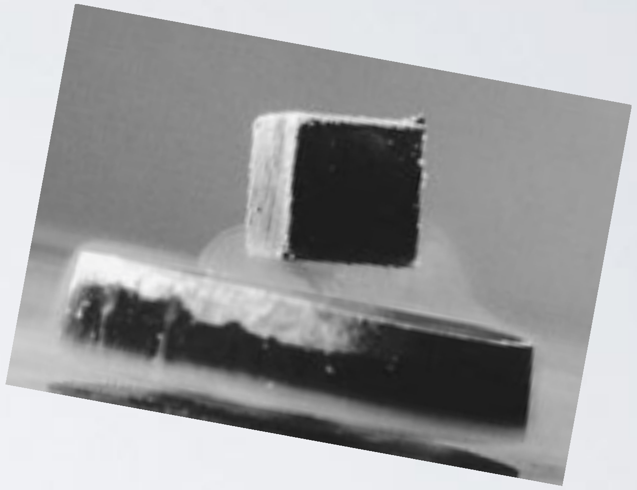
CONNECTING MICROSCOPICS TO EMERGENT PHENOMENA

Bryan Clark
University of Illinois at Urbana Champaign
Blue Waters Professor

Emergence

SIMPLE RULES

Emergent Phenomena



COMPLICATED BEHAVIOR

Strongly Correlated Systems!!

Dirac's Challenge

The fundamental laws necessary for the mathematical treatment of a large part of physics and the whole of chemistry are thus completely known, and the difficulty lies only in the fact that the application of these laws leads to equations that are too complex to solve.

- Paul Dirac

Is Blue Water's the solution to Dirac's Challenge?

Simulating quantum mechanics

Because we know the microscopic rules, we can write down the algorithm which solves exactly the problem we want.

There's only one problem….

n things (electrons, spins, etc) → **computational complexity: 2^n**

Underlined "Why?" Even the state of a quantum system can only be stored with 2^n numbers.

Exact Diagonalization

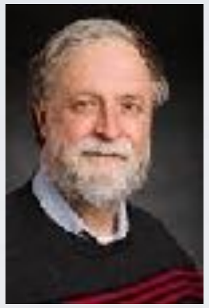
tensor networks

quantum Monte Carlo

Spin Liquids

Hitesh Changlani

Krishna Kumar



Eduardo Fradkin

Many-Body Localization

Xiongjie Yu

Benjamin Correa

David Luitz

David Pekker

Superconducting Materials

Katie Hyatt

Matthew Fisher

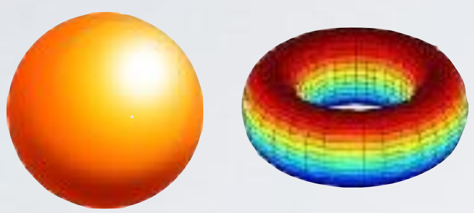
Chiral spin liquids

Topological

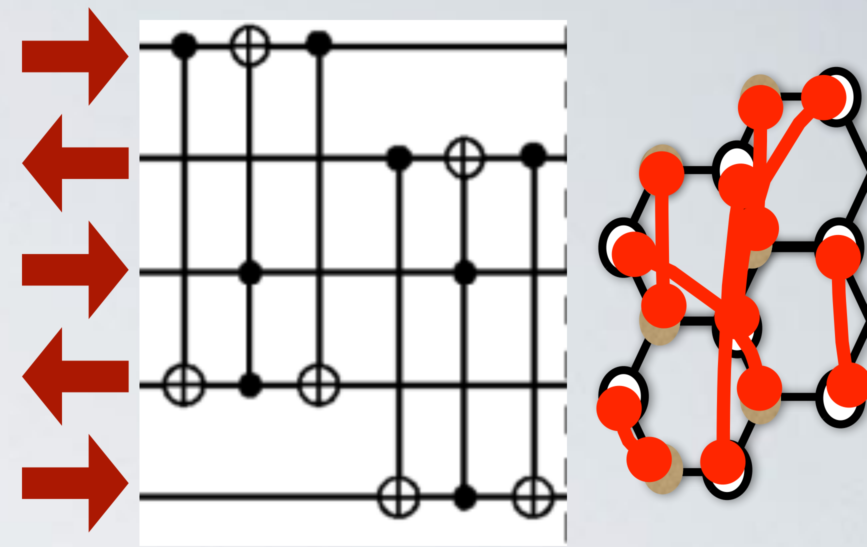
Magnets don't care what topology it's painted on.

Spin liquids do.

One vs. two ground states.



Long Range Entangled.



Spin liquids: Long quantum circuits to build spin liquid

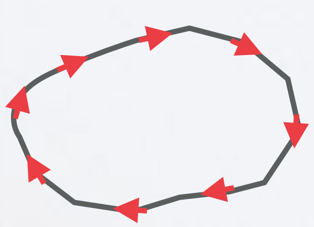
"No" symmetry breaking

Beyond Landau symmetry breaking paradigm

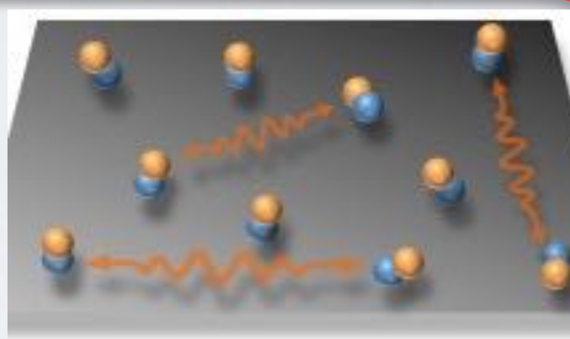
Still different phases.

Does break "chiral" symmetry

Edge modes



Fractional Excitations



Bosons => exchange: +1

Fermions => exchange: -1

Anyons => phase (or unitary matrix)

Useful for building a quantum computer.

H → Spin Liquids

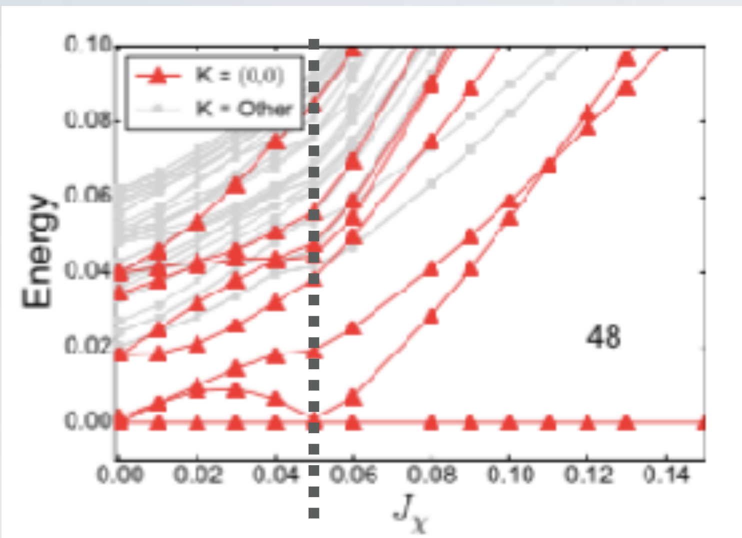
Question: What is my phas

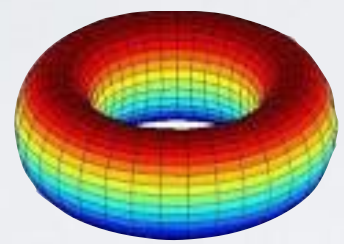
$$H_{XXZ} = \sum_{\langle i,j \rangle} J_{xy}\left(S_i^x S_j^x + S_i^y S_j^y\right) + J_z S_i^z S_j^z - h_B \sum_i S_i^z$$

