Quantum Diffusion and Delocalization for Random Band Matrices

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Two standard models of quantum disorder

Consider the two random Hamiltonians on $\mathbb{C}^N$ (one-dimensional lattice).

Random Schrödinger operator. On-site randomness + short-range hopping.

$$H = -\Delta + \sum_x v_x = \begin{pmatrix} v_1 & 1 & & & \\ 1 & v_2 & 1 & & \\ & 1 & \ddots & \ddots & \\ & & \ddots & v_{N-1} & 1 \\ & & & 1 & v_N \end{pmatrix}$$

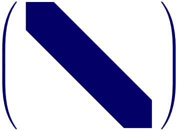
Eigenvectors are localized, local spectral statistics are Poisson.

Wigner random matrix. $H = (H_{xy})_{x,y=1}^N$ with random centred entries, i.i.d. up to the constraint $H = H^T$ or $H = H^*$. This is a mean-field model with no spatial structure.

Eigenvectors are delocalized, local spectral statistics are GOE/GUE.

Band matrices

Intermediate model: random band matrix. The elements H_{xy} are centred, independent (up to $H = H^*$), and satisfy $H_{xy} = 0$ for $|x - y| > W$. Here W is the band width.



Summary: If $W = O(1)$ then $H \sim$ random Schrödinger operator.

If $W = O(N)$ then $H \sim$ Wigner matrix.

Anderson transition for band matrices

- $W = O(1) \Longrightarrow$ eigenvectors are localized.
- $W = O(N) \Longrightarrow$ eigenvectors are delocalized.

Varying $1 \ll W \ll N$ provides a means to test the Anderson transition.

Conjecture (numerics, nonrigorous SUSY arguments)

The Anderson transition occurs at $W \sim N^{1/2}$.

Let ℓ denote the typical localization length of the eigenvectors of H. Then the conjecture means that $\ell \sim W^2$.

Rigorous results:

- $\ell / W \leqslant W^7$ (Schenker).
- $\ell / W \geqslant W^{1/6}$ (Erdős, K).

Conjecture for higher dimensions

If $d = 2$ then ℓ is exponential in W.
If $d \geqslant 3$ then $\ell = N$ (delocalization).

Assumptions

- Let $d \geqslant 1$ and $N \in \mathbb{N}$. Consider random matrices $H = (H_{xy})$ whose entries are indexed by $x, y \in \Lambda_N := \{-N, \dots, N\}^d$.
- Assume that the entries H_{xy} are independent (up to $H = H^*$) with variances given by

  $$\mathbb{E}|H_{xy}|^2 \;=\; \frac{1}{W^d} f\left(\frac{x-y}{W}\right).$$

  Here f is a probability density of zero mean on $\mathbb{R}^d$ (the "band shape").
- Assume that H_{xy} is symmetric and exhibits subexponential decay.

Note that $\sum_y \mathbb{E}|H_{xy}|^2 = 1$. Let $\{\lambda_\alpha\}$ be the family of eigenvalues of H. Then

$$\frac{1}{|\Lambda_N|} \sum_\alpha \mathbb{E}\lambda_\alpha^2 \;=\; \frac{1}{|\Lambda_N|} \mathbb{E} \operatorname{Tr} H^2 \;=\; \frac{1}{|\Lambda_N|} \sum_{x,y} \mathbb{E}|H_{xy}|^2 \;=\; 1\,,$$

i.e. the eigenvalues of H are of order 1. In fact, $\mathrm{Sp}(H) \to [-2, 2]$.

The diffusive scaling

Define the quantum transition probability from 0 to x in time t through

$$\varrho(t,x) \;:=\; \mathbb{E}\big|\big\langle \delta_x \,, \mathrm{e}^{-\mathrm{i}tH/2}\delta_0 \big\rangle\big|^2 \,.$$

Note that $\varrho(t,\cdot)$ is a probability on Λ_N for all t.

Consider the diffusive regime

$$t \;=\; \eta T \,, \qquad x \;=\; \eta^{1/2} W X \,,$$

for $\eta \to \infty$. Here X and T are of order one.

For $d = 1$, diffusion cannot hold for $x \gg W^2 \Longrightarrow$ choose $\eta = W^\kappa$ for $0 < \kappa < 2$.

