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Anomalous diffusive limit for a kinetic interface model[1]

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[1] Joint work with K. Bogdan (Wroclaw University) and T. Komorowski (IMPAN)

Our model: linearized Boltzmann equation

Aim: Study the asymptotic behaviour of a kinetic equation with random interface conditions

Outside the interface $\mathcal{I} := \{y = 0\}$, phonons dymanics is described in terms of a linearized Boltzmann equation:

$$\text{(KE):} \quad \begin{cases} \partial_t W(t,y,k) + \omega'(k)\partial_y W(t,y,k) = \gamma L_k W(t,y,k); \\ W(0,y,k) = W_0(y,k), \end{cases}$$

where

- $W(t,y,k)$ is the phonons energy density at position $y \in \mathbb{R}$ and frequency $k \in \mathbb{T} := [-\frac{1}{2}, \frac{1}{2}]_{/\sim}$;
- $\omega \in C^2(\mathbb{T}_*)$ even and unimodal (with infimum in 0), is the dispersion relation;
- $\gamma > 0$ is the scattering rate of phonons;
- the scattering operator L_k, acting only on the frequency variable k, is given by

$$L_k u(k) := \int_{\mathbb{T}} R(k,k') \left[u(k') - u(k)\right] \, dk',$$

for a symmetric scattering kernel $R \in C^2(\mathbb{T} \times \mathbb{T})$.

Our model: interface conditions

At the interface $\mathcal{I}$, the phonons undergo a random transmission-reflection-absorption mechanism:

$$\text{(IC):}\quad \begin{cases} W(t,0^+,k) = p_+(k)W(t,0^-,k) + p_-(k)W(t,0^+,-k) + p_0(k)T, & \text{for } k \in \mathbb{T}_+; \\ W(t,0^-,k) = p_+(k)W(t,0^+,k) + p_-(k)W(t,0^-,-k) + p_0(k)T, & \text{for } k \in \mathbb{T}_- \end{cases}$$

where

- $T \geq 0$ is the temperature preset of the system;
- $p_+, p_-, p_0 : \mathbb{T} \to [0,1]$ are even, continuous and such that $p_+(k) + p_-(k) + p_0(k) = 1$;

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Aim: To understand the right scaling index $\alpha > 0$ such that

$$W_\lambda(t,y,k) := W(\lambda t, \lambda^{1/\alpha} y, k), \qquad \lambda > 0;$$

satisfying the interface conditions (IC) and

$$(\text{KE}_\lambda): \begin{cases} \frac{1}{\lambda}\partial_t W_\lambda(t,y,k) + \frac{1}{\lambda^{1/\alpha}}\omega'(k)\partial_y W_\lambda(t,y,k) = \gamma L_k W_\lambda(t,y,k); \\ W_\lambda(0,y,k) = W_0(y,k) \end{cases}$$

admits the limit $\lim_{\lambda\to\infty} W_\lambda$ and characterise the limit function $\bar{W}$.

A problem in non-equilibrium statistical mechanics

Aim: To understand heat conduction in crystalline solids (from microscopic to macroscopic scales).

A prototypical example on $\mathbb{R}$ is the Fermi-Pasta-Ulam (FPU) β-chain whose Hamiltonian is:

$$\mathcal{H}(\mathfrak{p},\mathfrak{q}) := \underbrace{\frac{1}{2}\sum_{j\in\mathbb{Z}} \mathfrak{p}_j^2}_{\text{kinetic}} + \underbrace{\frac{\omega_0^2}{2}\sum_{j\in\mathbb{Z}} \mathfrak{q}_j^2}_{\text{pinning}} + \underbrace{\frac{1}{2}\sum_{j,k\in\mathbb{Z}} \alpha_{j-k}(\mathfrak{q}_j-\mathfrak{q}_k)^2}_{\text{harmonic}} + \underbrace{\frac{1}{4}\sum_{j,k\in\mathbb{Z}} \beta_{j-k}(\mathfrak{q}_j-\mathfrak{q}_k)^4}_{\text{anharmonic}},$$

where $(\mathfrak{p}_j,\mathfrak{q}_j)\in\mathbb{R}\times\mathbb{R}$ momentum and position of particle j and $\alpha_j, \beta_j\in\mathbb{R}$ suitable coupling parameters.

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$\rightsquigarrow$ Consider only the harmonic chain:

$$\text{(H):}\quad \begin{cases} \dot{\mathfrak{q}}_j(t) = \partial_{\mathfrak{p}_j}\mathcal{H}(\mathfrak{p},\mathfrak{q}) = \mathfrak{p}_j(t), & j\in\mathbb{Z},\ t>0 \\ \dot{\mathfrak{p}}_j(t) = -\partial_{\mathfrak{q}_j}\mathcal{H}(\mathfrak{p},\mathfrak{q}) = -(\bar{\alpha}\star\mathfrak{q}(t))_j, & \end{cases}$$

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$\rightsquigarrow$ ballistic transport!

