Quantum Diffusion in Fluctuating Media

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Joint work with Zak Tilocco and Shiwen Zhang
Quantum Diffusion

Outline

1. Quantum Diffusion Conjecture (Extended States)
2. Schrödinger equation with a Markov fluctuating potential
3. Comments on the proof
4. Open Quantum Systems
5. Conclusions
Consider the Schrödinger equation

\[ i\partial_t \psi(x) = H_\omega \psi_t(x) \]

where \( H_\omega \) is an RSO with a spatially homogeneous distribution. Under suitable hypotheses,\(^a\) a diffusive rescaling of the mean wave density \( \mathbb{E}(|\psi_t(x)|^2) \) should approximately solve a heat equation at large time:

\[
\mathbb{E}\left(|\psi_{Tt}(\sqrt{T}x)|^2\right) \sim \int_{\sigma(H_\omega)} \frac{1}{(D(E)t)^{d/2}} e^{-\frac{1}{4D(E)t}|x|^2} \, d\nu(E), \quad T \to \infty
\]

with \( D(E) > 0 \) in the center of the band — \( D(E) = 0 \) at the edges due to Lifshitz tails localization.

\(^a\)Weak disorder, dimension \( \geq 3 \), ...
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- In a multiple scattering picture

$$e^{-itH_\omega} = e^{-itH_0} - i\lambda \int_0^t e^{-i(t-s)H_0} V_\omega e^{-isH_0} ds + \ldots$$

suggests a build up of random phases.
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- classical random scattering $\implies$ diffusion (CLT?)
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In particular, recurrence is a huge problem. And in 1D —and maybe 2D—it is an essential obstacle.

Best results so far: Erdös, Salmhofer, Yau, proved diffusion in a limit with the “disorder strength” \( \lambda \propto T^{-\frac{1}{2}+\epsilon} \).
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Schrödinger equation with a Markov fluctuating potential

What if the potential fluctuates?

What are the long time dynamics for solutions to

$$\partial_t U(t, t_0) = -iH(t)U(t, t_0),$$

with $U(t_0, t_0) = I$ and $H(t) = H_0 + g \sum_x w(x, t) |x\rangle \langle x|$?
What kind of fluctuations?

Throughout we take

\[ w(x, t) = w(\tau_x \alpha_t) \]

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1. \( t \mapsto \alpha_t \) a Markov process on a nice space \( \Lambda \) with a unique invariant probability measure \( \nu \) and a "spectral gap."

- Take the initial value \( \alpha_0 \) distributed according to \( \nu \) (for simplicity).
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   - Take the initial value \( \alpha_0 \) distributed according to \( \nu \) (for simplicity).
2. \( \{\tau_x\}_{x \in \mathbb{Z}^d} \) an action of \( \mathbb{Z}^d \) on \( \Lambda \) as \( \nu \)-measure preserving maps
   - assume the distribution of the Markov process is invariant under \( \tau_x \).
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   - assume the distribution of the Markov process is invariant under \( \tau_x \).
3. \( w \) a non-constant, mean-zero function on \( \Lambda \) such that

\[
\lim_{x \to \infty} \int_{\Lambda} w(\tau_x \alpha) w(\alpha) \nu(d\alpha) = 0.
\]
Schrödinger equation with a Markov fluctuating potential

Huh?

If that was too much, think of the following:

Flip process

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Global resampling process

Take $w(x, 0)$ i.i.d. and use a single Poisson process. Resample the whole distribution of $w$ at each Poisson time.
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These are just a couple of simple examples. There are many fancier ones that you can use (if you want).
What sort of hopping?

Our methods apply to quite general hopping

\[ T\psi(x) = \sum_y h(x - y)\psi(y) \]

such that

1. \( \sum_y |y|^2 h(y) < \infty \), so that \( \hat{h}(k) = \sum_y h(y)e^{-ik\cdot y} \) is a \( C^2 \) function.
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- \( T \) has some ac spectrum, with ballistic transport. It may have infinitely degenerate imbedded eigenvalues (if \( \hat{h} \) is constant on some open sets of positive measure).
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- \( T \) has some ac spectrum, with ballistic transport. It may have infinitely degenerate imbedded eigenvalues (if \( \hat{h} \) is constant on some open sets of positive measure).
- If \( h \) is finite range, or exponentially bounded, then the spectrum is pure a.c. since \( \hat{h} \) is analytic.
Theorem (Kang and S. 2009)