Quantum diffusion

Theorem(Quantum diffusion) [Erdős, K]

Fix $0 < \kappa < 1/3$ and pick a test function $\varphi \in C_b(\mathbb{R}^d)$. Then

$$\lim_{W \to \infty} \sum_{x \in \Lambda_N} \varrho(W^{d\kappa} T, x) \, \varphi\left(\frac{x}{W^{1+d\kappa/2}}\right) \;=\; \int_{\mathbb{R}^d} \mathrm{d}X \; L(T,X) \, \varphi(X) \,,$$

uniformly in $N \geqslant W^{1+d/6}$ and $T \geqslant 0$ in compacts. Here

$$L(T,X) \;:=\; \int_0^1 \mathrm{d}\lambda \; \frac{4}{\pi} \frac{\lambda^2}{\sqrt{1-\lambda^2}} \, G(\lambda T, X)$$

is a superposition of heat kernels

$$G(T,X) \;:=\; \frac{1}{(2\pi T)^{d/2} \sqrt{\det \Sigma}} \, \mathrm{e}^{-\frac{1}{2T} \, X \cdot \Sigma^{-1} X} \,,$$

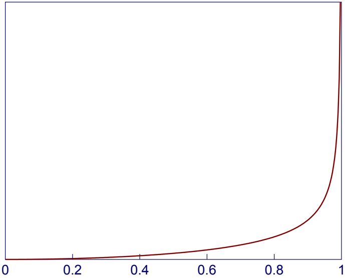
where $\Sigma = (\Sigma_{ij})$ is the covariance matrix of the probability density f:
$\Sigma_{ij} := \int_{\mathbb{R}^d} \mathrm{d}X \; X_i X_j f(X)$.

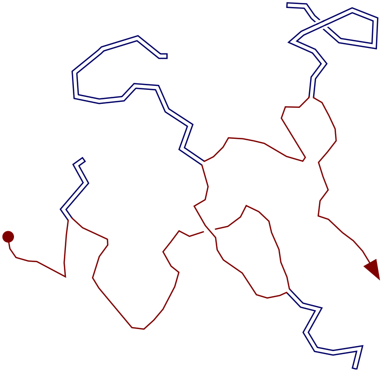
Interpretation of λ

The quantum particle spends a macroscopic time λT moving according to a random walk, with jump rate $O(1)$ in time t and transition kernel $p(y \leftarrow x) = \mathbb{E}|H_{xy}|^2$. The remaining fraction $(1-\lambda)T$ is the time the particle "wastes" in backtracking.

Probability density of λ:

$$\frac{4}{\pi}\frac{\lambda^2}{\sqrt{1-\lambda^2}}$$





Corollary: delocalization

Informally: fraction of eigenvectors localized on scales $\ell \leqslant W^{1+d\kappa/2}$ converges to 0.

Let $\{\psi_\alpha\}_{\alpha=1}^{|\Lambda_N|}$ be an orthonormal family of eigenvectors of H. Fix $K > 0$ and $\gamma > 0$ and define the random subset of eigenvectors

$$\mathfrak{B}_\ell^\omega \;:=\; \left\{\alpha \in \mathfrak{A} \,:\, \exists\, u \in \Lambda_N \;\sum_x |\psi_\alpha^\omega(x)|^2 \exp\left[\frac{|x-u|}{\ell}\right]^\gamma \leqslant K\right\}.$$

Theorem(Delocalization) [Erdős, K]

For any $\kappa < 1/3$ we have

$$\lim_{W \to \infty} \mathbb{E}\,\frac{|\mathfrak{B}_\ell|}{|\Lambda_N|} \;=\; 0\,,$$

where $\ell = W^{1+d\kappa/2}$.

