Resonant delocalization in random Schrödinger operators

(on graphs of rapid volume growth)

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Abstract (localization / delocalization & the third way)

Under certain conditions, Random Schrödinger operators may exhibit energy regimes (phases) in which extended states are formed from resonating local quasi-modes.

The corresponding eigenstates may be delocalized, in the sense of geometric spread, yet are also "non-ergodic", in the sense that they violate a heuristic version of the equidistribution principle.

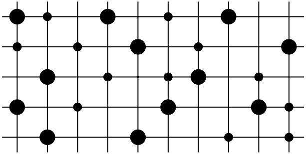
Indications of such phases were encountered in the analysis of the random Schrödinger operator on tree graphs (joint work with Simone Warzel). Related phenomena may also occur in many-particle systems which are among the goals of ongoing research (with Mira Shamis and Simone Warzel).

I shall discuss the key mechanism leading to such states, and describe some partial results which we obtained so far.

I. Some one-particle models

i. Quantum particle in a random potential on $\mathbb{Z}^d$ (or the finite $[-L, L]^d$)

Dynamics generated by **Schrödinger operator with random potential**



$\omega(x),\ x \in \mathbb{Z}^d$, i.i.d. random variables

Here:

$\mathbb{P}(\omega(x) \in dv) = \varrho(v)\, dv$ with $\varrho \in L^\infty$,

$$\boxed{H_\lambda(\omega) = T + \lambda\, V(\omega) \qquad \text{in} \qquad \ell^2(\mathcal{G})}$$

- $T\psi(x) := \sum_{|y-x|=1} \psi(y)$ the adjacency operator ($T = -\Delta + 2d\mathbb{I}$) .
- $V\psi(x) := \omega(x)\,\psi(x)$ the random potential (operator)
- Disorder parameter: $\lambda \geq 0$.

$H_\lambda(\omega)$ is a self-adjoint operator. The limit $L \to \infty$ is easy to make sense of, and spectral analysis is then of relevance for describing the unitary time evolution $e^{-itH_\lambda(\omega)}$, as well as the equilibrium states of systems of many noninteracting particles (with a one-body Hamiltonian).

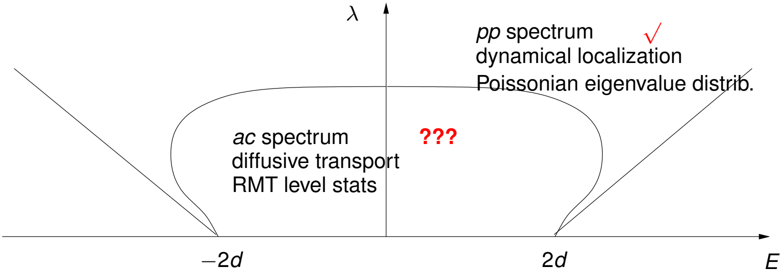
The expected Phase Diagram for $\boxed{H_\lambda(\omega) = T + \lambda\, V(\omega) \quad \text{in} \quad \ell^2(\mathcal{G})}$

T - absolutely continuous spectrum
extended (generalized) eigenfunctions ($\Psi_E = e^{-i\,k\cdot x} \notin \ell^2(\mathbb{Z}^d)$)

$V(\omega)$ - pure-point spectrum, $\sigma(V(\omega)) = \{V_x(\omega)\}_{x\in\mathbb{B}}$
localized eigenstates ($\{\delta_x\}_{x\in\mathbb{B}}$)

Dimension $\mathbf{d} = \mathbf{1}\checkmark$: *pp* only spectrum for **all** $\lambda > 0$ Goldsheid/Molchanov/Pastur '73.

The generally expected picture for $\mathbf{d} > \mathbf{2}$ (?): e.g. $\varrho(v) = 1_{[-\frac{1}{2},\frac{1}{2}]}(v)$

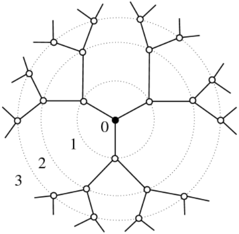


ii. Rand. Sch. Ops on Regular Tree Graphs ($\mathcal{G} = \mathbb{T}^{(k)}$)

- coordination number (degree) $= \; K + 1$
- $H_\lambda(\omega) = T \, + \, \lambda \, V(\omega) \qquad \text{in} \qquad \ell^2(\mathcal{G})$
- It is less immediate what finite graphs does $\mathbb{T}^{(k)}$ approximate. A sensible answer is:

  finite $(K+1)$ -regular graphs

  Globally these are not trees, but locally they look as such.



