Flatbands – a romance with disorder and 2+3 dimensions*

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Localization properties in disordered 2- and 3-dimensional Lieb lattices and their extensions

J Liu, C Danieli, J Zhong and RA Roemer

March 2021 / PCS IBS Daejeon

* with a nod to “Flatland – A Romance of Many Dimensions”, Adwin Abbott, 1884

Flat band physics – the fate of compactly localized states (CLS)

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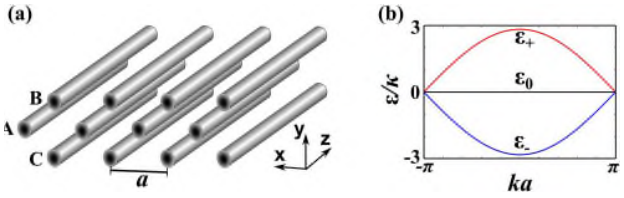
Flatband lattices—periodic media with at least one completely **dispersionless** Bloch **band** (*)

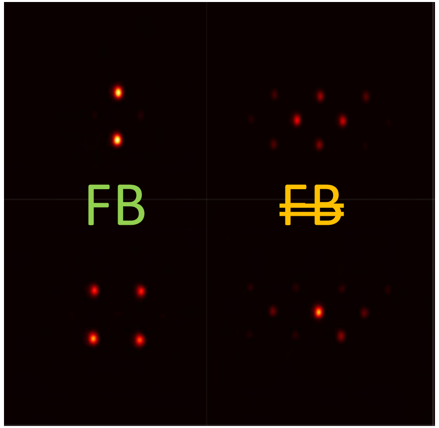
- **Strictly localized states**: B. Sutherland, “Localization of electronic wave functions due to local topology,” Phys. Rev. B 34, 5208 (1986)
- **Thm 2: large (magnetic) degeneracy for special topology (unsymmetric bipartite):** E. H. Lieb, “Two theorems on the Hubbard model”, Phys. Rev. Lett. **62**, 1201 (1989) [Thm 1, uniqueness …]
- Since then, much theoretical work from Mielke, Tasaki, Kohmoto, see D. Leykam, A. Andreanov, and S. Flach, Adv. Phys. X **3**, 677 (2018) for a review
- Experiments?

[(*) D. Leykam and S. Flach, APL Photonics **3**, 070901 (2018)]

Two experiments with **photonic lattices**

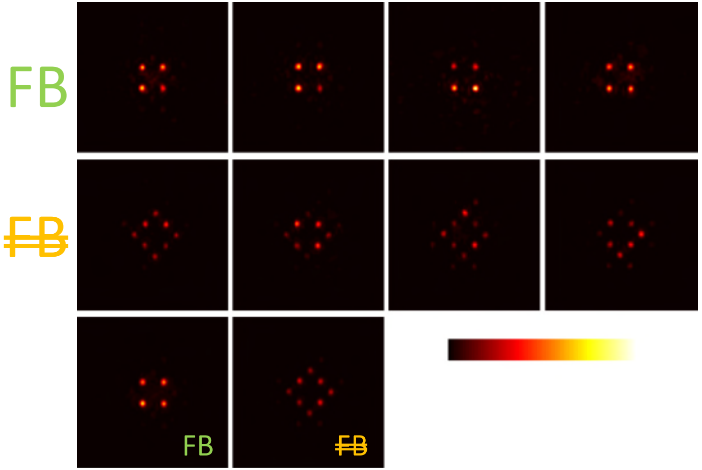
- **S. Mukherjee** and R. R. Thomson, Opt. Lett. **40**, 5443 (2015).

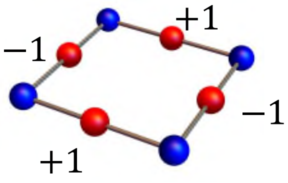




1D

- **S. Mukherjee**, A. Spracklen, D. Choudhury, N. Goldman, P. Öhberg, E. Andersson, and R. R. Thomson, Phys. Rev. Lett. **114**, 245504 (2015).





2D

11th International Workshop on Disordered Systems: From Localization to Thermalization and Topology

IBS Center for Theoretical Physics of Complex Systems, Daejeon, South Korea

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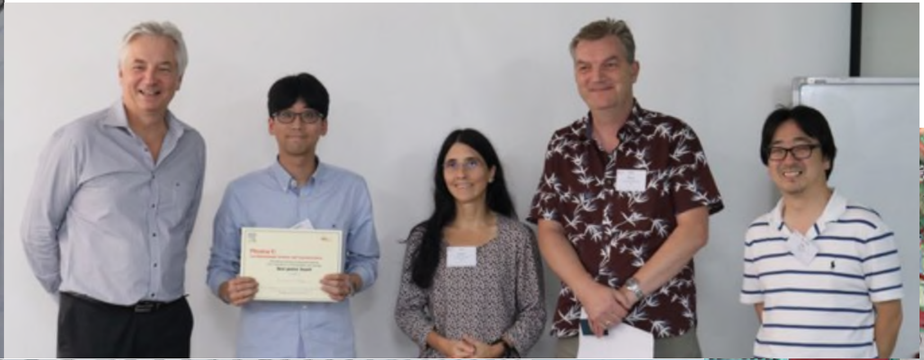
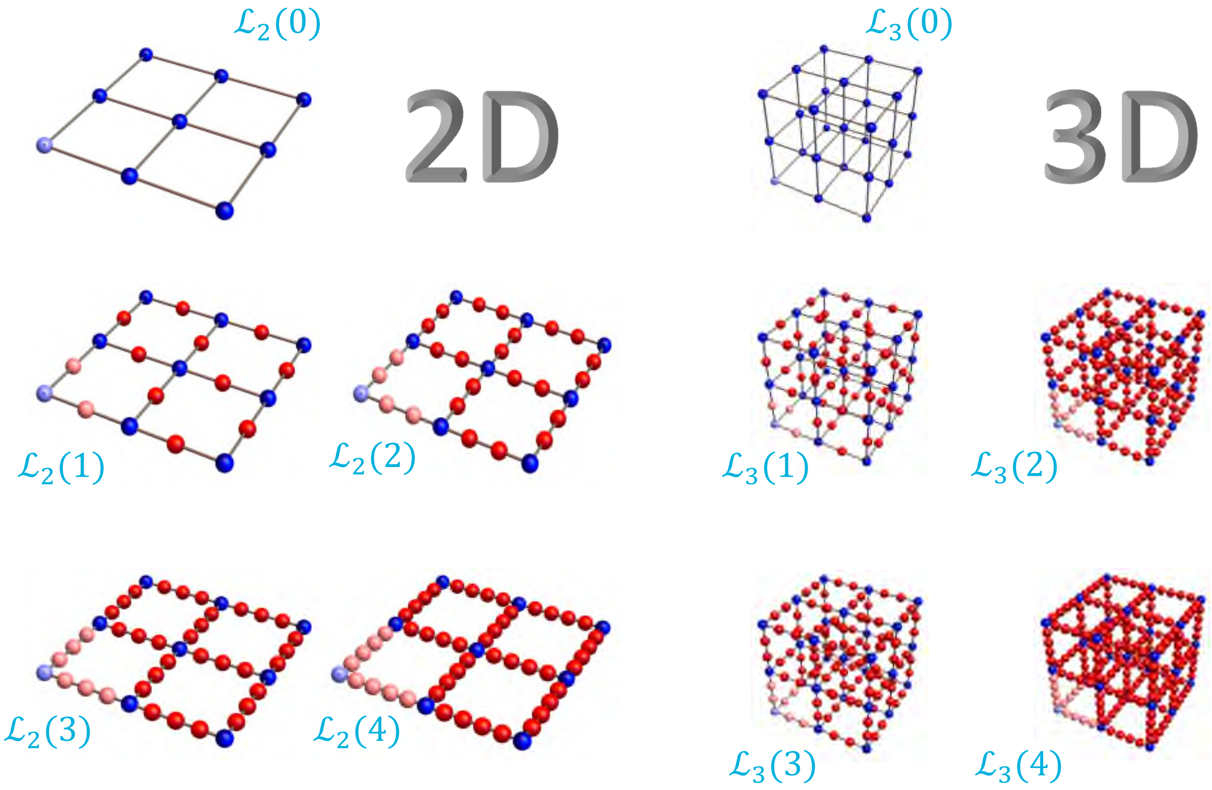


Lieb models $\mathcal{L}_d(n)$



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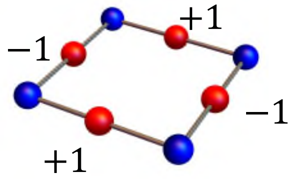
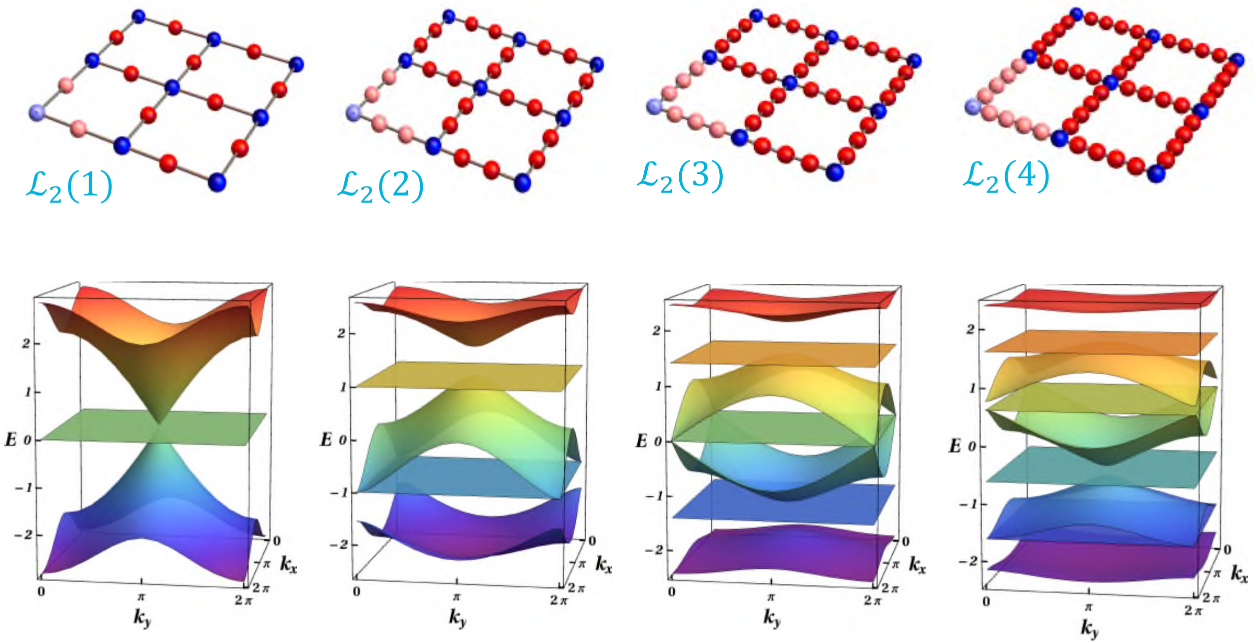
- Cubic systems with standard hub sites and additional rim sites
- The lighter shaded sites denote the unit cells.