If \( i\partial_t \psi_t(x) = T \psi_t(x) + gW(x, t)\psi_t(x) \) with, say, \( \psi_0(x) = \delta_0(x) \). Then

\[
\lim_{T \to \infty} \frac{1}{T} \sum_x x_i x_j \mathbb{E} \left( |\psi_t(x)|^2 \right) = D(g)_{i,j}
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\lim_{T \to \infty} \sum_x e^{-i \frac{1}{\sqrt{T}} k \cdot x} \mathbb{E} \left( |\psi_{Tt}(x)| \right)^2 = e^{-t \text{tr}(D(g)k \otimes k)},
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where \( D(g) \) is a \( d \times d \) positive definite matrix, and

\[
D(g) = \frac{1}{g^2} D_0 + O(1)
\]

as \( g \to 0 \).
A full central limit theorem follows from the result for the Fourier transform:

$$
\lim_{T \to \infty} \sum_x f(\frac{x}{\sqrt{t}}) \mathbb{E} \left( |\psi_t(x)|^2 \right) = C_d \int_{\mathbb{R}^d} f(r) e^{-\frac{1}{2} \text{tr}(D(g)^{-1} r \otimes r)} \, dr.
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If $T$ commutes with lattice rotations, then $D(g) = D(g) \mathbb{1}$, where $D(g) = \frac{1}{d} \text{tr} D(g)$ is the diffusion constant.
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For the global resampling process there is an explicit formula for $D_0$ in terms of the Green’s functions of $T$, suggesting that the asymptotics have to do with AC spectrum and ballistic transport.
Fast diffusion

\[ \lambda = 0, u = 1, \gamma = 1, \delta = 0.05 \]

Static Random Potential
Fluctuating Random Potential

time = 0

Probability
Position

-40 -30 -20 -10 0 10 20 30 40
Theorem (S. 2015)

Let $H_{\omega}$ be a RSO

$$i\partial_t \psi_t(x) = H_{\omega}\psi_t(x) + gW(x, t)\psi_t(x)$$

with, say, $

\psi_0(x) = \delta_0(x).$

Then

$$\lim_{T \to \infty} \sum_x e^{-i\frac{1}{\sqrt{T}} k \cdot x} \mathbb{E}(|\psi_{Tt}(x)|)^2 = e^{-t \operatorname{tr}(D(g)k \otimes k)},$$

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where $D(g)$ a $d \times d$ positive definite matrix. If $H_\omega$ has exponential dynamical localization then

$$D(g) = F_0 g^2 + o(g^2).$$
Slow diffusion

\[ \lambda=0, \ u=1, \ \gamma=1, \ \delta = 0.05 \]

- Static Random Potential
- Fluctuating Random Potential

Probability vs. Position for time = 0.
Schrödinger equation with a Markov fluctuating potential

Slow diffusion

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\begin{align*}
\text{Probability} \\
0 & \quad \quad 0.1 \quad \quad 0.2 \quad \quad 0.3 \quad \quad 0.4 \quad \quad 0.5 \quad \quad 0.6 \quad \quad 0.7 \quad \quad 0.8 \quad \quad 0.9 \quad \quad 1 \\
\text{Position} \\
-40 & \quad \quad -30 \quad \quad -20 \quad \quad -10 \quad \quad 0 \quad \quad 10 \quad \quad 20 \quad \quad 30 \quad \quad 40
\end{align*}
Conjecture

Let $H_0$ be an ergodic Schrödinger operator and suppose that the dynamics $e^{-itH_0}$ have a transport exponent $\nu$:

$$\sum_x x_j^2 |\psi_t(x)|^2 \sim C_j t^{2\nu}$$

with $0 < C_j < \infty$. Then solutions to $i\partial_t \psi(x) = H_0 \psi_t(x) + gW(x, t) \psi_t(x)$ are diffusive with diffusion matrix

$$D(g) = g^{2-4\nu} D_0 + o(g^{2-4\nu}).$$
Theorem (S., Tilocco, Zhang 2018, in preparation)

Let $H_0 = T + U$ where $U(x)$ is a periodic potential, and suppose that $H_0$ has ballistic transport.\(^a\) Then diffusion holds for solutions to

$$i\partial_t(x) = H_0\psi_t(x) + gW(x, t)\psi_t(x)$$

with

$$D(g) = \frac{1}{g^2} D_0 + O(1)$$

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A formal calculation suggests that
\[ D(g) = \frac{1}{g^2} D_0 + D_1 + o(1). \]
Schrödinger equation with a Markov fluctuating potential

Slow/Fast diffusion

\[\lambda=0, \ u=1, \ \gamma=1, \ \delta=0.05\]

Probability

Position

Static Random Potential
Fluctuating Random Potential

time = 0
$D$ versus $g$
Schrödinger equation with a Markov fluctuating potential

Literature.