⚠ Numerical simulations show different macroscopic heat behaviours for the FPU β-chain:

- diffusive transport in the pinned case, i.e. $\omega_0\neq 0$;
- super-diffusive transport in the unpinned case, i.e. $\omega_0 = 0$.

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A problem in non-equilibrium statistical mechanics

[BO05]: Replace anharmonicity with a random exchange of momenta between nearest neighbourhood particles:

$$\text{(wPH):}\begin{cases} d\mathfrak{q}_j(t) = \mathfrak{p}_j(t)dt, & j\in\mathbb{Z},\ t>0 \\ d\mathfrak{p}_j(t) = -(\bar{\alpha}\star\mathfrak{q}(t))_j dt + \frac{\varepsilon\gamma}{2}\Delta_d(p_{j+1}(t)+4p_j(t)+p_{j-1}(t))dt + \sqrt{\varepsilon\gamma}\sum_{k=-1,0,1}\mathcal{L}_{j+k}p_j(t)dw_{j+k}(t), & \end{cases}$$

where $\{w_j(t)\}_{j\in\mathbb{Z}}$ independent BMs on $\mathbb{R}$, $\varepsilon \ll 1$, Δ_d discrete Laplacian and vector fields

$$\mathcal{L}_j = (p_j - p_{j+1})\partial_{p_{j-1}} + (p_{j+1}-p_{j-1})\partial_{p_j} + (p_{j-1}-p_j)\partial_{p_{j+1}}.$$

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Main features of the random perturbations

- $\varepsilon \ll 1 \rightsquigarrow$ Boltzmann-Grad hypothesis (only a finite number of collisions at macroscopic scale);
- The infinitesimal generator of $\mathcal{B}^{\varepsilon}$ is given by

$$\frac{1}{2}\sum_{j\in\mathbb{Z}} (\mathcal{L}_j)^2,$$

$\rightsquigarrow$ local conservation of kinetic energy and momentum!

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[KO20]: Our interface model (KE) + (IC) emerges as the kinetic limit for the ”energy density” of (LwPH)!

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Related results: classical vs anomalous diffusive limits

⚠ Only in the case of nearest neighbourhood interactions, i.e. $\alpha_j = 0$ if $|j| > 1$, we know that

$$R(k) := \int_{\mathbb{T}} R(k,k')\,dk' \approx |k|^2, \qquad p_\iota(k) \approx p_\iota^* > 0, \qquad |k| \ll 1,\ \iota \in \{0, \pm\}$$

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- **[BKO19]** In the pinned case $\rightsquigarrow \omega'(k) \approx |k|$, the right scaling is diffusive: $\alpha = 2$ and

$$\lim_{\lambda\to\infty} W_\lambda(t,y,k) = \bar{W}(t,y) \quad \text{where} \quad \begin{cases} \partial_t \bar{W}(t,y) = \bar{\gamma}\partial^2_{yy}\bar{W}(t,y), & y \in \mathbb{R}_* \\ \bar{W}(t,0) = T. \end{cases}$$

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- **[KOR20]** In the unpinned case $\rightsquigarrow \omega'(k) \approx O(1)$, the right scaling is super-diffusive: $\alpha = 3/2$ and

$$\partial_t \bar{W}(t,y) = \bar{\gamma}\, \text{p.v.} \int_{yy'>0} q_{\frac{3}{2}}(y'-y)[\bar{W}(t,y') - \bar{W}(t,y)]\, dy'$$

$$+ \int_{yy'<0} q_{\frac{3}{2}}(y'-y)\{p_+^*[\bar{W}(t,y')-\bar{W}(t,y)] + p_-^*[\bar{W}(t,-y')-\bar{W}(t,y)] + p_0^*[T_o - \bar{W}(t,y)]\}\, dy', \qquad y \in \mathbb{R}_*$$

for explicitly given diffusion coefficients $\bar{\gamma} > 0$ and $q_\alpha(y) := c_\alpha |y|^{-(1+\alpha)}$;

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for explicitly given diffusion coefficients $\bar{\gamma} > 0$ and $q_\alpha(y) := c_\alpha |y|^{-(1+\alpha)}$;

⚠ frequency homogenisation happens at the limit : $\bar{W}(0,y) = \bar{W}_0(y) := \int_{\mathbb{T}} W_0(y,k)\,dk$.