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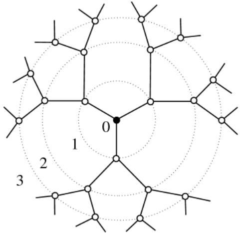

- Among the earliest studied models of Anderson localization

  Abou-Chacra/Anderson/Thouless '73, '74

  Relatively more accessible compared to $\mathbb{Z}^d$.
  Self-consistent approach to localization becomes exact ($\neq$ solvable !).
- Recently found surprises in the phase diagrams Aiz. / Warzel '11, Altshuler ..., Biroli/Teixeira/Tarzia '12
- Renewed interest as of relevance for the configuration space of systems with many particles (as suggested in Altshuler/Gefen/Kamenev/Levitov '97)

2. Some Graphs sharing features with Systems of Particles

Unlike the case of non-interacting particles, the question which are relevant for very large finite systems are not easily expressed in terms of the spectral properties of a self adjoint operator on an infinite graph (!).

> **Note:** The configuration space for a system of particles with hard core repulsion on a graph $\mathcal{G}$ can be presented as $\widetilde{Q}_{\mathcal{G}} = \{-1, 1\}^{\mathcal{G}}$. A relevant metric is: $\mathrm{dist}(x, y)$:= the min. number of moves transforming x into y.

The "Hamming cube": $Q_N = \{-1, 1\}^N$, with $\mathrm{dist}(\sigma, \sigma') = \sum_{j=1}^{N} \mathbb{I}[\sigma_j \neq \sigma_j']$,

where $\sigma_j = \pm 1$.

$$\boxed{H = \sum_{J=1}^{N} (\mathbb{I} - T_j) + \lambda \sqrt{N}\, V(\sigma)}$$

with $T_j =$ flip of σ_j, and V given by 2^N iid $\mathcal{N}(0, 1)$ gaussian variables.

A yet further simplification – the "Complete Graph" of $|\mathcal{G}| = M$ sites:

$$\boxed{H = |\Phi\rangle\langle\Phi| + \frac{\kappa}{\sqrt{\log_2 M}} V(\sigma)}$$

with $|\Phi\rangle := (1, 1, ...1)/\sqrt{M}$.

3. Boltzmann's 'Ergodic Hypothesis' / Equidistribution on the Energy Shell

The ergodic hypothesis (Boltzmann, 1898): Under the time evolution, the fraction of time spent by the system's trajectory in any region of the phase space of microstates with the same energy and number of particles converges to the "microcannonical volume" of this region.
(To be taken as a useful guiding principle, not at face value*.)

For (finite) classical systems this equivalent to the assumption that the time evolution is ergodic with respect to (almost every) "microcannonical state".

For quantum systems this can be taken as suggesting that in semiclassical representations, typically, the eigenfunctions (=stationary states) are as spread as the principle of equidistribution suggests.
The local manifestation of that is "eigenfunction thermalization".

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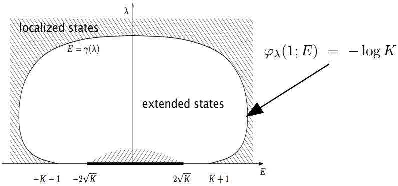
The local manifestation of that is "eigenfunction thermalization".

More precise statement can in some cases be formulated (& even proven !), e.g. for high energy eigenstates of chaotic billiard systems, in the semiclassical limit.

Note: Equidistribution is violated in Anderson localization.

4. A possible Equidistribution violation without Anderson localization

Theorem (Aiz./Warzel '11): For the Schrödinger operator on any regular tree, with unbounded random potential (supp $\rho = \mathbb{R}$, etc.), for $\lambda > 0$ the ac spectrum immediately extends up to $E = \pm(K+1)$, in particular, into the regime of Lifshitz tails.



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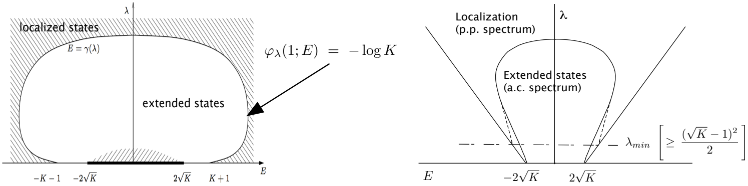

- The result supplements previous proofs of:
  - *ac* spectrum near the band $[-2\sqrt{K}, 2\sqrt{K}]$ (Klein ‘94, ASW ‘06, FHS ‘07)
  - localization in the outer region (Aiz. ‘94) *[both expressing continuity (!)]*