Mao, Liu, Zhong, and RAR, Physica E **124**, 114340 (2020).

J. Liu, X. Mao, J. Zhong, and RAR, PRB **102**, 174207 (2020).

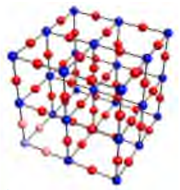
Lieb model in 2D and its extensions, **the clean case**



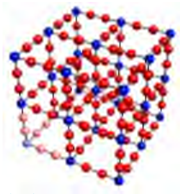
- $\mathcal{L}_2(n)$ exhibits
  - n flat bands and
  - $n+1$ dispersive bands
- Simple **“square lattice”** structure makes it straight-forward to study
- Ideal test case for **flat band physics**

[also Da Zhang, Yiqi Zhang, Hua Zhong, Changbiao Li, Zhaoyang Zhang, Yanpeng Zhang, Milivoj R. Belić, “New edge-centered photonic square lattices with flat bands”, Annals of Physics **382** (2017), 160-169]

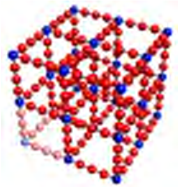
Lieb model in 3D and its extensions, **the clean case**



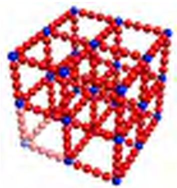
$\mathcal{L}_3(1)$



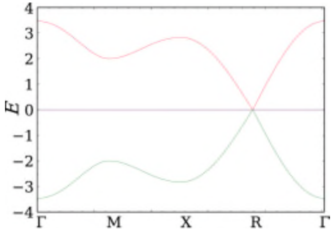
$\mathcal{L}_3(2)$



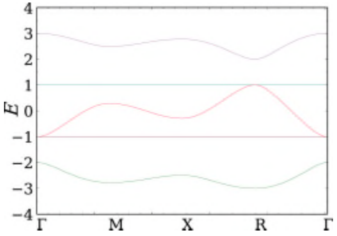
$\mathcal{L}_3(3)$



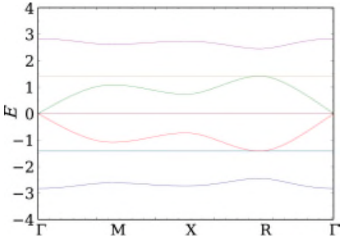
$\mathcal{L}_3(4)$



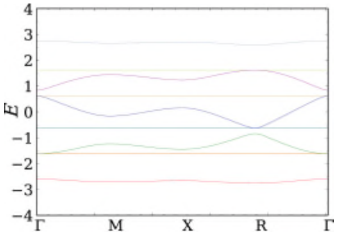
$(0,0,0)$



$(\pi,\pi,0)$



$(0,\pi,0)$



(π,π,π)

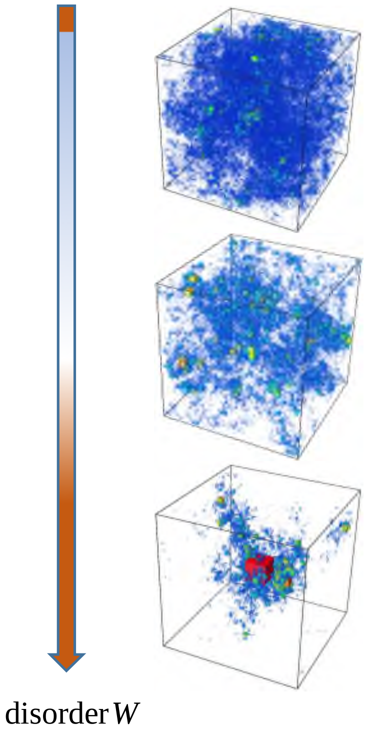
- $\mathcal{L}_3(n)$ exhibits
  - n flat bands and
  - $n+1$ dispersive bands
- Simple **"square lattice"** structure makes it straight-forward to study
- Ideal test case for **flat band physics in 3D**

$$H = \sum_{\boldsymbol{r}} \varepsilon_{\boldsymbol{r}} |\boldsymbol{r}\rangle\langle\boldsymbol{r}| - \sum_{\langle \boldsymbol{r} \neq \boldsymbol{r}' \rangle} t_{\boldsymbol{r},\boldsymbol{r}'} |\boldsymbol{r}\rangle\langle\boldsymbol{r}'|$$

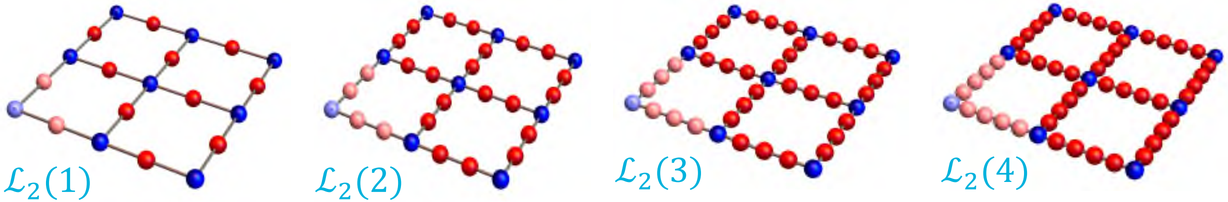
$$\varepsilon_r \in \left[-W/2, W/2\right]$$

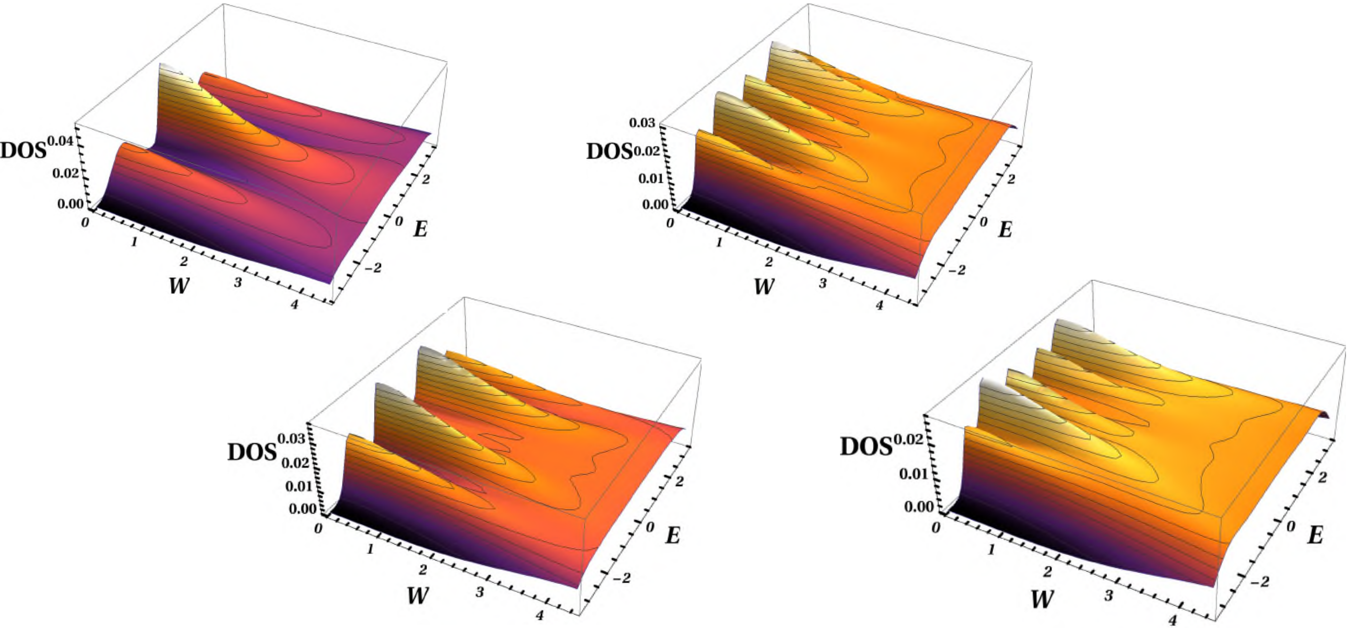
Question: what happens with [CLS-violating] disorder?

- 2D
  - X. Mao, J. Liu, J. Zhong, and R. A. Römer, Phys. E Low-Dimensional Syst. Nanostructures **124**, 114340 (2020).
- 3D
  - J. Liu, X. Mao, J. Zhong, and R. A. Römer, Phys. Rev. B **102**, 174207 (2020).
    1. MIT, energy-disorder phase diagram and the critical disorder strengths
    2. No region of localized states around the flat band energies for small disorders
    3. no change in the critical properties of the MIT
- 3D with CLS-preserving disorder?
  - Topic of ongoing work, partial results below …



Lieb model in 2D and its extensions, **the disordered DOS**





- $\mathcal{L}_2(n)$ exhibits
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- Flat bands immediately **broaden**
- At $W \approx 2$, only the **usual broad Anderson band** remains

Lieb models and the transfer matrix (TM) method

- Schrödinger equation

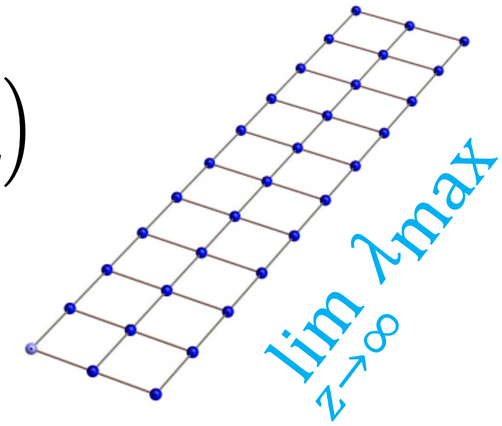
$$\psi_{z+1}(x) = \left(\frac{\varepsilon_{x,z}\mathbb{I} - E\mathbb{I}}{\boldsymbol{t}_{z+1}} - \frac{\boldsymbol{t}_x}{\boldsymbol{t}_{z+1}}\right)\psi_z(x) - \frac{\boldsymbol{t}_z}{\boldsymbol{t}_{z=1}}\psi_{z-1}(x)$$

- TM equation

$$\begin{pmatrix}\psi_{z+1}(x) \\ \psi_z(x\end{pmatrix} = \underbrace{\begin{bmatrix}\left(\frac{\varepsilon_{x,z}\mathbb{I} - E\mathbb{I}}{\boldsymbol{t}_{z+1}} - \frac{\boldsymbol{t}_x}{\boldsymbol{t}_{z+1}}\right) & -\frac{\boldsymbol{t}_z}{\boldsymbol{t}_{z=1}} \\ 1 & 0\end{bmatrix}}_{\boldsymbol{T}_z}\begin{pmatrix}\psi_z(x) \\ \psi_{z-1}(x\end{pmatrix}$$

