Thermal conductivity for a chain of harmonic oscillators in a magnetic field

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Stochastic Dynamics Out of Equilibrium

Joint work with Keiji Saito and Shuji Tamaki (Keio University)

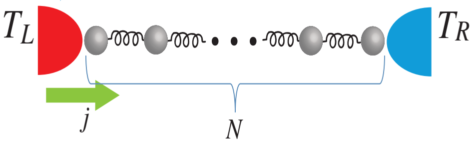
Introduction

Microscopic Model : System of oscillators (Hamiltonian dynamics) + magnetic field + stochastic noise

Goal : Understand

- Behavior of macroscopic energy diffusion
- In particular, the anomalous diffusion in $d = 1, 2$
- In this talk, we only consider the order of the divergence of thermal conductivity
- Role of "momentum conservation"
- Role of "sound velocity"

Transport of energy



Thermal conductivity in a stationary non-equilibrium state:

$$\kappa_N = \frac{NJ}{(T_L - T_R)} \sim N^{\alpha}$$

J: current per a particle

Normal transport : $\alpha = 0$, $\kappa_N \to \kappa < \infty$
Fourier's law : $j(x,t) = -\kappa \partial_x T(x,t)$
Diffusion equation : $\partial_t T(x,t) = \frac{\kappa}{c} \Delta T(x,t)$

Anomalous transport : $0 < \alpha < 1$ (or $\kappa_N \sim \log N$)
Diffusion equation: $\partial_t T(x,t) = -c(-\Delta)^{c_\alpha} T(x,t)$??

(Ballistic transport : $\alpha = 1$)

Model : system of harmonic oscillators (periodic b.c.)

- $\mathbb{Z}_N^d = \mathbb{Z}^d / N\mathbb{Z}^d$
- $q_x, p_x \in \mathbb{R}^{d^*}$, $x \in \mathbb{Z}_N^d$ (d^* is not necessarily equal to d)
- $H = \sum_x \{ \frac{|p_x|^2}{2} + \sum_{|y-x|=1} \frac{|q_x - q_y|^2}{4} \} =: \sum_x \mathcal{E}_x$

Hamiltonian dynamics (deterministic) :

$$(0) \begin{cases} \dfrac{dq_x^k}{dt} = \partial_{p_x^k} H = p_x^k & (k = 1, \ldots, d^*) \\ \dfrac{dp_x^k}{dt} = -\partial_{q_x^k} H = (\Delta q^k)_x & (k = 1, \ldots, d^*) \end{cases}$$

where $(\Delta F)_x = \sum_{|y-x|=1} (F_y - F_x)$ for $F : \mathbb{Z}_N^d \to \mathbb{R}$

* The energy transport is ballistic for the deterministic dynamics

Magnetic field for $d^* = 2$

Consider the system in a magnetic field with strength B and its direction is orthogonal to the plane where oscillators move.

Model (I) : Uniform

- Each oscillator has a uniform charge
- Operator : $G^I = \sum_x (p_x^2 \partial_{p_x^1} - p_x^1 \partial_{p_x^2})$
- Generator of the deterministic part : $L = A + BG^I$

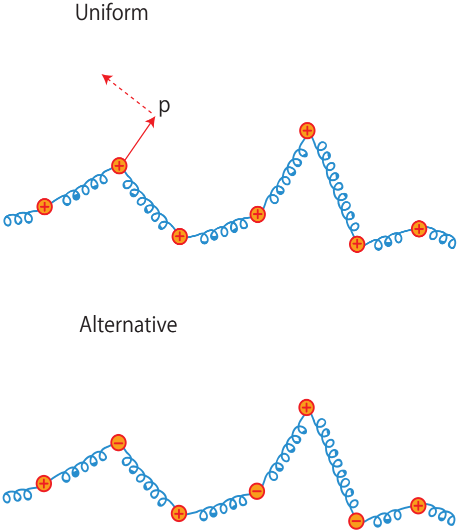
Model (II) : Alternative

- Assume N is even and $d = 1$
- Each oscillator has a charge with uniform absolute value but its sign is alternative in x
- Operator : $G^{II} = \sum_x (-1)^x (p_x^2 \partial_{p_x^1} - p_x^1 \partial_{p_x^2})$
- Generator of the deterministic part : $L = A + BG^{II}$

Remark

We can also consider the term G comes from Coriolis force in Model (I).