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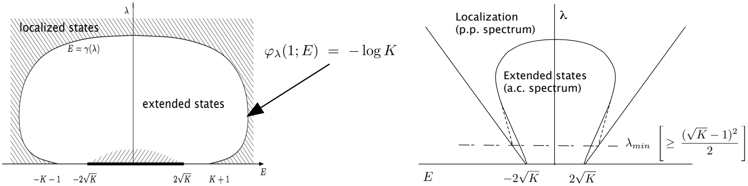

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  - localization in the outer region (Aiz. '94) *[both expressing continuity (!)]*
- The surprise here is that extended states occur also in regimes of extremely low density of states (which in the gaussian case is of the order of e^{-C/λ^2}).
- The extended states seem to consist of resonating localized quasi-modes. These are sensitive to the details of the Hamiltonian as the localized states are, yet in those states, for every $x \in \mathcal{G}$:

$$\mathrm{Prob}_\Psi\,(X(T) = x) \equiv \left(\Psi, e^{itH} P_{x_0} e^{-itH}\,\Psi\right) \to 0$$

(for $\lim_{L\to\infty}$, $\lim_{T\to\infty}$, in any order, and suitable averages over the potential).

5. Heuristics – fluctuation enabled resonant tunneling

The mechanism at work here:

States which locally appear to be localized have arbitrarily close energy gaps (ΔE) with other states (at distances R), to which the tunneling amplitudes are exponentially small (as $\approx e^{-L_\lambda(E)R}$) .

Mixing between two levels occurs if $\boxed{\Delta E \ll e^{-L(\lambda(E)R}}$.

Since the volume grows exponentially fast (as K^R),

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Essential enabling conditions:

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• For the tight criteria use is also made of the large deviations theory (applied to the Green function).

• The proof requires to go beyond the divergence of the mean, and establish that with positive probability the number of resonant sites is actually of the order of the mean. (The Paley - Zygmund second moment test, etc.)

Quasimodes & their tunneling amplitude

Definition:

1. A quasi-mode (qm) with discrepancy d for a self-adjoint operator H is a pair (E, ψ) s.t.

$$\boxed{\|(H - E)\psi\| \leq d\|\psi\| \,.}$$

2. For a collection of orthogonal qm's (E_j, ψ_j), the pairwise tunneling amplitude at energy E is $\tau_{jk}(E)$ in:

$$\boxed{P_{jk} \frac{1}{(H-E)} P_{jk} = \begin{bmatrix} e_j + \sigma_{jj}(E) & \tau_{jk}(E) \\ \tau_{kj}(E) & e_k + \sigma_{kk}(E) \end{bmatrix}^{-1} .}$$

(recall the Schur complement formula).

A seemingly reasonable rule of thumb:

If the typical **gap size** for quasi-modes is $\Delta(E)$, the condition for their **resonant delocalization** is:

$$\boxed{\Delta(E) \precsim |\tau_{jk}(E)| \,.}$$

A 2×2 calculation for: $\quad H = \begin{pmatrix} E_1 & \tau \\ \tau^* & E_2 \end{pmatrix}$

Energy gap: $\Delta E := E_1 - E_2$ **Tunneling amplitude:** τ.

- Case $|\Delta E| \gg |\tau|$: **Localization**

$$\psi_1 \approx (1, 0) , \qquad \psi_2 \approx (0, 1) .$$

- Case $|\Delta E| \ll |\tau|$: **Delocalization**

$$\psi_1 \approx \frac{1}{\sqrt{2}} (1, 1) , \qquad \psi_2 \approx \frac{1}{\sqrt{2}} (1, -1) .$$

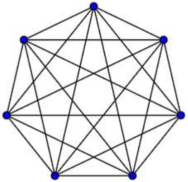
Questions beyond 2×2:

1) large deviations (lead to the ℓ^1 condition)...
2) interference between more than 2 quasi-modes (2nd moment test)
3) possibility of a hierarchical organization (?)

6. The case of the complete graph

Complete graph over M sites:

$$\boxed{H_M = -|\varphi_0\rangle\langle\varphi_0| + \kappa_M \; V}$$



with:

- $\langle\varphi_0| = (1, 1, \ldots, 1)/\sqrt{M}$,
- $V_1, V_2, \ldots V_M$ iid standard Gaussian rv's, i.e.

$$\varrho(v) = \frac{1}{\sqrt{2\pi}} e^{-v^2/2},$$

- $\kappa_M := \lambda \big/ \sqrt{2 \log M}$.