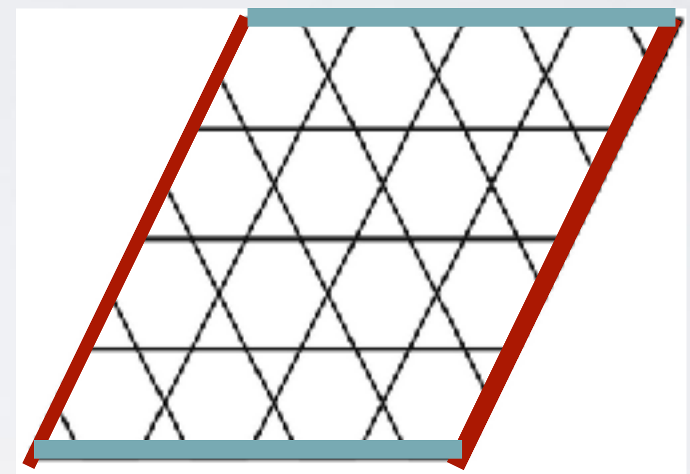
$$m = 2/3$$

H → Spin Liquids

Two locally indistinguishable states



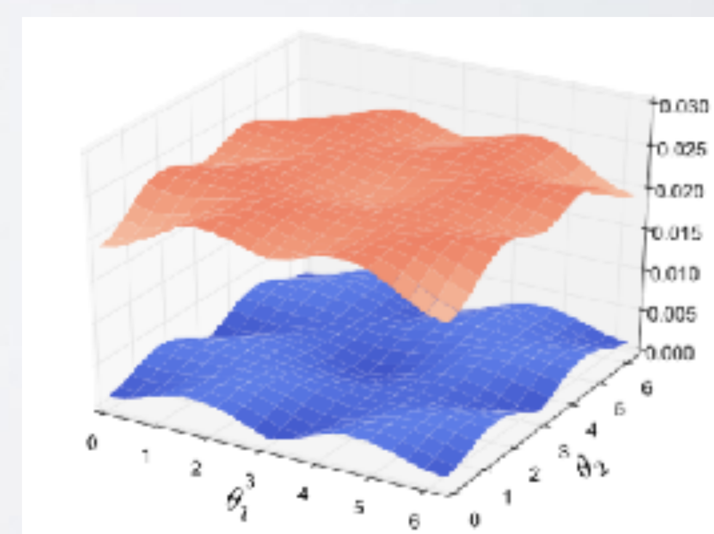




Twisting the boundaries….

When you walk off the edge you might not end up in the same place, but could come back with a phase.

You want your energy vs. phase to be gapped.



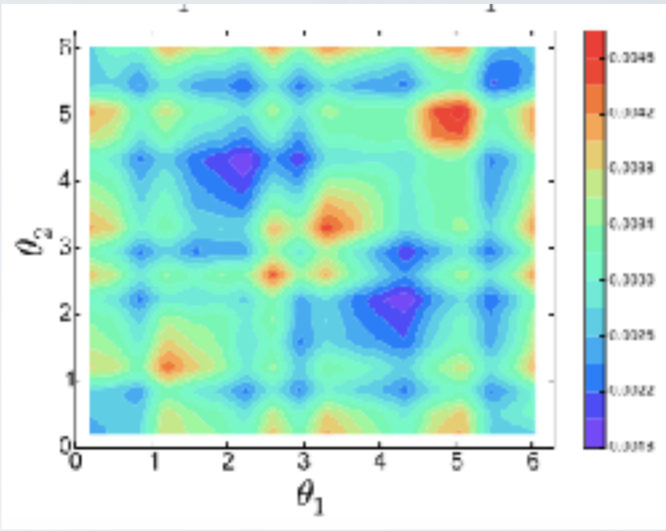
E

Two smoking guns...

Chern Number

$$C = \frac{1}{2\pi}\int_0^{2\pi}\int_0^{2\pi} B(\theta_1,\theta_2)d\theta_1 d\theta_2$$

$$\begin{aligned} B(\theta_1,\theta_2) = \mathbf{Log}\{ &\langle\psi(\theta_1,\theta_2)|\psi(\theta_1+\delta\theta_1,\theta_2)\rangle \\ &\times\langle\psi(\theta_1+\delta\theta_1,\theta_2)|\psi(\theta_1+\delta\theta_1,\theta_2+\delta\theta_2)\rangle \\ &\times\langle\psi(\theta_1+\delta\theta_1,\theta_2+\delta\theta_2)|\psi(\theta_1,\theta_2+\delta\theta_2)\rangle \\ &\times\langle\psi(\theta_1,\theta_2+\delta\theta_2)|\psi(\theta_1,\theta_2)\rangle\,\} \end{aligned}$$

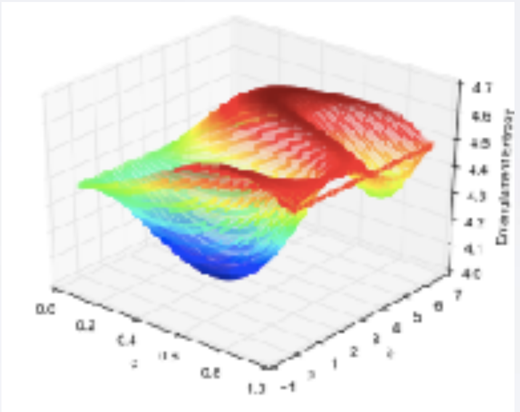


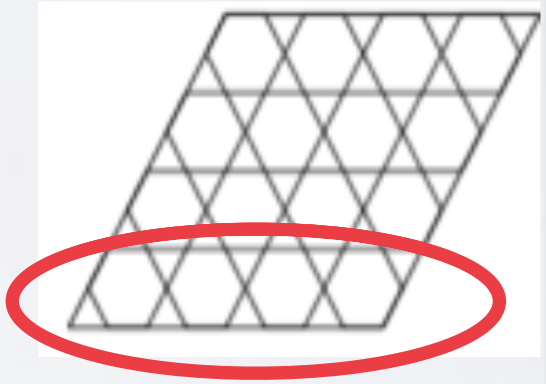
A new chiral spin liquid!

Modular S-Matrix

Build minimally entangled states

$$\Psi_{\mathrm{MES}} = \alpha_1\Psi_1 + \alpha_2\Psi_2$$





$$\mathcal{S} = \frac{1}{\sqrt{2}}\begin{pmatrix}1 & 1\\ 1 & -1\end{pmatrix}, \qquad \mathcal{U} = e^{i\frac{2\pi}{24}1}\begin{pmatrix}1 & 0\\ 0 & i\end{pmatrix}$$

$$\mathcal{S} = \begin{pmatrix}0.705 & 0.694\\ 0.694 & -0.736e^{-i0.088}\end{pmatrix} \qquad \mathcal{U} = e^{i\frac{2\pi}{24}1.014}\begin{pmatrix}1.000 & 0.000\\ 0.000 & ie^{0.053i}\end{pmatrix}$$

