Thermal Conductivity and Fourier Law from Microscopic Dynamics

Collège de France, Paris
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Stefano Olla

in collaboration with:

G. Basile, C. Bernardin, M. Jara, T. Komorowski, C. Liverani, H. Spohn, R. Livi

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Noise can conserve *energy*, or *energy + momentum*.

Conservative Noise

Energy + momentum conserved:

$$Y_{x,y}^{i,j} = (p_x^i - p_y^i)(\partial_{p_x^j} - \partial_{p_y^j}) - (p_x^j - p_y^j)(\partial_{p_x^i} - \partial_{p_y^i})$$

$$Y_{x,y}^{i,j}(\mathbf{p}_x + \mathbf{p}_y) = 0 \qquad Y_{x,y}^{i,j}(|\mathbf{p}_x|^2 + |\mathbf{p}_y|^2) = 0$$

$$S = \sum_{|x-y|=1} \sum_{i,j}^{\nu} (Y_{x,y}^{i,j})^2$$

$$L = \{\mathcal{H}, \cdot\} + \gamma S$$

Energy Current

Total energy is conserved by the bulk dynamics: $\mathcal{H}_N = \sum_{\mathbf{x}} e_{\mathbf{x}}$

$$e_{\mathbf{x}} = \frac{\mathbf{p}_{\mathbf{x}}^2}{2} + \frac{1}{2} \sum_{\mathbf{y}:|\mathbf{y}-\mathbf{x}|=1} V(\mathbf{q}_{\mathbf{x}} - \mathbf{q}_{\mathbf{y}}) + W(\mathbf{q}_{\mathbf{x}})$$ Energy of atom $\mathbf{x}$.

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$$Le_{\mathbf{x}} = \sum_{k=1}^{d} \nabla_{\mathbf{e}_k}^* j_{\mathbf{x},\mathbf{x}+\mathbf{e}_k}$$ local conservation of energy.

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In dimension 1, if $W = 0$, we have 2 other conserved quantities

$$\sum_x r_x = \sum_x (q_{x+1} - q_x), \qquad \sum_x p_x$$

Hyperbolic scaling

$d = 1$, $W = 0$ (unpinned):

$$\epsilon \sum_x G(\epsilon x) \begin{pmatrix} r_x(\epsilon^{-1}t) \\ p_x(\epsilon^{-1}t) \\ e_x(\epsilon^{-1}t) \end{pmatrix} \xrightarrow[N\to\infty]{\text{probability}} \int G(y) \begin{pmatrix} \mathfrak{r}(t,y) \\ \mathfrak{p}(t,y) \\ \mathfrak{e}(t,y) \end{pmatrix} dy$$

$$\partial_t \mathfrak{r} = \partial_y \mathfrak{p}$$

$$\partial_t \mathfrak{p} = \partial_y P(\mathfrak{r}, \mathfrak{e} - \mathfrak{p}^2/2) \qquad P(r,u) = -\frac{\partial_r s(r,u)}{\partial_u s(r,u)}$$

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O.-Yau-Varadhan (1993), O. Basile (2007)

(Relative Entropy, smooth solutions).

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$$\kappa(T) = \lim_{t\to\infty} \frac{1}{2\bar{e}^2 t} \sum_x x^2 \left(< e_x(t) e_0(0) >_\beta - \bar{e}^2\right)$$

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$$= \frac{1}{2\bar{e}^2} \int_0^\infty \sum_x \left\langle j^a_{x,x+1}(t) j^a_{0,1}(0) \right\rangle_\beta \, dt$$

Green-Kubo formula.

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and there are some surprises about the decay of $\left\langle j^a_{x,x+1}(t) j^a_{0,1}(0) \right\rangle_\beta$, at least in dimension 1.

