Thermal boundaries for energy superdiffusion

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Thermal boundaries

Thermal boundaries appear in macroscopic equations for the evolution of energy or temperatures profiles.



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Basic example: *heat equation* for a material in contact with heat bath at the boundaries:

$$\partial_t u(t, y) = \partial_y (D(u)\partial_y u(t, y)), \qquad y \in [0, L]$$

$$u(t, 0) = T_+, \qquad u(t, L) = T_-.$$

But superdiffusion associated to fractional Laplacian can appear, and BC are more delicate.

Consider the usual heat equation with temperature fixed at y = 0:

$$\partial_t u(t, y) = D\Delta_y u(t, y), \qquad y \in \mathbb{R} \setminus \{0\}$$

$$u(t, 0) = T.$$

This is very easy problem, and left side does not exchange energy with the right side.

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What about, for $\alpha < 1$,

$$\partial_t u(t, y) = -D|\Delta_y|^{\alpha} u(t, y), \qquad y \in \mathbb{R} \setminus \{0\}$$
$$u(t, 0) = T ?$$

There are many different definition of the BC for the fractional Laplacian. Which one emerges from the microscopic dynamics?

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$$\mathfrak{p} = \{\mathfrak{p}_x, x \in \mathbb{Z}\}, \mathfrak{q} = \{\mathfrak{q}_x, x \in \mathbb{Z}\}$$
$$\mathcal{H}(\mathfrak{p}, \mathfrak{q}) \coloneqq \frac{1}{2} \sum_x \mathfrak{p}_x^2 + \frac{1}{2} \sum_{x,x'} \alpha_{x-x'} \mathfrak{q}_x \mathfrak{q}_{x'}$$

 $d\mathfrak{q}_{X}(t) = \mathfrak{p}_{X}(t)dt, \quad X \in \mathbb{Z}$

 $d\mathfrak{p}_{x}(t) = -(\alpha * \mathfrak{q}(t))_{x} dt + \left(-\gamma \mathfrak{p}_{0}(t) dt + \sqrt{2\gamma T} dw(t)\right) \delta_{0,x},$

where $\{w(t), t \ge 0\}$ is a standard Wiener process.

Microscopic modeling: Poisson-Maxwell thermostats

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- $\{N(t), t \ge 0\}$ is a standard Poisson process,
- $\{\tilde{p}_j\}$ i.i.d. $\mathcal{N}(0, T)$,

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$$\rho(\mu) = \frac{\sqrt{2\mu-1}}{\mu}$$
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- for $\mu \to \infty$ it converges to the Langevin thermostat.
- for $\mu = 1/2$ flip sign of the velocity at Poisson times.

$$\hat{f}(k) = \sum_{x} f_{x} e^{-i2\pi kx} \qquad k \in \Pi \sim [0,1]$$

•
$$\hat{\alpha}(k) \in \mathbb{C}^{\infty}(\Pi)$$
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• $\omega(k) = \sqrt{\hat{\alpha}(k)}$: dispersion relation.

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$$\hat{\psi}(t,k) = e^{-i\omega(k)t}\hat{\psi}(0,k) - i\gamma \int_0^t e^{-i\omega(k)(t-s)}\mathfrak{p}_0(s)ds + i\sqrt{2\gamma T} \int_0^t e^{-i\omega(k)(t-s)}dw(t)ds + i\sqrt{2\gamma T} \int_0^t e^{-i\omega(k)(t-s)}dw(t)dt + i\sqrt{2\gamma T} \int_0^t e^{-i\omega(k)(t-s)}dw(t)dt + i\sqrt{2\gamma T} \int_0^t e^{-i\omega(k)(t-s)}dw(t)dt + i\sqrt{2\gamma T} \int_0^t e^{-i\omega(k)}dw(t)dt + i\sqrt{2\gamma T} \int_0^t e$$