Chain of Oscillators in a magnetic field ($d = 1, d^* = 2$)



Model : system of harmonic oscillators in a magnetic field with uniform charge

- $B \neq 0$: strength of the magnetic field
- $q_x, p_x \in \mathbb{R}^{d^*}$, $x \in \mathbb{Z}_N^d$ $\quad (d^* \geq 2)$
- $H = \sum_x \{ \frac{|p_x|^2}{2} + \sum_{|y-x|=1} \frac{|q_x - q_y|^2}{4} \}$

Hamiltonian dynamics + magnetic field (deterministic) :

$$(I) \begin{cases} \dfrac{dq_x^k}{dt} = \partial_{p_x^k} H = p_x^k & (k = 1, \ldots, d^*) \\ \dfrac{dp_x^1}{dt} = -\partial_{q_x^1} H + B p_x^2 = (\Delta q^1)_x + B p_x^2 & \\ \dfrac{dp_x^2}{dt} = -\partial_{q_x^2} H - B p_x^1 = (\Delta q^2)_x - B p_x^1 & \\ \dfrac{dp_x^k}{dt} = -\partial_{q_x^k} H = (\Delta q^k)_x & (k = 3, \ldots, d^*) \end{cases}$$

Model : system of harmonic oscillators in a magnetic field with alternative charge

- $B \neq 0$: strength of the magnetic field
- N : even, $d = 1$
- $q_x, p_x \in \mathbb{R}^{d^*}$, $x \in \mathbb{Z}_N$ $(d^* \geq 2)$
- $H = \sum_x \{ \frac{|p_x|^2}{2} + \sum_{|y-x|=1} \frac{|q_x - q_y|^2}{4} \}$

Hamiltonian dynamics + magnetic field (deterministic) :

$$(II) \begin{cases} \dfrac{dq_x^k}{dt} = \partial_{p_x^k} H = p_x^k & (k = 1, \ldots, d^*) \\ \dfrac{dp_x^1}{dt} = -\partial_{q_x^1} H + (-1)^x B p_x^2 = (\Delta q^1)_x + (-1)^x B p_x^2 \\ \dfrac{dp_x^2}{dt} = -\partial_{q_x^2} H - (-1)^x B p_x^1 = (\Delta q^2)_x - (-1)^x B p_x^1 \\ \dfrac{dp_x^k}{dt} = -\partial_{q_x^k} H = (\Delta q^k)_x & (k = 3, \ldots, d^*) \end{cases}$$

Conserved quantities

- $\mathcal{E}_x := \frac{|p_x|^2}{2} + \sum_{|y-x|=1} \frac{|q_x - q_y|^2}{4}$: energy of x
- $H = \sum_x \mathcal{E}_x$

Model (0): $\sum_x \mathcal{E}_x, \quad \sum_x p_x^k \ (k = 1, 2, \dots, d^*)$

Model (I) : $\sum_x \mathcal{E}_x, \quad \sum_x p_x^k \ (k = 3, \dots, d^*), \ \sum_x (p_x^1 - Bq_x^2),$
$\sum_x (p_x^2 + Bq_x^1)$

Model (II) : $\sum_x \mathcal{E}_x, \quad \sum_x p_x^k \ (k = 3, \dots, d^*),$
$\sum_{x:even}(p_x^1 + p_{x+1}^1 - Bq_x^2 + Bq_{x+1}^2), \ \sum_{x:even}(p_x^2 + p_{x+1}^2 + Bq_x^1 - Bq_{x+1}^1)$

- $\sum_x p_x^1$ and $\sum_x p_x^2$ are not conserved for both (I) and (II)
- The number of conserved quantities are same for all models
- Precisely, there are infinitely many conserved quantities without the stochastic noise

Micro-canonical state space and micro-canonical measure

- $\Omega_{N,\mathcal{E}} := \{(q_x, p_x) \in (\mathbb{R}^{2d^*})^{N^d}; \sum_x q_x = 0, \sum_x p_x = 0, \sum_x \mathcal{E}_x = \mathcal{E} N^d\}$
- $\mu_{N,\mathcal{E}}$: Uniform measure on $\Omega_{N,\mathcal{E}}$.
- $\langle \cdot \rangle_{N,\mathcal{E}}$: Expectation w.r.t. $\mu_{N,\mathcal{E}}$

- $\Omega_{N,\mathcal{E}}$ and $\mu_{N,\mathcal{E}}$ are invariant for Model (0) and (I)
- For Model (II), we do not consider the micro-canonical state space for simplicity.
- For the coordinates (q_x, p_x) with periodic b.c., $\int \exp(-\beta H(q,p)) dqdp = \infty$ for any $\beta > 0$, so we can not consider the canonical measure.