Cost on Blue Waters for exact-diagonalization

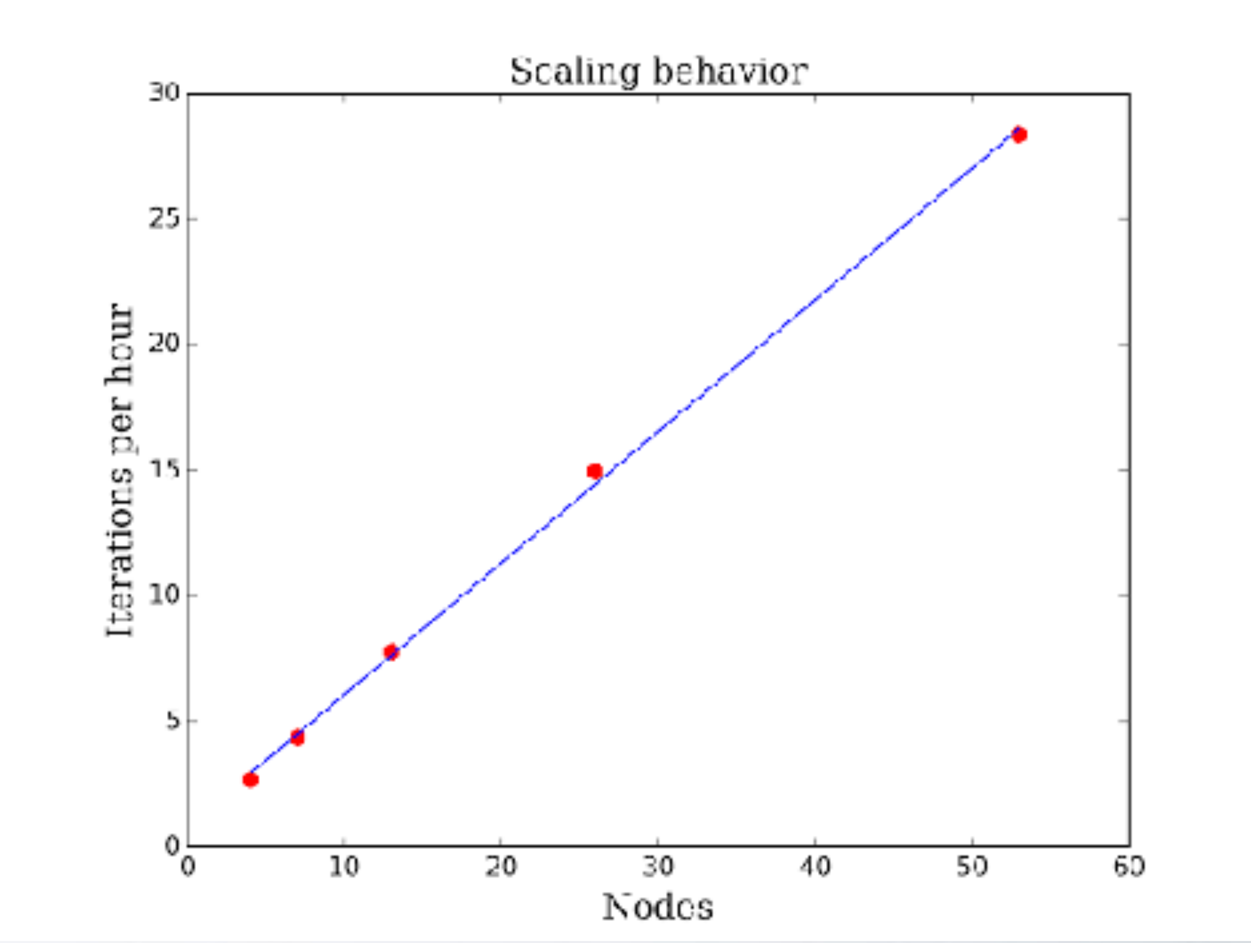
400 points.

Each point is ~150 node hours per block

~30 blocks (embarrassingly parallel)

Matrix size: 377 million x 377 million

Goal: Get a single point, in wall-clock time of a few hours



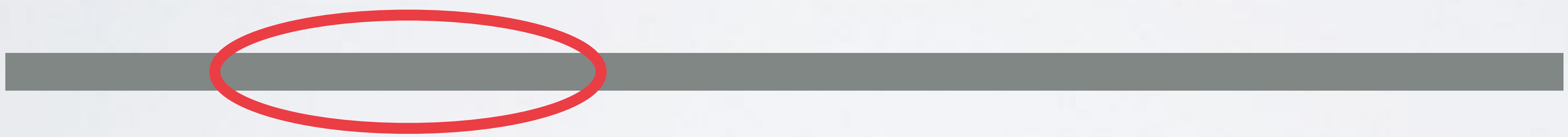
Many Body Localization

<u>Stat Mech 101</u>

That coffee cup eventually cools down until it reaches the temperature of the room.

We would be shocked if the coffee cup stayed hot forever.

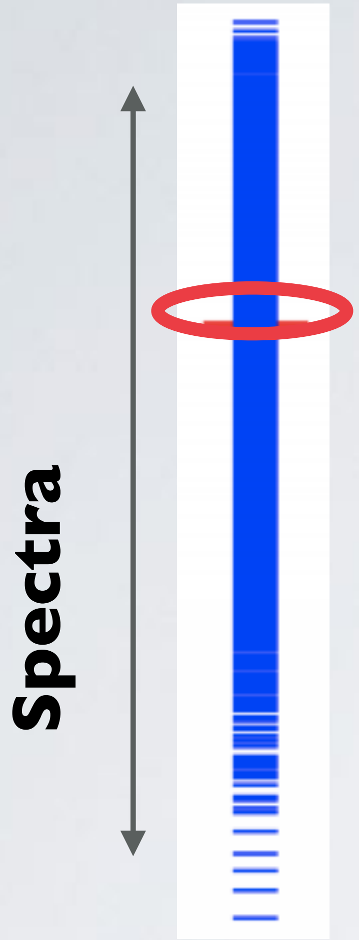
But that's exactly what happens in MBL systems.



The rest of the system doesn't act as a heat bath for this part of the system.

How can we understand this?

Understand MBL



2N Eigenstates in the interior of a spectra.

Average spacing:

20 sites: 3×10^{-5}

100 sites: 7×10^{-30}

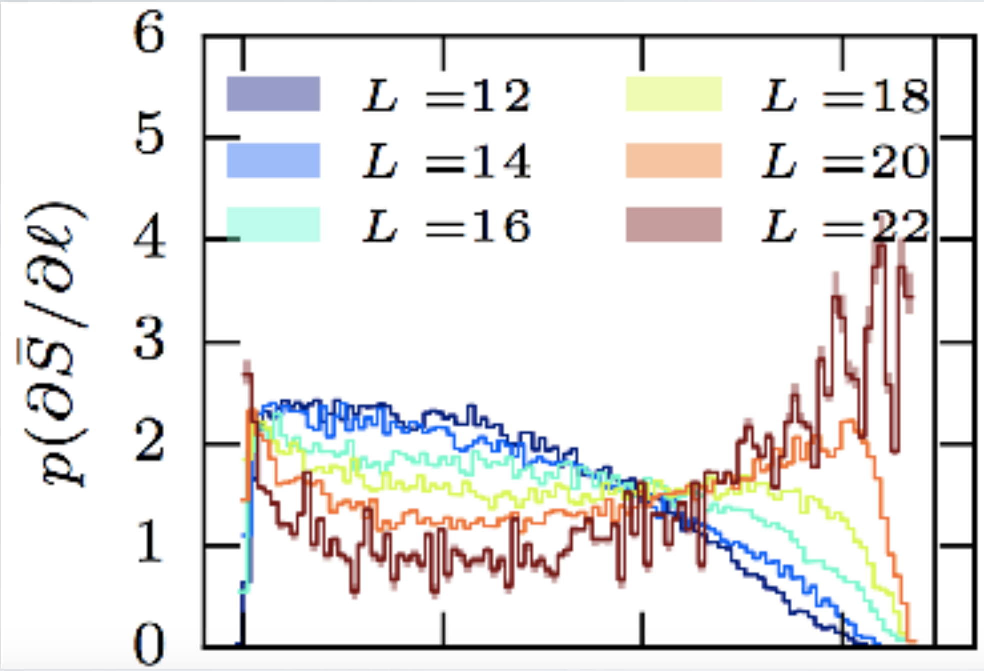
The "order parameter" of the MBL phase is studied by measuring interior eigenstates.

Need hundreds or thousands of such samples.