- Localization length

$$\lambda_{\max} = \min[\mathrm{EV}\,\boldsymbol{\tau}^T(\boldsymbol{T}_z\boldsymbol{T}_{z-1}\cdots\boldsymbol{T}_1)]^{-1/2M}$$



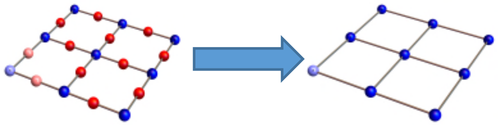
$$\lim_{M\to\infty}\lambda_{\max}$$

Lieb models and the transfer matrix (TM) method

$\mathcal{L}_2(1)$:

$$\begin{pmatrix} \psi^B_{x+1} \\ \psi^A_x \end{pmatrix} = \begin{pmatrix} \left(\frac{\varepsilon_{x,y}-E}{t} - \frac{t}{\varepsilon_{x,y-1}-E} - \frac{t}{\varepsilon_{x,y+1}-E}\right)\mathbf{1}_M - \frac{\mathbf{t}_y}{\varepsilon_{x,y-1}-E} - \frac{\mathbf{t}_y^\dagger}{\varepsilon_{x,y+1}-E} & -\mathbf{1}_M \\ \mathbf{1}_M & \mathbf{0}_M \end{pmatrix} \begin{pmatrix} \psi^A_x \\ \psi^B_{x-1} \end{pmatrix}$$

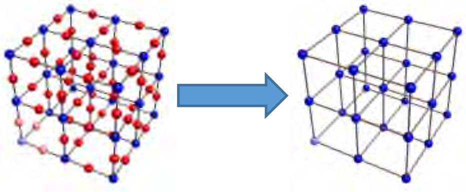
Renormalization:



$\mathcal{L}_3(1)$:

$$\begin{pmatrix} \Psi^{\mathrm{D}}_{z+1} \\ \Psi^{\mathrm{A}}_z \end{pmatrix} = \mathbf{T}_{\mathrm{A}\to\mathrm{D}} \begin{pmatrix} \Psi^{\mathrm{A}}_z \\ \Psi^{\mathrm{D}}_{z-1} \end{pmatrix}$$

$$= \begin{pmatrix} \mathcal{E}\mathbf{1}_{M^2} - \frac{1}{\epsilon_{z,x-1,y}-E}\mathbf{t}_{x-} - \frac{1}{\epsilon_{z,x+1,y}-E}\mathbf{t}_{x+} - \frac{1}{\epsilon_{z,x,y-1}-E}\mathbf{t}_{y-} - \frac{1}{\epsilon_{z,x,y+1}-E}\mathbf{t}_{y+} & -\mathbf{1}_{M^2} \\ \mathbf{1}_{M^2} & \mathbf{0}_{M^2} \end{pmatrix} \begin{pmatrix} \Psi^{\mathrm{A}}_z \\ \Psi^{\mathrm{D}}_{z-1} \end{pmatrix},$$



$$\mathcal{E} = \frac{\epsilon_{z,x,y}-E}{t} - \frac{t}{\epsilon_{z,x-1,y}-E} - \frac{t}{\epsilon_{z,x+1,y}-E} - \frac{t}{\epsilon_{z,x,y-1}-E} - \frac{t}{\epsilon_{z,x,y+1}-E},$$

Finite-size scaling of reduced localization lengths $\Lambda_M = \lambda_M / M$

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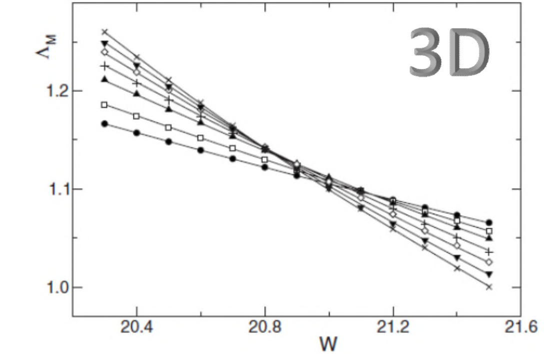
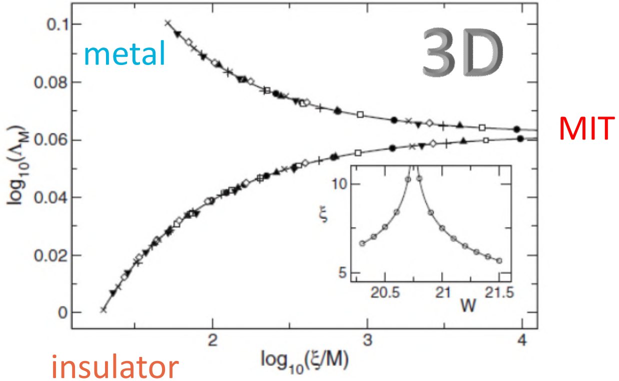
- $\Lambda_M = f\left(\frac{M}{\xi}\right)$ depends on energy and disorder only through the localization length for the infinite system via

$$\xi(E, W)$$

- Hence data for various E and W should fall onto the same curve $f\left(\frac{M}{\xi}\right)$
  - -> the $\lambda_M(E, W)$ scale!
- Divergence of $\xi(E_c, W)$ or $\xi(E, W_c)$ indicates MIT



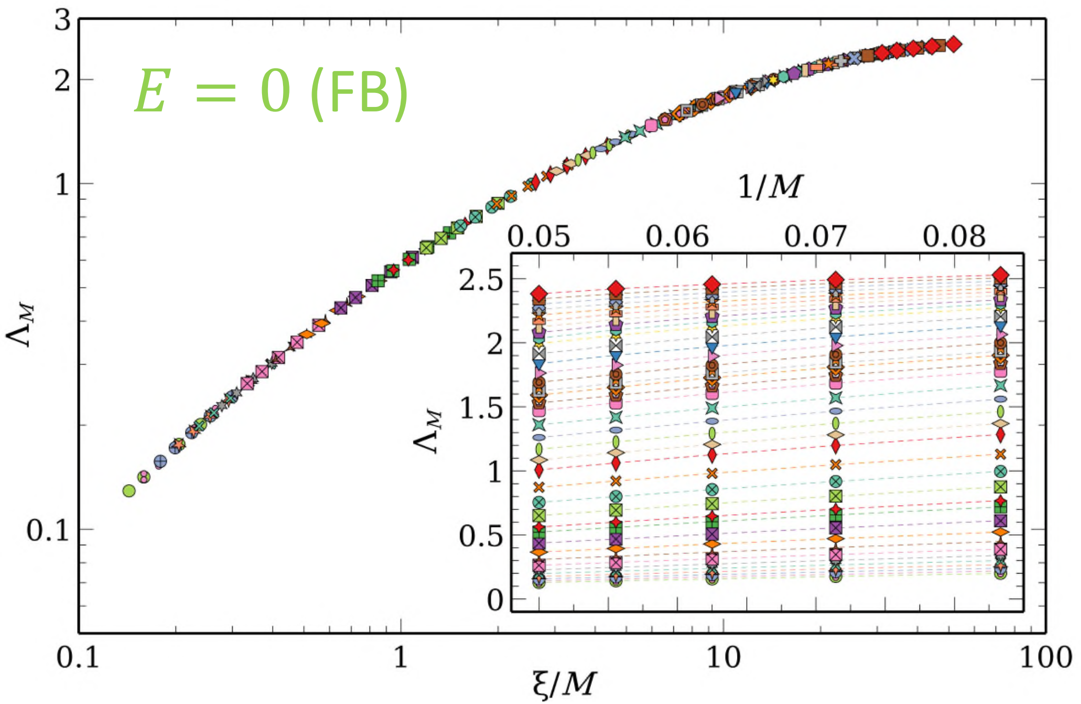


[A. Eilmes, A. M. Fischer, and R. A. Römer, Phys. Rev. B **77**, 245117 (2008)]

Localization lengths in **2D**

- Increasing disorders $W = 1, 1.01, \ldots, 10$ leads to reduced $\Lambda_M = \lambda_M / M$ values, i.e. more localization
- Increasing system widths $M = 10, 12, \ldots, 20$ leads to reduced Λ_M values, i.e. more localization
- Finite-size scaling gives single scaling curve with localized branch only

