Many-Body Localization Landscape

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Foundation Announces Simons Collaboration on Localization of Waves

July 24, 2018

The Simons Foundation is pleased to announce the establishment of the Simons Collaboration on Localization of Waves, directed by Svitlana Mayboroda of University of Minnesota.

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MATHEMATICAL PHYSICS

Mathematicians Tame Rogue Waves, Lighting Up Future of LEDs

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The mathematician Svitlana Mayboroda and collaborators have figured out how to predict the behavior of electrons — a mathematical discovery that could have immediate practical effects.

Outline

- Single-particle localization landscape
  - Numerical surprises and “miracles” in the Schrödinger equation
    - Hidden structure of localization
    - Calculating spectrum without solving eigenvalue problems
  - The mathematical structure behind the surprising numerics
    - Universal bound on the wave-function
    - Agmon inequalities

- Generalization to interacting many-body systems
  - Fock-space graph and many-body localization landscape
  - Generalized universal bound
  - Fock-Agmon distance and generalized inequalities
  - Locator expansion and proof of a weak form of MBL

- Many ideas for future work (including “UQM models”)

Introduction to single-particle localization landscape

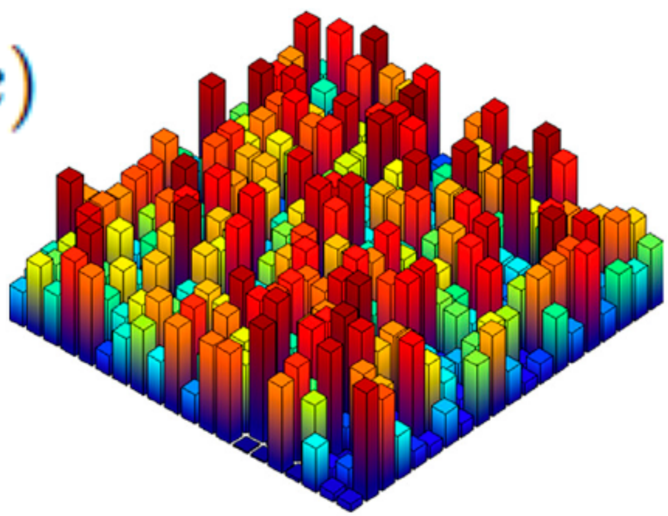
The setup: the good old Schrödinger equation

$$\mathcal{H} = -\nabla^2 + V(\boldsymbol{x})$$

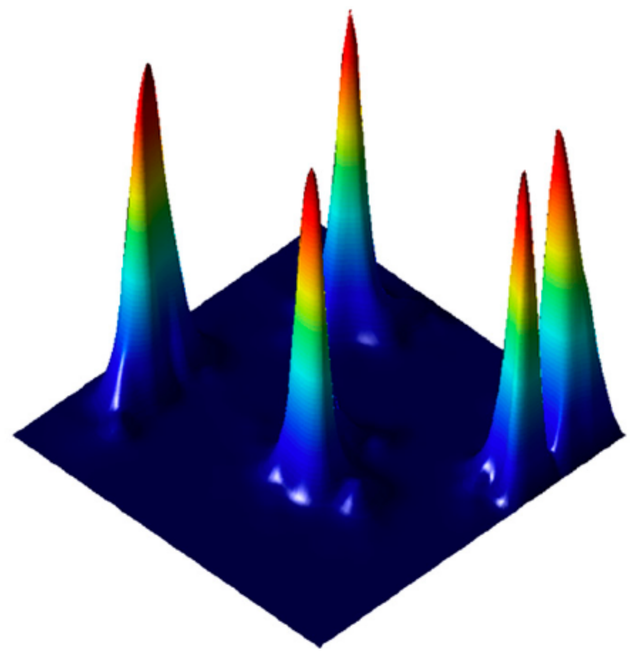
$$\mathcal{H}\psi(\boldsymbol{x}) = E\psi(\boldsymbol{x}), \quad \boldsymbol{x} \in \Omega \subset \mathbb{R}^d$$

$$\psi(\boldsymbol{x})\Big|_{\partial\Omega} = 0$$ - Dirichlet boundary conditions

$V(\boldsymbol{x})$



We focus on random potentials



First 5 (localized) states

Marcel Filoche and Svitlana Mayboroda, PNAS 2012

Where do the localized states actually reside?

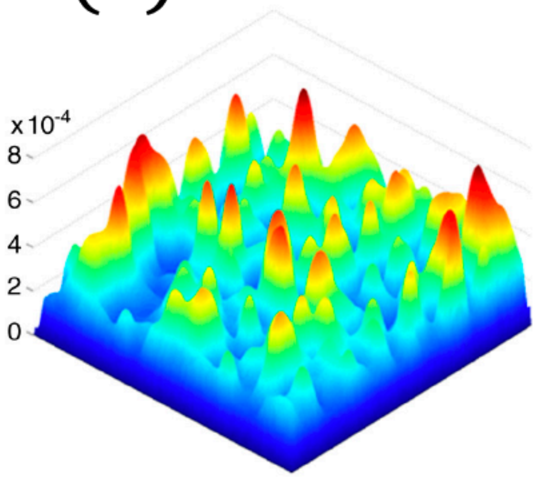
- Answer: there is a simple structure hidden in plain sight that represents an effective (~classical) localization pseudopotential.

