}_{\mathbf{x}} \cdot \mathbf{p}_{\mathbf{y}}$$
(58)

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 $\{1, \ldots, d\}$. Summation by

parts can be performed (without outcoming boundary terms since we are on the torus) and we get

$$Au_{\lambda,N} = \frac{\alpha}{\gamma} \sum_{\mathbf{x}} [(\alpha \Delta - \nu I)g_{\lambda,N}](\mathbf{x} - \mathbf{y})\mathbf{q}_{x}\mathbf{q}_{\mathbf{y}} + \frac{\alpha}{\gamma} \sum_{\mathbf{y},\mathbf{x}} g_{\lambda,N}(\mathbf{x} - \mathbf{y})\mathbf{p}_{\mathbf{x}} \cdot \mathbf{p}_{\mathbf{y}}$$
(59)

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:

$$Au_{\lambda,N} = \sum_{\mathbf{x},\mathbf{y}} \{a_1(\mathbf{x} - \mathbf{y})\mathbf{p}_{\mathbf{x}} \cdot \mathbf{p}_{\mathbf{y}} + a_2(\mathbf{x} - \mathbf{y})\mathbf{q}_{\mathbf{x}} \cdot \mathbf{q}_{\mathbf{y}}\}$$
(60)

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 $\ell \in \{1, \ldots, d\}$ then

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

Since the action of S is only on the **p**'s, we have

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

where in the last line, we performed a summation by parts. Since $g_{\lambda,N}$ is solution of (56), we have

$$\lambda u_{\lambda,N} - \gamma S u_{\lambda,N} = \frac{\alpha}{2} \sum_{\mathbf{x}} \mathbf{p}_{\mathbf{x}} \cdot (\mathbf{q}_{\mathbf{x}+\mathbf{e}_1} - \mathbf{q}_{\mathbf{x}-\mathbf{e}_1}) = -\sum_{\mathbf{x}} j^a_{\mathbf{x},\mathbf{x}+\mathbf{e}_1} \qquad (61)$$

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

$$\hat{v}(\xi) = \sum_{\mathbf{z} \in \mathbb{T}_N^d} v(\mathbf{z}) \exp(2i\pi \xi \cdot \mathbf{z}/N)$$
(62)

The inverse transform is given by

$$v(\mathbf{z}) = \frac{1}{N^d} \sum_{\xi \in \mathbb{T}_N^d} \hat{v}(\xi) \exp(-2i\pi \xi \cdot \mathbf{z}/N)$$
(63)

Similarly on \mathbb{Z}^d we define:

$$\hat{v}(\mathbf{k}) = \sum_{\mathbf{z} \in \mathbb{Z}^d} v(\mathbf{z}) \exp(2i\pi \mathbf{k} \cdot \mathbf{z}) \qquad \mathbf{k} \in \mathbb{T}^d$$
(64)

and its inverse by

$$v(\mathbf{z}) = \int_{\mathbb{T}^d} \hat{v}(\mathbf{k}) \exp(-2i\pi \mathbf{k} \cdot \mathbf{z})$$

For $\eta > 0$, let $G_{\eta,N}$ be the solution in \mathbb{T}_N^d of the equation

$$\frac{2\eta}{\gamma}G_{\eta,N}(\mathbf{z}) - 4\Delta G_{\eta,N}(\mathbf{z}) = \delta_0(\mathbf{z}) - 1, \quad d \ge 2 \quad (65)$$
$$\frac{2\eta}{\gamma}G_{\eta,N}(z) - \frac{1}{3}\Delta \left(4G_{\eta,N}(z) + G_{\eta,N}(z+1) + G_{\eta,N}(z-1)\right) = \delta_0(z) - 1$$
$$d = 1$$

and in all cases, we have $g_{\eta,N}(\mathbf{x}) = G_{\eta,N}(\mathbf{x} + \mathbf{e}_1) - G_{\eta,N}(\mathbf{x} - \mathbf{e}_1)$. Then we have

$$\hat{G}_{\eta,N}(\xi) = \frac{1 - \delta_0(\xi)}{\frac{2\eta}{\gamma} + 16\sum_{k=1}^d \sin^2(\pi\xi^k/N)}, \quad \text{if } d \ge 2$$

and

$$\hat{G}_{\eta,N}(\xi) = \frac{1 - \delta_0(\xi)}{\frac{2\eta}{\gamma} + \frac{8}{3} \sin^2(\pi \xi/N) \left(1 + 2\cos^2(\pi \xi/N)\right)}, \quad \text{if } d = 1$$