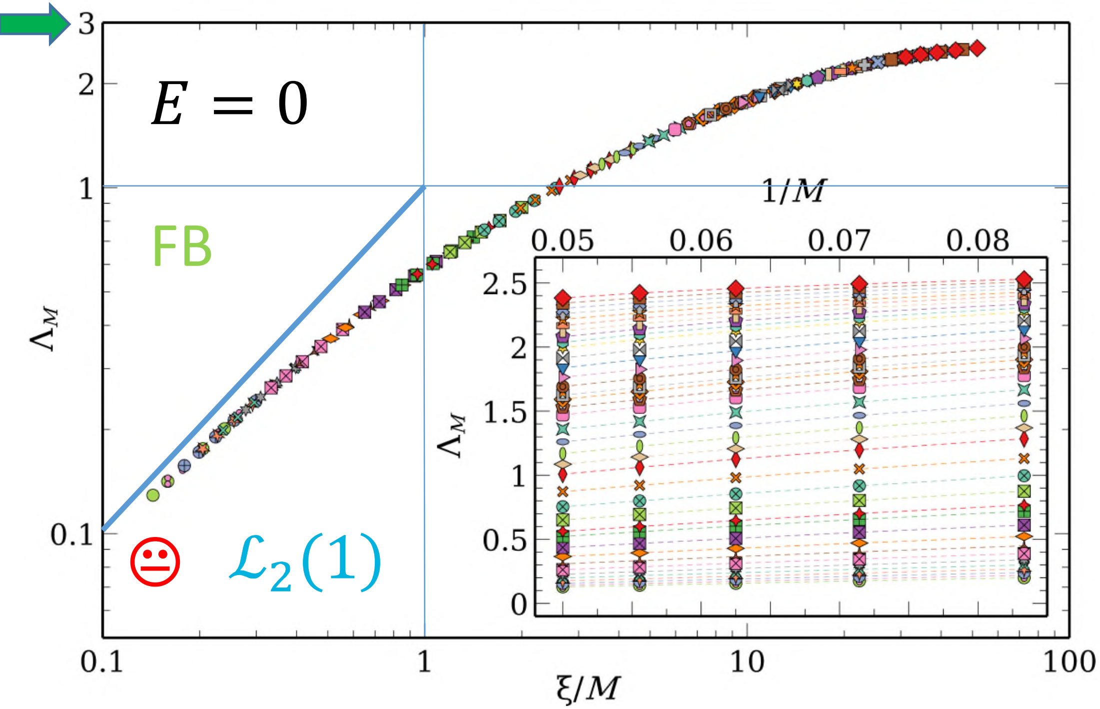
$\mathcal{L}_2(1)$



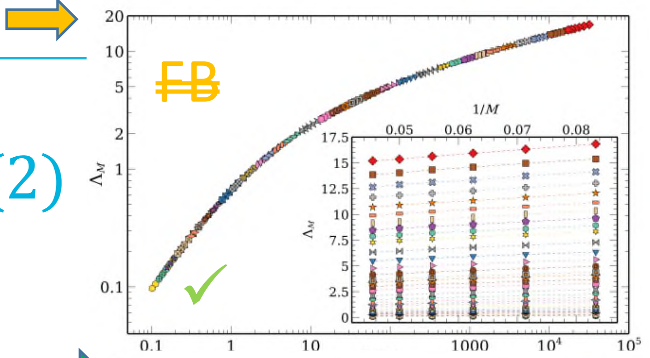
Localization lengths in **2D**

$E = 0$

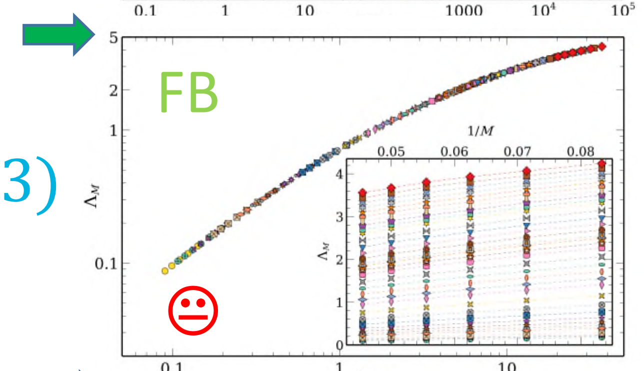
$\xi/_M \cong \Lambda_M = \lambda/_M$ for large W!



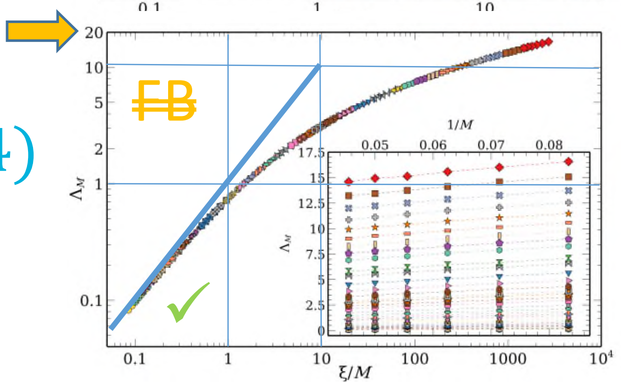
$\mathcal{L}_2(2)$



$\mathcal{L}_2(3)$



$\mathcal{L}_2(4)$

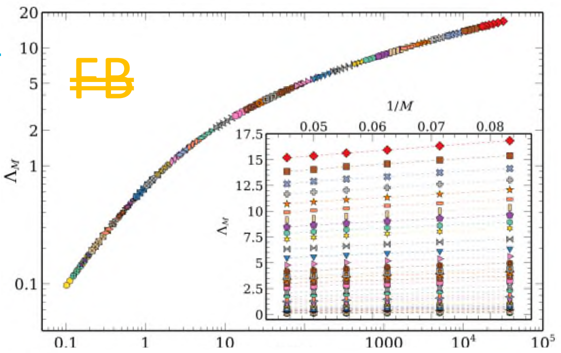


Localization lengths in **2D**

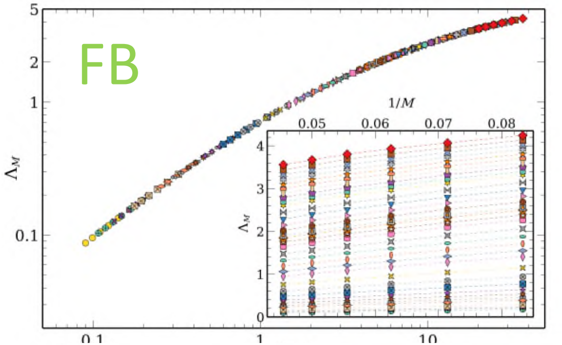
$E = 0$

$\mathcal{L}_2(1)$ $\quad {}^{\xi}/_{M} \cong \Lambda_M = {}^{\lambda}/_{M}$ for large W!

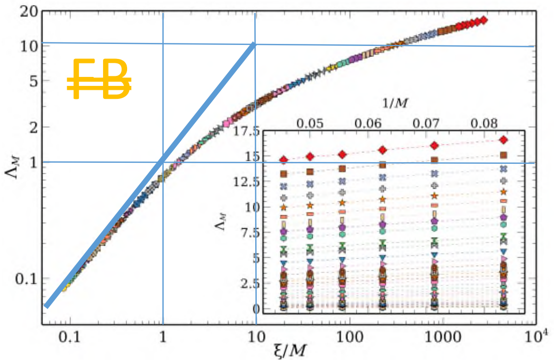
$\mathcal{L}_2(2)$



$\mathcal{L}_2(3)$



$\mathcal{L}_2(4)$



- Flat bands **localize differently** from dispersive bands:
  - At FB energies, the localization **lengths** $\boldsymbol{\lambda}$ are much **smaller** than for dispersive bands (DB) at the same disorder values
  - At FB energies, the **scaling behaviour** for $\Lambda_M = {}^{\lambda}/_{M}$ **does not** yet **follow** ${}^{\xi}/_{M} \cong \Lambda_M$ for disorders up to $W = 10$.

Localization lengths in **2D**

- 1D: $\xi = {}^{105}/_{W^2}$

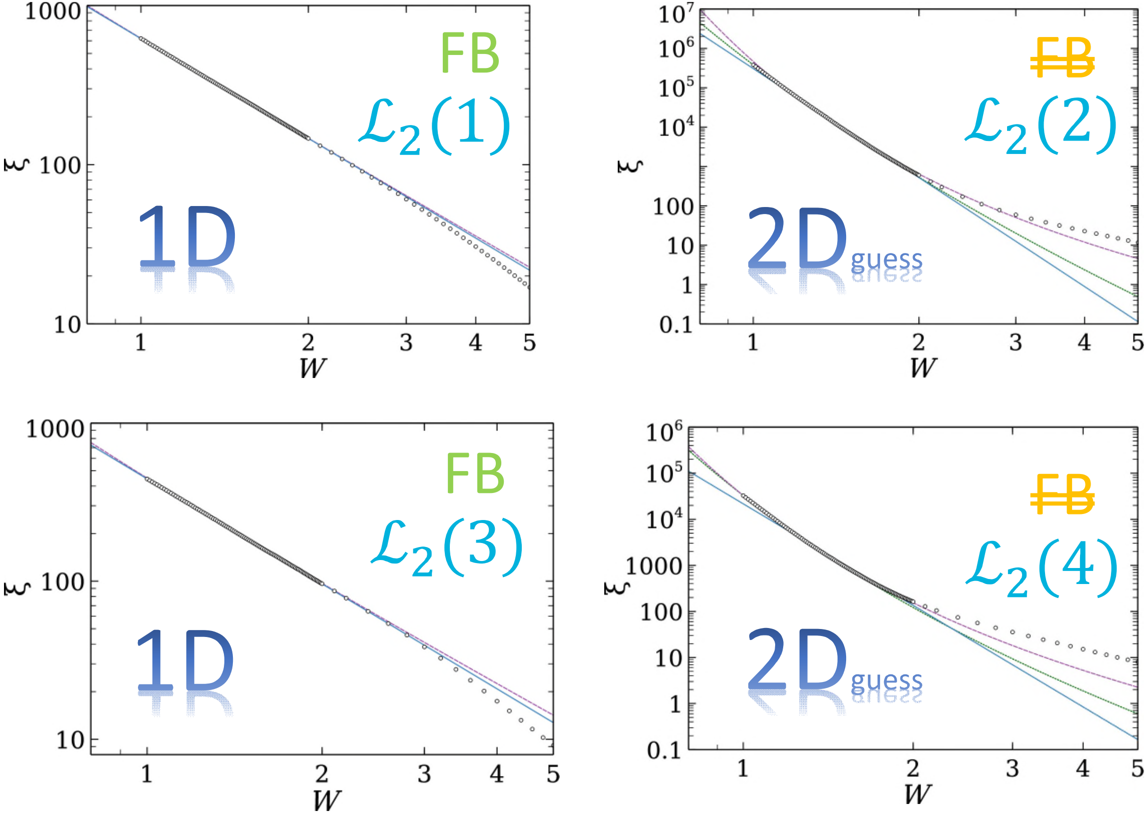
[Edwards+Thouless, JPC **5**, 807 (1972)]

- 2D: $\xi = aW^{-\alpha}\exp(\beta W^{-\gamma})$

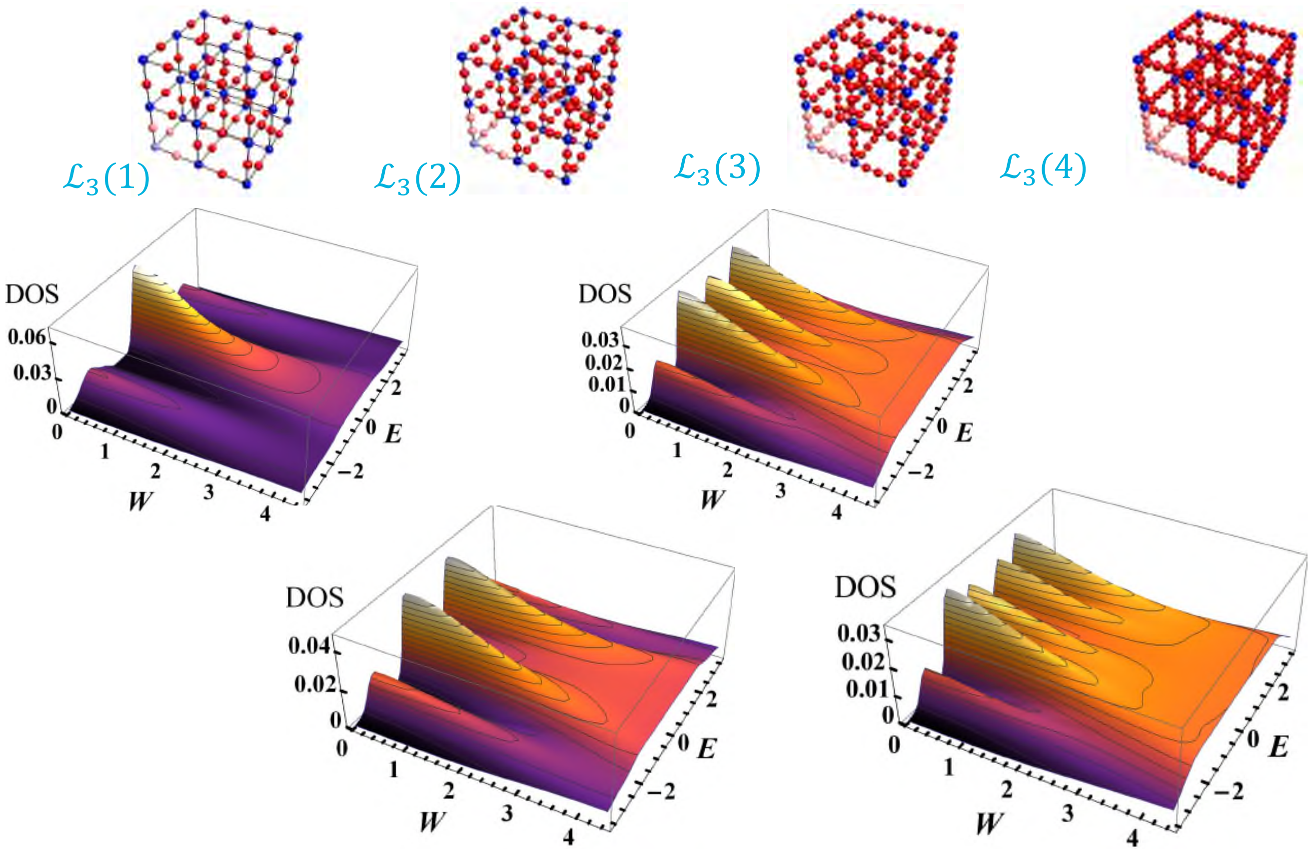
[Kramer+MacKinnon, Rep Prog Phys **56**, 1469 (1993)]

