Diffusion of wave packets in a Markov random potential

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Outline

The problem

"Obvious" fact

Waves in a disordered environment diffuse.

Problem:

Despite experience and the rich physical theory surrounding this fact, we are very far from having a good mathematical understanding of this phenomenon.[1]

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$$i\partial_t \psi(x) \;=\; -\sum_{|y-x|=1} \psi(y) + \lambda v_\omega(x)\psi(x), \quad \psi \in \ell^2(\mathbb{Z}^d),$$

- λ small
- v_ω random

Does

$$\lim_{t\to\infty} \frac{1}{t} \sum_x |x|^2 |\psi_t(x)|^2 \;=\; D > 0?$$

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- multiple scattering $\implies$ build up of random phases
- build up of random phases $\implies$ loss of coherence
- loss of coherence $\implies$ "classical" propagation (absence of interference)
- classical random scattering $\implies$ diffusion (central limit theorem)

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Recurrence

One key difficulty is *recurrence*: the wave packet may return often to regions visited previously.

- Makes loss of coherence imprecise
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So let's get rid of recurrence:
Make the potential time dependent with short correlations.

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Make the potential time dependent with short correlations.

Time dependent potentials

- Why?
  - Applications to signal propagation in optical fibers (Mitra & Stark, Nature 411 (2001); Green, Littlewood, Mitra, Wegener PRE 66 (2002))
  - More fundamentally reason: to have a rigorous mathematical model of wave diffusion.
- It is more or less clear that one should expect diffusion (and only diffusion) from time dependent models[1].
  Can we prove it?
  - Ovvchinnikov and Erikhman (JETP 40 (1974)):
    Gaussian white noise potential $\Longrightarrow$ diffusion.
  - Pillet (CMP 102 (1985)):
    Transience of the wave packet.
    A *very useful formula* for a Markov potential.
  - Tcheremchantsev (CMP 187 (1997), CMP 196 (1998)):
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Outline

Markov process

A random path $\omega(t)$ in some topological space Ω:

- Distribution of $\omega(\cdot + t)$ given $\omega(s)$, $0 \le s \le t$, depends *only* on $\omega(t)$.
- Precise definition with σ-algebras and transition measures.
- The increments of the process have no memory — $\omega(t)$ and $\omega(s)$ can still be correlated.

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Markov tight binding Schroedinger equation

$$\mathrm{i}\partial_t \psi_t(x) = \sum_{\zeta} h(\zeta)\psi(x-\zeta) + u_x(\omega(t))\psi(x)$$

with

- $\sum_{\zeta} |\zeta|^2 |h(\zeta)| < \infty$
- ω a Markov process.[1]
- $u_x : \Omega \to \mathbb{R}$ bounded measurable functions

Question

What do we need to know about h, u_x and ω to prove diffusion?

[1] with cádlág paths.

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Simple Example

The "flip" model

- Suppose $\Omega = \{-1, 1\}^{\mathbb{Z}^d}$, so each element ω is a field of ± 1 spins.
- Let $u_x(\omega) = \omega(x) =$ spin at x.
- Let $\omega(x)$ evolve in time, independently of all other spins, so that it flips at the times $0 < t_1(x) < t_2(x) < \cdots$ of a Poisson process. Then

$$\lim_{\tau \to \infty} \sum_x \mathrm{e}^{-\mathrm{i}\frac{1}{\sqrt{\tau}}\mathbf{k}\cdot x} \mathbb{E}\left(|\psi_{\tau t}(x)|^2 \right) = \|\psi_0\|^2 \mathrm{e}^{-t \sum_{i,j} D_{i,j}\mathbf{k}_i \mathbf{k}_j}.$$

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Diffusion

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$$\Longrightarrow \quad \lim_{\tau\to\infty}\tau^{\frac{d}{2}}\sum_\zeta w(\sqrt{\tau}\mathbf{r}-\zeta)\mathbb{E}\left(|\psi_{\tau t}(\zeta)|^2\right) \to \|\psi_0\|^2\frac{1}{(\pi D t)^{\frac{d}{2}}}e^{-\frac{|\mathbf{r}|^2}{Dt}}.$$

in the sense of distributions.

- Mean square amplitude of the wave packet converges in a scaling limit to the fundamental solution of a heat equation.
- We also show that

$$\lim_{t\to\infty}\frac{1}{t}\sum_x |x|^2\mathbb{E}\left(|\psi_t(x)|^2\right) = D.$$

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Conditions

1. (*Stationarity*): Invariant probability measure μ on Ω
   - Bernoulli with $p = 1/2$ in the flip model.
2. (*Translation invariance*): $u_x = u_0 \circ \tau_x$ with $\tau_x : \Omega \to \Omega$ measure preserving maps, $\tau_x \circ \tau_y = \tau_{x+y}$
3. (*Markov generator*):

$$S_t f(\omega) = \mathbb{E}\left(f(\omega(t))|\omega(0) = \omega\right)$$

defines a *strongly continuous contraction semi-group* on $L^2(\Omega)$, so we have $S_t = e^{-tB}$ for some *maximally dissipative operator* B.