Wigner distribution

 $\eta \in \mathbb{R}, \; \varepsilon > 0$ -hyperbolic rescaling of space–time

$$\begin{split} \widehat{W}_{\varepsilon}(t,\eta,k) &:= \frac{\varepsilon}{2} \mathbb{E}\left[\hat{\psi}^*\left(\varepsilon^{-1}t,k-\frac{\varepsilon\eta}{2}\right)\hat{\psi}\left(\varepsilon^{-1}t,k+\frac{\varepsilon\eta}{2}\right)\right] \\ &\widehat{W}_{\varepsilon}(t,\eta,k) &:= \widehat{W}_{\varepsilon}(t,-\eta,k)^* \end{split}$$

and the inverse Fourier transform in $\boldsymbol{\eta}$

$$W_{\varepsilon}(t,y,k) = \int \widehat{W}_{\varepsilon}(t,\eta,k) e^{i2\pi\eta y} d\eta \in \mathbb{R}, \qquad y \in \mathbb{R},$$

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$$W_{\varepsilon}(t,y,k) \stackrel{\sim}{\underset{\varepsilon \to 0}{\rightarrow}} W(t,y,k) \ge 0$$
, as distribution

When $\gamma = 0$ it is easy to prove that

$$\partial_t W(t,y,k) + \frac{\omega'(k)}{2\pi} \partial_y W(t,y,k) = 0$$

$$\hat{\psi}(t,k) = \hat{\psi}(0,k)e^{-i\omega(k)t}$$

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$$\hat{\psi}(t,k) = \hat{\psi}(0,k)e^{-i\omega(k)t}$$
$$\widehat{W}_{\varepsilon}(t,\eta,k) := e^{i\left[\omega\left(k-\frac{\varepsilon\eta}{2}\right)-\omega\left(k+\frac{\varepsilon\eta}{2}\right)\right]\varepsilon^{-1}t}\widehat{W}_{\varepsilon}(0,\eta,k)$$
$$\underset{\varepsilon \to 0}{\sim} e^{-i\omega'(k)\eta t}\widehat{W}(0,\eta,k)$$

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$$\underset{\varepsilon \to 0}{\sim} e^{-i\omega'(k)\eta t}\widehat{W}(0,\eta,k)$$
$$W(t,y,k) = W\left(0,y-\frac{\omega'(k)}{2\pi}t,k\right)$$

Phonon of wave number k moves freely with velocity $\frac{\omega'(k)}{2\pi}$.

$\gamma > 0$ Explicit solution (microscopic)

$$J(t) = \int_{\mathbb{T}} \cos(\omega(k)t) \ dk,$$

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$\gamma > 0$ Explicit solution (microscopic)

$$J(t) = \int_{\mathbb{T}} \cos(\omega(k)t) \ dk,$$

The Laplace transform of J(t) is given by

$$\begin{split} \tilde{J}(\lambda) &= \int_0^\infty e^{-\lambda t} J(t) dt = \int_{\mathbb{T}} \frac{\lambda}{\lambda^2 + \omega^2(k)} dk. \\ \tilde{g}(\lambda) &= \left(1 + \gamma \tilde{J}(\lambda)\right)^{-1} = \int_0^\infty e^{-\lambda t} g(dt). \qquad |\tilde{g}(\lambda)| < 1 \\ \phi(t,k) &= \int_0^t e^{i\omega(k)\tau} g(d\tau) \underset{t \to \infty}{\longrightarrow} \tilde{g}(-i\omega(k)) \coloneqq \nu(k) \\ t,k) &= e^{-i\omega(k)t} \Big[\hat{\psi}(0,k) - i\gamma \int_a^t \phi(t-s,k) e^{i\omega(k)s} \mathfrak{p}_0^0(s) \, ds \end{split}$$

$$\hat{\psi}(t,k) = e^{-i\omega(k)t} \Big[\hat{\psi}(0,k) - i\gamma \int_0^t \phi(t-s,k) e^{i\omega(k)s} \mathfrak{p}_0^0(s) \, ds \\ +i\sqrt{2\gamma T} \int_0^t \phi(t-s,k) e^{i\omega(k)s} \, dw(s) \Big]$$

 $\mathfrak{p}_0^0(i)$: moment of particle 0 under the free evolution for $\gamma = 0$.