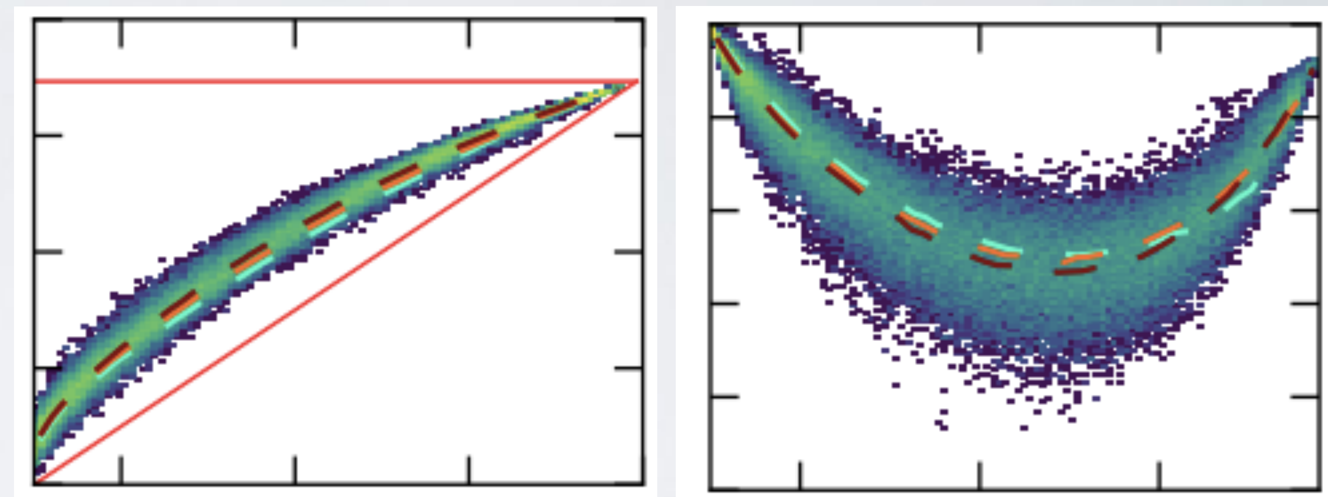
N~20 Shift and Invert

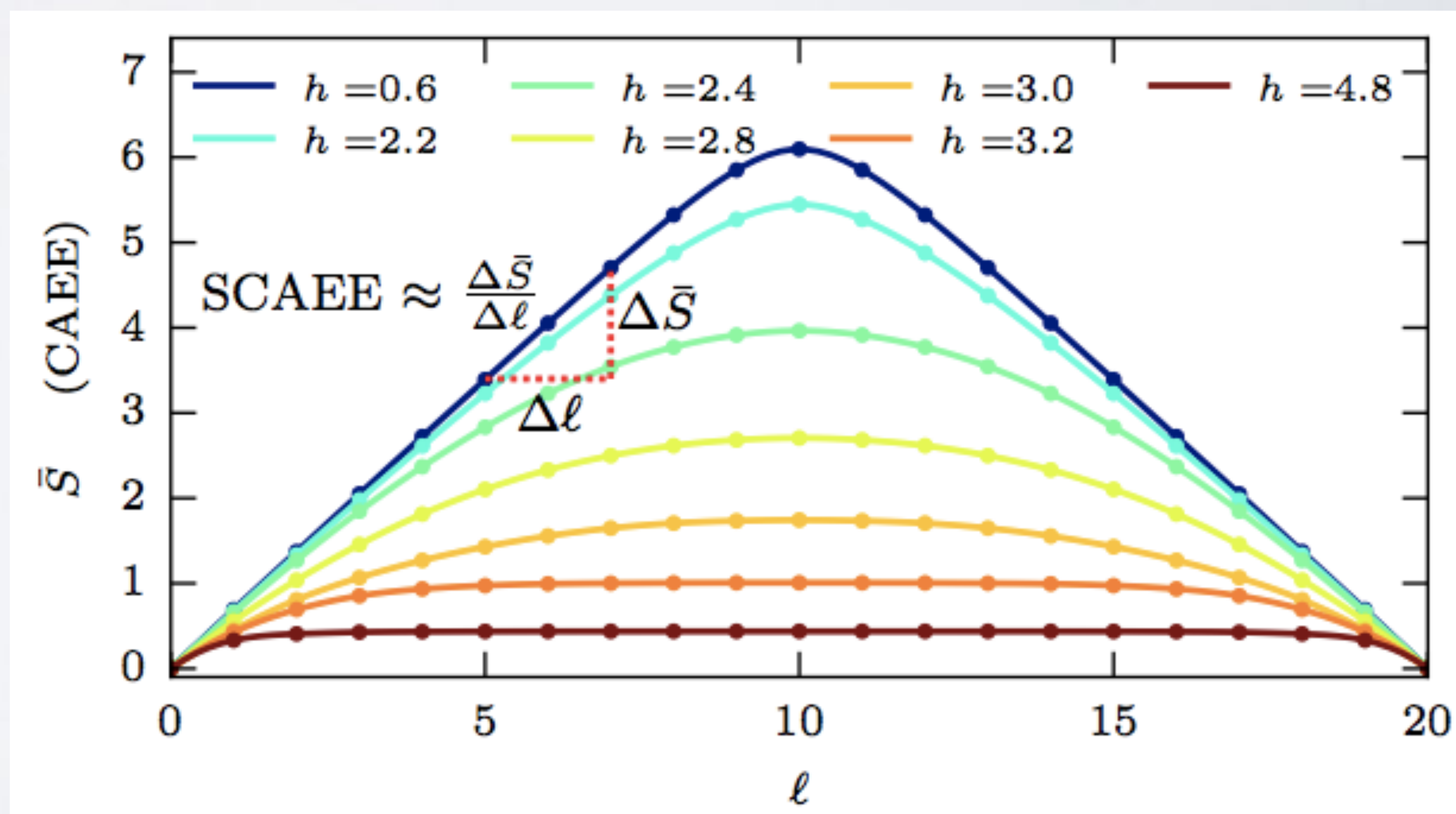
N~100 Matrix Product States

Bimodality in the critical region of MBL.