Proof. Expand $\mathrm{e}^{-\mathrm{i}tH/2}\delta_0 = \sum_\alpha \overline{\psi_\alpha(0)}\,\mathrm{e}^{-\mathrm{i}t\lambda_\alpha/2}\,\psi_\alpha$. □

Naive (and doomed) attempt: power series expansion of $\mathrm{e}^{-\mathrm{i}tH/2}$

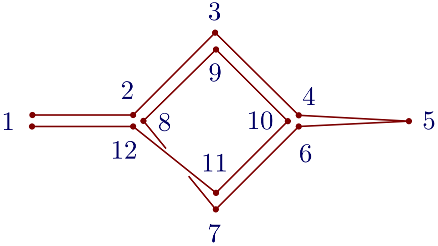
The moment method (Wigner 1955: semicircle law, . . .) involves computing

$$\mathbb{E}\,\mathrm{Tr}\,H^n \;=\; \sum_{x_1,\dots,x_n} \mathbb{E}\,H_{x_1x_2}H_{x_2x_3}\cdots H_{x_nx_1}$$

for large n. Because of $\mathbb{E}H_{xy} = 0$, nonzero terms have a complete pairing (or a higher-order lumping).

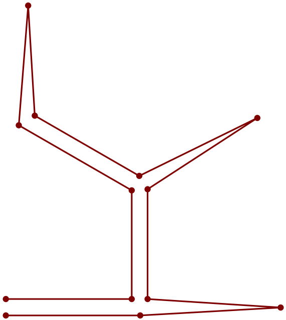
Graphical representation: path $x_1, x_2, \dots, x_n, x_1$.

- The path is nonbacktracking if $x_i \neq x_{i+2}$ for all i.
- The path is fully backtracking if it can be obtained from x_1 by successive replacements of the form $a \mapsto aba$. (This generates "double-edged trees".)



A fully backtracking path is paired by construction; its contribution is 1.

Proof. Sum over all vertices, starting from the leaves. Each summation yields a factor $\sum_y \mathbb{E}|H_{xy}|^2 = 1$. ☐



Fully backtracking paths give the leading order contribution as $W \to \infty$. Wigner's original derivation of the semicircle law involved counting the number of fully backtracking paths.

Applying this strategy to ϱ leads to trouble: the expansion

$$\varrho(t,x) \;=\; \sum_{n,n' \geqslant 0} \frac{\mathrm{i}^{n-n'} t^{n+n'}}{2^{n+n'} n! n'!} \mathbb{E} H_{0x}^n H_{x0}^{n'}$$

is unstable as $t \to \infty$. The main contribution comes from fully backtracking graphs, whose number is of the order $4^{n+n'}$. The main contribution to the sum over n, n' comes from $n + n' \sim t$ (Poisson), diverges like e^{4t} as $t \to \infty$.

Getting rid of the trees: perturbative renormalization

Simple example: Let $z = E + \mathrm{i}\eta$ with $\eta > 0$ and compute

$$\mathbb{E}G_{ii}(z) \;=\; \mathbb{E}(H-z)^{-1}_{ii}\,.$$

Assuming that the semicircle law holds, we know what to expect:

$$\mathbb{E}G_{ii}(z) \;=\; \mathbb{E}\frac{1}{N}\sum_j G_{jj}(z) \;=\; \mathbb{E}\frac{1}{N}\sum_\alpha \frac{1}{\lambda_\alpha - z} \;=\; \mathbb{E}m_N(z) \;\approx\; m(z)$$

where $m_N(z)$ is the Stieltjes transform of the empirical eigenvalue density $N^{-1}\sum_\alpha \delta_{\lambda_\alpha}$, and

$$m(z) \;:=\; \int \frac{1}{x-z}\,\frac{\sqrt{4-x^2}}{2\pi}\,\mathrm{d}x$$

is the Stieltjes transform of the semicircle law.

Note: $m(z)$ is uniquely characterized by

$$z + m(z) + \frac{1}{m(z)} \;=\; 0\,, \qquad |m(z)| \;<\; 1 \qquad (z \notin [-2,2])\,.$$

Choose $\mu \equiv \mu(z) \in \mathbb{C}$ and expand $G(z)$ around μ^{-1}:

$$\frac{1}{H-z} = \frac{1}{\mu + H - \mu - z} = \frac{1}{\mu} + \frac{1}{\mu}\sum_{n=1}^{\infty}\left(\frac{\mu+z}{\mu} - \frac{H}{\mu}\right)^n .$$

Thus we get

$$\mathbb{E}G_{ii} = \frac{1}{\mu} + \frac{1}{\mu^2}(\mu+z) + \frac{1}{\mu^3}\big((\mu+z)^2 + \mathbb{E}H_{ii}^2\big) + \frac{1}{\mu^4}(\cdots) + \cdots .$$

Choose μ so that red terms cancel:

$$\frac{1}{\mu^2}(\mu+z) = -\frac{1}{\mu^3}\mathbb{E}H_{ii}^2 = -\frac{1}{\mu^3} \qquad \Longleftrightarrow \qquad z + \mu + \frac{1}{\mu} = 0 .$$

We need $|\mu| > 1$ for convergence: choose $\mu = m^{-1}$.