Precise assumptions on our model

[MK]: the scattering kernel is non-symmetric but of multiplicative form:

$$R(k, k') = R_1(k)R_2(k')$$

for (normalised) even, non-negative R_1, R_2 in $C(\mathbb{T})$;

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[S]: We consider abstract scaling features:

$$R_j(k) \approx |k|^{\beta_j}, \qquad S(k) := \frac{|\omega'(k)|}{\gamma R_1(k)} \approx |k|^{-\beta_3} \qquad k \ll 1, \ j = 1, 2$$

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[D]: the absorption probability has a logarithmic decay of order $\kappa > 0$ at 0:

$$p_0(k) \approx |\log|k||^{-\kappa}, \qquad k \ll 1$$

[ND]: the transmission probability is non-zero on $\mathbb{T}$:

$$\inf_{k\in\mathbb{T}} p_+(k) \neq 0$$

$\rightsquigarrow$ We introduce the scaling parameter:

$$\alpha := \frac{1+\beta_2}{\beta_3} \in (1,2)$$

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Associated function spaces

In order to state our main result, we need to introduce:

- the space $\mathcal{C}_T$ of the interface admissible configurations, composed by all $\phi \in C_b(\mathbb{R}_* \times \mathbb{T}_*)$ satisfying (IC) and which can be continuously extended to $\bar{\mathbb{R}}_\iota \times \mathbb{T}_*$, for $\iota \in \{+,-\}$;

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- the space $\mathcal{H}_o$ of the limit admissible configurations as the completion of $C_c^\infty(\mathbb{R}_*)$ under the seminorm $\|\cdot\|_{\mathcal{H}_o}$ given by

$$\|u\|_{\mathcal{H}_o} := \sqrt{\hat{\mathcal{E}}[u]},$$

for any Borel function $u\colon \mathbb{R}_* \to \mathbb{R}$ and with the following Dirichlet form:

$$\hat{\mathcal{E}}[u] := \frac{1}{2}\int_{yy'>0} (u(y') - u(y))^2 q_\alpha(y' - y)\, dydy' \\ + \frac{1}{2}\int_{yy'<0} q_\alpha(y' - y)\left\{p_+^*[u(y') - u(y)]^2 + p_-^*[u(-y') - u(y)]^2\right\} dydy';$$

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- the scattering invariant measure π on $\mathbb{T}$ associated with the scattering operator L_k:

$$\pi(dk) := \frac{R_2(k)}{R_1(k)}\, dk.$$

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Our main result

Let W_0 be a "suitable" initial condition: $W_0 \in \mathcal{C}_T$ and $\bar{W}_0 - T \in \mathcal{H}_o$ where

$$\bar{W}_0(y) \ := \int_{\mathbb{T}} W_0(y,k)\, \pi(dk) \ \in \ L^2(\mathbb{R}).$$

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$$\bar{W}_0(y) := \int_{\mathbb{T}} W_0(y,k)\,\pi(dk) \in L^2(\mathbb{R}).$$

Existence of super-diffusive limit and its characterisation

Let $W_\lambda(t,y,k)$ be the classical solution to $(\mathrm{KE}_\lambda) + (\mathrm{IC})$. Then,

$$\lim_{\lambda\to+\infty} \langle W_\lambda(t), F\rangle_{L^2(\mathbb{R}\times\mathbb{T})} = \langle \bar{W}(t), F\rangle_{L^2(\mathbb{R}\times\mathbb{T})}, \qquad F \in C_c^\infty(\mathbb{R}\times\mathbb{T}).$$

Moreover, the limit function $\bar{W}$ is the unique weak solution to

$$(\mathrm{LE}): \begin{cases} \partial_t \bar{W}(t,y) = \bar{\gamma}\,\mathrm{p.v.}\displaystyle\int_{yy'>0} q_\alpha(y'-y)[\bar{W}(t,y') - \bar{W}(t,y)]\,dy' \\ \qquad\qquad + \displaystyle\int_{yy'<0} q_\alpha(y'-y)\{p_+^*[\bar{W}(t,y') - \bar{W}(t,y)] + p_-^*[\bar{W}(t,-y') - \bar{W}(t,y)]\}\,dy'; \\ \bar{W}(t,0) = T, \qquad \bar{W}(0,y) = \bar{W}_0(y), \end{cases}$$

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Sketch of the proof: Probabilistic interpretation

1) We construct the skeleton random sequences in terms of $\{\tau_n\}_{n\geq 0}$ i.i.d. such that $\sim \exp(1)$:

- the frequency and position chains as $K_0(k) = k$ and $\{K_n\}_{n\in\mathbb{N}}$ i.i.d. on $\mathbb{T}$ such that

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$$\mathfrak{T}_n(k) := \sum_{j=0}^{n} \mathfrak{t}(K_j(k))\tau_j \quad \text{where} \quad \mathfrak{t}(k) := \frac{1}{\gamma R_1(k)}.$$

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4) As $\lambda \to +\infty$, the solution W_λ to (KE$_\lambda$) + (IC) weakly converges to solution $\bar{W}$ of (LE) if

> the processes $\{Y^o_\lambda(t,y,k)\}_\lambda$ weakly converge to $\eta^o(t,y)$ over $\mathcal{D}[0,+\infty)$ with the M_1-topology.