- 2D guess:
  $\xi = aW^{-2}\exp(\beta W^{-\gamma})$
- -> clear **differences in localization** properties for FB and DB states/energies
- FB states are more (compactly?) localized for weak disorder

$E = 0$



Lieb model in 3D and its extensions, **the disordered case**



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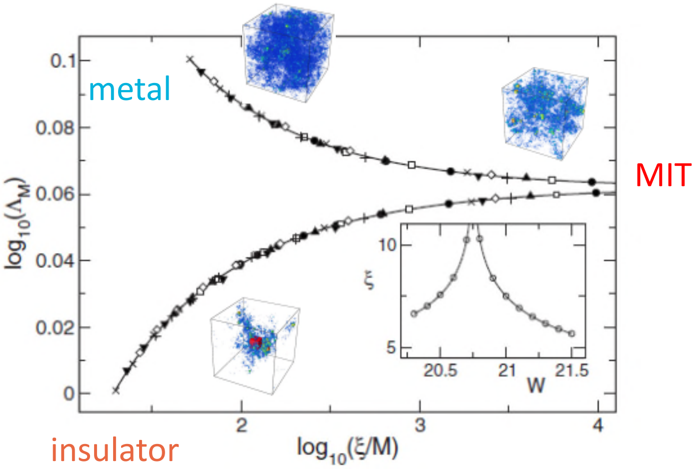
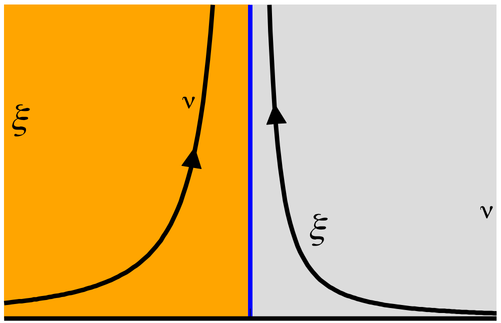
- At $W \approx 2$, only the **usual broad Anderson band** remains

The 3D Anderson model with disorder



- Divergent localization length

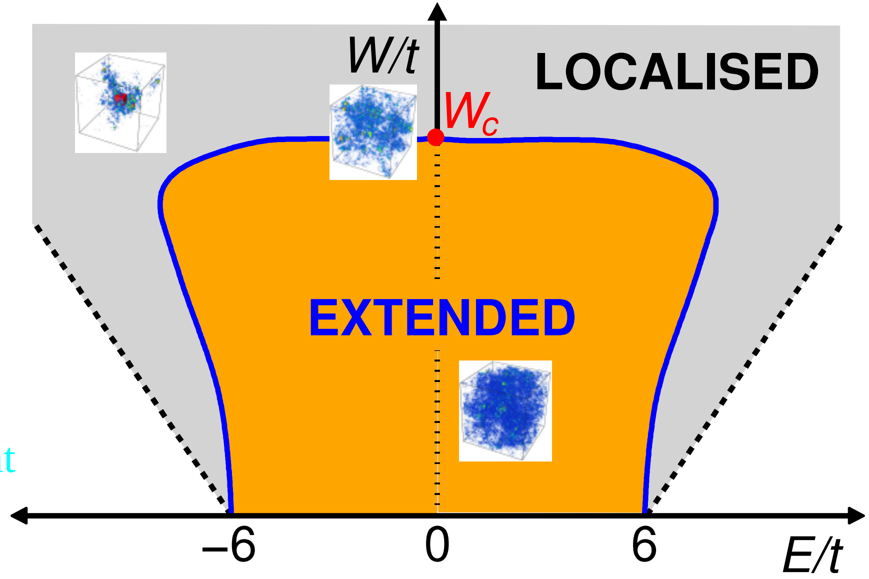


$$\xi \sim |X - X_c|^{-\upsilon}$$

with $X = E$ or W

υ = critical exponent

- Phase diagram in 3D



Disorderd and extended Lieb models in 3D (J Liu, Monday talk)

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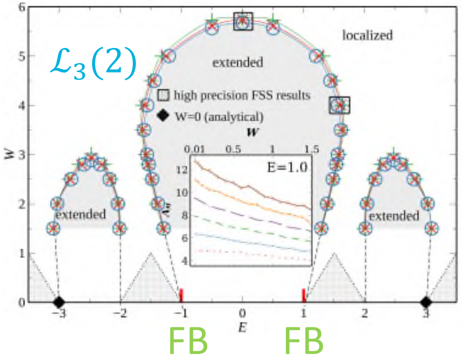
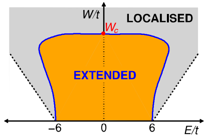
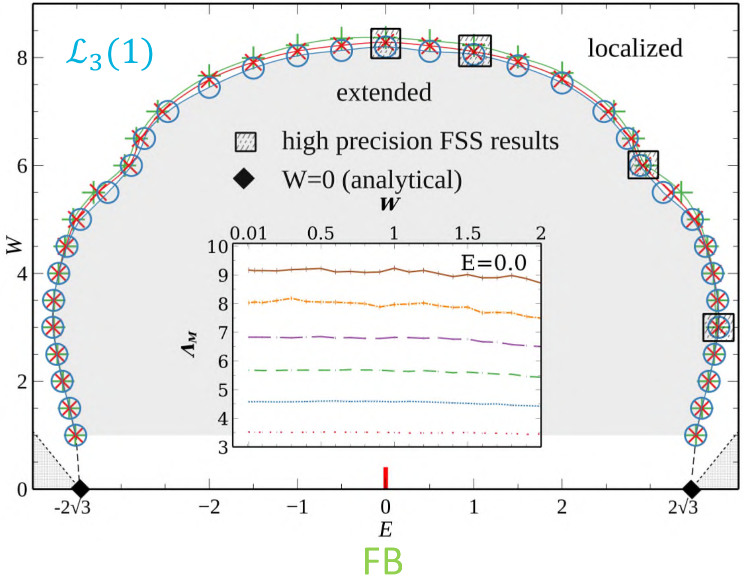
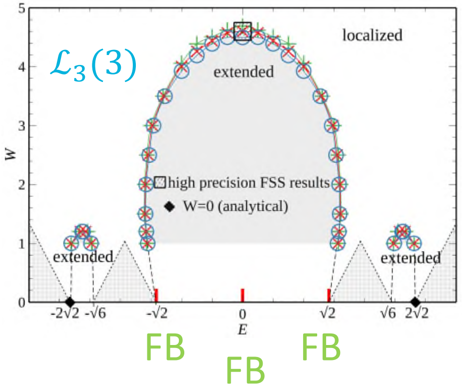
- Phase boundaries determined from scaling behavior with small $M^2 = 6^2, 8^2, 10^2 = 36, 64, 100$ (1%)
- High-precision checks up to $M^2 = 20^2 = 400$ (0.1%)

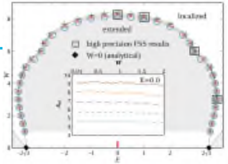


- Disjoint “lakes” of extended states for small $W \lesssim 1$
- FB energies do not seem to lead to more localization when $W \to 0$