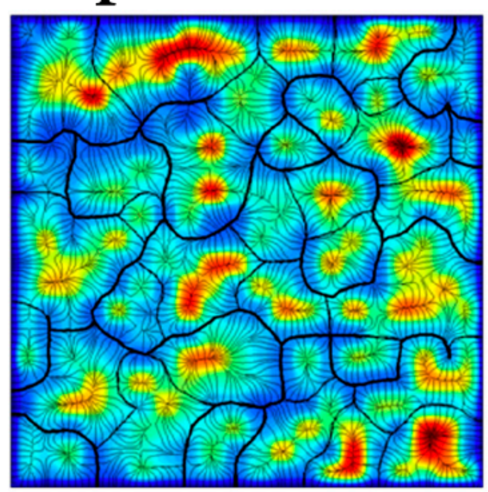
$$\mathcal{H} = -\nabla^2 + V(\boldsymbol{x})$$

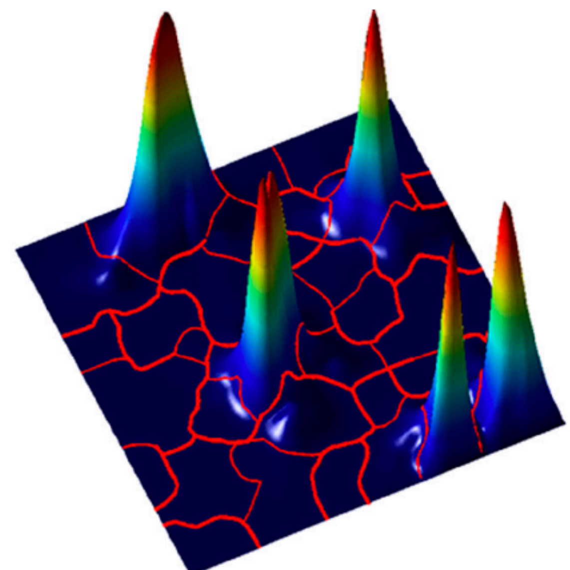
$$\boxed{\mathcal{H}u(\boldsymbol{x}) = 1} \qquad u(\boldsymbol{x})\Big|_{\partial\Omega} = 0$$

Localization landscape

- $u^{-1}(x)$ is an effective potential.



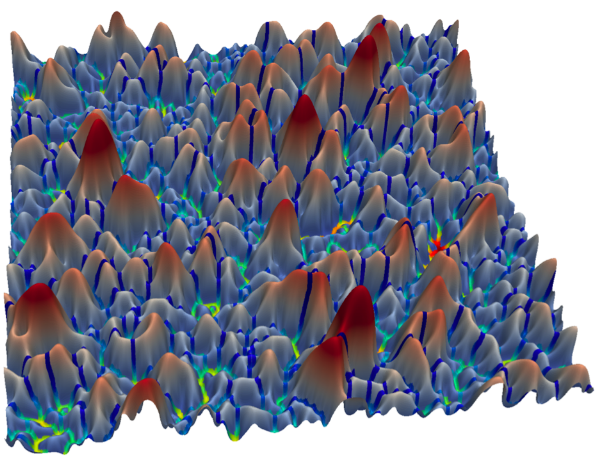


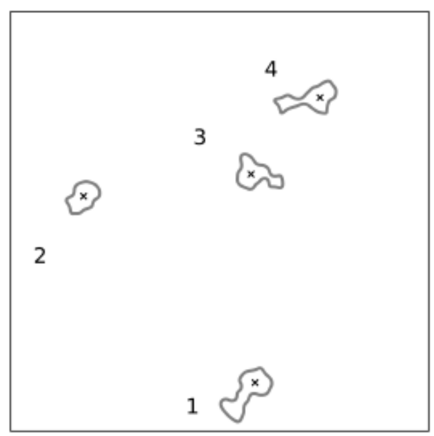


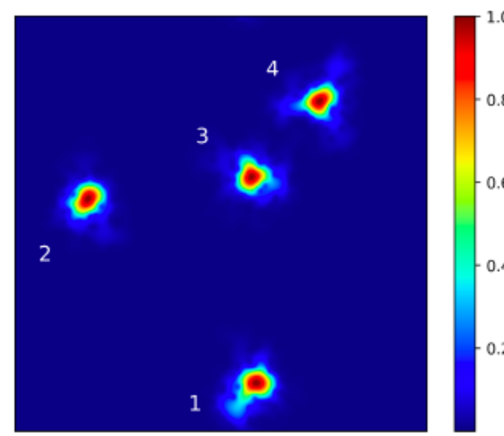
Marcel Filoche and Svitlana Mayboroda, PNAS 2012

A more impressive numerical example

- Bernoulli potential: $V(x) = \begin{cases} 1, \textit{with probability}, p \\ 0, \textit{otherwise} \end{cases}$

