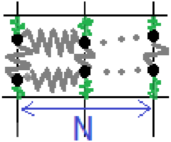
Non-equilibrium statistical mechanics of crystals in medium

Andrey Dymov (Université de Cergy-Pontoise)

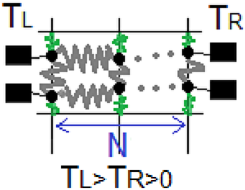
Saint Petersbourg, June 4, 2015



Let $\Lambda \subset \mathbb{Z}^d$, $d \geq 1$, be a bounded set,
$(p, q) = (p_j, q_j)_{j \in \Lambda}$, the Hamiltonian

$$H^\nu = \sum_{j \in \Lambda} \left(\frac{p_j^2}{2} + \frac{q_j^2}{2} \right) + \frac{\nu}{2} \sum_{j,k \in \Lambda : |j-k|=1} V(q_j, q_k),$$

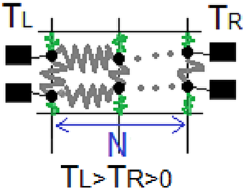
where $\nu > 0$,
$V(q_j, q_k) \equiv V(q_k, q_j)$ is smooth.



Let $\Lambda \subset \mathbb{Z}^d$, $d \geq 1$, be a bounded set, $(p,q) = (p_j, q_j)_{j \in \Lambda}$, the Hamiltonian

$$H^\nu = \sum_{j \in \Lambda} \left(\frac{p_j^2}{2} + \frac{q_j^2}{2} \right) + \frac{\nu}{2} \sum_{j,k \in \Lambda : |j-k|=1} V(q_j, q_k),$$

where $\nu > 0$,
$V(q_j, q_k) \equiv V(q_k, q_j)$ is smooth.



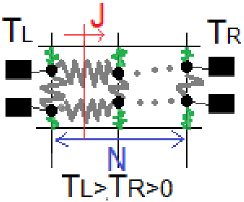
Let $\Lambda \subset \mathbb{Z}^d$, $d \geq 1$, be a bounded set, $(p, q) = (p_j, q_j)_{j \in \Lambda}$, the Hamiltonian

$$H^\nu = \sum_{j \in \Lambda} \left(\frac{p_j^2}{2} + \frac{q_j^2}{2} \right) + \frac{\nu}{2} \sum_{j,k \in \Lambda : |j-k|=1} V(q_j, q_k),$$

where $\nu > 0$,
$V(q_j, q_k) \equiv V(q_k, q_j)$ is smooth.

1. **Existence and uniqueness of a stationary measure μ? Convergence of solutions to it as $t \to \infty$?**

   Eckmann, Pillet, Rey-Bellet '98



Let $\Lambda \subset \mathbb{Z}^d$, $d \geq 1$, be a bounded set, $(p, q) = (p_j, q_j)_{j\in\Lambda}$, the Hamiltonian

$$H^\nu = \sum_{j\in\Lambda}\left(\frac{p_j^2}{2} + \frac{q_j^2}{2}\right) + \frac{\nu}{2}\sum_{j,k\in\Lambda:|j-k|=1} V(q_j, q_k),$$

where $\nu > 0$,
$V(q_j, q_k) \equiv V(q_k, q_j)$ is smooth.

1. **Existence and uniqueness of a stationary measure μ? Convergence of solutions to it as $t \to \infty$?**

   Eckmann, Pillet, Rey-Bellet '98

2. **Fourier law?**

$$\langle \mu, J\rangle \overset{N\gg 1}{\approx} \kappa(T)\frac{T_L - T_R}{N},$$

where J is the energy flow through some cross section, $T = (T_L + T_R)/2$ and κ is the conductivity.

Linear case: Rieder, Lebowitz, Lieb '67 ($\kappa = \infty$)
Non-linear case: no results

Toy models: each particle is perturbed by sufficiently strong noise

Basile, Bernardin, Bonetto, Lebowitz, Liverani, Lukkarinen, Olla, . . .

The Fourier law is studied only for the linear case.

Toy models: each particle is perturbed by sufficiently strong noise

Basile, Bernardin, Bonetto, Lebowitz, Liverani, Lukkarinen, Olla, ...

The Fourier law is studied only for the linear case.

Stochastic perturbation $\to 0$?

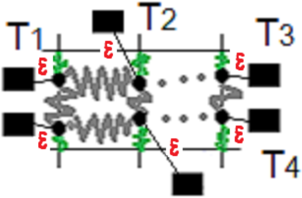
Toy models: each particle is perturbed by sufficiently strong noise

Basile, Bernardin, Bonetto, Lebowitz, Liverani, Lukkarinen, Olla, . . .

The Fourier law is studied only for the linear case.

Stochastic perturbation $\to 0$?

Crystal weakly interacting with medium



$\varepsilon \to 0$?