- Ovchinnikov and Erikhman (JETP 1974)
- Pillet (CMP 1985)
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Pillet (CMP 1985)
Tcheremchantsev (CMP 1997, CMP 1998)
Kang & S. (JSP 2009); Hamza, Kang & S. (LMP 95 2010); S. (CMP 2015)
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Augmented space formalism

- We use the “Augmented space formalism” with disorder variables in the Hilbert space:

$$\mathbb{E} \left( |\psi_t(x)|^2 \right) = \langle \delta_x \times \delta_x \times 1 | e^{-tG} | \delta_0 \times \delta_0 \times 1 \rangle_{\mathcal{H} \times \mathcal{H} \times L^2(\Lambda)}$$

- $\mathcal{H} = \ell^2(\mathbb{Z}^d)$
- $G = i[H, \cdot] + B$ (non self adjoint),
- $H = H_0 + gw(\tau_x \alpha)$ (No time dependence!)
- $B =$ Markov process generator.
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Generator $\mathcal{G}$ commutes with translations

$$\delta_x \times \delta_y \times f(\omega) \mapsto \delta_{x + \xi} \times \delta_{y + \xi} \times f(S_\xi \omega).$$
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\[ \delta_x \times \delta_y \times f(\omega) \mapsto \delta_{x+\xi} \times \delta_{y+\xi} \times f(S_\xi \omega). \]

In the periodic case, this is a subgroup of possible translations.
Sketch of the Proof

- Make a Bloch-Floquet transform

\[
\sum_{x \in P \mathbb{Z}^d} e^{-i k \cdot x} \mathbb{E} \left( |\psi_t(x)|^2 \right)
= \sum_{y \in P} \langle \delta_0 \times \delta_y \times 1 | e^{-t \hat{G}_k} | \delta_0 \times \delta_0 \times 1 \rangle_{\mathcal{H} \times \ell^2(P) \times L^2(\Lambda)},
\]

where
- \( P \) is the periodicity cell for the periodic potential,
- \( \hat{G}_k \) is an explicit fiber operator (non SA), with hopping in disorder space.
- \( \hat{G}_0 \) has a simple zero eigenvector (conservation of probability) and a spectral gap.
Basic perturbation theory shows that $\hat{G}_k$ has a simple near zero eigenvector $E(k)$ and a spectral gap.
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$$\nabla E(0) = 0$$

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Proof for the random operator case is a bit different. There is no gap, but we can use the resolvent $(\eta + \hat{G}_k)^{-1}$ to prove the result.
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Estimating $D$ at small $g$ takes more work.
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- Most work relies on Fermi Golden Rule (quantum Markov formalism).
- Some recent mathematical physics literature:
  - D. Spehner and J. Bellissard (JSP 2001);
  - W. De Roeck and J. Fröhlich (CMP 2011);
  - Fröhich and S. (JMP 2016);
Theorem (Fröhlich, S. 2016)

\[ \partial_t \rho_t = -i [H_\omega, \rho_t] + u \mathcal{L}(\rho_t), \]

with \( H_\omega = T + \lambda V_\omega \) and a suitable\(^a\) Lindbladian \( \mathcal{L} \). Then

\[ D = \lim_{t \to \infty} \frac{1}{t} \sum_x |x|^2 \mathbb{E}(\langle x | \rho_t | x \rangle) \]

exists and satisfies \( 0 < D < \infty \).
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exists and satisfies \( 0 < D < \infty \).

1. If \( \lambda = 0 \) (no disorder), then \( D = \frac{C}{u} \) for all \( u > 0 \).
2. If \( H_\omega \) exhibits localization, then

\[ D = \Delta u + o(u) \]

where \( 0 < \Delta < (\text{loc. length})^2 \).
The Lindblad generator

Describes a hopping process for the particle momentum:

\[
\rho^W(X, p) = \sum_\xi e^{ip \cdot \xi} \langle \frac{X + \xi}{2} \left| \rho \left| \frac{X - \xi}{2} \right. \rangle,
\]

\[
\mathcal{L}\rho^W(X, p) = \int \hat{r}(p, q) \left[ \rho^W(X, q) - \rho^W(X, p) \right] dq,
\]

\[
\hat{r}(p, q) = \hat{r}(q, p),
\]

and

\[
\int\int \hat{r}(p, q) \left| f(p) - f(q) \right|^2 dp dq \geq c \int\int \left| f(p) - f(q) \right|^2 dp dq.
\]
Conclusions

Outline

1. Quantum Diffusion Conjecture (Extended States)
2. Schrödinger equation with a Markov fluctuating potential
3. Comments on the proof
4. Open Quantum Systems
5. Conclusions
Summary

- Diffusion is universal in the presence of time dependent fluctuations. (Quantitative analysis)
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- The speed of diffusion for weak noise carries information about the transport properties of the underlying time independent system. (Qualitative analysis)
Open Problems

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2. Operators $H_0$ with anomalous diffusion.
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If not, does it make sense to look at the limit in distribution.
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   \[ \mathbb{E} \left( \langle \psi_t | X^2 | \psi_t \rangle - \langle \psi_t | X | \psi_t \rangle^2 \right) \]?

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1. Diffusion in an open quantum system without the Markov approximation.
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   - How to prove that decoherence emerges and memory in the bath decays?
2. Diffusion for weak disorder (without fluctuations)
   - Recurrence is the problem.
   - Can fluctuations help?
Thank you!