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Conditions on the generator

4. (*Gap condition*): A strict spectral gap for the generator B

$$\mathrm{Re}\,\langle f, Bf\rangle_{L^2(\Omega)} \geq \frac{1}{T}\langle f, f\rangle_{L^2(\Omega)} \;, \quad \text{if } \int_\Omega f(\omega)\mathrm{d}\mu(\omega) = 0.$$

5. (*Sectoriality*):

$$|\mathrm{Im}\,\langle f, Bf\rangle|_{L^2(\Omega)} \;\leq\; \gamma\,\mathrm{Re}\,\langle f, Bf\rangle_{L^2(\Omega)}$$

Exponential return to equilibrium

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Result

Theorem (Kang and S. 2009)

Under the above assumptions, if for all $x \neq y$

$$\inf_{x \neq y} \left\| B^{-1}(u_x - u_y) \right\|_{L^2(\Omega)} > 0, \qquad (\star)$$

and if the hopping is non-trivial,[1] *then*

$$\lim_{\tau \to \infty} \sum_x \mathrm{e}^{-\mathrm{i}\frac{1}{\sqrt{\tau}}\mathbf{k}\cdot x} \mathbb{E}\left(|\psi_{\tau t}(x)|^2 \right) = \mathrm{e}^{-t\sum_{i,j} D_{i,j}\mathbf{k}_i\mathbf{k}_j} \|\psi_0\|^2$$

with $D_{i,j}$ a positive definite matrix.

- $B^{-1}u_x$ and $B^{-1}u_y$ independent (as in the flip model) $\implies (\star)$:

$$\left\| B^{-1}(u_x - u_y) \right\|^2 = \mathrm{var}(B^{-1}u_x) + \mathrm{var}(B^{-1}u_y) = 2\,\mathrm{var}(B^{-1}u_0).$$

[1] $\sum_\zeta (\mathbf{k}\cdot\zeta)^2 h(\zeta) \neq 0$ for all $\mathbf{k} \in \mathbb{R}^d \setminus \{0\}$.

Periodic potentials

Theorem (Hamza, Kang and S. 2009)

In place of $(\star)$ suppose that u_x is periodic, $u_{x+L\zeta} = u_x \quad \forall \zeta \in \mathbb{Z}^d$ with some $L \geq 2$ and

$$\min_{x \in \Lambda_L \setminus \{0\}} \left\| B^{-1}(u_x - u_0) \right\|_{L^2(\Omega)} > 0, \qquad (\star\star)$$

where $\Lambda_L = [0, L]^d$. Then

$$\lim_{\tau \to \infty} \sum_x \mathrm{e}^{-\mathrm{i}\frac{1}{\sqrt{\tau}}\mathbf{k}\cdot x} \mathbb{E}\left(|\psi_{\tau t}(x)|^2 \right) = \int_{(0,2\pi]^d} \mathrm{e}^{-t\sum_{i,j} D_{i,j}(\mathbf{p})\mathbf{k}_i \mathbf{k}_j} w_{\psi_0}(\mathbf{p}) \mathrm{d}\mathbf{p}$$

with $D_{i,j}(\mathbf{p})$ positive definite for all $\mathbf{p}$ and $w_{\psi_0}(\mathbf{p}) \geq 0$.

- Superposition of diffusions.
- Example: translate a periodic potential by a continuous time random walk.

Outline

Density matrix

$$\rho_t(x,y) \;=\; \psi_t(x)\psi_t(y)^*,$$

- $\rho_t(x,x) = |\psi_t(x)|^2$.
- Linear evolution:

$$\partial_t \rho_t(x,y) \;=\; -\mathrm{i}\sum_{\zeta} h(\zeta)\left[\rho_t(x-\zeta,y) - \rho_t(x,y+\zeta)\right] \\ - \mathrm{i}\left(u_x(\omega(t)) - u_y(\omega(t))\right)\rho_t(x,y).$$

Feynman-Kac and Augmented space

Pillet 1985

$$\mathbb{E}(\rho_t(x,y)) = \left\langle \delta_x \otimes \delta_y \otimes 1, \mathrm{e}^{-tL}\rho_0 \otimes 1 \right\rangle_{L^2(\mathbb{Z}^d \times \mathbb{Z}^d \times \Omega)}.$$