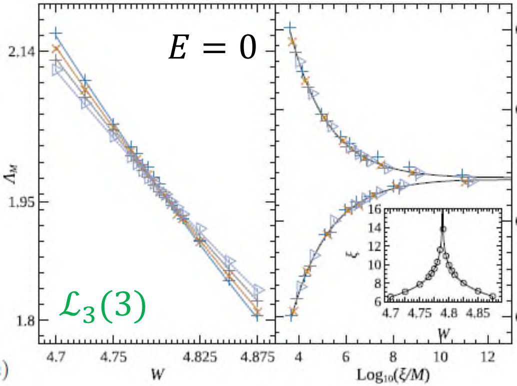


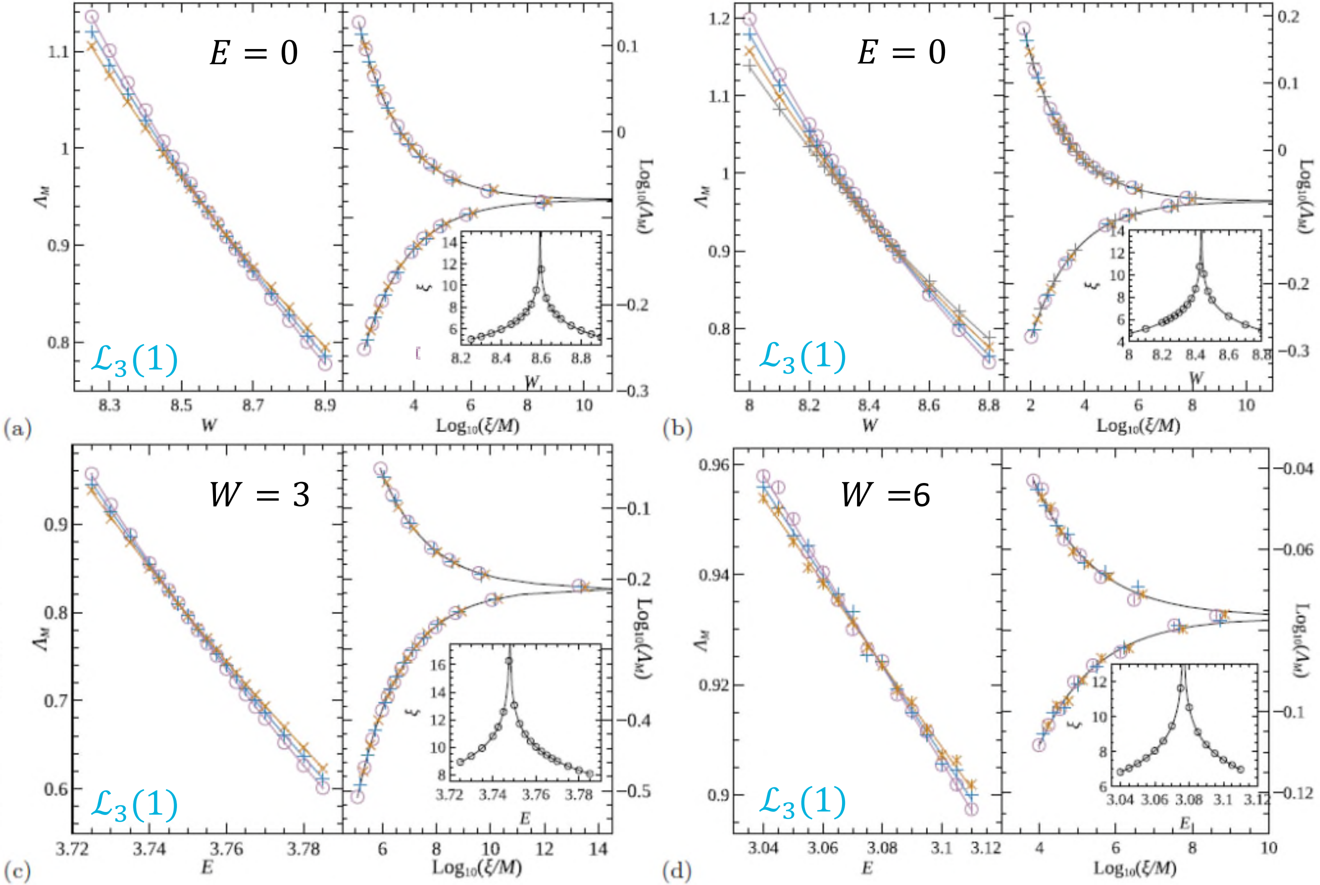




FSS for the disordered extended Lieb models in 3D

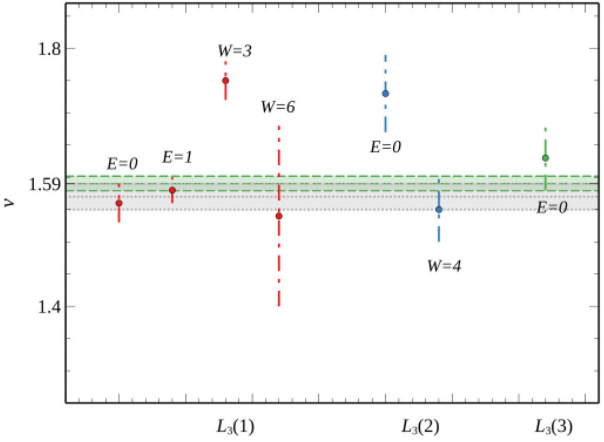
- Excellent FSS for all E and W value in $\mathcal{L}_3(1)$
- Excellent FSS for all other $\mathcal{L}_3(n)$ as well.





Critical properties of extended Lieb models in 3D

- $\xi \sim |X - X_c|^{-\nu}$ with $X = E$ or W
- $\nu = 1.59 \pm 0.1$



					$\mathcal{L}_3(1)$				
ΔM	E	δW	n_r	m_r	W_c	$\mathrm{CI}(W_c)$	ν	$\mathrm{CI}(\nu)$	p
16–20	0	8.25–8.9	3	1	*8.594*	[8.585,8.604]	*1.57*	[1.49,1.65]	0.15
16–20	0	8.25–8.9	2	2	8.598	[8.586,8.610]	1.55	[1.46,1.63]	0.08
16–20	0	8.25–8.9	3	2	8.595	[8.582,8.607]	1.57	[1.48,1.66]	0.13
Averages:					8.596(4)		1.56(3)		
ΔM	E	δW	n_r	m_r	W_c	$\mathrm{CI}(W_c)$	ν	$\mathrm{CI}(\nu)$	p
14–20	1	8.0–8.8	3	1	*8.435*	[8.429,8.441]	*1.60*	[1.54,1.65]	0.18
14–20	1	8.0–8.8	2	2	8.439	[8.432,8.447]	1.57	[1.53,1.62]	0.19
14–20	1	8.0–8.8	2	3	8.438	[8.431,8.446]	1.57	[1.53,1.62]	0.21
Averages:					8.437(3)		1.58(2)		
ΔM	W	δE	n_r	m_r	E_c	$\mathrm{CI}(E_c)$	ν	$\mathrm{CI}(\nu)$	p
16–20	3	3.725–3.785	2	1	*3.748*	[3.747,3.749]	*1.75*	[1.68,1.82]	0.88
16–20	3	3.725–3.785	2	2	3.748	[3.747,3.749]	1.76	[1.67,1.84]	0.86
16–20	3	3.725–3.785	3	1	3.748	[3.747,3.749]	1.75	[1.68,1.82]	0.86
Averages:					3.748(1)		1.75(3)		
ΔM	W	δE	n_r	m_r	E_c	$\mathrm{CI}(E_c)$	ν	$\mathrm{CI}(\nu)$	p
16–20	6	3.04–3.11	1	1	*3.077*	[3.070,3.083]	*1.54*	[1.08,2.01]	0.14
16–20	6	3.04–3.11	2	1	3.076	[3.069,3.082]	1.54	[1.09,1.99]	0.24
16–20	6	3.04–3.11	2	2	3.077	[3.069,3.084]	1.54	[1.07,2.00]	0.21
Averages:					3.077(3)		1.54(14)		
					$\mathcal{L}_3(2)$				
ΔM	E	δW	n_r	m_r	W_c	$\mathrm{CI}(W_c)$	ν	$\mathrm{CI}(\nu)$	p
12,14,18	0	5.85–6.05	2	2	*5.964*	[5.958,5.969]	*1.75*	[1.57,1.92]	0.08
12,14,18	0	5.85–6.05	2	3	5.965	[5.959,5.970]	1.70	[1.51,1.89]	0.08
12,14,18	0	5.85–6.05	3	2	5.963	[5.956,5.971]	1.75	[1.57,1.92]	0.07
Averages:					5.964(3)		1.73(6)		
ΔM	W	δE	n_r	m_r	E_c	$\mathrm{CI}(W_c)$	ν	$\mathrm{CI}(\nu)$	p
10,12,14	4	1.6–1.8	2	1	*1.704*	[1.701,1.708]	*1.55*	[1.43,1.68]	0.18
10,12,14	4	1.6–1.8	1	3	1.705	[1.701,1.709]	1.56	[1.43,1.70]	0.1
10,12,14	4	1.6–1.8	2	2	1.703	[1.700,1.707]	1.53	[1.40,1.66]	0.2
Averages:					1.704(2)		1.55(5)		
					$\mathcal{L}_3(3)$				
ΔM	E	δW	n_r	m_r	W_c	$\mathrm{CI}(W_c)$	ν	$\mathrm{CI}(\nu)$	p
12–18	0	4.7–4.875	2	1	*4.79*	[4.786,4.794]	*1.63*	[1.48,1.78]	0.49
12–18	0	4.7–4.875	1	2	4.791	[4.786,4.795]	1.63	[1.48,1.78]	0.47
12–18	0	4.7–4.875	2	2	4.791	[4.786,4.795]	1.63	[1.48,1.78]	0.47
Averages:					4.790(2)		1.63(5)		

Conclusions 1: Extended and disordered Lieb models in 2 and 3D

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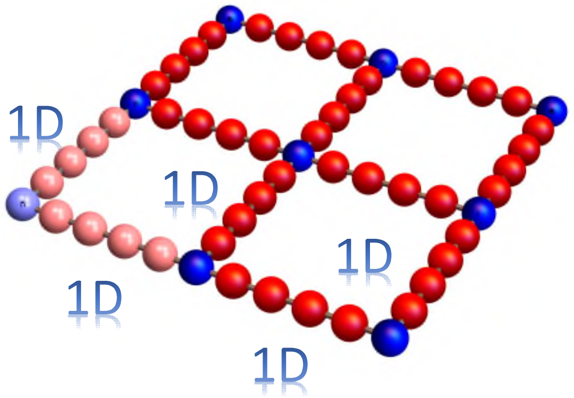
- At FB energies, localization behavior can be different (2D); phase diagrams (3D) do not develop regions of localized states down to $W = 0.01$
- FB states change phase diagrams and localization length values, but universal properties remain unchanged!
- Rim sites in Lieb model act as additional 1D localizers, 1D localization is strong (un-avoidable), hence Lieb models, even more so extensions, lead to stronger localization $(W_c(\text{Lieb}) < W_c(\text{Anderson}))$
- BORING?😐



And then what!

11th International Workshop on Disordered Systems: From Localization to Thermalization and Topology

IBS Center for Theoretical Physics of Complex Systems, Daejeon, South Korea

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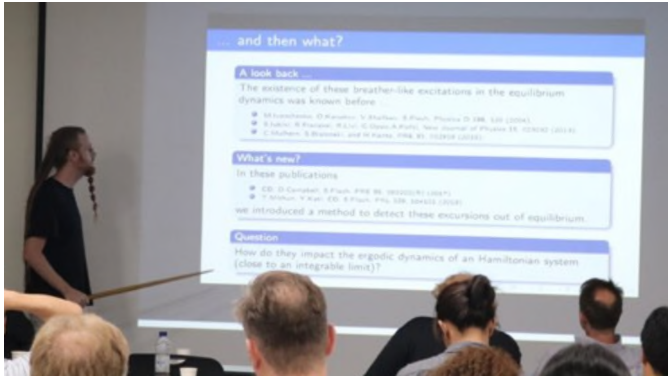
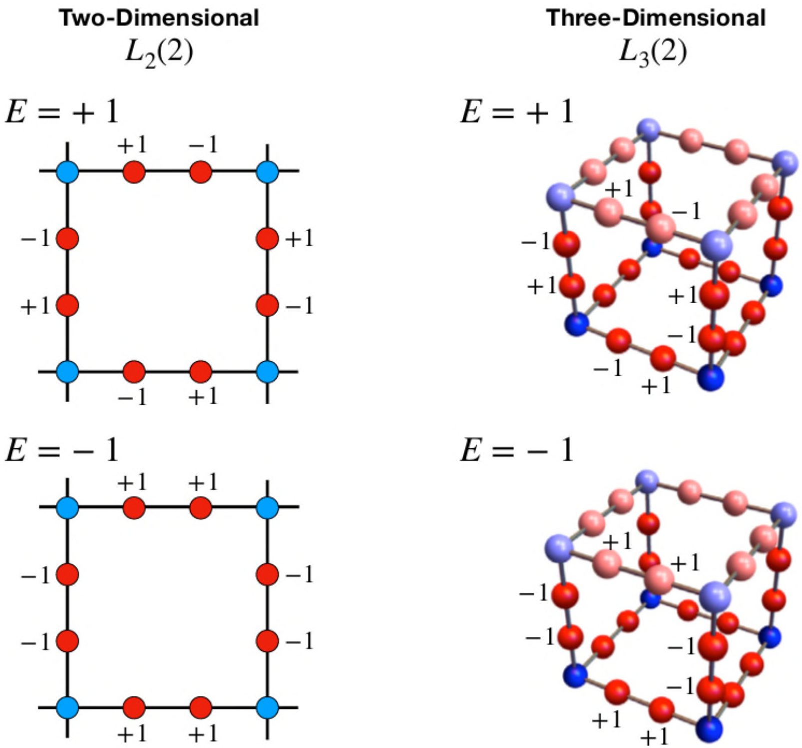
- Carlo Danieli, referee for PRB:

  "Make special disorder at hub sites only, no disorder at rim sites -> CLS will survive!"