Using a graphical expansion, one can check that this choice of μ leads to a systematic cancellation of leading-order pairings (trees) up to all orders. What remains are higher-order corrections of size $O(W^{-d})$. In particular, $\mathbb{E}G_{ii} = m + o(1)$.

This is essentially two-legged subdiagram renormalization in perturbative field theory. Works also for more complicated objects like $\mathbb{E}|G_{ij}|^2$.

Renormalization using Chebyshev polynomials

A more systematic and powerful renormalization: use a beautiful algebraic identity due to Bai, Yin, Feldheim, Sodin, $\dots$.

Define the n-th nonbacktracking power of H through

$$H^{(n)}_{x_0 x_n} \; := \sum_{x_1, \dots, x_{n-1}} H_{x_0 x_1} \cdots H_{x_{n-1} x_n} \prod_{i=0}^{n-2} \mathbf{1}(x_i \neq x_{i+2})\,.$$

Assume from now on that

$$H_{xy} = \frac{\mathbf{1}(1 \leqslant |x-y| \leqslant W)}{\sqrt{W^d}}\, \mathrm{Unif}(S^1)\,.$$

We shall see later how to relax this condition.

Lemma[Bai, Yin]

$$H^{(n)} \;=\; HH^{(n-1)} - H^{(n-2)}$$

Proof. Introduce $1 = \mathbf{1}(x_0 \neq x_2) + \mathbf{1}(x_0 = x_2)$ into $(HH^{(n-1)})_{x_0 x_n}$. ☐

Feldheim and Sodin inferred that $H^{(n)} = \widetilde{U}_n(H)$, where $\widetilde{U}_n(\xi) = U_n(\xi/2)$ and U_n is the standard Chebyshev polynomial of the second kind. Indeed, we have

$$\widetilde{U}_n(\xi) \;=\; \xi \widetilde{U}_{n-1}(\xi) - \widetilde{U}_{n-2}(\xi)\,.$$

Thus, we expand the propagator $\mathrm{e}^{-\mathrm{i}tH/2}$ in terms of Chebyshev polynomials:

$$\mathrm{e}^{-\mathrm{i}t\xi} \;=\; \sum_{n \geqslant 0} \alpha_n(t) U_n(\xi)\,.$$

We can compute the coefficients

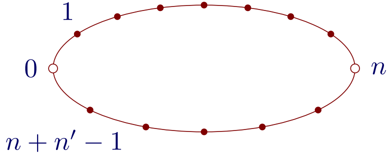
$$\alpha_n(t) \;=\; \frac{2}{\pi} \int_{-1}^{1} \mathrm{e}^{-\mathrm{i}t\xi} U_n(\xi) \sqrt{1-\xi^2}\, \mathrm{d}\xi \;=\; 2(-\mathrm{i})^n \frac{n+1}{t} J_{n+1}(t)\,,$$

where J_n is the n-th Bessel function of the first kind.

The graphical representation

The Chebyshev expansion yields $\varrho(t,x) \;=\; \sum_{n,n' \geqslant 0} \alpha_n(t)\overline{\alpha_{n'}(t)}\,\mathbb{E} H^{(n)}_{0x} H^{(n')}_{x0}\,.$

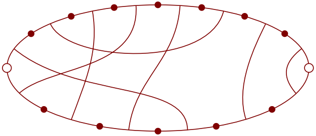
Represent matrix multiplication by loop; upper edge represents $H^{(n)}_{0x}$ and lower edge $H^{(n')}_{x0}$.