Universality in the critical region of MBL

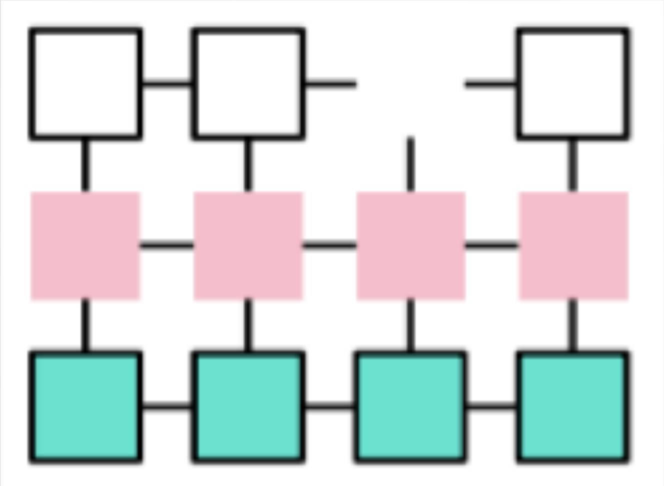


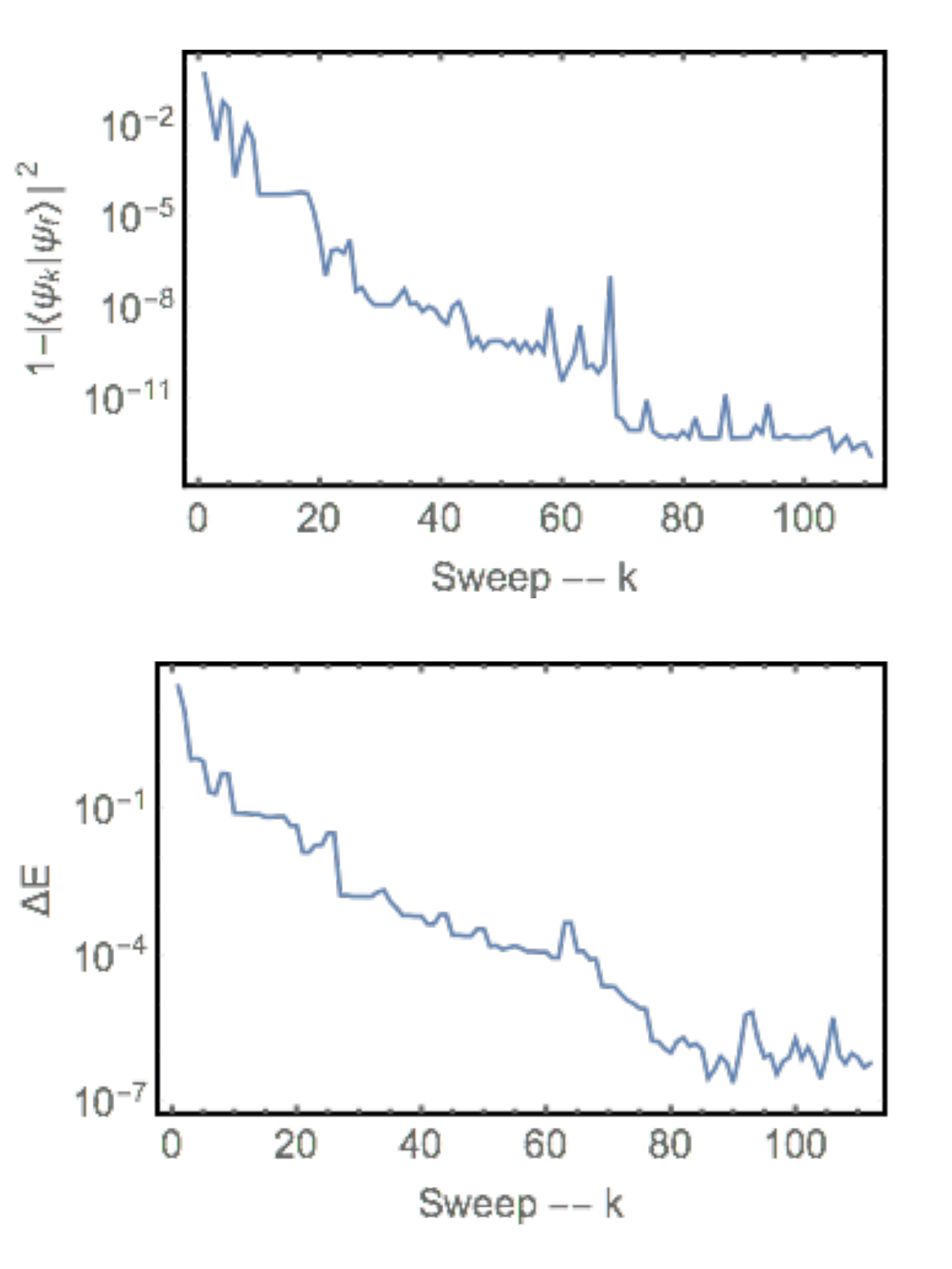


ES DMRG

Typical DMRG: For a site produce an effective Hamiltonian H' and solve for the ground state of H'

Modified DMRG: For a site produce an effective Hamiltonian H' and choose the eigenstate of H' closest to the current energy of your state.





How well does it work?