Remarks:

- Scaling of the potential: $\quad \|V\|_\infty = \sqrt{2 \log M} + \mathcal{O}(1)$.
- The spectrum of H on the macroscopic scale for $M \to \infty$:

$$\sigma(H_M) \longrightarrow [-\lambda, \lambda] \cup \{-1\}\,.$$

Interlacing of eigenvalues with potential values!

Resonant delocalization

Quasi-modes: $(U_j\,,\delta_j)$ where $U_j := \kappa_M V_j$, i.e., $\|(H_M - U_j)\delta_j\| = 1/\sqrt{M}$.

Density of quasi-modes at $E \in \mathbb{R}$: $\mu(E) = \frac{\varrho(E/\kappa_M)}{\kappa_M}$.

Gap size: $\Delta(E) = \frac{1}{M\,\mu(E)} = \Theta\big(\kappa_M\, M^{(E/\lambda)^2 - 1}\big)$

Tunneling amplitude: $\tau_{jk}(E) = \frac{1}{M}\left(1 - \frac{1}{M}\sum_{n \neq i,j} \frac{1}{\kappa_M V_n - E}\right)^{-1}$

$$\frac{\Delta(E)}{\tau_{i,j}(E)} = M\Delta(E)\Big(1 - \underbrace{\fint \frac{\varrho(v)\,dv}{\kappa_M v - E}}_{=: \frac{1}{\kappa_M}\,\overline{\varrho}\left(\frac{\mathcal{E}}{\kappa_M}\right)}\Big) + \mathcal{O}(1)$$

(Hilbert transform)

Condition for resonant delocalization:

$$\boxed{M\Delta(E)\left(1 - \frac{1}{\kappa_M}\,\overline{\varrho}\left(\frac{E}{\kappa_M}\right)\right) \lesssim 1}$$

Q: *For which E does this condition hold?* *(blackboard)*

Resonant deloc. at scaling limits:

Scaling windows: centered at some sequence of energies E_M with:

$$\text{limiting value} \quad E \in [-\lambda, \lambda], \quad \text{and} \qquad |E_M - E| \leq C\kappa_M^2 .$$

The rescaled eigenvalues process $\boxed{u_{n,M} \;:=\; \dfrac{e_{n,M} - E_M}{\Delta(E)} .}$

<u>Theorem</u> (Aiz., Shamis, Warzel '13) If either

- $E = 0$, or
- $E = -1$, in which case we also suppose that $\lambda > \sqrt{2}$.

and additionally the limit

$$\alpha := \lim_{M\to\infty} M\Delta(E) \left(1 - \frac{1}{\kappa_M}\,\overline{\varrho}\left(\frac{E_M}{\kappa_M}\right)\right)$$

exists, then:

1. the rescaled eigenvalue point process $(u_{n,M})$ converges in distribution as $M \to \infty$ to the α - BGS (Bogomolny-Gerland-Schmit) point process
2. the corresponding eigenfunctions (at energies within the scaling window) are almost surely all ℓ^1-delocalized (and delocalized "geographically "):

$$\lim_{M\to\infty} \frac{\|\psi_{n,M}\|_1}{\|\psi_{n,M}\|_\infty} \;=\; \infty \qquad \text{for all } |n| < \infty.$$

Yet the eigenfunctions are localized in the ℓ^2-sense, with a non-degenerate limit for the distribution of $\frac{\|\psi_{n,M}\|_2^2}{\|\psi_{n,M}\|_\infty^2}$.

The Bogomolny-Gerland-Schmit process

Given a Poisson process ω of constant intensity 1, the following sum converges almost surely, and defines for us the Stieltjes-Poisson random function

$$F_{SP}(u;\omega) := \lim_{w\to\infty} \sum_n \frac{1[|\omega_n - u| \le w]}{\omega_n - u} .$$

Definition: We refer to the point set of solutions of:

$$F_{SP}(u;\omega) = \alpha \,, \qquad \alpha \in [-\infty, \infty] \,,$$

as the α-BGS point process, at level $\alpha \in [-\infty, +\infty]$).

Remarks:

- Limiting cases $\alpha = \pm\infty$ yield the original Poisson process.
- At $|\alpha| < \infty$ the process shows intermediate statistics: level repulsion at short distances, with Poisson fluctuations of level numbers in large intervals.

  Bogomolny/Gerland/Schmit 2001
- The Stieltjes transform of point processes converges under more general conditions.
  Curiosity: Quite generally – for shift invariant point processes the value of $F(E)$ has the Cauchy distribution.