System of harmonic oscillators (periodic b.c.) for (r, p)-coordinates

- $d = 1$
- $r_x, p_x \in \mathbb{R}^{d^*}$, $x \in \mathbb{Z}_N$
- Change the coordinates with $r_x = q_{x+1} - q_x$ formally in the dynamics (but $q_{x+N} = q_x$ does not hold here)

Hamiltonian dynamics (deterministic) :

$$(0) \begin{cases} \dfrac{dr_x^k}{dt} = p_{x+1}^k - p_x^k & (k = 1, \ldots, d^*) \\ \dfrac{dp_x^k}{dt} = r_x^k - r_{x-1}^k & (k = 1, \ldots, d^*) \end{cases}$$

System of harmonic oscillators in a magnetic field for (r, p)-coordinates with uniform charge

- $B \neq 0$
- $d = 1$
- $r_x, p_x \in \mathbb{R}^{d^*}$, $x \in \mathbb{Z}_N$ $\quad (d^* \geq 2)$

Hamiltonian dynamics + magnetic field (deterministic) :

$$(I) \begin{cases} \dfrac{dr_x^k}{dt} = p_{x+1}^k - p_x^k & (k = 1, \ldots, d^*) \\ \dfrac{dp_x^1}{dt} = r_x^1 - r_{x-1}^1 + Bp_x^2 & \\ \dfrac{dp_x^2}{dt} = r_x^2 - r_{x-1}^2 - Bp_x^1 & \\ \dfrac{dp_x^k}{dt} = r_x^k - r_{x-1}^k & (k = 3, \ldots, d^*) \end{cases}$$

System of harmonic oscillators in a magnetic field for (r, p)-coordinates with alternative charge

- $B \neq 0$
- N : even, $d = 1$
- $r_x, p_x \in \mathbb{R}^{d^*}$, $x \in \mathbb{Z}_N$ $\quad (d^* \geq 2)$

Hamiltonian dynamics + magnetic field (deterministic) :

$$
(II) \begin{cases} \dfrac{dr_x^k}{dt} = p_{x+1}^k - p_x^k & (k = 1, \dots, d^*) \\ \dfrac{dp_x^1}{dt} = r_x^1 - r_{x-1}^1 + (-1)^x B p_x^2 & \\ \dfrac{dp_x^2}{dt} = r_x^2 - r_{x-1}^2 - (-1)^x B p_x^1 & \\ \dfrac{dp_x^k}{dt} = r_x^k - r_{x-1}^k & (k = 3, \dots, d^*) \end{cases}
$$

Conserved quantities

Model (0): $\sum_x \mathcal{E}_x$, $\sum_x p_x^k$ $(k = 1, 2, \ldots, d^*)$, $\sum_x r_x^k$ $(k = 1, 2, \ldots, d^*)$

Model (I) : $\sum_x \mathcal{E}_x$, $\sum_x p_x^k$ $(k = 3, \ldots, d^*)$, $\sum_x r_x^k$ $(k = 1, 2, \ldots, d^*)$

Model (II) : $\sum_x \mathcal{E}_x$, $\sum_x p_x^k$ $(k = 3, \ldots, d^*)$, $\sum_x r_x^k$ $(k = 1, 2, \ldots, d^*)$,
$\sum_{x:even}(p_x^1 + p_{x+1}^1 + Br_x^2)$, $\sum_{x:even}(p_x^2 + p_{x+1}^2 - Br_x^1)$

- $\sum_x(p_x^1 - Bq_x^2)$ and $\sum_x(p_x^2 + Bq_x^1)$ are not functions of (r, p)
- The number of conserved quantities are different between Model (0),(II) and Model (I)
- If $d = 1$ and $d^* = 2$, Model (0) and (II) have five conserved quantities, but Model (I) has only three conserved quantities