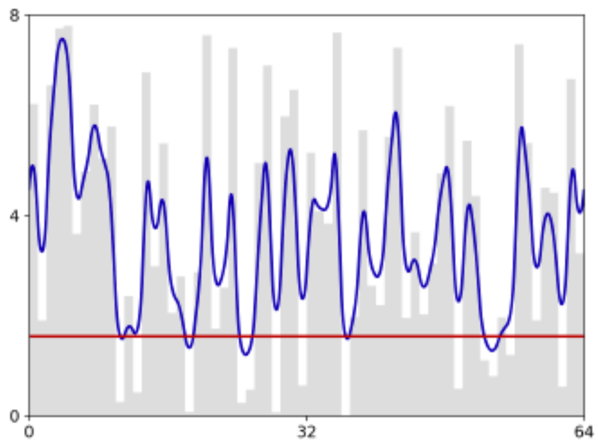


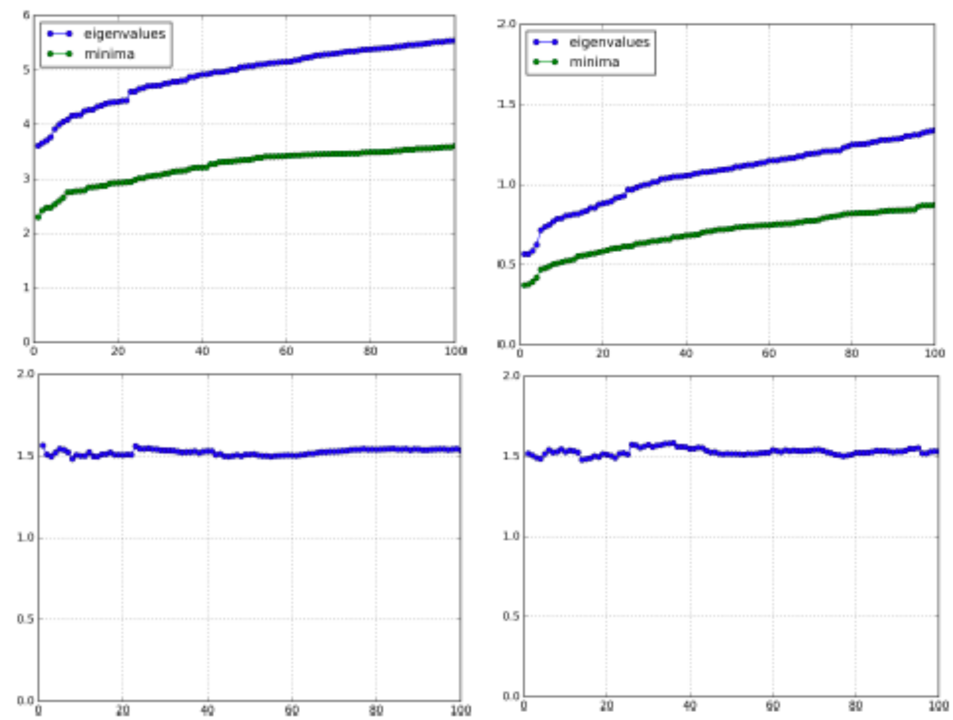




Images: courtesy of S. Mayboroda (International Congress of Mathematicians, 2018)
Douglas Arnold *et al*., *Journal of Scientific Computing 2019*

From surprises to "miracles"





$$E_n \approx \left(1+\frac{d}{2}\right) n^{th} \min_x [u^{-1}(x)]$$

Douglas Arnold *et al*., *Journal of Scientific Computing 2019*

Society for Industrial and Applied Mathematics

SIAM Journal on Scientific Computing, 2019, Vol. 41, No. 1 : pp. B69-B92

Computing Spectra without Solving Eigenvalue Problems

Douglas N. Arnold, Guy David, Marcel Filoche, David Jerison, and Svitlana Mayboroda

https://doi.org/10.1137/17M1156721

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Hidden landscape of an Anderson insulator

Posted in Journal Articles on August 30, 2019 at 10:29 am by JCCMP

Computing spectra without solving eigenvalue problems
Authors: Douglas N. Arnold, Guy David, Marcel Filoche, David Jerison, and Svitlana Mayboroda
SIAM J. Sci. Comput. 41, B69 (2019); DOI: 10.1137/17M1156721
arXiv:1711.04888

Recommended with a commentary by Carlo Beenakker, Leiden University
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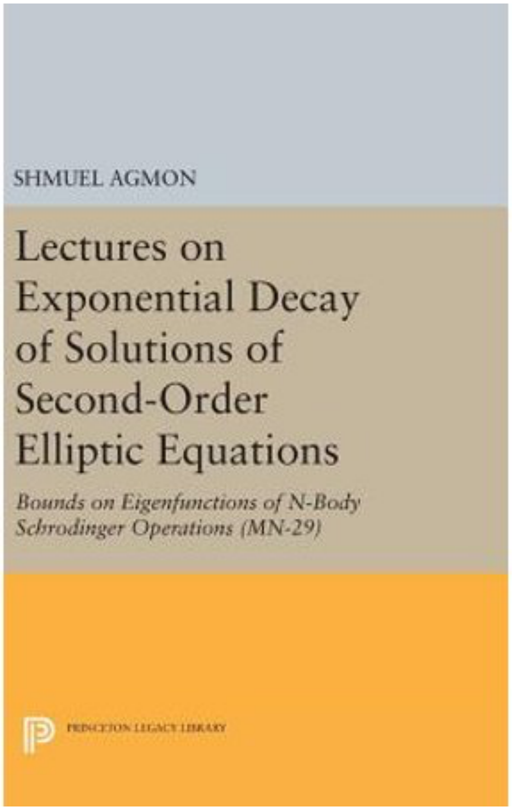
JCCM_August_2019_01

The origin of some of the surprises can be elucidated through a sequence of simple (in retrospect) theorems and so-called Agmon inequalities.



Important statements and theorems

- Consider an arbitrary elliptic operator, $\hat{L}$ (i.e., a properly generalized Laplacian, see e.g. Wikipedia), then

  $$\frac{|\psi(\boldsymbol{x})|}{\max_{\boldsymbol{x}\in\Omega}|\psi(\boldsymbol{x})|} \leq \lambda \cdot u(\boldsymbol{x})$$

  where $\hat{L}\psi(\boldsymbol{x}) = \lambda\psi(\boldsymbol{x}), \boldsymbol{x} \in \Omega$

  and $u(\boldsymbol{x})$ is the landscape: $\hat{L}u(\boldsymbol{x}) = 1$

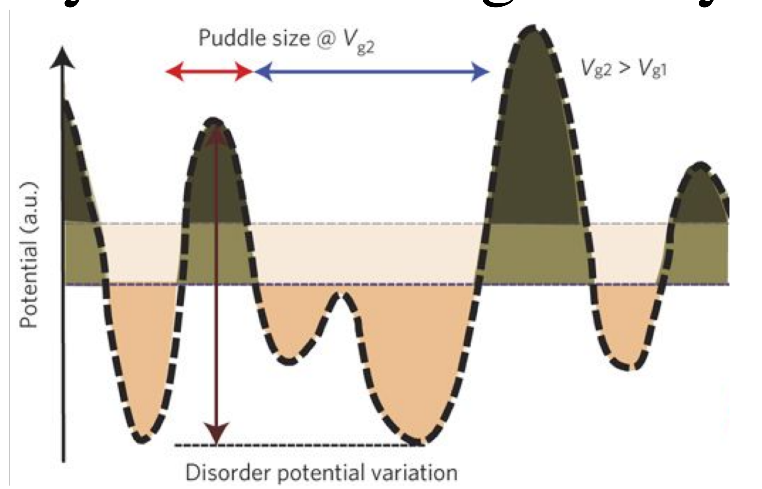
- Minimum principle: $u(\boldsymbol{x})$ is pointwise positive.
- Inverse landscape is an effective potential in the deformed Schrödinger equation (here, assume, $\hat{L} = -\nabla^2 + V$)

$$-\frac{\hbar^2}{2m}\left[\frac{1}{u^2}\text{div}\left(u^2\nabla\psi\right)\right] + \frac{1}{u}\psi = E\psi$$