Results in presence of the Langevin thermostat in 0 ($\gamma > 0$)

$$\nu(k) = (1 + \gamma \tilde{J}(-i\omega(k)))^{-1}, \qquad \tilde{J}(\lambda) = \int_{\mathbb{T}} \frac{\lambda}{\lambda^2 + \omega^2(k)} dk.$$

Re $\nu(k) = (1 + \frac{\gamma \pi}{|\omega'(k)|}) |\nu(k)|^2$

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$$\operatorname{Re} \nu(k) = \left(1 + \frac{\gamma \pi}{|\omega'(k)|}\right) |\nu(k)|^2$$

$$\mathfrak{g}(k) = \frac{2\pi \gamma |\nu(k)|^2}{|\omega'(k)|} \qquad \text{absorbtion probability}$$

$$p_+(k) = \left|1 - \frac{\gamma \pi \nu(k)}{|\omega'(k)|}\right|^2 \qquad \text{transmission probability}$$

$$p_-(k) = \left|\frac{\gamma \pi \nu(k)}{|\omega'(k)|}\right|^2 \qquad \text{reflection probability}$$

$$\mathfrak{g}(k) + p_+(k) + p_-(k) = 1$$

T.Komorowski, L.Ryzhik, S.O., H.Spohn, ARMA (2020)

$$\partial_t W(t, y, k) + \frac{\omega'(k)}{2\pi} \partial_y W(t, y, k) = 0, \qquad y \in \mathbb{R} \setminus \{0\}$$

with boundary conditions:

$$\begin{split} &W(t,0^+,k) = p_-(k)W(t,0^+,-k) + p_+(k)W(t,0^-,k) + \mathfrak{g}(k)T, \quad 0 < k < 1/2 \\ &W(t,0^-,k) = p_-(k)W(t,0^-,-k) + p_+(k)W(t,0^+,k) + \mathfrak{g}(k)T, \quad -1/2 < k < 0 \end{split}$$

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Since $\mathfrak{g}(k) + p_+(k) + p_-(k) = 1$, we have that

W(t, y, k) = T is a stationary solution.

No dispersion in the macroscopic scattering!

T.Komorowski, S.O., arXiv:2101.04360 (2021)

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with boundary conditions 0 < k < 1/2:

$$W(t,0^{+},k) = p_{-}(k)W(t,0^{+},-k) + p_{+}(k)W(t,0^{-},k) + p_{abs}\mathfrak{g}(k)T$$
$$+\mathfrak{g}(k)\int_{0}^{1/2}W(t,0^{-},\ell)p_{sc}(\ell)d\ell + \mathfrak{g}(k)\int_{0}^{1/2}W(t,0^{+},-\ell)p_{sc}(\ell)d\ell$$

$$p_+(k) + p_-(k) + p_{abs}\mathfrak{g}(k) + \mathfrak{g}(k) \int_0^1 p_{sc}(\ell) d\ell = 1$$

Dispersion in the macroscopic scattering!

 $p_{\rm abs} \rightarrow 1$ and $p_{\rm sc}(\ell) \rightarrow 0$ as $\mu \rightarrow \infty$ (converges to the Langevin scattering).

When random bulk scattering is present

If we add a (slow) random scattering in the bulk of the system: random flip of sign of velocities, random exchange of velocity of n.n. particles, with rates ~ $\gamma' \varepsilon$.

T. Komorowski, S.O. (J. Funct. Analys. 2020)

$$\partial_t W(t, y, k) + \frac{\omega'(k)}{2\pi} \partial_y W(t, y, k) = \gamma' L W(t, y, k)$$

$$LW(k) = \int \mathfrak{R}(k, k') \left(W(k') - W(k) \right)$$
$$R(k, k') = R(K)R(k'), \qquad R(k) \sim |k|^2, \ k \sim 0$$

same boundary conditions:

$$\begin{split} & W(t,0^+,k) = p_-(k)W(t,0^+,-k) + p_+(k)W(t,0^-,k) + \mathfrak{g}(k)T, \quad 0 < k < 1/2 \\ & W(t,0^-,k) = p_-(k)W(t,0^-,-k) + p_+(k)W(t,0^+,k) + \mathfrak{g}(k)T, \quad -1/2 < k < 0 \end{split}$$

Without the thermostat: Basile, O., Spohn, ARMA 2009.