Equations of motion

$$\frac{d}{dt}q_j = p_j, \quad \frac{d}{dt}p_j = -\partial_{q_j} H^\nu(p,q) \overbrace{-\varepsilon p_j + \sqrt{2\varepsilon T_j}\frac{d}{dt}B_j}^{\text{Langevin thermostat}}, \quad j \in \Lambda,$$

where $(B_j)_{j\in\Lambda}$ are standard independent Brownian motions, $T_j > 0$ are temperatures.

Equation above has a unique stationary measure, which is mixing.

Equations of motion

$$\frac{d}{dt}q_j = p_j, \quad \frac{d}{dt}p_j = -\partial_{q_j} H^\nu(p,q) \overbrace{-\varepsilon p_j + \sqrt{2\varepsilon T_j}\frac{d}{dt}B_j}^{\text{Langevin thermostat}}, \quad j \in \Lambda,$$

where $(B_j)_{j\in\Lambda}$ are standard independent Brownian motions, $T_j > 0$ are temperatures.

Equation above has a unique stationary measure, which is mixing.

Scaling

$$\nu = \varepsilon$$

Natural time scale is $t \sim \varepsilon^{-1} \Rightarrow$ slow time $\tau = \varepsilon t$, $\tau \sim 1$

Equations of motion

$$\frac{d}{dt}q_j = p_j, \quad \frac{d}{dt}p_j = -\partial_{q_j} H^\nu(p,q) \overbrace{-\varepsilon p_j + \sqrt{2\varepsilon T_j}\frac{d}{dt}B_j}^{\text{Langevin thermostat}}, \quad j \in \Lambda,$$

where $(B_j)_{j\in\Lambda}$ are standard independent Brownian motions, $T_j > 0$ are temperatures.

Equation above has a unique stationary measure, which is mixing.

Scaling

$$\nu = \varepsilon$$

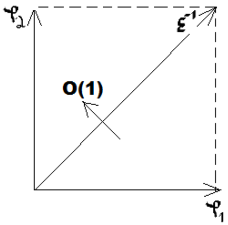
Natural time scale is $t \sim \varepsilon^{-1} \Rightarrow$ slow time $\tau = \varepsilon t$, $\tau \sim 1$

Equations of motion in the slow time

$$\dot{q}_j = \varepsilon^{-1} p_j,\ \dot{p}_j = -\varepsilon^{-1} q_j - \sum_{k\in\Lambda:|j-k|=1} \partial_{q_j} V(q_j, q_k) - p_j + \sqrt{2T_j}\dot{B}_j,\ j \in \Lambda, \tag{1}$$

where the dot denotes the derivative w.r.t. τ.

Limiting as $\varepsilon \to 0$ behavior of solutions of eq. (1)



Action-angle variables for H^0 are $(I, \varphi) \in \mathbb{R}^{|\Lambda|} \times \mathbb{T}^{|\Lambda|}$, where

$$I_j = \frac{p_j^2 + q_j^2}{2}, \quad \varphi_j = \arg(p_j + iq_j), \quad j \in \Lambda.$$

Equations of motion

$$\dot{I}_j = O(1), \quad \dot{\varphi}_j = \varepsilon^{-1} + O(1) \quad , \quad j \in \Lambda$$

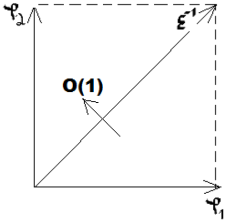
Averaging of the I-eq. along the diagonal $\mathbf{1} = (1, 1, \dots, 1)$ of the torus $\mathbb{T}^{|\Lambda|}$

$$=$$

the resonant averaging

$$\langle f \rangle_R = \frac{1}{2\pi} \int_0^{2\pi} f(I, \varphi + \theta \mathbf{1})\, d\theta$$

Limiting as $\varepsilon \to 0$ behavior of solutions of eq. (1)



Action-angle variables for H^0 are $(I, \varphi) \in \mathbb{R}^{|\Lambda|} \times \mathbb{T}^{|\Lambda|}$, where

$$I_j = \frac{p_j^2 + q_j^2}{2}, \quad \varphi_j = \arg(p_j + iq_j), \quad j \in \Lambda.$$

Equations of motion

$$\dot{I}_j = O(1), \quad \dot{\varphi}_j = \varepsilon^{-1} + O(1) \cdot I_j^{-1}, \quad j \in \Lambda$$

Averaging of the I-eq. along the diagonal $\mathbf{1} = (1, 1, \ldots, 1)$ of the torus $\mathbb{T}^{|\Lambda|}$

$$=$$

the resonant averaging

$$\langle f \rangle_R = \frac{1}{2\pi} \int_0^{2\pi} f(I, \varphi + \theta \mathbf{1})\, d\theta$$

Singularities $\Rightarrow$ Guess an effective equation such that for its solution $(p, q)(\tau)$ we have $I(p, q)(\tau)$ satisfies $\langle I\text{-eq.}\rangle_R$.