Agmon inequalities

- Agmon inequalities are results (1979 onwards) from the field of mathematical analysis, which are rigorous pointwise bounds on solutions to (Schrödinger-like) differential equations
- The initial construction is motivated by WKB approximation, but instead of asymptotic expansions, Agmon uses WKB to prove exact (non-asymptotic) bounds on the wave-function.
- Essentially, given a potential valley surrounded by hills, they bound wave-functions in the classically forbidden regions by

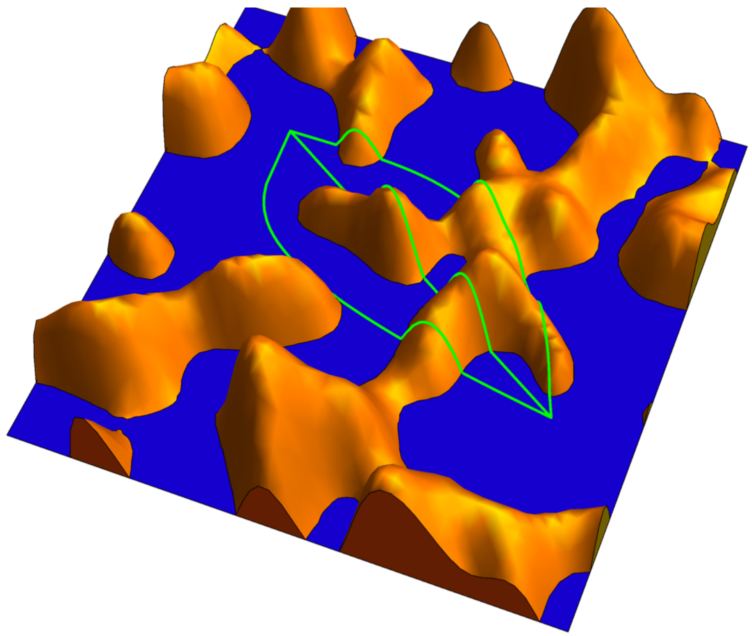
$$|\psi(x)| < C \cdot exp\left[-\int |"p"(x)|dx\right]$$



Agmon distance

- The key to Agmon construction is Agmon's distance

$$d(x,y) = \min_{\gamma:x\to y} \int_0^1 \sqrt{\min\{0, V[\gamma(t)] - E\}\gamma'(t)dt}$$



- The standard Agmon estimate for a decay of ψ, localized in a quantum well: take any point x_0 in the classically allowed region within the well, then "roughly" $|\psi(x)| < C\, e^{-d(x_0,x)}$

Limitations of the standard Agmon construction

- In many cases (of relevance to localization), the standard Agmon estimates are useless. E.g., the potential may not be smooth enough for the theorems to apply, or/and the classical regions can percolate (the Agmon distance hence is just 0).

Still the wave-functions exponentially localize!

- The key to Mayboroda et al's construction is that they replace the physical "bare" potential with the effective one – the inverse landscape. It is always smooth and the classical regions do not percolate (at least for some low-E states).

Mayboroda-Agmon distance (my terminology)

- Instead of bounding solutions to the standard Schrödinger equation, consider the "deformed" equation

$$-\frac{\hbar^2}{2m}\left[\frac{1}{u^2}\text{div}\left(u^2\nabla\psi\right)\right]+\frac{1}{u}\psi=E\psi$$

- With the landscape, $u(x)$, defined again as follows

$$\left[-\frac{\hbar^2\nabla^2}{2m}+V(x)\right]u(x)=0, \text{with } u(x)|_{x\in\Omega}=0$$

- Then, the new distance (let's call it S – an "action") is

$$S(x_0,x)=\min_{\gamma:x_0\to x}\int_0^1\sqrt{\min\left\{0,u^{-1}[\gamma(t)]-E\right\}\gamma'(t)dt}$$

- <u>The wave-function is exponentially bounded by it</u>

$$|\psi(x)|<Ce^{-S(x)}$$

Single-particle summary so far

- Universal bound (always true)

$$\frac{|\psi(\boldsymbol{x})|}{\max_{\boldsymbol{x}\in\Omega}|\psi(\boldsymbol{x})|} \leq E \cdot u(\boldsymbol{x})$$

- Stronger exponential bound away from a 1/landscape well

$$|\psi(x)| < Ce^{-S(x)}$$

$$S(x_0, x) = \min_{\gamma: x_0 \to x} \int_0^1 \sqrt{\min\left\{0, u^{-1}[\gamma(t)] - E\right\}}\gamma'(t)dt$$

- Importantly, there is a series of theorems that show that the inverse landscape is colloquially-speaking a smoother, deeper, and "better" potential than the original one.
- The theorems and numerics suggest that it is the "*actual*" potential where localization takes place.

Generalization to interacting

many-body problems (including MBL):

Many-body localization landscape

Localization (an unnecessary reminder)

- Usual Anderson model

$$H = -t \sum_{\langle i,j \rangle} c_i^\dagger c_j + \sum_i \epsilon_i n_i, \text{ with } \epsilon_i \text{ random}$$

- Anderson's original paper used locator expansion (pertubative expansion in the hopping) to argue the existence of localization.
- The locator expansion diverges due to resonances. Reasonable resummation schemes exist but they are not exact (apart from the Bethe lattice).
- Localization has been rigorously proven in 1D, but not in higher dimensions. But on physical grounds, the picture seems clear.