Diffusive and superdiffusive behavior for $\gamma' > 0$, $\gamma = 0$

For random exchange of nearest neighbor velocities

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$$R(k, k') = R(K)R(k'), R(k) \sim |k|^2, \qquad k \sim 0$$

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. Without thermal boundary:

• if $\omega'(k) \sim k$ (optical chain) : $D < +\infty$, diffusive behaviour $W(\lambda^2 t, \lambda y, k) \xrightarrow{}{\lambda \to 0} e(t, y)$ $\partial_t e = D \partial_{yy} e, \qquad D = \frac{1}{4\pi^2 \gamma'} \int \frac{\omega'(k)^2}{R(k)} dk$

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- if ω'(k) ~ 1 (acustic chain) : D = +∞, superdiffusive behaviour (Jara-Komorowski-Olla AAP 2009, Basile-Bovier MPRF 2010):

$$\begin{split} W(\lambda^{3/2}t,\lambda y,k) &\xrightarrow[\lambda \to 0]{} e(t,y) \\ \partial_t e &= -\hat{c} |\Delta|^{3/4} e, \end{split}$$

Giada Basile, Tomasz Komorowki, S.O., **Kinetic and Related Models**, AIMS, (2019) In the cases of bulk diffusive behavior: $\omega'(k) \sim k$ (optical chain)

$$W(\lambda^2 t, \lambda y, k) \xrightarrow{\lambda \to 0} e(t, y)$$

$$\partial_t e = D \partial_{yy} e, \qquad y \neq 0, \qquad D = \frac{1}{4\pi^2 \gamma'} \int \frac{\omega'(k)^2}{R(k)} dk$$
$$e(t, 0^+) = T = e(t, 0^-)$$

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$$e(t, 0^+) = T = e(t, 0^-)$$

Reflection and transmission of phonons are irrelevant in this time scale: phonons gets absorbed and created such that energy density is T at y = 0.

Superdiffusive behaviour with thermal boundary

Tomasz Komorowki, S.O., Lenya Rhyzik, Ann. of Prob. (2020) *Situation is different in the super-diffusive case.*

$$\begin{aligned} \partial_{t}W(t,y,k) &+ \frac{\omega'(k)}{2\pi} \partial_{y}W(t,y,k) = \int \Re(k,k') \left(W(k') - W(k) \right) \\ R(k,k') &= R(K)R(k'), \qquad R(k) \sim |k|^{2}, \qquad |\omega'(k)| \sim 2, \qquad k \sim 0, \\ W(t,0^{+},k) &= p_{-}(k)W(t,0^{+},-k) + p_{+}(k)W(t,0^{-},k) + \mathfrak{g}(k)T, \qquad 0 < k < 1/2 \\ W(t,0^{-},k) &= p_{-}(k)W(t,0^{-},-k) + p_{+}(k)W(t,0^{+},k) + \mathfrak{g}(k)T, \qquad -1/2 < k < 0. \end{aligned}$$

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$$\begin{aligned} \partial_t W(t, y, k) &+ \frac{\omega'(k)}{2\pi} \partial_y W(t, y, k) = \int \Re(k, k') \left(W(k') - W(k) \right) \\ R(k, k') &= R(K) R(k'), \qquad R(k) \sim |k|^2, \qquad |\omega'(k)| \sim 2, \qquad k \sim 0, \\ W(t, 0^+, k) &= p_-(k) W(t, 0^+, -k) + p_+(k) W(t, 0^-, k) + \mathfrak{g}(k) T, \qquad 0 < k < 1/2 \\ W(t, 0^-, k) &= p_-(k) W(t, 0^-, -k) + p_+(k) W(t, 0^+, k) + \mathfrak{g}(k) T, \qquad -1/2 < k < 0 \\ R(k, k') \sim 0, \qquad k \sim 0, \end{aligned}$$

the phonon is crossing the thermostat when $k \sim 0$.