Taking the expectation yields a lumping (or partition) Γ of the edges:

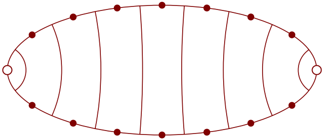
$$\mathbb{E} H^{(n)}_{0x} H^{(n')}_{x0} \;=\; \sum_{\Gamma \in \mathscr{G}_{n,n'}} V_x(\Gamma)\,.$$

Each lump $\gamma \in \Gamma$ contains at least two edges.
The most important lumpings are the pairings; their contribution estimates the contribution of all other lumpings (see later).



The ladder pairings

The leading order contribution to ϱ is given by the ladder pairings $L_0, L_1, L_2, \ldots$:



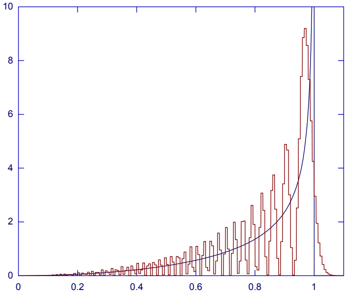
$$\varrho_{\text{ladder}}(t, x) \;=\; \sum_{n \geqslant 0} |\alpha_n(t)|^2 \, V_x(L_n)$$

The family of weights $\{|\alpha_n(t)|^2\}_{n=0}^{\infty}$ is a t-dependent probability distribution on $\mathbb{N}$ (since the family $\{U_n\}_{n=0}^{\infty}$ is orthonormal).

The number $|\alpha_n(t)|^2$ is the probability that the particle performs n steps of a random walk during the time t. The steps of the random walk have the transition kernel

$$p(y \leftarrow x) \;=\; \mathbb{E}|H_{xy}^2| \;=\; \frac{1}{W^d} f\left(\frac{x-y}{W}\right).$$

The distribution of the number of jumps does not concentrate at $n \approx t$ because of possible delays due to backtracking.



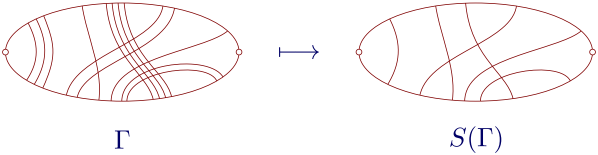
The function $\lambda \mapsto t\,|\alpha_{[\lambda t]}(t)|^2$ for $t = 150$ (brown), and its weak limit $\frac{4}{\pi}\frac{\lambda^2}{\sqrt{1-\lambda^2}}$ (blue) as $t \to \infty$.

The non-ladder lumpings

We have to prove that the sum of the contributions of all non-ladder lumpings vanishes. This is the main work!

- First, we estimate the contribution of all non-pairings in terms of the contribution of all non-ladder pairings.
  $\Longrightarrow$ It is enough to show that the contribution of all non-ladder pairings vanishes as $W \to \infty$.
- Problem: The summation labels are associated with vertices, but edges are paired. We need to extract conditions on the vertex labels from a pairing of the edges.
- Basic philosophy: The more complicated a pairing, the more constraints it induces on the vertex labels, and therefore the smaller its contribution. This fights against the larger number of complicated pairings.
  $\Longrightarrow$ We need a means of quantifying the combinatorial complexity of a pairing.
- Observation: A group of parallel lines has a large contribution, but a trivial combinatorics $\Longrightarrow$ parallel lines should not contribute to the combinatorial complexity of a pairing.

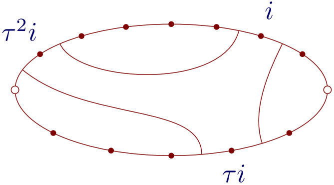
Step 1. Collapse the parallel lines. We assign to each pairing Γ its skeleton pairing $S(\Gamma)$ obtained from Γ by collapsing all parallel lines of Γ.



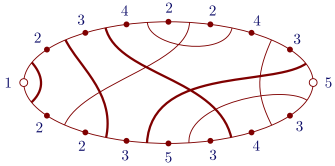
The size $2m$ of $S(\Gamma)$ is the correct notion of complexity for Γ.

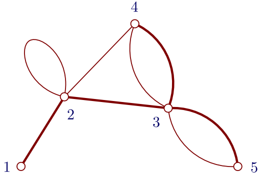
We recover Γ by replacing each line σ of $S(\Gamma)$ with a number ℓ_σ of parallel lines. The contribution of ℓ_σ parallel lines is given by a random walk with ℓ_σ steps $\Longrightarrow$ use heat kernel bounds on each line of $S(\Gamma)$ (local CLT).