Since

$$\hat{g}_{\eta,N}(\xi) = -2i\sin(2\pi\xi^{1}/N)\hat{G}_{\eta,N}(\xi)$$

the following bound follows wasily by Parseval relation:

$$\sum_{\mathbf{x}\in\mathbb{T}_N^d} (g_{\eta,N}(\mathbf{x}))^2 \le \frac{\gamma^2}{\eta^2}$$
(66)

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

$$\hat{\Gamma}_N(\xi) = \frac{1 - \delta_0(\xi)}{\nu + 4\alpha \sum_{k=1}^d \sin^2(\pi \xi^k / N)}$$
(67)

and it follows the well known estimates

- $\Gamma_N(0)$ is of order N if $d = 1, \nu = 0$.
- $\begin{aligned} \Gamma_N(0) & \text{is of order } \log N \text{ if } d = 2, \nu = 0. \\ \Gamma_N(0) & \text{is of order } 1 \text{ if } d \geq 3 \text{ or } \nu > 0. \end{aligned}$ (68)

As $N \to \infty$ we have $G_{\eta,N} \to G_{\eta}$ (resp. $g_{\eta,N} \to g_{\eta}$) solution of the same equations (65) (resp. (56,57)) but on \mathbb{Z}^d . The convergence is understood pointwise and in \mathbb{L}^2 .

We can compute then, for d = 1,

$$G_{\eta}(0) + G_{\eta}(1) = \gamma \int_{0}^{1} \frac{\cos^{2}(\pi k)}{\eta + \gamma/3 \sin^{2}(\pi k) \left(1 + 2\cos^{2}(\pi k)\right)} dk$$
(69)

Moreover we have for d = 1

$$\sum_{z} g_{\eta}(z) \left(\Gamma(z+1)\right) - \Gamma(z-1)\right) = \frac{\gamma}{2} \int_{0}^{1} \frac{\sin^{2}(2\pi k)}{\left(\eta + 4\gamma/3 \sin^{2}(\pi k)(1+2\cos^{2}(\pi k))\right) \left(\nu + 4\alpha \sin^{2}(\pi k)\right)} dk$$
(70)

and for $d \geq 2$

$$= 2\gamma \int_{\mathbb{T}^d} \frac{\sin^2(2\pi k^1)}{\left(\eta + 8\gamma \sum_{j=1}^d \sin^2(\pi k^j)\right) \left(\nu + 4\alpha \sum_{j=1}^d \sin^2(\pi k^j)\right)} d\mathbf{k}$$
(71)

The limits as $\eta \to 0$ 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.

References

- [1] G. Basile, C. Bernardin, S. Olla, A momentum conserving model with anomalous thermal conductivity in low dimension, cond-mat/0509688, (2005).
- [2] C. Bernardin, S. Olla, Fourier's law for a microscopic model of heat conduction, J. Stat. Phys. 121, N. 3/4, (2005).
- [3] P. Diaconis, D. Freedman, A dozen de Finetti style results in search of a theory, Ann. Inst. H. Poincaré (Probabilités et Statistiques), 23, 397-423, (1987).
- [4] Z. Rieder, J.L. Lebowitz, E. Lieb, Properties of harmonic crystal in a stationary non-equilibrium state, J. Math. Phys. 8, 1073-1078 (1967).

6. FORMULAIRE

Some formulas we use:

$$S\mathbf{p}_{\mathbf{x}} = 2\Delta \mathbf{p}_{\mathbf{x}} \qquad d \ge 2$$
 (72)

$$Sp_x = \frac{1}{6}\Delta \left(4p_x + p_{x+1} + p_{x-1}\right) \qquad d = 1$$
(73)

$$Se_{\mathbf{x}} = S\mathbf{p}_{\mathbf{x}}^2/2 = \Delta \mathbf{p}_{\mathbf{x}} \qquad d \ge 2$$
 (74)

$$Se_x = Sp_x^2/2 = \frac{1}{6}\Delta \left(4p_x^2 + p_{x+1}^2 + p_{x-1}^2\right) \qquad d = 1$$
(75)

DIP. DI MATEMATICA U. DINI, UNIVERSITÀ DI FIRENZE, VIALE MORGAGNI 67A, 50134 FIRENZE - ITALY. basile@math.unifi.it

UMPA, UMR-CNRS 5669 ENS-LYON, 46, ALLÉE D'ITALIE, 69364 LYON CEDEX 07 - FRANCE. Cedric.Bernardin@umpa.ens-lyon.fr http://w3umpa.ens-lyon.fr/~cbernard/

CEREMADE, UMR CNRS 7534 UNIVERSITÉ DE PARIS DAUPHINE, PLACE DU MARÉCHAL DE LATTRE DE TASSIGNY 75775 PARIS CEDEX 16 - FRANCE. olla@ceremade.dauphine.fr http://www.ceremade.dauphine.fr/~olla