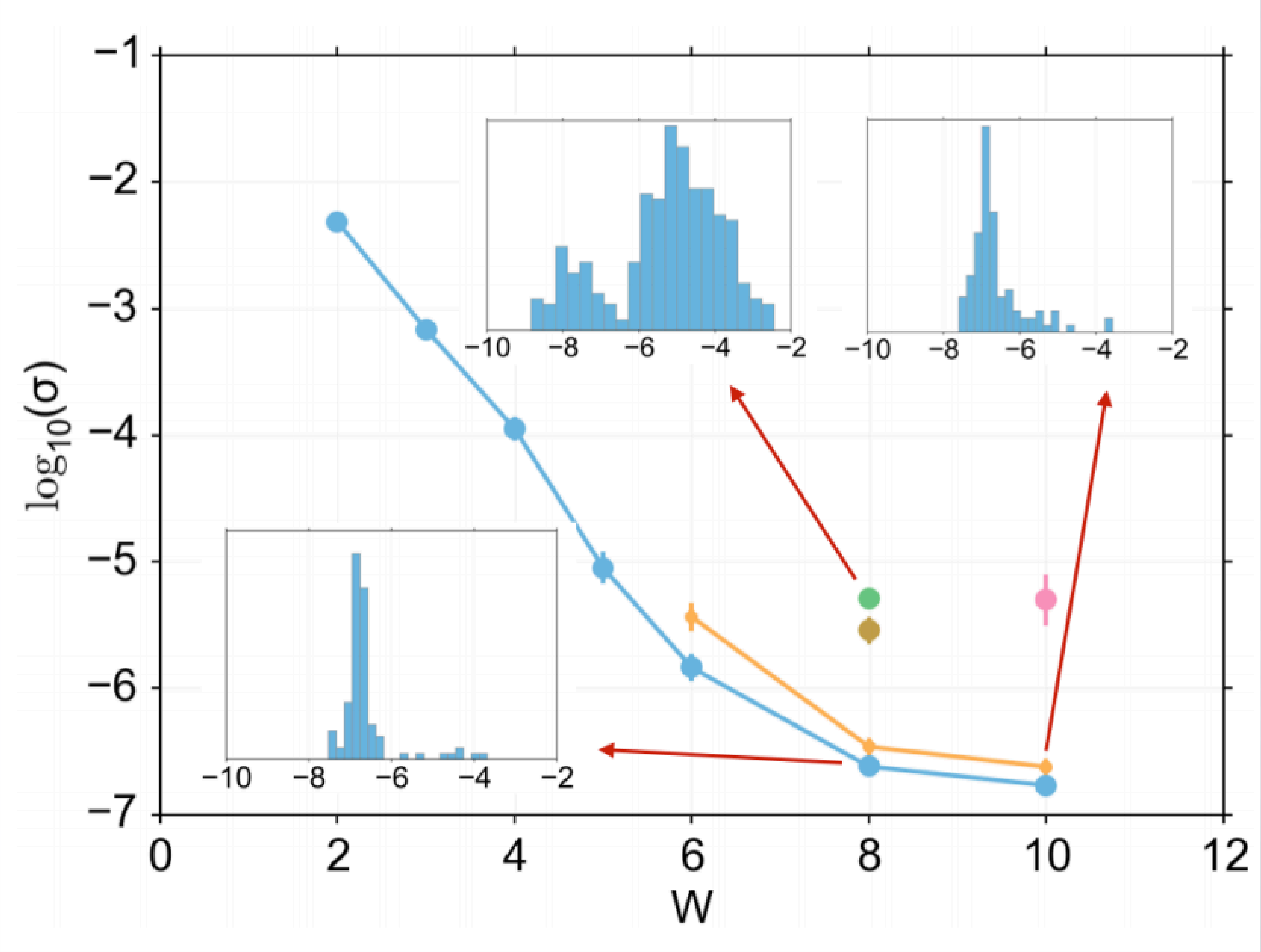
N=100 ES-DMRG

N=30 - SIMPS M=20

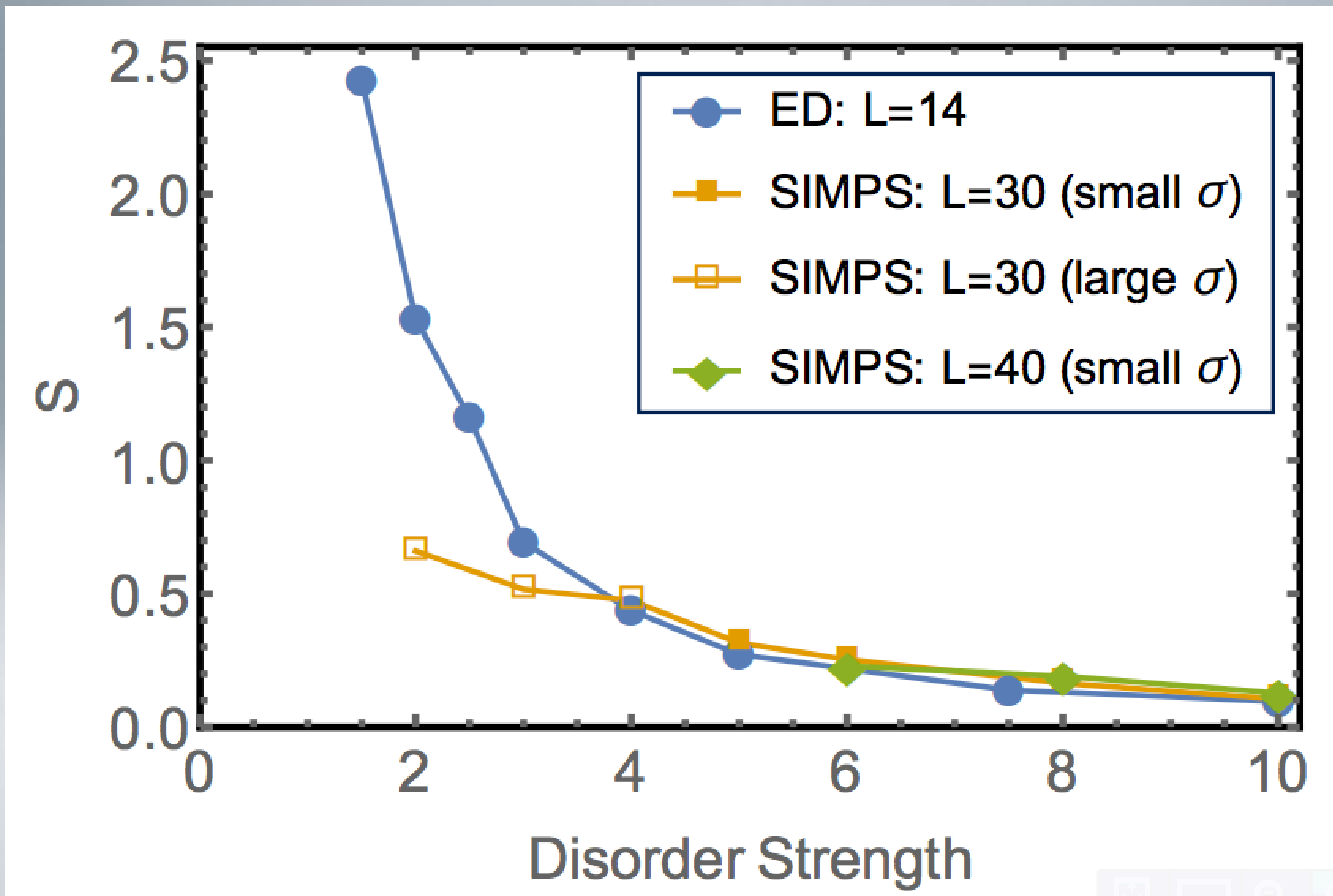
N=30 - ES-DMRG M=20

N=30 - SIMPS M=60

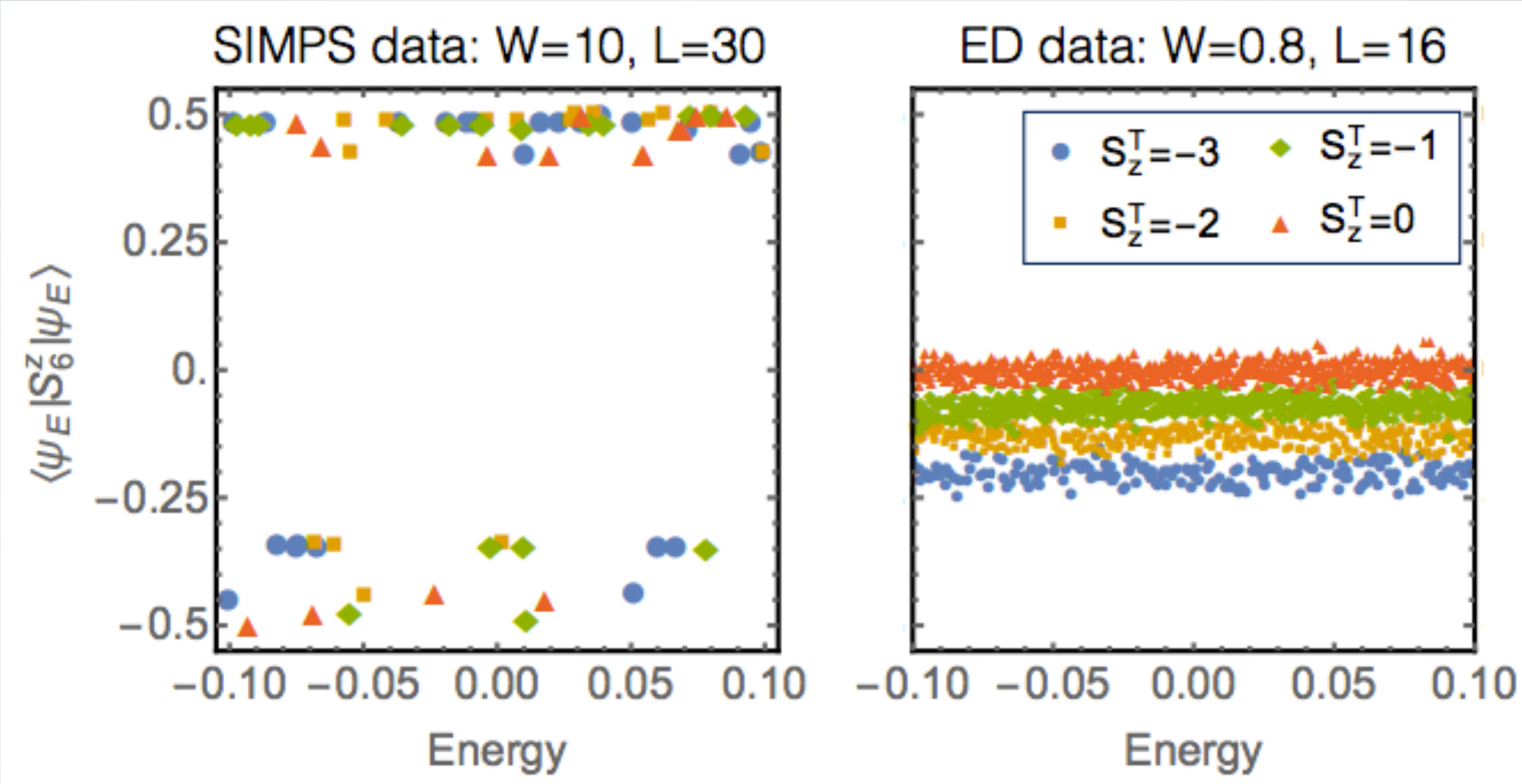
N=40 - SIMPS M=60

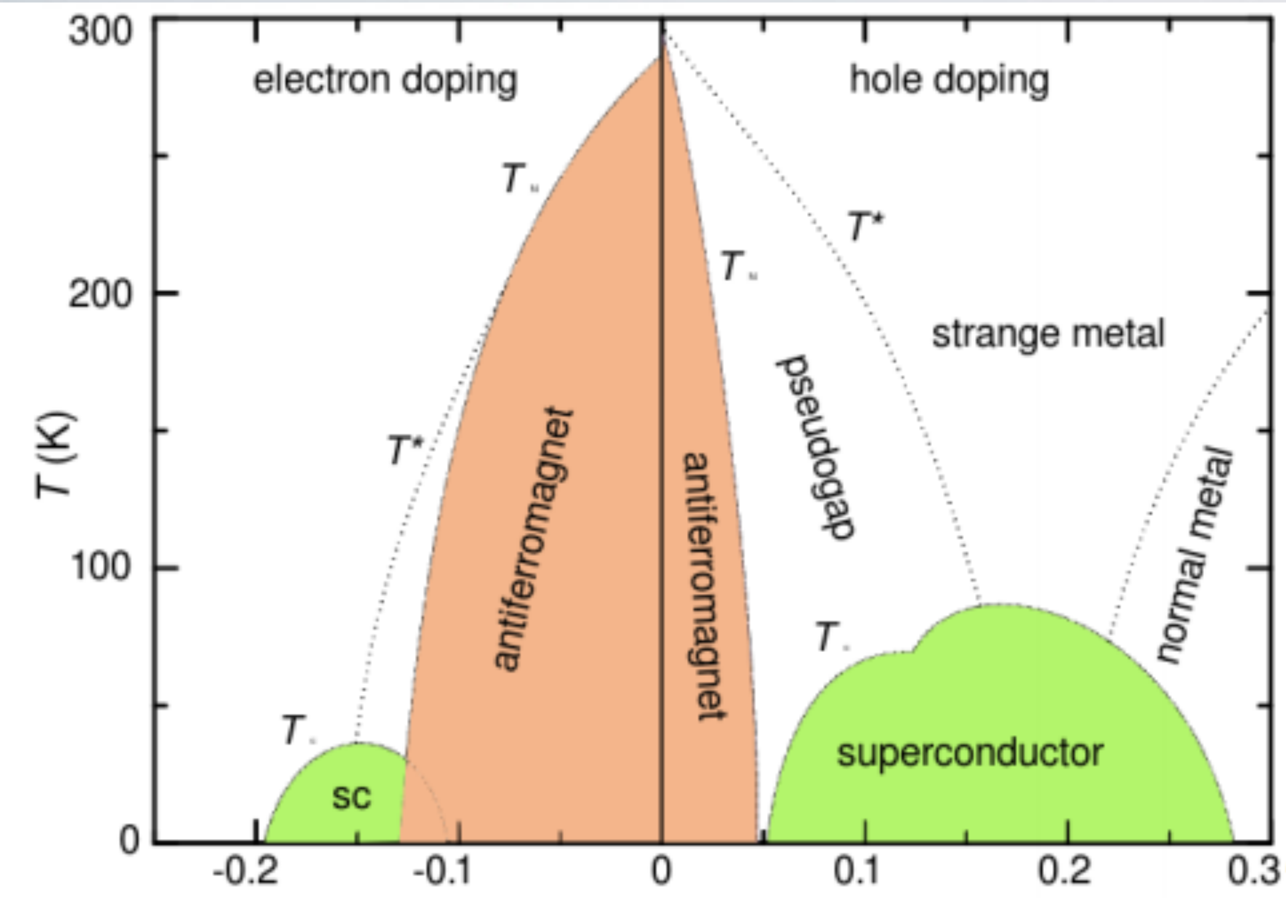


How does entanglement scale?



Breakdown of thermalization





Pseudogap and Strange metal are not understood - even qualitatively.

Understanding them is (widely regarded) as the key to understanding high Tc.

Superconducting Materials

Broad Mechanism for superconductivity:

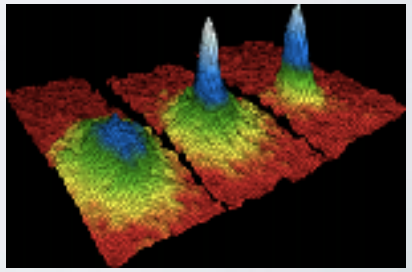
Electrons "pair together" into bosons

Bosons condense and superconduct

Above the superconducting dome:

ARPES shows paired bosons but uncondensed.

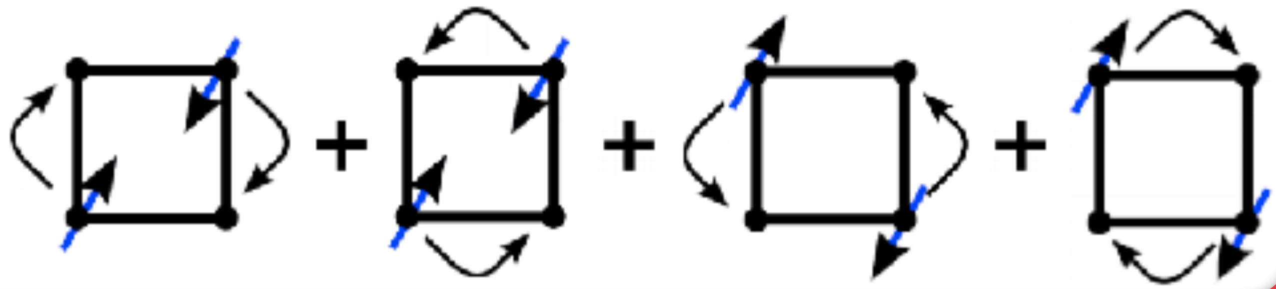