Step 2. Estimate the number of free labels in a skeleton: the $2/3$ rule. Since parallel lines are forbidden, each vertex label must appear at least three times. Thus, the number L of free labels satisfies $3L \leqslant 2m$, i.e. $L \leqslant 2m/3$.



Step 3. Encode the skeleton as a multigraph and sum everything up using heat kernel bounds.





Each edge σ of the multigraph carries a random walk of ℓ_σ steps. To sum up the graph, choose a spanning tree of the multigraph. Apply heat kernel bounds:

- ℓ^1-bound for each tree edge ($\to$ factor 1)
- ℓ^∞-bound for each nontree edge ($\to$ factor $\ell_\sigma^{-d/2} W^{-d}$).

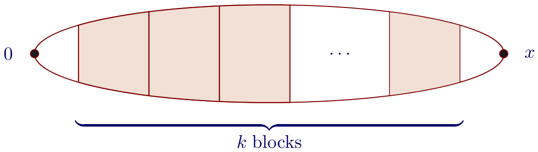
The $2/3$ rule implies that the number of nontree edges is at least $m/3$.
$\Longrightarrow$ Contribution of skeletons of size m is (roughly) bounded by

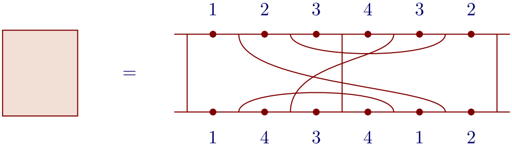
$$\binom{n}{m} m! \, (W^{-d})^{m/3} \, .$$

This is summable for $n \leqslant t \ll W^{d/3}$.

The necessity of the condition $\kappa < 1/3$

The following family $\Sigma_1, \Sigma_2, \Sigma_3, \dots$ of skeletons is critical; Σ_k is defined as





The bound in the $2/3$ rule is saturated: each vertex label occurs exactly three times ($6k$ edges and $4k$ free labels).

It is not hard to see that the contribution of all such skeletons diverges as $\kappa \to 1/3$.
$\Longrightarrow$ going beyond $\kappa = 1/3$ requires (i) resummations of terms with different n, n', or (ii) a more refined use of heat kernel bounds.

General band matrices

So far we assumed that $H_{xy} = W^{-d/2}\mathbf{1}(1 \leqslant |x-y| \leqslant W)\,\mathrm{Unif}(S^1)$, which was necessary for the algebraic identity

$$H^{(n)} \;=\; H H^{(n-1)} - H^{(n-2)} \tag{1}$$

to hold.

If the entries of H are general, the algebraic relation (1) is no longer exact; the RHS of (1) receives the error terms $-\Phi_2 H^{(n-2)} - \Phi_3 H^{(n-3)}$, where

$$(\Phi_2)_{xy} \;:=\; \delta_{xy} \sum_z \bigl(|H_{xz}|^2 - \mathbb{E}|H_{xz}|^2\bigr)\,, \qquad (\Phi_3)_{xy} \;:=\; |H_{xy}|^2 H_{xy}\,.$$

Strategy: Φ_3 is small by power counting (easy), Φ_2 has zero expectation (hard).

The rigorous treatment requires a considerably more complicated class of graphs; out of the simple “loop” grow backtracking “branches”. The cancellation of backtracking paths is no longer complete.

The organization of the expansion of the backtracking branches is quite involved. The threshold $t \ll W^{d/3}$ is again necessary.

Summary

- The quantum time evolution generated by $\mathrm{e}^{-\mathrm{i}tH/2}$ is diffusive up to time scales $t \ll W^{d/3}$. The dynamics is given by a superposition of delayed heat kernels.
- Eigenvectors of H are delocalized on scales $\ell \geqslant W^{1+d/6}$.
- Proof. Expansion in nonbacktracking powers $H^{(n)}$ of $H \Longleftrightarrow$ self-energy renormalization. Use that $H^{(n)} = U_n(H)$. Control the expectation using a graphical expansion.