- "Augmented" space: $L^2(\mathbb{Z}^d \times \mathbb{Z}^d \times \Omega) = \ell^2(\mathbb{Z}^d) \otimes \ell^2(\mathbb{Z}^d) \otimes L^2(\Omega)$.
- Generator

$$L\Psi(x,y,\omega) = \underbrace{\mathrm{i}\sum_\zeta h(\zeta)\left[\Psi(x-\zeta,y,\omega) - \Psi(x,y+\zeta,\omega)\right]}_{K\Psi(x,y,\omega)} + \underbrace{\mathrm{i}\left(u_x(\omega) - u_y(\omega)\right)\Psi(x,y,\omega)}_{V\Psi(x,y,\omega)} + B\Psi(x,y,\omega)$$

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Translation Symmetry

$$[S_\xi, L] = \mathrm{i}[S_\xi, K] + \mathrm{i}[S_\xi, V] + [S_\xi, B] = 0$$

$$S_\xi \Psi(x, y, \omega) = \Psi(x - \xi, y - \xi, \tau_\xi \omega).$$

- Fourier transform

$$\widehat{\Psi}(x, \omega, \mathbf{k}) = \sum_\zeta \mathrm{e}^{-\mathrm{i}\mathbf{k}\cdot\zeta} S_\zeta \Psi(x, 0, \omega) = \sum_\zeta \mathrm{e}^{-\mathrm{i}\mathbf{k}\cdot\zeta} \Psi(x - \zeta, -\zeta, \tau_\zeta \omega).$$

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Bloch decomposition

$$\mathbb{E}\left(\rho_t(x,y)\right) = \int_{\mathbb{T}^d} \mathrm{e}^{-\mathrm{i}\mathbf{k}\cdot y} \left\langle \delta_{x-y} \otimes 1, \mathrm{e}^{-t\widehat{L}_{\mathbf{k}}} \widehat{\rho}_{0;\mathbf{k}} \otimes 1 \right\rangle_{L^2(\mathbb{Z}^d \times \Omega)} \mathrm{d}\ell(\mathbf{k}).$$

- Generator

$$\widehat{L}_{\mathbf{k}}\phi(x,\omega) = \underbrace{\mathrm{i}\sum_{\zeta} h(\zeta)\left[\phi(x-\zeta,\omega) - \mathrm{e}^{-\mathrm{i}\mathbf{k}\cdot\zeta}\phi(x-\zeta,\tau_\zeta\omega)\right]}_{\widehat{K}_{\mathbf{k}}\phi(x,\omega)} + \mathrm{i}\underbrace{\left(u_x(\omega) - u_0(\omega)\right)\phi(x,\omega)}_{\widehat{V}\phi(x,\omega)} + B\phi(x,\omega).$$

- $\widehat{\rho}_{0;\mathbf{k}}(x) = \sum_\zeta \mathrm{e}^{-\mathrm{i}\mathbf{k}\cdot\zeta}\rho_0(x-\zeta,-\zeta).$

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$$\widehat{L}_{\mathbf{k}}\phi(x,\omega) = \underbrace{\mathrm{i}\sum_{\zeta} h(\zeta)\left[\phi(x-\zeta,\omega) - \mathrm{e}^{-\mathrm{i}\mathbf{k}\cdot\zeta}\phi(x-\zeta,\tau_\zeta\omega)\right]}_{\widehat{K}_{\mathbf{k}}\phi(x,\omega)} + \mathrm{i}\underbrace{(u_x(\omega) - u_0(\omega))\phi(x,\omega)}_{\widehat{V}\phi(x,\omega)} + B\phi(x,\omega).$$

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Diffusively rescaled Feynman-Kac

$$\sum_x e^{-i\frac{1}{\sqrt{\tau}}\mathbf{k}\cdot x}\mathbb{E}\left(\rho_t(x,x)\right) = \left\langle \delta_0 \otimes 1, e^{-\tau t \widehat{L}_{\mathbf{k}/\sqrt{\tau}}}\widehat{\rho}_{0;\mathbf{k}/\sqrt{\tau}} \otimes 1 \right\rangle_{L^2(\mathbb{Z}^d \times \Omega)}.$$

- Diffusion = good control over $e^{-t\widehat{L}_{\mathbf{k}}}$ for $\mathbf{k} \approx 0$.
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  1. Understand $\mathbf{k} = 0$.
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Block decomposition for $\widehat{L}_0$