- We are interested in the interacting model (switching to spins)

$$H = -t \sum_{\langle i,j \rangle} \sigma_i^+ \sigma_j^- + \sum_i \epsilon_i n_i + \sum_{i,j} V(|i-j|) n_i n_j$$

What do we know about MBL?

- Problem #1 is lack of clear definition: what is MBL? Options:
  1. Persistence of localization of some states (partial MBL)
  2. Persistence of localization of all states in 1D and 2D
  3. Emergent integrability and ergodicity breaking
  4. Poisson level statistics
- Basko, Aleiner, & Altshuler examined locator expansion with interactions& concluded that (partial) localization (in Fock space) persists. A MIT was found. *But there is no rigorous proof*.
- Numerics in 1D disordered spin chains (e.g., Oganesyan & Huse) suggested full MBL. *Finite size effects make results inconclusive*.
- John Imbrie presented a proof of MBL in 1D (per definition #3) with math rigor, but *has an ad hoc assumption Re: lack of level attraction*.
- Some cold atom experiments support existence of MBL. *Not a proof*.

There is an overwhelming evidence for MBL but no rigorous proof.

Fock space graph

- We consider a model defined on an arbitrary (bipartite) lattice

$$H = -t \sum_{\langle i,j \rangle} \sigma_i^+ \sigma_j^- + \sum_i \epsilon_i n_i + \sum_{i,j} V(|i-j|) n_i n_j$$

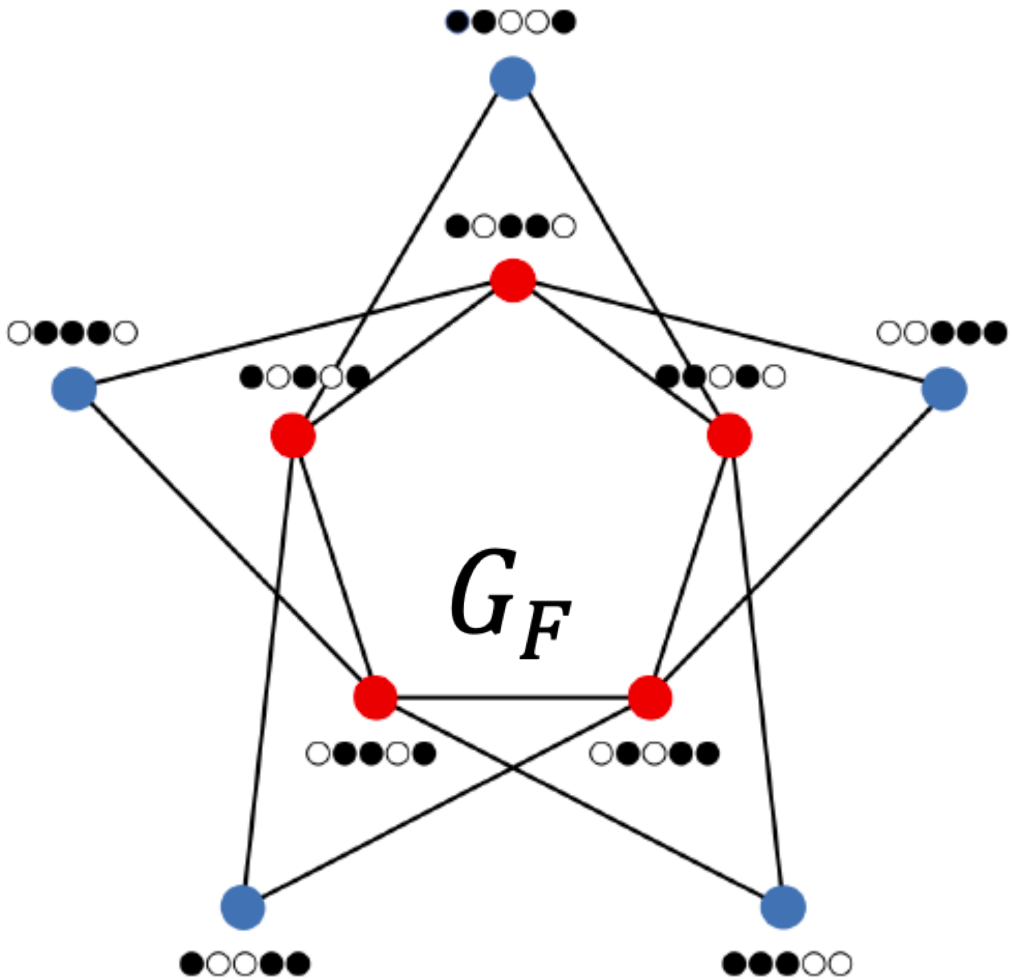
- Let L be the total number of sites and N number of occupied sites

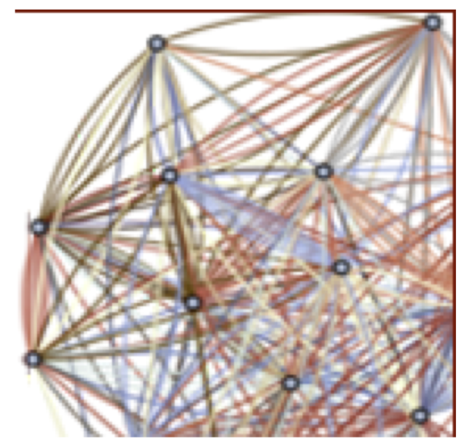
- Consider the occupation number basis with $M = \binom{L}{N}$ basis vectors.

- Fock space graph, G_F:
  - Associate with each many-body basis vector, $|\alpha >$, *a vertex*, α
  - Associate with each two vertices, connected by hopping, *an edge*

Simple example of G_F

- To illustrate, consider a model with L=5 and N=3 & periodic bc's.