Canonical state space and canonical measure

- $\Omega_N := \{(r_x, p_x) \in (\mathbb{R}^{2d^*})^N\} = \mathbb{R}^{2d^* N}$
- $\mu_{N,\beta}(drdp) = \frac{1}{Z_\beta} \exp(-\beta \sum_x \mathcal{E}_x) drdp =$ $\Pi_x \Pi_{k=1}^{d^*} \frac{\beta}{2\pi} \exp(-\beta \frac{(r_x^k)^2 + (p_x^k)^2}{2}) dr_x^k dp_x^k$ for $\beta > 0$.
- $\langle \cdot \rangle_{N,\beta}$: Expectation w.r.t. $\mu_{N,\beta}$

- $\mu_{N,\beta}$ is invariant for Model (0),(I) and (II)
- The measure is product because $d = 1$

Stochastic noise (momentum exchange)

For each $k \in \{1, \dots, d^*\}$ and a pair $x, y \in \mathbb{Z}_N^d$ satisfying $|x - y| = 1$, exchange $p_x^k \leftrightarrow p_y^k$ with rate $\gamma > 0$.

- Every conserved quantity is also conserved by the stochastic noise
- Micro-canonical (resp. canonical) state spaces and measures are still invariant with the stochastic noise

Full generator of our dynamics: $L = A + BG + \gamma S$ where

$$G^{(I)} = \sum_x (p_x^2 \partial_{p_x^1} - p_x^1 \partial_{p_x^2}), \quad G^{(II)} = \sum_x (-1)^x (p_x^2 \partial_{p_x^1} - p_x^1 \partial_{p_x^2})$$

$$Sf = \sum_{k=1}^{d^*} \sum_x \sum_{|y-x|=1} (f(q, p^{x,y,k}) - f(q, p))$$

$$\text{or } \sum_{k=1}^{d^*} \sum_x \sum_{|y-x|=1} (f(r, p^{x,y,k}) - f(r, p))$$

Thermal conductivity

Infinite system (Formal argument)

- $S(x,t) := \langle (\mathcal{E}_x(t) - \mathcal{E})(\mathcal{E}_0(0) - \mathcal{E}) \rangle$ where $\mathcal{E} = \langle \mathcal{E}_0 \rangle$
- $\langle \cdot \rangle$: expectation w.r.t. some shift-invariant equilibrium measure
- $\kappa^{k,l} := \lim_{t\to\infty} \frac{1}{2\mathcal{E}^2 t} \sum_{x\in\mathbb{Z}^d} x^k x^l S(x,t)$

Green-Kubo formula :

$$\kappa^{k,l} = \lim_{t\to\infty} \frac{1}{2t\mathcal{E}^2} \sum_{x\in\mathbb{Z}^d} \langle (\int_0^t j_{x,x+e_k}(s)ds)(\int_0^t j_{0,e_l}(s')ds') \rangle$$

$$= \frac{1}{\mathcal{E}^2} \sum_{x\in\mathbb{Z}^d} \int_0^\infty \langle j_{x,x+e_k}(t) j_{0,e_l}(0) \rangle dt = \delta_{k,l}\kappa^{1,1} = \kappa\delta_{k,l}$$

- $j_{x,x+e_k}(t)$: energy current from x to $x+e_k$ at time t
- If the energy fluctuation diffuses normally, $0 < \kappa < \infty$
- By the symmetry (even for $B \neq 0$), $\kappa^{k,k} = \kappa$ for any $k = 1, 2, \ldots, d$

Thermal conductivity: Finite size approximation

Periodic b.c.

$$\kappa_N(t) := \frac{1}{2t\mathcal{E}^2} \sum_{x \in \mathbb{Z}_N^d} \langle (\int_0^t j_{x,x+e_1}(s)ds)(\int_0^t j_{0,e_1}(s')ds') \rangle_{N,\mathcal{E}(\beta)}$$

$$= \frac{1}{2t\mathcal{E}^2 N^d} \int_0^t \int_0^t \langle J(s)J(s') \rangle_{N,\mathcal{E}(\beta)} dsds'$$

where $J(s) = \sum_{x \in \mathbb{Z}_N^d} j_{x,x+e_1}(s)$
Formally $\kappa = \lim_{t \to \infty} \lim_{N \to \infty} \kappa_N(t)$

The stationary non-equilibrium state

$$\kappa_N := \lim_{|T_L - T_R| \to 0, T_L, T_R \to T(\mathcal{E})(T(\beta))} \frac{N \langle J_N \rangle}{T_L - T_R}$$

where J_N is the stationary energy flux with system size N per a particle.