Effective equation

$$\dot{q}_j = \partial_{p_j} H^{res} - \frac{q_j}{2} + \sqrt{T_j}\dot{B}_j^1, \quad \dot{p}_j = -\partial_{q_j} H^{res} - \frac{p_j}{2} + \sqrt{T_j}\dot{B}_j^2, \qquad (2)$$

where $B_j^{1,2}$ are standard independent Brownian motions and

$$H^{res} = \Big\langle \frac{1}{2} \sum_{k,j\in\Lambda:|k-j|=1} V(q_j, q_k) \Big\rangle_R .$$

Let (p_0, q_0) be some "not very bad" random initial conditions. Fix $\mathcal{T} > 0$.

Theorem

1. *Let $(p^\varepsilon, q^\varepsilon)(\tau)$ be a unique solution of eq. (1) and $(p,q)(\tau)$ be that of eq. (2), satisfying $(p^\varepsilon, q^\varepsilon)(0) = (p,q)(0) = (p_0, q_0)$. Then*

$$\mathcal{D}\big(I(p^\varepsilon, q^\varepsilon)(\cdot)\big) \overset{\varepsilon\to 0}{\rightharpoonup} \mathcal{D}\big(I(p,q)(\cdot)\big) \quad in \quad C([0,\mathcal{T}], \mathbb{R}^{|\Lambda|})$$

   uniformly in $|\Lambda|$.

2. *Let μ^ε be a unique stationary measure of eq. (1) and μ be that of eq. (2). Then $\mu^\varepsilon \overset{\varepsilon\to 0}{\rightharpoonup} \mu$. Under some additional assumption this convergence holds uniformly in $|\Lambda|$.*

Limiting as $\varepsilon \to 0$ energy transport in eq. (1)

Scaling

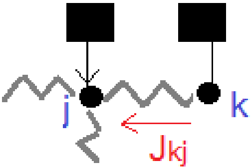
$$\nu = \varepsilon\lambda, \quad \text{where} \quad \lambda \ll 1 \quad \text{is independent from} \quad \varepsilon.$$

small low temperature oscillations

Scaling

$$\nu = \varepsilon\lambda, \quad \text{where} \quad \lambda \ll 1 \quad \text{is independent from} \quad \varepsilon.$$

small low temperature oscillations



$J_{kj} := p_k \partial_{q_k} V(q_k, q_j) - p_j \partial_{q_j} V(q_k, q_j)$
is the Hamiltonian energy flow from the k-th oscillator to the j-th one.

$$\langle \mu^\varepsilon, J_{kj} \rangle \to \,? \quad \text{as} \quad \varepsilon \to 0$$

Here μ^ε is the unique stationary measure of eq. (1).

Theorem

There exists a function $\kappa : \mathbb{R}_+^2 \mapsto \mathbb{R}_+$, $\kappa(x, y) \equiv \kappa(y, x)$, *which is*

- *smooth,*
- *strictly positive,*

such that for any $k, j \in \Lambda$ *satisfying* $|k - j| = 1$ *we have*

$$\langle \mu^\varepsilon, J_{kj} \rangle \to \lambda\kappa(T_k, T_j)(T_k - T_j) + o(\lambda) \quad \textit{as} \quad \varepsilon \to 0 \quad \textit{uniformly in } |\Lambda|.$$

Theorem

There exists a function $\kappa : \mathbb{R}_+^2 \mapsto \mathbb{R}_+$, $\kappa(x, y) \equiv \kappa(y, x)$, *which is*

- *smooth,*
- *strictly positive,*

such that for any $k, j \in \Lambda$ *satisfying* $|k - j| = 1$ *we have*

$$\langle \mu^{\varepsilon}, J_{kj} \rangle \to \lambda\kappa(T_k, T_j)(T_k - T_j) + o(\lambda) \quad \text{as} \quad \varepsilon \to 0 \quad \text{uniformly in } |\Lambda|.$$

This resembles the Fourier law. However, it is not.

Theorem

There exists a function $\kappa : \mathbb{R}^2_+ \mapsto \mathbb{R}_+$, $\kappa(x,y) \equiv \kappa(y,x)$, *which is*

- *smooth,*
- *strictly positive,*

such that for any $k, j \in \Lambda$ *satisfying* $|k-j| = 1$ *we have*

$$\langle \mu^\varepsilon, J_{kj} \rangle \to \lambda \kappa(T_k, T_j)(T_k - T_j) + o(\lambda) \quad \text{as} \quad \varepsilon \to 0 \quad \text{uniformly in } |\Lambda|.$$

This resembles the Fourier law. However, it is not.

Proof.

1. Theorem 1 implies $\langle \mu^\varepsilon, J_{kl} \rangle \to \langle \mu, J_{kl} \rangle$ as $\varepsilon \to 0$, where μ is the unique stationary measure of the effective equation.

2. $\mu = \mu^0 + \lambda \mu^1 + o(\lambda)$.

3. $\langle \mu^0, J_{kj} \rangle = 0$, $\langle \mu^1, J_{kj} \rangle = \kappa(T_k, T_j)(T_k - T_j)$.