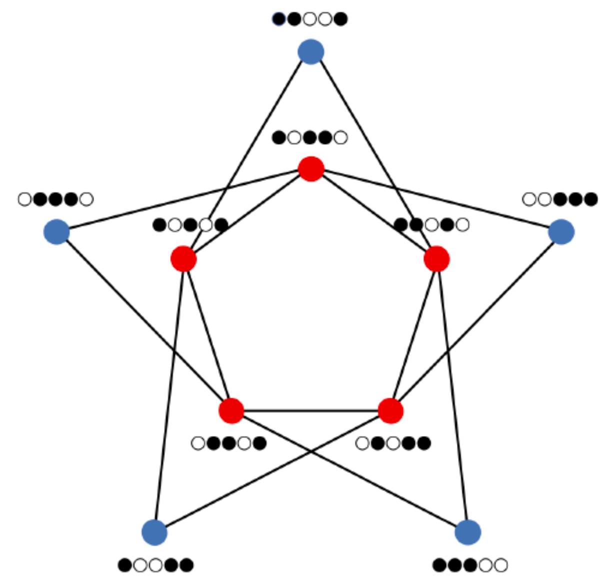




- For the nearest-neighbor hopping, the connectivity of the graph is limited: roughly, it is between $O\left(N^{1-\frac{1}{d}}\right)$ and $O(N)$

Many-body localization landscape (MBLL)

- The goal is to generalize landscape construction to interacting Hamiltonians defined on the Fock space graph.



- The definition is simple

$$\mathcal{H}\,|u\rangle = |1\rangle$$

where <1|=(1,1,1,…,1) is the vector of all ones

- Here the action of the Hamiltonian in the Fock space on an arbitrary many-body wave-function, $|v\rangle = \sum_\alpha v_\alpha |\alpha\rangle$, is defined as

$$\langle\alpha|\mathcal{H}|v\rangle = -t \sum_{\beta\in N(\alpha)} v_\beta + \left(\sum_{i=1}^{L} V n_i^{(\alpha)} n_{i+1}^{(\alpha)} + \epsilon_i n_i^{(\alpha)}\right) v_\alpha$$

Off-diagonal part

Diagonal part

Generalization of key theorems to MBLL

- Pointwise (in Fock space) positivity of landscape, $u_\alpha > 0, \forall \alpha \in G_F$

- "Deformed" many-body Schrödinger equation. The landscape incorporates interactions and disorder in a non-perturbative way.

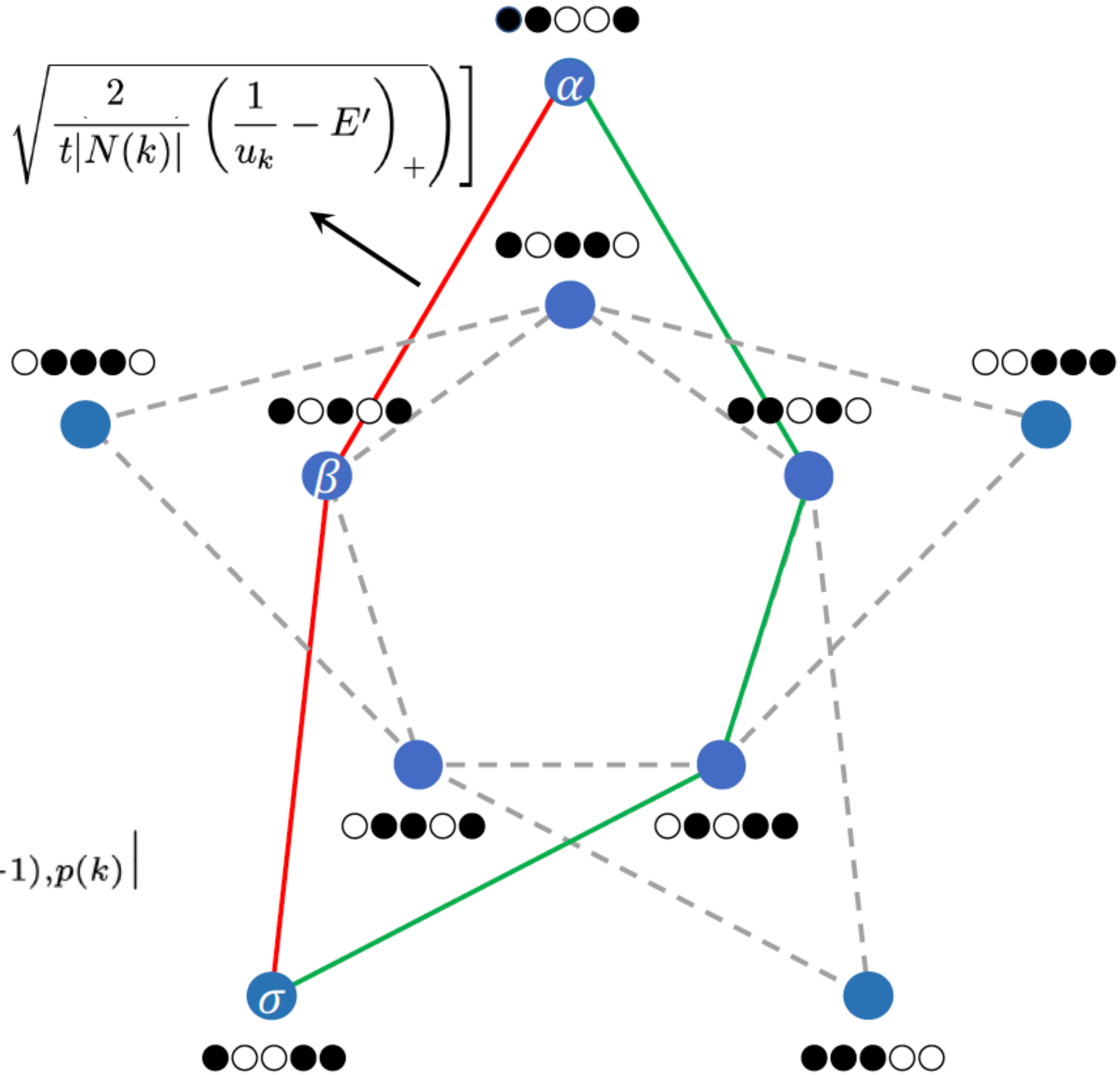
$$-t \sum_{\beta \in N(\alpha)} u_\beta u_\alpha \left(\frac{\psi_\beta}{u_\beta} - \frac{\psi_\alpha}{u_\alpha} \right) + \psi_\alpha = E' u_\alpha \psi_\alpha.$$