Relation between κ, $\kappa_N(t)$ and κ_N

Assume the limit $\lim_{N\to\infty} \kappa_N(t) := \kappa(t)$ exists.

In the regime $\kappa < \infty$, the following is generally expected:

- $\lim_{t\to\infty} \kappa(t) = \lim_{N\to\infty} \kappa_N = \kappa$

In the regime $\kappa = \infty$, the followings are generally expected:

- $\lim_{t\to\infty} \kappa(t) = \lim_{N\to\infty} \kappa_N = \infty$
- If $\kappa(t) \sim t^\beta$ and $\kappa_N \sim N^\alpha$ and the sound velocity is not zero, then $\beta = \alpha$
- More generally, $\kappa(t_N) \sim \kappa_N$ as $N \to \infty$ where t_N is a proper time scaling
- If the energy spreads with t^δ in width at time t, then $(t_N)^\delta \sim N$ since at time t_N, the periodic boundary starts to effect
- Therefore, heuristically, $t_N \sim N$ if the sound velocity is not zero
- If the sound velocity is vanishing, we can not predict the relation of β and α so far

Dispersion relation and the sound velocity

Model (0): $B = 0$

- $\omega_\theta = \sqrt{4 \sum_{k=1}^{d} \sin^2(\pi\theta^k)}$
- $v_s := \lim_{\theta\to 0} |\partial_{\theta^1}\omega_\theta| > 0$

Model (I) $d^* = 2$

- $\tilde{\omega}_\theta = \sqrt{\omega_\theta^2 + (\frac{B}{2})^2} \pm \frac{B}{2}$
- $v_s = \lim_{\theta\to 0} |\partial_{\theta^1}\tilde{\omega}_\theta| = \lim_{\theta\to 0} |\frac{4\pi\sin(\pi\theta^1)\cos(\pi\theta^1)}{\sqrt{\omega_\theta^2 + (\frac{B}{2})^2}}| = 0$

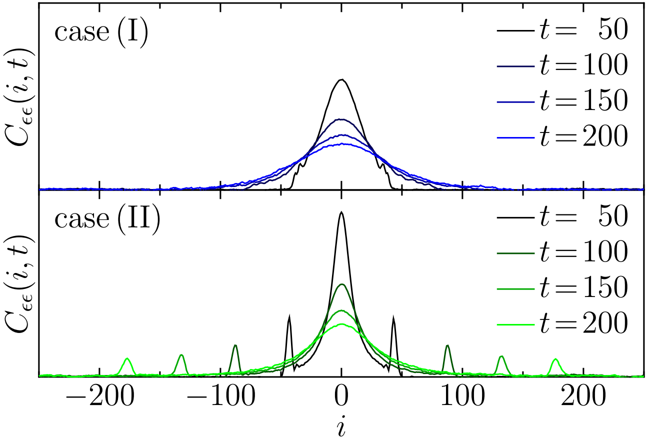
Model (I) $d^* \geq 3$

- $\tilde{\omega}_\theta, \omega_\theta$
- $v_s > 0$ and $v_s = 0$

Model (II)

- $\tilde{\omega}_\theta = \pm\sqrt{\frac{4+B^2-\sqrt{(4+B^2)^2-16\omega(\theta)^2}}{2}} \sim \pm\frac{4}{4+B^2}\omega_\theta$ as $\theta \to 0$
- $v_s = \lim_{\theta\to 0} |\partial_\theta\tilde{\omega}_\theta| > 0$

Sound speed in Model (I) and (II) in $d = 1, d^* = 2$



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Previous results for Model (0) and related models

Model (0) (Basile-Bernardin-Olla(06,09), Jara-Komorowski-Olla(15))

- For $d = 1$, $\kappa(t) \sim t^{1/2}$ as $t \to \infty$
- For $d = 2$, $\kappa(t) \sim \log t$ as $t \to \infty$
- For $d \geq 3$, $\lim_{t\to\infty} \kappa(t) < \infty$