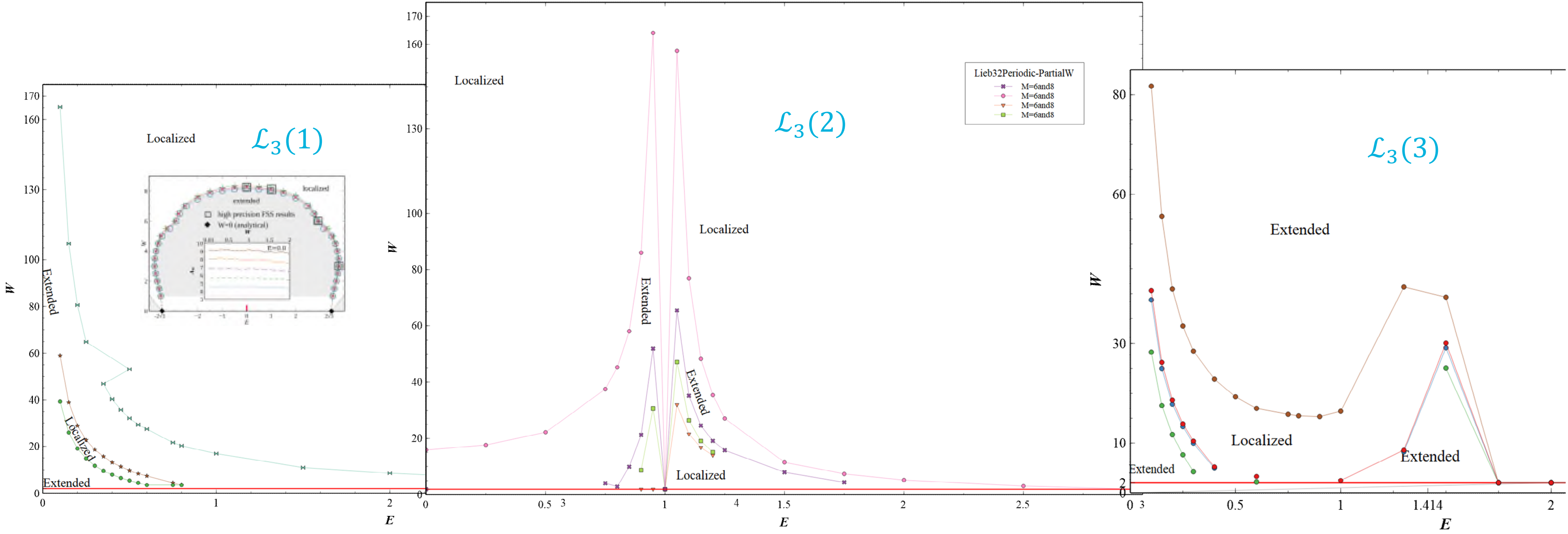




TMM, again … but … wait …

- Again, we look for crossings as small M to establish rough phase boundaries

- Disorder on hub sites
- No disorder on rim sites



Extended Lieb models in 2 and 3D with CLS-preserving disorder

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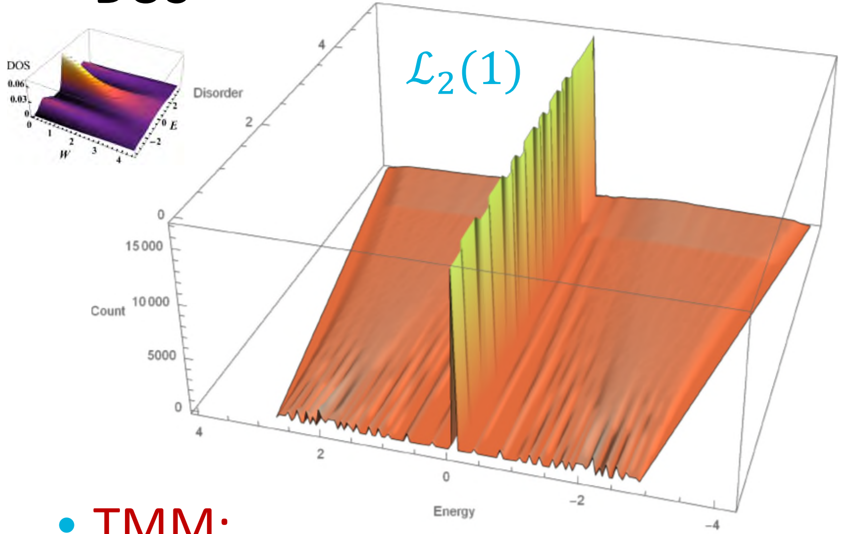
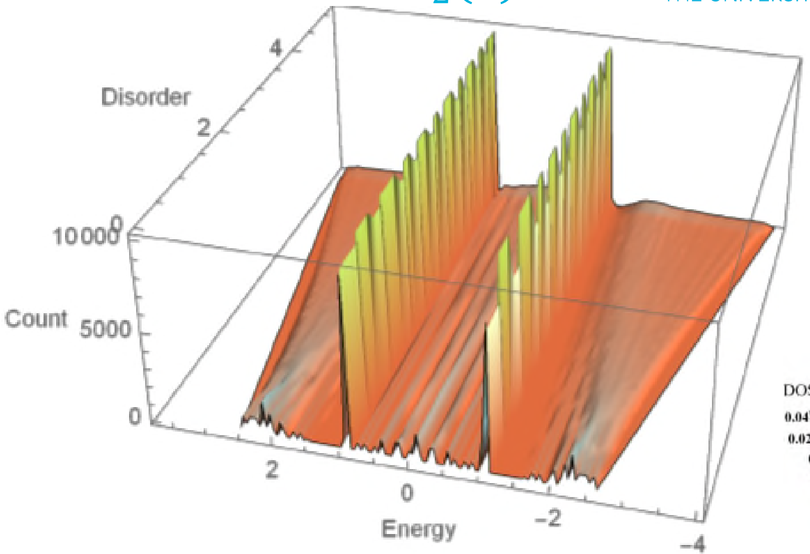
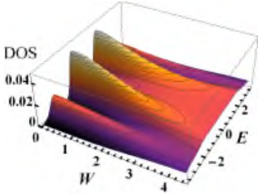
- DOS

$\mathcal{L}_2(1)$



$\mathcal{L}_2(2)$





- TMM:
  - much harder since effectively less disorder on renormalized sites, hence harder to converge
- How to compute modified phase diagrams for CLS-preserving disorder?

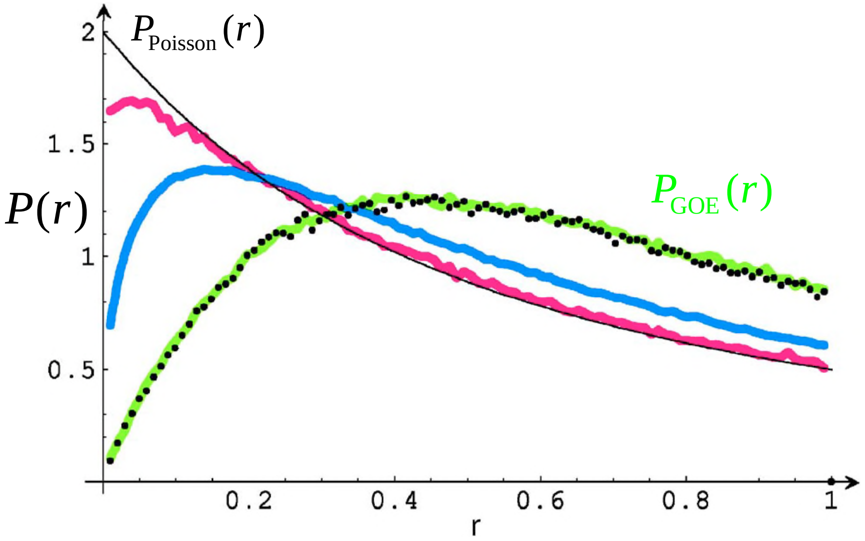
Energy-level statistics without unfolding

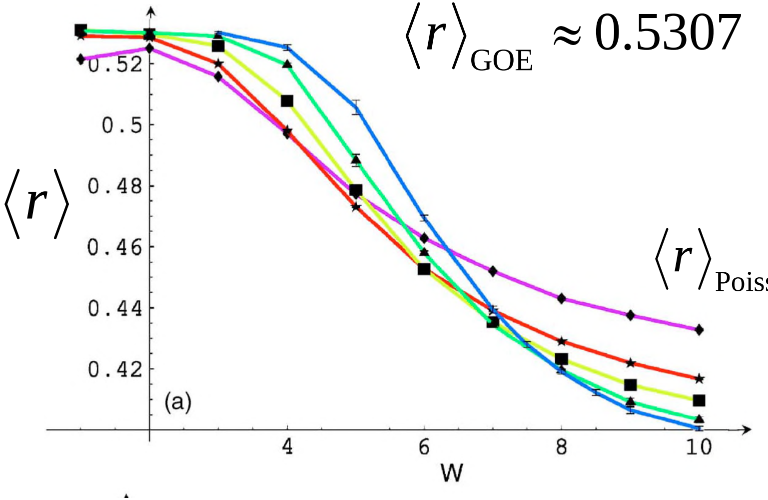
V. Oganesyan and D. A. Huse,
Phys. Rev. B **75**, (2007):