- Universal (weak) pointwise bound $\dfrac{|\psi_\alpha|}{\max_\beta |\psi_\beta|} \leq E' u_\alpha$

- Locality theorems: given a landscape with "valleys" and "hills" in G_F, the wave-functions solved for and localized in individual valleys are close enough to true eigenstates (if not resonant).

An Agmon-like metric on the Fock-space graph

$$|\mathcal{L}_{\alpha,\beta}| = \min_{k=\alpha,\beta}\left[\log\left(1+\sqrt{\frac{2}{t|N(k)|}\left(\frac{1}{u_k}-E'\right)_+}\right)\right]$$

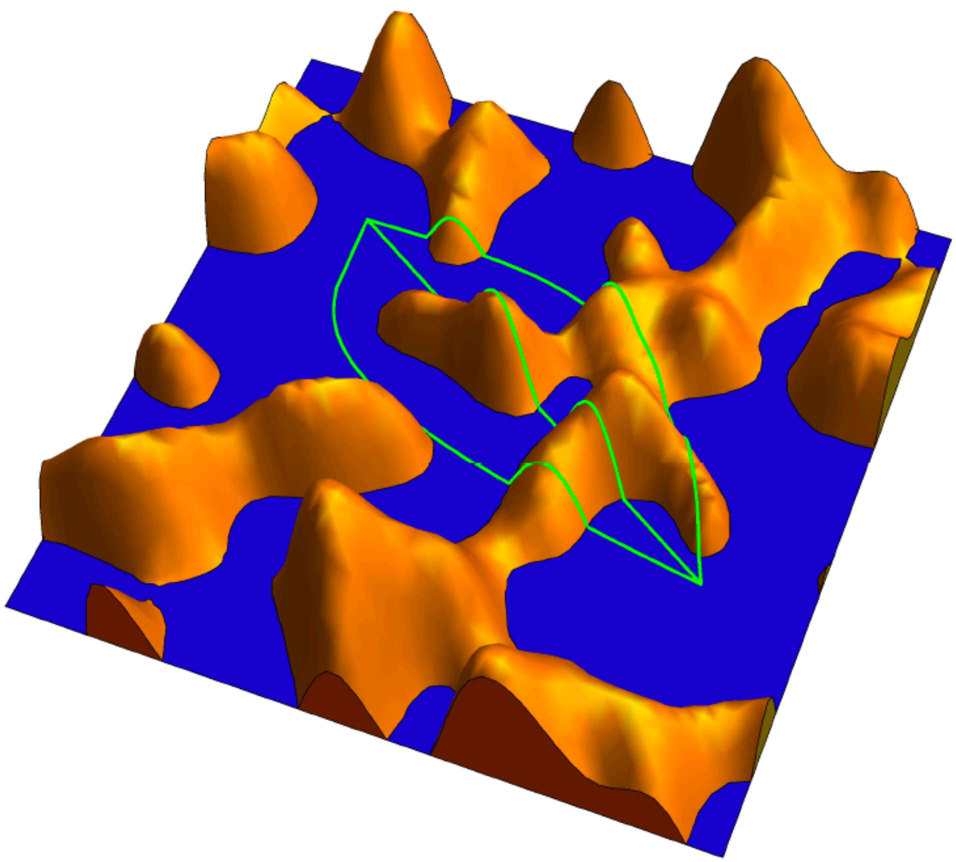


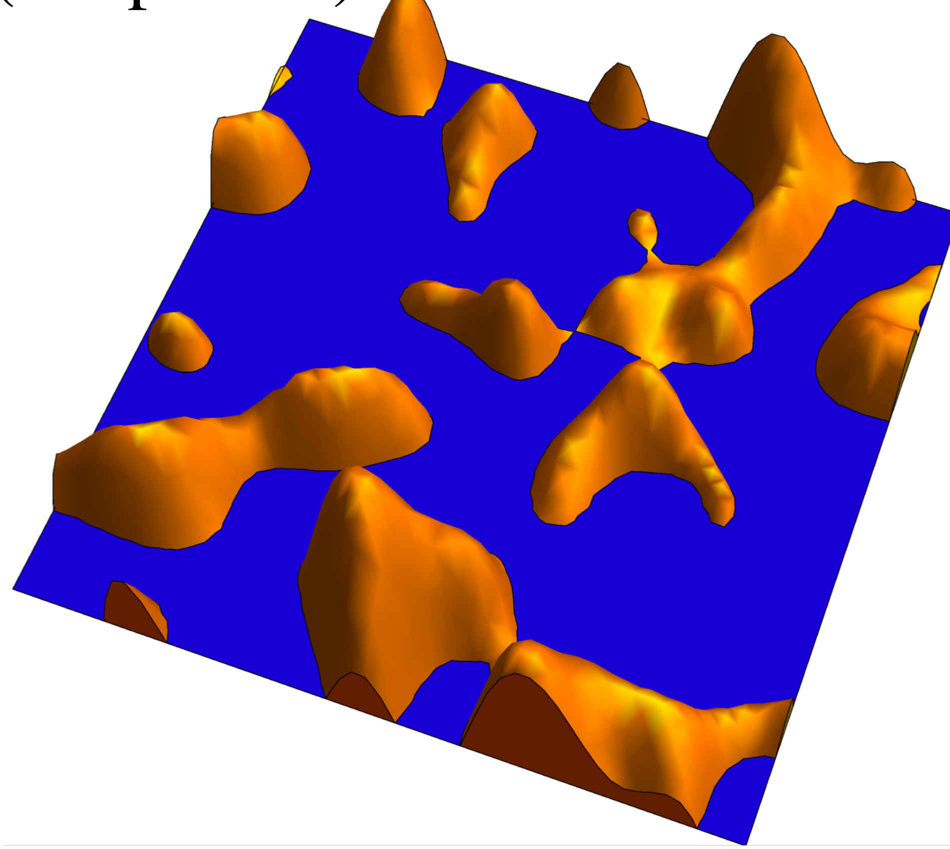
$$S_\sigma = \min \sum_k \left|\mathcal{L}_{p(k-1),p(k)}\right|$$