+ pinning potential (Basile-Bernardin-Olla(06,09), Jara-Komorowski-Olla(15))

- For $d \geq 1$, $\lim_{t\to\infty} \kappa(t) < \infty$

The momentum flip noise (Simon(13), Komorowski-Olla-Simon(16))

- For $d \geq 1$, $\lim_{t\to\infty} \kappa(t) < \infty$

non-acoustic interaction potential (Komorowski-Olla(16))

- For $d \geq 1$, $\lim_{t\to\infty} \kappa(t) < \infty$

- d^* does not play any role (Only the case $d = d^*$ has been studied)
- Fractional heat eq. or heat eq. are derived rigorously for all models in $d = 1$.

Role of momentum conservation and the sound velocity

Model (0)

$v_s \neq 0$, $\sum_x p_x^k$ are conserved $\Rightarrow$ Anomalous

Model (0) + pinning potential

$v_s = 0$, $\sum_x p_x^k$ are not conserved $\Rightarrow$ Normal

velocity flip noise

$v_s \neq 0$, $\sum_x p_x^k$ are not conserved $\Rightarrow$ Normal

non-acoustic chain

$v_s = 0$, $\sum_x p_x^k$ are conserved $\Rightarrow$ Normal

Model (I) and Model (II)

$v_s = 0$ (or $v_s > 0$), $\sum_x p_x^k$ are not conserved $\Rightarrow$ Normal??

Main result

Theorem (Saito-S,2017)

Model (I), $d^* = 2$

- For $d = 1$, $\kappa(t) \sim t^{1/4}$ as $t \to \infty$
- For $d = 2$, $\kappa(t) \sim \log t$ as $t \to \infty$
- For $d \geq 3$, $\limsup_{t \to \infty} \kappa(t) < \infty$

Model (I), $d^* \geq 3$

- For $d = 1$, $\kappa(t) \sim t^{1/2}$ as $t \to \infty$
- For $d = 2$, $\kappa(t) \sim \log t$ as $t \to \infty$
- For $d \geq 3$, $\limsup_{t \to \infty} \kappa(t) < \infty$

- For the case $d^* = 2$ where $v_s = 0$ and $\sum_x p_x^k$ are not conserved, anomalous behavior appears.
- New universality class appears.
- For $d^* \geq 3$ the conservation of $\sum_x p_x^k (k \geq 3)$ plays some role
- The result holds for micro-canonical and canonical measures.

Main result

Theorem (Saito-S,2017)

Model (II), $d^* \geq 2$

Assume $B^2 + 4 > 16\gamma^2$. Then,

- *For $d = 1$, $\kappa(t) \sim t^{1/2}$ as $t \to \infty$*

- Even for the case $d^* = 2$ where $\sum_x p_x^k$ are not conserved for any k, the order $t^{1/2}$ appears.
- The condition on the parameter may be technical.

Current-Current correlation

Let $C(t) = \lim_{N\to\infty} \frac{1}{N^d}\langle J(t)J(0)\rangle$.

Theorem (Saito-S,2017)

Model (I) For any d and $d^* \geq 2$,

$$C(t) = C_1(t) + C_2(t) + C_3(t) + (d^* - 2)C_4(t)$$

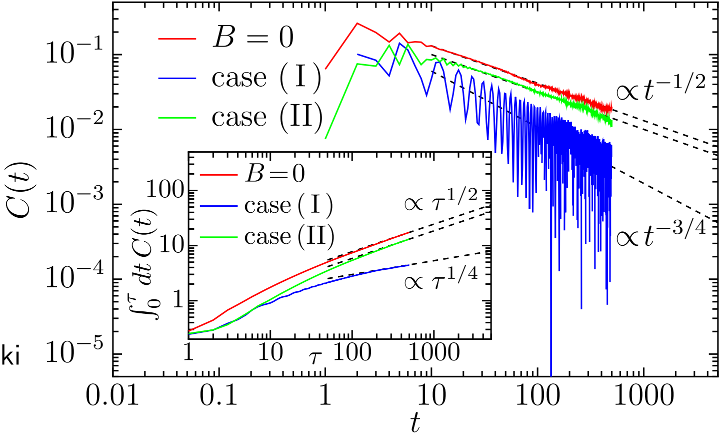
where $C_1(t) \sim t^{-d/2}\cos(Bt)$, $C_2(t) \sim t^{-d/2-1}$, $C_3(t) \sim t^{-d/4-1/2}$, $C_4(t) \sim t^{-d/2}$.