Diffusive scaling

The ultimate goal is to prove that

$$\epsilon \sum_x G(\epsilon x) e_x(\epsilon^{-2} t) \underset{\epsilon \to 0}{\longrightarrow} \int G(u) T(t,u)\, du$$

with $T(t,u)$ satisfying a (eventually non-linear) heat equation

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3 approaches:

- Weak coupling limit
- Kinetic limit
- Hydrodynamic limit

Weak coupling limit

in collaboration with C. Liverani

- $V(\mathbf{q}_{x+1} - \mathbf{q}_x) \longrightarrow \epsilon V(\mathbf{q}_{x+1} - \mathbf{q}_x)$

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- stochastic perturbation acting independently on each particle conserving $|\mathbf{p}_x|^2$, dimension $\nu \geq 2$.

$$L = A_\epsilon + S, \qquad A = \{\mathcal{H}_\epsilon, \cdot\} \qquad \text{Poisson brackets}$$

$$S = \sum_x \sum_{i,j}^{\nu} (Y_{x;i,j})^2 \qquad Y_{x;i,j} = p_x^j \partial_{p_x^i} - p_x^i \partial_{p_x^j}$$

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$$dp_x^i(t) = \partial_{q_x^i} \mathcal{H}_\epsilon \, dt - \nu p_x^i \, dt + \sum_j^{\nu} p_x^j \, dw_{i,j}(t), \quad w_{i,j} = -w_{j,i}$$

Weak coupling limit

Theorem: $e_x^\epsilon(\epsilon^{-2}t) \longrightarrow \tilde{e}_x(t)$, solution of the system of SDE:

$$d\tilde{e}_x(t) = \sum_{|y-x|=1} \alpha(\tilde{e}_x(t), \tilde{e}_y(t))\, dt + \sum_{|y-x|=1} \gamma(\tilde{e}_x(t), \tilde{e}_y(t))\, dw_{x,y}(t)$$

$$\alpha(\tilde{e}_x, \tilde{e}_y) = -\alpha(\tilde{e}_y, \tilde{e}_x) = (\partial_{\tilde{e}_x} - \partial_{\tilde{e}_y})\gamma(\tilde{e}_x(t), \tilde{e}_y(t))^2, \qquad w_{x,y} = -w_{y,x}$$

$$\widetilde{L} = \frac{1}{2} \sum_{x,y:|x-y|=1} (\partial_{\tilde{e}_x} - \partial_{\tilde{e}_y})\gamma(\tilde{e}_x, \tilde{e}_y)^2(\partial_{\tilde{e}_x} - \partial_{\tilde{e}_y})$$

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Non-gradient Ginzburg-Landau model

$$\gamma(\tilde{e}_x, \tilde{e}_y)^2 = \int_0^\infty < j_{x,y}^a(t) j_{x,y}^a(0) >_{\epsilon=0,\tilde{e}_x,\tilde{e}_y} \; dt$$

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$$\begin{aligned} d\tilde{e}_x(t) &= \sum_{|y-x|=1} -(\tilde{e}_x(t) - \tilde{e}_y(t))\, dt + \sum_{|y-x|=1} \sqrt{\tilde{e}_x(t)\tilde{e}_y(t)}\, dw_{x,y}(t) \\ &= \Delta \tilde{e}_x(t)\, dt + \sum_{|y-x|=1} \sqrt{\tilde{e}_x(t)\tilde{e}_y(t)}\, dw_{x,y}(t) \end{aligned}$$

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$$\delta^\nu \sum_x G(\delta x)\tilde{e}_x(\delta^{-2} t) \underset{\delta \to 0}{\longrightarrow} \int G(u) T(t,u)\, du, \qquad \partial_t T = \Delta T$$

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In the non-harmonic case, $\alpha(\tilde{e}_x, \tilde{e}_y)$ is not a gradient, but Varadhan's non-gradient technique for hydrodynamic limit can be applied (with some difficulties) and

$$\delta^\nu \sum_x G(\delta x)\tilde{e}_x(\delta^{-2}t) \underset{\delta \to 0}{\longrightarrow} \int G(u)T(t,u)\, du, \qquad \partial_t T = \nabla \tilde{\kappa}(T) \nabla T$$

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$$Y_{x,y}^{i,j} = (p_x^i - p_y^i)(\partial_{p_x^j} - \partial_{p_y^j}) - (p_x^j - p_y^j)(\partial_{p_x^i} - \partial_{p_y^i})$$