$$0 \le r_n = \min\{s_n, s_{n-1}\} / \max\{s_n, s_{n-1}\} \le 1$$

$$(s_n = E_n - E_{n-1})$$

$$\text{mean}: \langle r \rangle = \int_0^1 P(r) r \, \mathrm{d} r$$



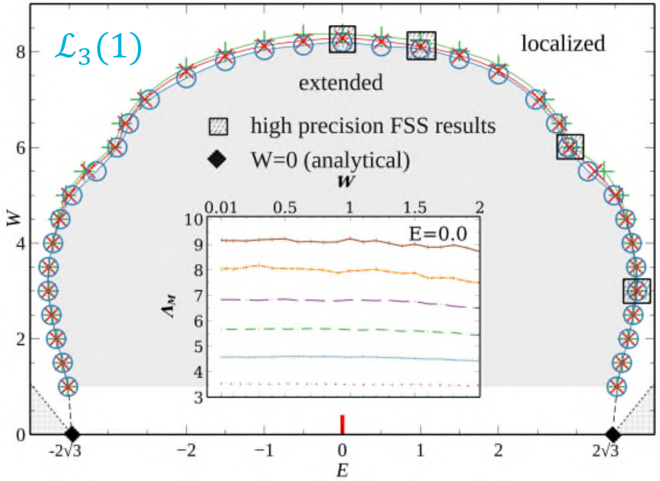


$$\langle r \rangle_{\text{GOE}} \approx 0.5307$$

$$\langle r \rangle_{\text{Poisson}} = 0.386$$

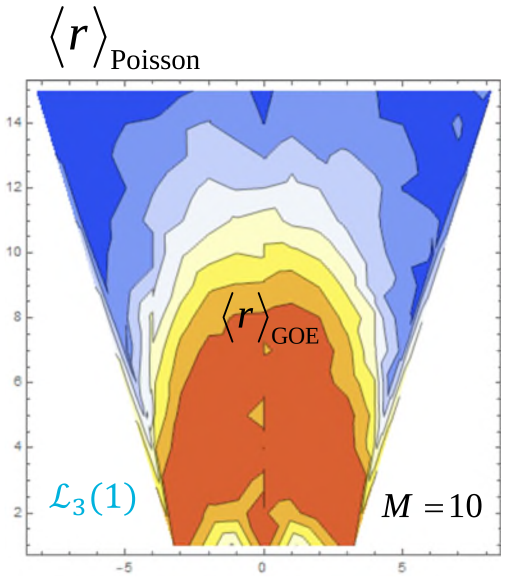
Does it work? Testing for the full disorder, equal on hub and rim

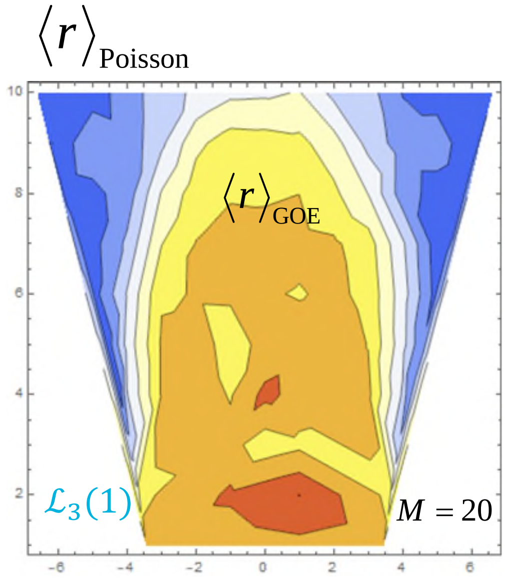
- TMM:
  - Phase boundaries determined from scaling behavior with small $M^2 = 6^2, 8^2, 10^2 = 36, 64, 100$ (1%)



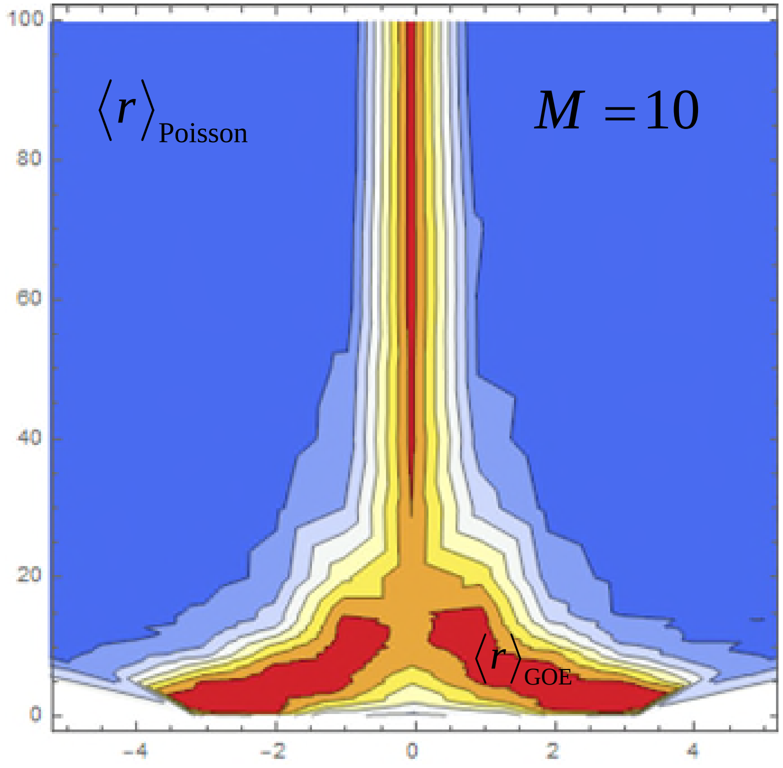
- Sparse-diagonalization
  - Phase boundaries determined from <r> for M=10, 20, i.e. sites

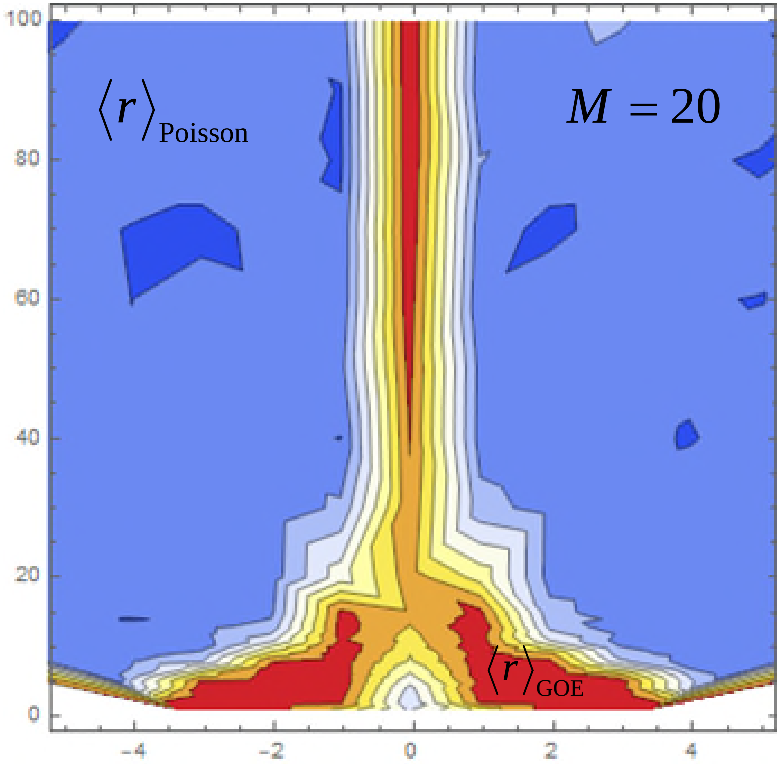
$$N = (3*10)^3 = 27000, (3*20)^3 = 216000$$



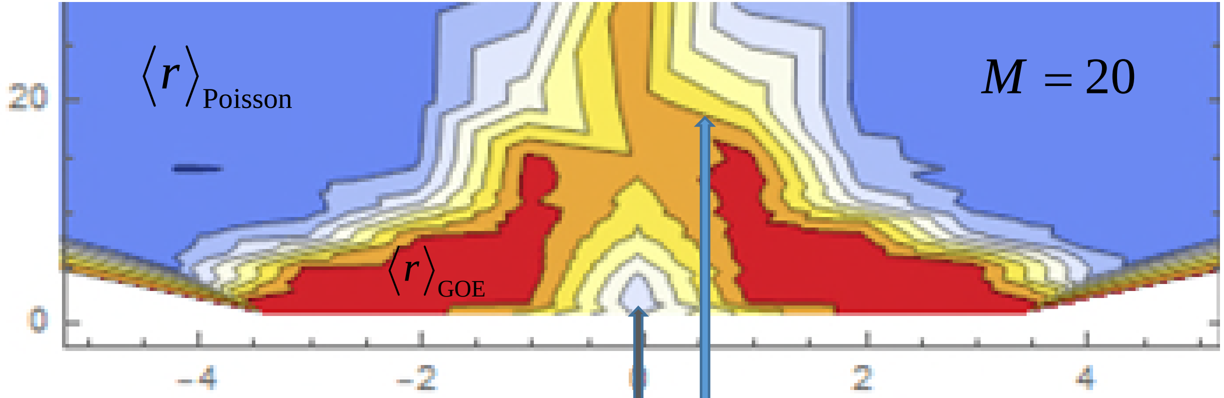


3D Lieb model with CLS-preserving disorder, 1st results





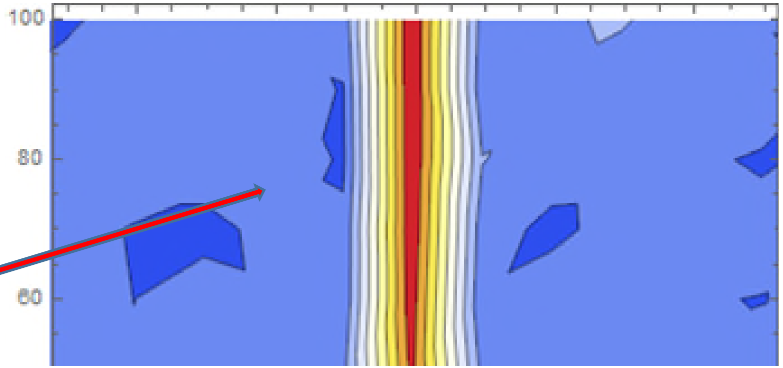
3D Lieb model with CLS-preserving disorder, 1st results



- BORING?

No more!

- “inverse” Anderson transition
- CLS states stop delocalization at FB energy E=0!?
- Why do CLS appear to show <r> values for GOE? Superposition of CLS?



Conclusions 2: Extended and disordered Lieb models in 2 and 3D

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- ~~At FB energies, localization behavior can be different (2D); phase diagrams (3D) do not develop regions of localized states down to $W = 0.01$~~
- FB states change phase diagrams and localization length values, **expect** universal properties to remain unchanged!
- Rim sites in Lieb models act as additional 1D localizers
- CLS-preserving disorder is weaker (in terms of critical disorder larger) and stronger (in terms of inverse Anderson transition) – much more work needed
- Someone to discover these (extended) systems in a material.