Further comments on the complete graph

- Ossipov '13 found evidence of ℓ^2-localization near $E = 0$ using SUSY-calculation.
- Resonant delocalisation also near $E_{-1,M} := -1 - \kappa_M^2 + o(\kappa_M^2)$, i.e. the unique solution of $1 = \frac{1}{\kappa_M} \overline{\varrho}\left(\frac{E}{\kappa_M}\right)$ near -1.
- Proof makes use of rank-one perturbation theory:

$$\text{Eigenvalues}: \quad \frac{1}{M} \sum_n \frac{1}{\kappa_M V_n - E} = 1 \quad (*)$$

$$\text{Eigenvectors}: \quad \psi_{j,E} = \frac{1}{\kappa_M V_j - E} \quad \text{up to normalization}$$

In (*) distinguish between **tail sum** and **principle value** contributions.

Complete graph summary: heuristic delocalization criterion applies and yields a correct picture for the phase diagram:

1. Resonant delocalization of a macroscopic number of levels:
   - near $E = 0$, and
   - near $E = -1$ in case $\lambda > \sqrt{2}$.
2. The corresponding eigenstates are
   - **spatially delocalised** (ℓ^1-delocalization),
   - ℓ^2**-localized** (finite inverse participation ratio).

   They hence violate the equidistribution principle.
3. Localization elsewhere (also proven).
4. First-order transition of ground-state at $\lambda = 1$.

Among the natural next questions: the "Hamming cube": $Q_N = \{-1, 1\}^N$,

$$\boxed{H = \sum_{J=1}^{N} (\mathbb{I} - T_j) \; + \lambda \sqrt{N} \, V(\sigma)}$$

with $\sigma_j = \pm 1$, $T_j =$ flip of σ_j,
and V given by 2^N iid $\mathcal{N}(0, 1)$ gaussian variables, or a more interesting process.

The results for tree graphs were presented in the following joint works with S. Warzel

1. “Extended States in a Lifshitz Tail Regime for Random Schrödinger Operators on Trees", Phys. Rev. Lett. **106**, 136804 (2011).

2. “Absence of Mobility Edge for the Anderson Random Potential on Tree Graphs at Weak Disorder”, Euro. Phys. Lett. **96**, 37004 (2011).

3. “Resonant delocalization for random Schrödinger operators on tree graphs", J. Euro. Math. Soc., **15**, 1167 (2013).

4. “Absolutely continuous spectrum implies ballistic transport for quantum particles in a random potential on tree graphs”, J. Math. Phys. **53**, 095205 (2012).

The concepts developed there are currently being extended to other systems in works in progress with M. Shamis and S. Warzel.

Of related interest:

5. A. Pal, and D. Huse: “The many-body localization phase transition”, Phys. Rev. **B 82**, 174411 (2010).

6. G. Biroli, A. C. Ribeiro Teixeira, and M. Tarzia: “Difference between level statistics, ergodicity and localization transitions on the Bethe lattice” (Preprint, Dec. 2012).

7. M. Shamis: “Resonant delocalization on the Bethe strip”, (2013 preprint, arXiv:1304.4461)

... and then you tell'em what you told them

1. Some one-particle models (with disorder)
2. Some graphs sharing features with systems of particles
3. Boltzmann's 'Ergodic Hypothesis' / Equidistribution on the Energy Shell
4. A possible equidistribution violation without Anderson localization
5. Heuristics fluctuation enabled resonant tunneling
6. Results for some finite systems

For further attention:

- The question of a second phase transition for tree graphs (within the region enclosed by the mobility edge) versus crossover.
- Possible signature in the spectral gap statistics, e.g. for *d*-regular graphs (?)
- A question of interest: possible implications for many particle systems.

Thank you for your attention!

Notions of localization on sequences of finite graphs $\mathcal{G}_M$

On the complete graph the spatial structure is rather degenerate.

(De)localization quantified in ℓ^q-sense:

1. **Inverse participation ratio** with $q = 2$ (or higher)

$$P_q(\psi) := \frac{\sum_x |\psi(x)|^{2q}}{\left[\sum_x |\psi(x)|^2\right]^q}$$

- Relation to the norm ratio $r(\psi) := \|\psi\|_\infty / \|\psi\|_2$ through the bounds:

$$r(\psi)^{2q} \leq P_q(\psi) \leq r(\psi)^{2(q-1)}.$$

- extreme localization $P_q(\psi) = 1$
  ——— delocalization $P_q(\psi) = |\mathcal{G}_M|^{-q}$

2. ℓ^1**-delocalization:** $P_q(\psi)$ diverges in the distributional sense (for eigenfunctions in a specified range) for all $q \in (0, 1/2]$.