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$$\widehat{L}_0 = \begin{pmatrix} 0 & \mathrm{i} P_0 \widehat{V} \\ \mathrm{i} \widehat{V} P_0 & P_0^{\perp} \widehat{L}_0 P_0^{\perp} \end{pmatrix}$$

over $\mathcal{H}_0 \oplus \mathcal{H}_0^{\perp}$ with

$$\mathcal{H}_0 = \ell^2(\mathbb{Z}^d) \otimes \{1\}, \quad \mathcal{H}_0^{\perp} = \left\{ \phi(x,\omega) \; : \; \int_{\Omega} \phi(x,\omega) \mathrm{d}\mu(\omega) = 0 \right\}.$$

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Spectral gap for $\widehat{L}_0$

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- $\operatorname{Re} P_0^\perp \widehat{L}_0 P_0^\perp = P_0^\perp B P_0^\perp \geq \frac{1}{T} P_0^\perp$.
- Schur:[1] *If* $\operatorname{Re} z < 1/T$ *then* $\widehat{L}_0 - z$ *is invertible if and only if*

$$\Gamma(z) = P_0 \widehat{V} \left(P_0^\perp \widehat{L}_0 P_0^\perp - z \right)^{-1} \widehat{V} P_0 - z$$

is invertible.

$$\operatorname{Re} \Gamma(z) \geq \sigma^2 \frac{1 - T \operatorname{Re} z}{T} \frac{\|u\|_\infty^2}{1 + 4 \left(T \|\widehat{h}\|_\infty + 2T \|u\|_\infty + 1 \right)^2} (1 - \Pi_0),$$

- $\Pi_0 =$ projection onto $\delta_0 \otimes 1$.

[1] or Feshbach, or Krein ...

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Spectral gap for $\widehat{L}_0$

Lemma

There is $\delta > 0$ *such that*

$$\sigma(\widehat{L}_{\mathbf{0}}) \;=\; \{0\} \cup \Sigma_+ \tag{1}$$

where

1. 0 *is a non-degenerate eigenvalue, and*
2. $\Sigma_+ \subset \{z \;:\; \operatorname{Re} z > \delta\}$.

Furthermore, if $Q_0 =$ *orthogonal projection onto* $\delta_0 \otimes 1$*, then*

$$\left\| \mathrm{e}^{-t\widehat{L}_{\mathbf{0}}} (1 - Q_0) \right\| \;\le\; C_\epsilon \mathrm{e}^{-t(\delta - \epsilon)}.$$

Perturbation theory for $\widehat{L}_{\mathbf{k}}$

Lemma

If $|\mathbf{k}|$ is sufficiently small, the spectrum of $\widehat{L}_{\mathbf{k}}$ consists of:

1. *A non-degenerate eigenvalue $E(k)$ contained in $H_0 = \{z \,:\, |z| < c|\mathbf{k}|\}$.*
2. *The rest of the spectrum is contained in the half plane $H_1 = \{z : \operatorname{Re} z > \delta - c|\mathbf{k}|\}$ such that $H_0 \cap H_1 = \emptyset$.*

Furthermore, $E(\mathbf{k})$ is C^2 in a neighborhood of 0,

$$E(0) = 0, \quad \nabla E(0) = 0,$$

and

$$\partial_i \partial_j E(0) \;=\; 2 \operatorname{Re} \left\langle \partial_i \widehat{K}_0 \delta_0 \otimes 1, \frac{1}{\widehat{L}_0} \partial_j \widehat{K}_0 \delta_0 \otimes 1 \right\rangle,$$

is positive definite.

Putting it together

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$$= \mathrm{e}^{-\tau t E(\mathbf{k}/\sqrt{\tau})}\left\langle \delta_0 \otimes 1, Q(\mathbf{k})\widehat{\rho}_{0;\mathbf{k}/\sqrt{\tau}} \otimes 1 \right\rangle_{L^2(\mathbb{Z}^d\times\Omega)} + O(\mathrm{e}^{-c\tau t})$$

$$= \mathrm{e}^{-t\sum_{i,j}\frac{1}{2}\partial_i\partial_j E(0)\mathbf{k}_i\mathbf{k}_j}\left\langle \delta_0 \otimes 1, \widehat{\rho}_{0;0} \otimes 1\right\rangle_{L^2(\mathbb{Z}^d\times\Omega)} + o(1).$$

$\frac{1}{2}\partial_i\partial_j E(0) =$ Diffusion matrix □

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Comments

- Diffusion in a Markov potential can be seen in an elementary fashion.
- If u_x is periodic there is a further Bloch decomposition, with diffusion in each fiber.
- If $\lambda =$ disorder strength

$$D \sim \frac{1}{\lambda^2}\left[D_0 + \lambda Q(\lambda)\right]$$

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