An exponential decay on a graph

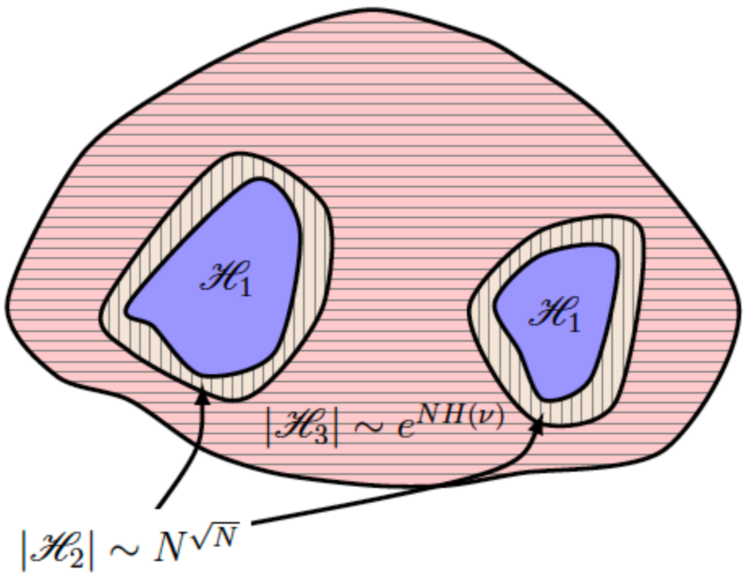
$$|\psi_\alpha| < \frac{C}{\sqrt{{}^{1}/_{u_\alpha} - E}} \cdot e^{-S_\alpha}$$

Attractive possibility: percolating classical regions in the landscape may indicate the mobility edge (not proven)





Structure of wave-function decay



- $\mathscr{H}_1$: Fixing a value of the many-body energy E', this region covers classically allowed regions of $\mathcal{G}_F$ where the wavefunction behaves like a constant.
- $\mathscr{H}_2$: This region is an annulus of thickness $N^{1/2}$ around $\mathscr{H}_1$ regions. It corresponds to the intermediate region in which there exist portions that do not decay at a rate scaling with the system size. In the thermodynamic limit, we will not observe decay
- $\mathscr{H}_3$: This region is outside of $\mathscr{H}_1$ and $\mathscr{H}_2$, in which eigenstates almost surely decay at a rate that scales with some increasing function in the system size.

- The proven estimates may likely be improved, so that the actual structure of MBL is different from (localization is stronger than) what the bounds, proven so far, establish.
- But in any case, the MBLL shows that there is a potentially large variety of MBL structures in the Fock space and the current terminology and classification are insufficient to describe them.

Locator expansion converges

- From Anderson's Nobel lecture, explaining his original work

In this case one takes E_i as the big term, and the starting eigenfunctions and eigen-energies are just

$$\varphi_i^0 = \varphi_i,\ E_i^0 = E_i \tag{18}$$

and V_{ij} is the perturbation. In this case, (which Larry Walker suggested I call "cisport") we use a "locator" instead of a "propagator" series, for the "locator" G_{ii} not the "propagator" G_{kk}:

Anderson's locator expansion diverges due to resonances (loops).

- Key observation: locator series for landscape is convergent

$$\langle\alpha|u\rangle = \frac{1}{\mathcal{E}_\alpha}\sum_{n=0}^{\infty}\sum_{\alpha_1=\alpha,\alpha_2,\ldots,\alpha_{n+1}}\frac{\langle\alpha_1|(T+V)|\alpha_2\rangle}{\mathcal{E}_{\alpha_2}}\times \frac{\langle\alpha_2|(T+V)|\alpha_3\rangle}{\mathcal{E}_{\alpha_3}}\cdots\frac{\langle\alpha_n|(T+V)|\alpha_{n+1}\rangle}{\mathcal{E}_{\alpha_{n+1}}}.$$

No resonances $(E-E')^{-1}$ are present.

- This (with other theorems) establishes a weak version of MBL.

Summary so far

- There are strong indications that both single-particle and many-body landscape represent an effective “classical” potential where localized states reside.

- It is important because inverting a matrix is easier full diagonalization. Larger systems are accessible than ED.

- MBLL is a tool that seems capable of rigorously proving a weak version of (partial) MBL.

- It exposes a rich variety of possible MBL structures in Fock space and may be used to classify those.

Open problems and ideas; connection to UQM

- Many-body mobility edge (percolation on the landscape network?)
- What's really behind the relation between the LL and the spectrum
- Proper LL path integral and improving the bounds. Agmon instantons?
- Generating a series of useful theorems for differential equations as a continuum limit of lattice models.
- Landscape structure and level statistics (connections to RMT)
- Integrability and localization. KAM theorem and LL
- LL in billiards

- Classification of MBL structures in Fock space
- Generalization to time-dependent models including Floquet (e.g., minimal solvable model of many-body chaos – Prosen)
- Is landscape useful for ergodic models?
- SYK-type models
- Landscape and topology (the role of boundary conditions)

Thank you!