This is a very unnatural state of bosons. Bosons want to condense (or insulate).



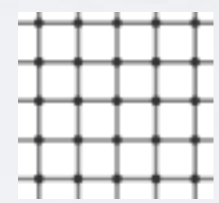
The *key* stumbling block: a microscopic model which starts with fermions and gives conducting, uncondensed bosons.

The Model

$$\hat{H} = K\sum_{\mathbf{r}} c^\dagger_{\mathbf{r}\uparrow} c_{\mathbf{r}+\hat{\mathbf{x}},\uparrow} c^\dagger_{\mathbf{r}+\hat{\mathbf{x}}+\hat{\mathbf{y}},\downarrow} c_{\mathbf{r}+\hat{\mathbf{y}},\downarrow} + \uparrow\leftrightarrow\downarrow + \text{h.c.}$$



- Electrons live on a a square lattice.



- Only one electron per site
- Up and down electrons ring exchange.

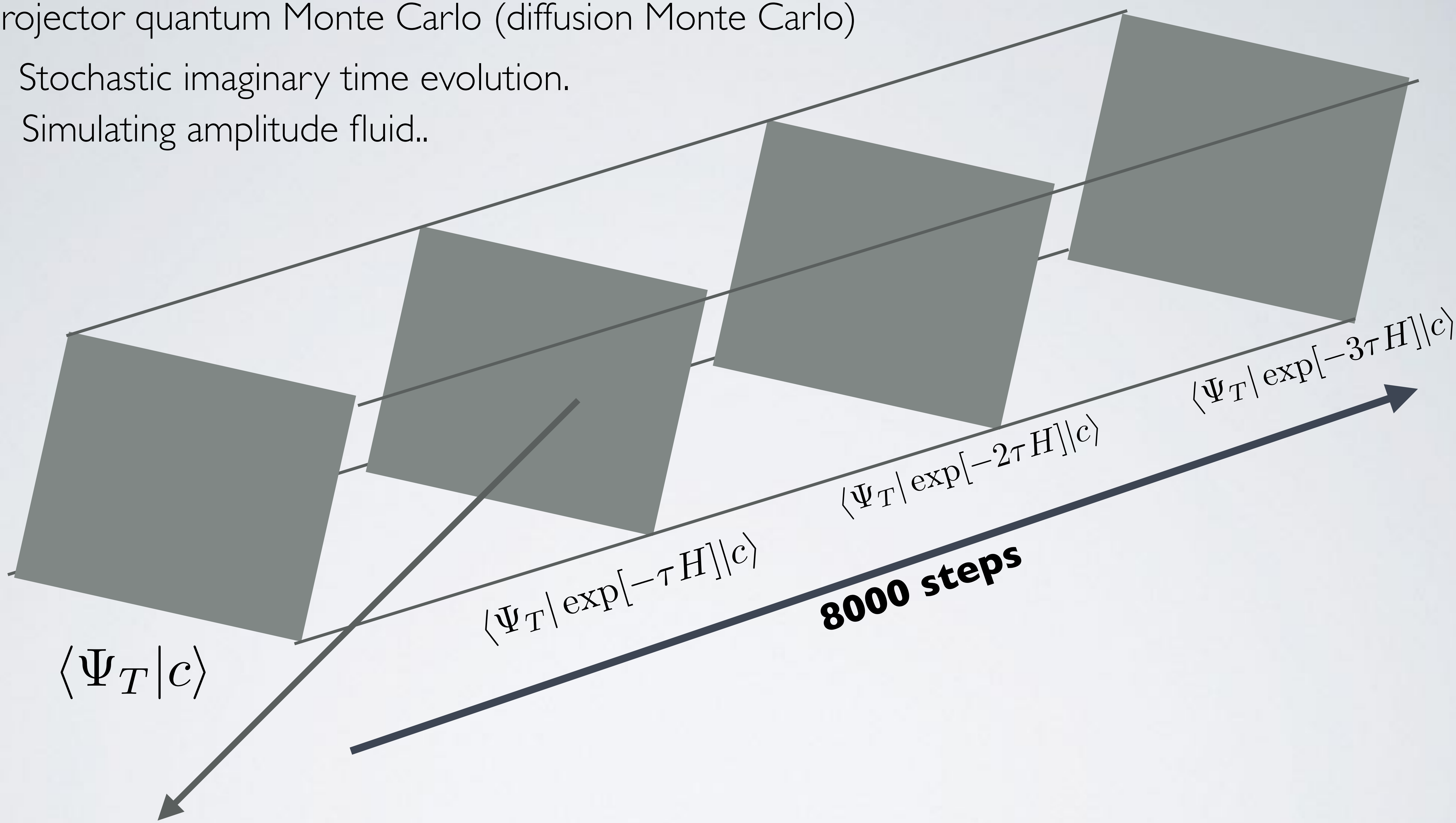
Fermions typically have sign problems..what about this?