Model (II) For $d = 1$ and $d^* \geq 2$,

$$C(t) \sim t^{-1/2}$$

- From above, the behavior of $\kappa(t)$ follows straightforwardly.
- $C_1(t)$ is the oscillation term

Numerical simulation for the decay of the current-current correlation in $d = 1, d^* = 2$



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“Pinning type effect” of magnetic field for Model (I)

Let $P^1 := \sum_x p_x^1$ and $P^2 := \sum_x p_x^2$. Then,

$$\begin{cases} \dfrac{dP^1}{dt} = BP_2 \\ \dfrac{dP^2}{dt} = -BP^1. \end{cases}$$

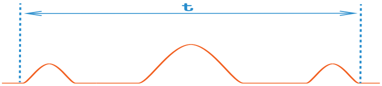
Namely, if the dynamics is in equilibrium $\langle P^1 \rangle = \langle P^2 \rangle = 0$.

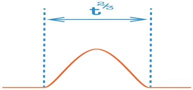
Since the current of the conserved quantity r_x^k is p_x^k, it implies there is no Euler scaling dynamics for $k = 1, 2$. Moreover, form the above, the current-current correlation for r^k is explicitly calculated as $\cos(Bt)$.

Relation between $\kappa(t)$ and κ_N for $d = 1$, $d^* = 2$

Model (I)

Numerical simulation for the system in a stationary non-equilibrium state shows that $\kappa_N \sim N^{3/8}$ which implies $t_N \sim N^{3/2}$. It may imply that the heat mode spreads in the width $t^{2/3}$ at time t. But so far, it is not clear what is the role of α, β and δ where $t_N = N^\delta$ in the macroscopic equation for the energy fluctuation diffusion.





Model (II)

Numerical simulation for the system in a stationary non-equilibrium state shows that $\kappa_N \sim N^{1/2}$ which implies $t_N \sim N$. This is consistent with the non-vanishing sound velocity.

Numerical simulation for κ_N

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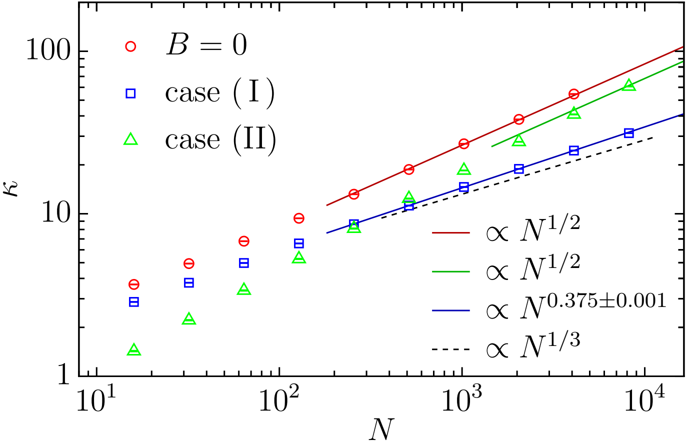

Sketch of the proof

- Follow the strategy of Basile-Bernardin-Olla (2006)
- Solve a poisson equation $(\lambda - L)u = J$ explicitly
- Asymptotic analysis of the inverse Laplace transform of the current-current correlation function

Summary and open problems

Summary

- Our model in a magnetic field : the momentum is not conserved, the sound velocity is vanishing for some case
- Question : Anomalous behavior of the thermal conductivity of the energy in $d = 1, 2$ appears or not?
- Result : Anomalous behavior appears. Moreover, a new universality class appears at least in the sense of the asymptotic behavior of the thermal conductivity
- Conclusion 1 : the momentum conservation is not necessary for the anomalous behavior
- Conclusion 2 : the non-vanishing sound velocity is not necessary for the anomalous behavior

Open problems

- What is the equation for the diffusion of the macroscopic energy fluctuation? Proper space-time scaling? (in progress)
- How to predict t_N?
- NFHT can be applied to this class with some generalization?