Tomasz Komorowki, S.O., Lenya Rhyzik, Ann. of Prob. (2020) For $k \to 0$, $\mathfrak{g}(k) \to \mathfrak{g}_0 > 0$, $p_-(k) \to p_-(0) > 0$.

$$W(\lambda^{3/2}t,\lambda y,k) \xrightarrow[\lambda \to 0]{} e(t,y)$$

$$\begin{aligned} \partial_t e(t,y) &= -\hat{c} |\Delta|^{3/4} e(t,y) \\ &+ \hat{c} \mathfrak{g}_0 \int_{yy' < 0} q(y - y') (T - e(t,y')) dy' \\ &+ \hat{c} p_-(0) \int_{yy' < 0} q(y - y') (e(t, -y') - e(t,y)) dy'. \\ &q(y) &= \frac{c}{|y|^{5/4}} \quad \text{kernel of } |\Delta|^{3/4}. \end{aligned}$$

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$$\mathfrak{p} = \{\mathfrak{p}_x, x \in \mathbb{Z}\}, \ \mathfrak{q} = \{\mathfrak{q}_x, x \in \mathbb{Z}\}$$
$$\mathcal{H}(\mathfrak{p}, \mathfrak{q}) \coloneqq \frac{1}{2} \sum_x \mathfrak{p}_x^2 + \frac{1}{2} \sum_{x, x'} \alpha_{x-x'} \mathfrak{q}_x \mathfrak{q}_{x'}$$

$$d\mathfrak{q}_{x}(t) = \mathfrak{p}_{x}(t)dt, \quad x \in \mathbb{Z}$$

$$d\mathfrak{p}_{x}(t) = -(\alpha * \mathfrak{q}(t))_{x} + \left(-\gamma \mathfrak{p}_{0}(t)dt + \sqrt{2\gamma T}dw(t)\right)\delta_{0,x},$$

$$\mathcal{E}_{x} = \frac{\mathfrak{p}_{x}^{2}}{2} + \frac{\mathfrak{q}_{x}\left(\alpha \star \mathfrak{q}\right)_{x}}{2}$$



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$$\mathcal{E}_{[\lambda y]}(\lambda^{-3/2}t) \stackrel{\sim}{\underset{\lambda \to 0}{\rightarrow}} e(t,y)$$
 weakly

Direct Hydrodynamic Limit

$$\mathcal{E}_{x} = \frac{\mathfrak{p}_{x}^{2}}{2} + \frac{\mathfrak{q}_{x} (\alpha \star \mathfrak{q})_{x}}{2}, \qquad x \in \mathbb{Z}$$
$$\mathcal{E}_{[\lambda y]}(\lambda^{-3/2}t) \stackrel{\sim}{\xrightarrow[\lambda \to 0]{}} e(t, y) \qquad \text{weakly} \quad y \in \mathbb{R}.$$

$$\begin{split} \partial_t \tilde{e}(t,y) &= \mathfrak{L} \tilde{e}(t,y), \qquad \tilde{e}(t,0) = 0, \\ \mathfrak{L} &\sim - (-\Delta_y)^{3/4} \end{split}$$

- Without the thermostat: M.Jara, T.Komoroswki, S.Olla, CMP (2015).
- With the thermostat, still open.

at distance
$$N = [\lambda^{-1}]$$
.

$$d\mathfrak{q}_{x}(t) = \mathfrak{p}_{x}(t)dt, \qquad x \in \mathbb{Z}$$

$$d\mathfrak{p}_{x}(t) = -(\alpha * \mathfrak{q}(t))_{x} \qquad + \left(-\gamma \mathfrak{p}_{0}(t)dt + \sqrt{2\gamma T_{-}}dw_{1}(t)\right)\delta_{0,x}$$

$$+ \left(-\gamma \mathfrak{p}_{N}(t)dt + \sqrt{2\gamma T_{+}}dw_{2}(t)\right)\delta_{N,x}$$

If $T_+ \neq T_-$: non-equilibrium stationary state.

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- Process Y(t) is generated by the linear Boltzmann equation (continuous trajectories),
- Process Z(t) is a pure jump Levy process obtained from Y(t), characterized by a Levy measure r(y) given by the law of

$$\frac{\bar{\omega}'(K)}{R(K)}$$

where K is a random variable on S^1 with law R(k)dk. We only need to control the convergence of Z(t)! A review article:

T. Komorowski, S. Olla, Thermal Boundaries in Kinetic and Hydrodynamic Limits, http://arxiv.org/abs/2010.04721, to appear in "Recent advances in kinetic equations and applications", F. Salvarani ed., Springer INdAM Series, 2021.

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- T. Komorowski, S. Olla, L. Ryzhyk, H. Spohn High frequency limit for a chain of harmonic oscillators with a point Langevin thermostat., Arch. Rational Mech. An., 237, 497543 (2020).
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