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Diffusive Limit and Fourier's Law for the Discrete Schrödinger eq.

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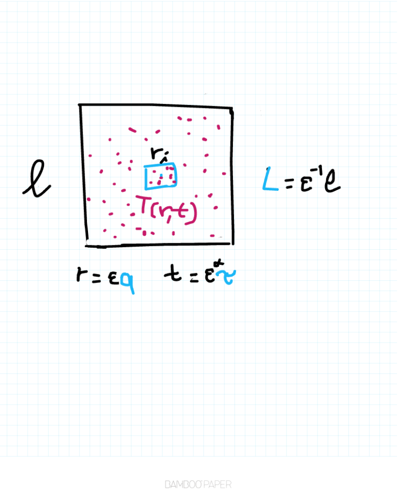
Physics Motivation

- Non-equilibrium systems
- Transport phenomena
- Fourier's law
  J(r)=-k $\nabla T(r)$

"Heat, like gravity, penetrates every substance of the universe, its rays occupy all parts of space. The object of our work is to set forth the mathematical laws which this element obeys. The theory of heat will hereafter form one of the most important branches of general physics." Joseph Fourier, The Analytical Theory of Heat

Local thermal equilibrium

- Local thermal equilibrium hypothesis (LTE).
  1. "Micro” : every small cube is at equilibre at $T(r_i, t)$
  2. "Macro" : since the variations of $T_0(r)$ are ϵ, then for $t > 0$ the system will be close to *LTE* with $T(r, t)$ solution of Fourier’s law.
- Hydrodynamic limit.
- Mathematical difficulty : the ergodic property !



The microscopic model : Discrete Schrödinger eq.

- Atoms are labeled by $x \in \mathbb{T}_N$ where $\mathbb{T}_N = 1, ..., N$ is the lattice torus of lenght N, corresponding to periodic boundary conditions.
- The configuration space is $\Omega^N = \mathbb{C}^{\mathbb{T}_N}$ and a generic element is $\{\psi(x)\}_{x\in\mathbb{T}_N}$, where $\psi(x)$ characterize the amplitude of the wave function of each particle.
- The hamiltonian

$$\mathcal{H}_N = \sum_{x=1}^{N-1} (\psi(x)\psi(x+1)^* + \psi(x)^*\psi(x+1)) + 2\sum_{x=1}^{N} |\psi(x)|^2 \tag{1}$$

- The total "mass"

$$M_N(\psi) = \sum_{x\in\mathbb{T}_N} |\psi(x)|^2 \tag{2}$$

is the only conserved quantity

The microscopic model : continuity equation

Let us define the density of particle x as

$$\rho_x = |\psi(x)|^2, \tag{3}$$

locally the conservation of mass generates an istantaneous current

$$\mathcal{L}_N \rho_x = j_{x-1,x} - j_{x,x+1} \tag{4}$$

with

$$j_{x,x+1} = -i\{\psi_x \psi^*_{x+1} - \psi^*_x \psi_{x+1}\}. \tag{5}$$

The hybrid model

- Hamiltonian $+$ stochastic noise : an hybrid model.
- Why ? We need *good* ergodic properties !
- The dynamics is described by the following system of stochastic differential equation for $x = 1, ..., N$

$$\begin{cases} d\psi(x,t) = -\, i\triangle\psi(x,t)dt - \dfrac{\gamma}{2}\psi(x,t)dt + i\psi(x,t)\sqrt{\gamma}dw_x \\ d\psi^*(x,t) = +i\triangle\psi^*(x,t)dt - \dfrac{\gamma}{2}\psi^*(x,t)dt - i\psi^*\sqrt{\gamma}dw_x \end{cases} \tag{6}$$

where $w_x(t)$ are real independent standard brownian motions.

The hybrid model

The generator is defined by $\mathrm{L}_N = \mathcal{A}_N + \mathcal{S}_N$ where

$$\mathcal{A}_N = \sum_{x \in \mathbb{T}_N} \{ i \triangle \psi^* \partial_{\psi(x)} - i \triangle \psi \partial_{\psi^*(x)} \} \tag{7}$$

is the Liouville operator and

$$\mathcal{S}_N = \frac{\gamma}{2} \sum_{x \in \mathbb{T}_N} \partial^2_{\theta(x)}. \tag{8}$$

is the diffusive operator corresponding to the noise part.

The hydrodynamic limit

Theorem

Let $(\mu_N)_N$ be a sequence of probability measures on Ω^N associated to a bounded initial density profile ρ_0. Then for every $t > 0$, the sequence of random measures

$$\pi_t^N(du) = \frac{1}{N} \sum_{x \in \mathbb{T}} \rho_t(x) \delta_{x/N}(du) \tag{9}$$

converges in probability to the absolutely continuous measure $\pi_t(du) = \rho(t,u)du$ whose density is the solution of the heat equation :

$$\begin{cases} \partial_t \rho = \frac{1}{\gamma} \triangle \rho \\ \rho(0,\cdot) = \rho_0(\cdot). \end{cases} \tag{10}$$

Strategy of the proof

1. Limit identification : under the empirical measure Q^N for every smooth function $G : \mathbb{T}_N \to \mathbb{C}$, the quantity

$$\langle \pi_t^N, G \rangle = \frac{1}{N} \sum_{x \in \mathbb{T}_N} G(\frac{x}{N}) \rho_t(x), \tag{11}$$

   converges weakly to

$$\langle \pi_t^N, G \rangle = \langle \pi_0^N, G \rangle + \frac{1}{\gamma N} \sum_{x \in \mathbb{T}_N} \int_0^t (\triangle_N G)(x/N) \rho_s(x) ds + o(N). \tag{12}$$

2. Relative compactness of Q^N
3. Uniqueness of limit points Q^*, concentrated on deterministic paths $\{\rho(t,u)du, 0 \leq t\}$
4. Uniqueness of weak solution of heath equation.

Stationary state

- $x \in \{1, ..., N\}$ atoms attached at their extremities to particle reservoirs of Langevin type at two different densities μ_l and μ_r.
- The generator of the dynamics is $\mathcal{L} = \mathcal{L}_N + \mathcal{L}_L + \mathcal{L}_R$

$$\begin{aligned}\mathcal{L}_L &= + \frac{\delta}{2}\{\mu_l(\partial^2_{\psi_{r(1)}} + \partial^2_{\psi_{i(1)}}) - (\psi_{r(1)}\partial_{\psi_{r(1)}} + \psi_{i(1)}\partial_{\psi_{i(1)}})\},\\ \mathcal{L}_R &= \frac{\delta}{2}\{\mu_r(\partial^2_{\psi_{r(N)}} + \partial^2_{\psi_{i(N)}}) - (\psi_{r(N)}\partial_{\psi_{r(N)}} + \psi_{i(N)}\partial_{\psi_{i(N)}})\}\end{aligned} \tag{13}$$

- The currents are

$$\begin{aligned} j_{x,x+1} &= -i\{\psi_x\psi^*_{x+1} - \psi^*_x\psi_{x+1}\} \text{ for } x = 2, ..., N-1,\\ j_{0,1} &= (2\mu_l - \rho_1),\\ j_{N,N+1} &= -(2\mu_r - \rho_N)\end{aligned} \tag{14}$$

Results

Theorem

(Fourier's law). For any $\gamma > 0$

$$\lim_{N\to\infty} N\langle j_{x,x+1}\rangle = \frac{2}{\gamma}(\mu_r - \mu_l) \tag{15}$$

Theorem

(Total mass).

$$\lim_{N\to\infty} \frac{\langle M_N(\psi)\rangle}{N} = (\mu_r + \mu_l) \tag{16}$$