Sketch of the proof: Semigroup analysis

5) Introducing $\theta := \mathbb{E}[\mathfrak{t}(K_1)]$, one can show that

$$\lim_{\lambda \to +\infty} \sup_{t \in [0, t_*]} \left| \tilde{\mathfrak{T}}_\lambda^{-1}(t, k) - \frac{t}{\theta} \right| = 0, \quad \mathbb{P}\text{-a.s.}$$

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6) Let us consider the corresponding Markov semigroups:

$$\tilde{P}_t^{o,\lambda}u(y) := \mathbb{E}[u(\tilde{Z}_\lambda^o(t,y,k)),\ t < \tilde{\mathfrak{t}}_{y,\mathfrak{f}}^\lambda];$$
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The weak convergence of $\tilde{Z}_\lambda^o(t,y,k)$ to $\zeta^o(t,y) := \eta^o(\theta t,y)$ now follows from:

As $\lambda\to+\infty$, the semigroups $\{\tilde{P}_t^{o,\lambda}\}_{\lambda>0}$ strongly L^2-converges, uniformly on compact time intervals, to P_t^o

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⚠ $\tilde{Z}_\lambda^o(t,y,k)$ is deterministic until first scattering $\rightsquigarrow$ construct a Markov process $\hat{Z}_\lambda^o(t,y)$ which is "close" to it:

$$\mathbb{P}\left(y Z_1^\lambda(y,k) < 0 \right) \le \exp\left\{ -\frac{|y|\lambda^{1/\alpha}}{|S(k)|} \right\},$$

where $Z_1^\lambda(y,k)$ is the position after the first jump of a phonon started in y.

Sketch of the proof: Dirichlet forms

7) To show the the L^2-convergence of the semigroups, we rely on the corresponding Dirichlet forms:

$$\tilde{\mathcal{E}}_\lambda[u] := \lim_{t\to0+} \frac{1}{t}\int_{\mathbb{R}} \left[u(y) - \tilde{P}^o_t u(y)\right] u(y)\, dy$$

$$\mathcal{E}^o[u] := \lim_{t\to0+} \frac{1}{t}\int_{\mathbb{R}} [u(y) - P^o_t u(y)]\, u(y)\, dy$$

Mosco convergence for Dirichlet forms

A family of Dirichlet forms $\mathcal{E}_\lambda$ is M-convergent to a Dirichlet form $\mathcal{E}_\infty$, as $\lambda \to +\infty$, if for any $u \in L^2(\mathbb{R})$:

- for any $\{u_\lambda\}_{\lambda>0}$ weakly convergent to u in $L^2(\mathbb{R})$, it holds that

$$\liminf_{\lambda\to+\infty} \mathcal{E}_\lambda[u_\lambda] \geq \mathcal{E}_\infty[u];$$

- there exists $\{v_\lambda\}_{\lambda>0}$ strongly convergent to u in $L^2(\mathbb{R})$ such that

$$\limsup_{\lambda\to+\infty} \mathcal{E}_\lambda[v_\lambda] \leq \mathcal{E}_\infty[u];$$

[M94]: The Dirichlet forms $\hat{\mathcal{E}}_\lambda$ M-converge to $\hat{\mathcal{E}}$ if and only if the associated Markov semigroups strongly L^2-converge, uniformly on compact intervals.

Where the scaling index α comes from?

- Without the interface, the f.d.d. convergence of $Y_\lambda(t, y, k)$ essentially relies on:

$$Y(s, y, k) \approx Y(\mathfrak{T}_n, y, k) = y - \int_0^{\mathfrak{T}_n} \omega'(K(r, k))\, dr = y - \sum_{j=1}^{n} \mathfrak{t}(K_j)\omega'(K_j)\tau_j, \qquad \text{for } \mathfrak{T}_n \le s < \mathfrak{T}_{n+1};$$

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$\rightsquigarrow$ Our abstract framework: $S(k) = \mathfrak{t}(k)\omega'(k) \approx |k|^{-\beta_3}$ and $\tilde{\pi}(dk) = R_2(k)dk \approx |k|^{\beta_2} dk$. Thus,

$$\alpha := \frac{1+\beta_2}{\beta_3}$$

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Some literature on the topic

[BBJKO15]: G. Basile, C. Bernardin, M. Jara, T. Komorowski, S. Olla, *Thermal conductivity in harmonic lattices with random collisions.*, in *Thermal Transport in Low Dimensions*, Springer, 2015;

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[BO05]: C. Bernardin, S. Olla, *Fourier's law for a microscopic model of heat conduction*, J. Stat. Phys., 2005;

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Thank you for your attention!