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Boltzmann phonon equation

$$a(\mathbf{k},t) = \frac{1}{\sqrt{2}}\left(\sqrt{\omega(\mathbf{k})}\hat{q}(\mathbf{k},t) + \frac{i}{\sqrt{\omega(\mathbf{k})}}\hat{p}(\mathbf{k},t)\right)$$

where $\omega(\mathbf{k})$ is the *dispersion relation* of the harmonic chain:

$$\omega(\mathbf{k}) = \left(\omega_0^2 + 4\sum_j^d \sin^2(\pi k^j)\right)^{1/2}, \qquad \int |a(\mathbf{k},t)|^2 d\mathbf{k} = \sum_x e_x$$

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Wigner distribution (in space-time scaling $\epsilon^{-1}x, \epsilon^{-1}t$):

$$W^\epsilon(y,k,t) = \left(\frac{\epsilon}{2}\right)^d \int_{(\mathbb{T}/\epsilon)^d} d\eta e^{i2\pi y\cdot\eta} \left\langle a(k-\epsilon\eta/2, t/\epsilon)^* a(k+\epsilon\eta/2, t/\epsilon)\right\rangle^\epsilon$$

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$$R(k,k') = R(k',k) \geq 0,$$

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- $R(k,k') \geq 1/2$ if only energy is conserved
- $R(k,k') \sim_{k \to 0} k^2$ if energy + momentum are conserved.

Boltzmann phonon equation

$$W^{\epsilon}(y,k,t) \underset{\epsilon \to 0}{\longrightarrow} W(y,k,t)$$

$$\partial_t W(\mathbf{k},x,t) + \nabla_k \omega(\mathbf{k}) \cdot \nabla_x W(\mathbf{k},x,t) = \int dk' R(\mathbf{k},\mathbf{k}')(W(\mathbf{k}') - W(\mathbf{k}))$$

$$R(k,k') = R(k',k) \geq 0,$$

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Harmonic case: $V(\mathbf{q_x} - \mathbf{q_y}) = \|\mathbf{q_x} - \mathbf{q_y}\|^2$, $W(\mathbf{q_x}) = \omega_0^2\|\mathbf{q_x}\|^2$.

G. Basile, C. Bernardin, S. O., **Phys. Rev. Lett. 96 (2006)**

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$$\sum_{\mathbf{x}\in\mathbb{Z}^d} \left\langle j^a_{\mathbf{x},\mathbf{x}+\mathbf{e}_1}(t) j^a_{0,\mathbf{e}_1}(0) \right\rangle_T = \frac{e^2}{4\pi^2 d} \int_{[0,1]^d} (\partial_{k_1} \omega(\mathbf{k}))^2 \, e^{-t\gamma\psi(\mathbf{k})} \, d\mathbf{k}$$

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$$\kappa^{1,1} = \frac{\gamma}{d} + \frac{1}{2e^2} \int_0^\infty C_{1,1}(t)\, dt$$
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Results for (some) an-harmonic case

If $0 < c_0 \le V'' \le C_0 < \infty$

$$\sup_{\lambda > 0} \int_0^\infty e^{-\lambda t} \sum_{\mathbf{x}} \left\langle j^a_{\mathbf{x},\mathbf{x}+\mathbf{e}_1}(t) j^a_{0,\mathbf{e}_1}(0) \right\rangle_T dt \ \le \ C(\gamma)$$

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We can prove the existence of the limit only for the self-consistent thermostats model (Bonetto-Lukkarinen-Lebowitz-O.)

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with Milton Jara, Tomasz Komorowski (2007)

In dimension 1 and 2, if noise conserve energy and momentum, and the interaction is harmonic and unpinned,

thermal conductivity is infinite and energy fluctuations superdiffuse!

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The exact results on the decay of the correlation suggest that the right scaling is

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unpinned 1-d system with energy+momentum conserving noise,

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- In the harmonic case $a = 0.48$ ($a = 0.5$ exact solution).

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More simulation for **Toda Lattice, rotors**