The algorithm...

Projector quantum Monte Carlo (diffusion Monte Carlo)

Stochastic imaginary time evolution.

Simulating amplitude fluid..



10^4 to 10^6 samples from a possible 2^{228} possibilities,

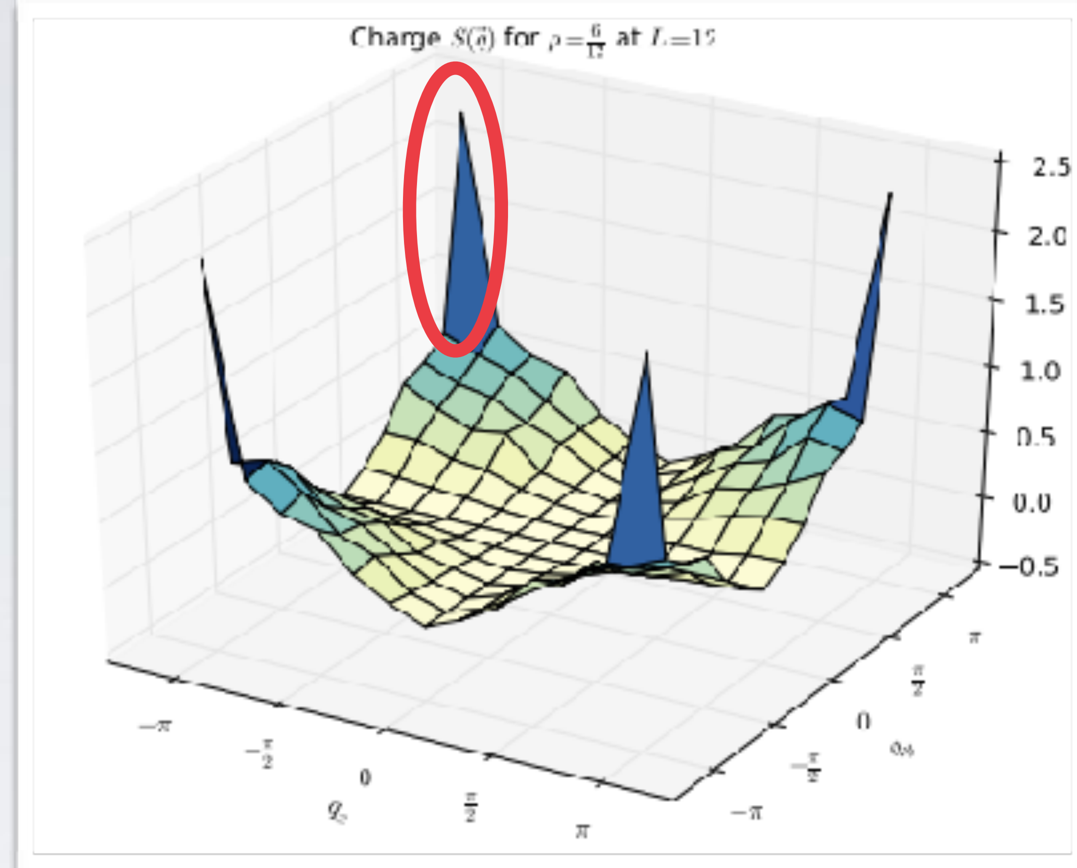
Forward walking

What should we look at?

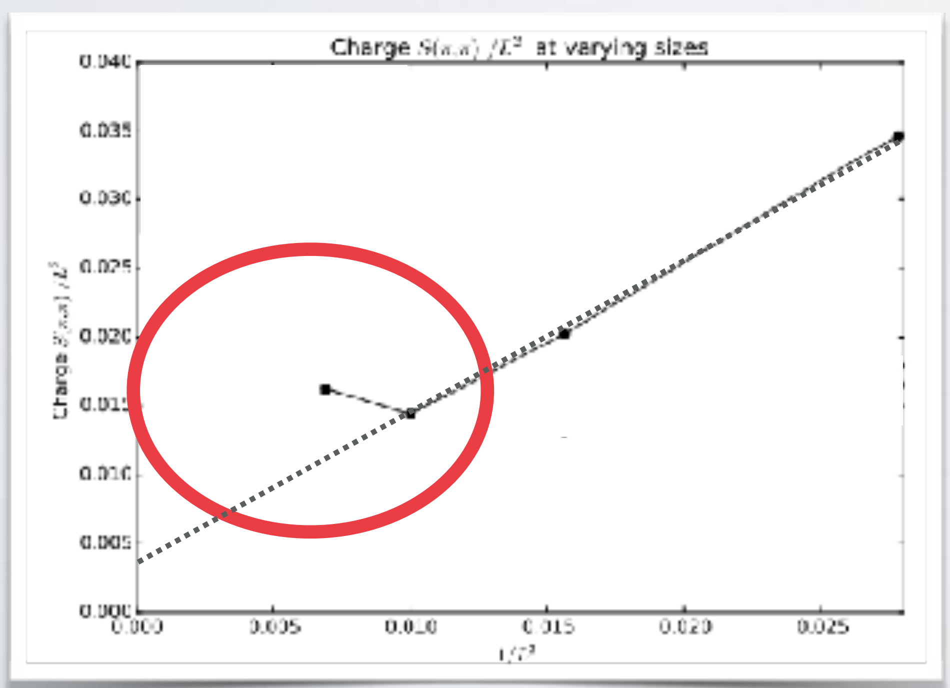
Structure Factor

$$S_C(\mathbf{q}) = \frac{1}{L^2} \sum_{\mathbf{r}_i, \mathbf{r}_j} e^{i\mathbf{q}\cdot(\mathbf{r}_i - \mathbf{r}_j)} \left(\langle \hat{n}_i \hat{n}_j \rangle - \bar{n}^2 \right)$$

Peaks in the structure factor <=> charge density wave



Density: Half Filling

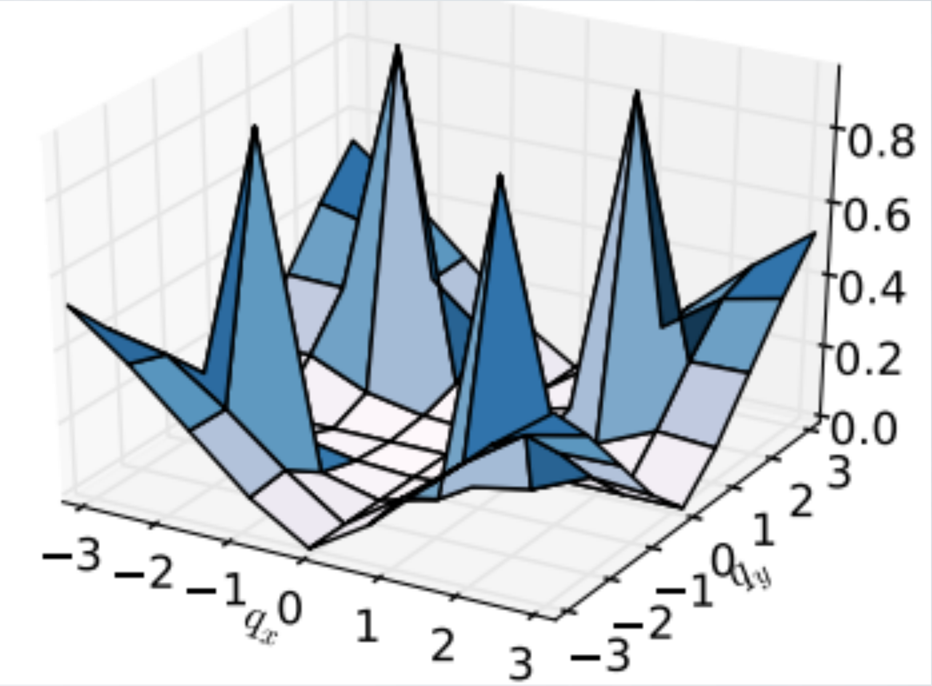


Does not extrapolate to zero.

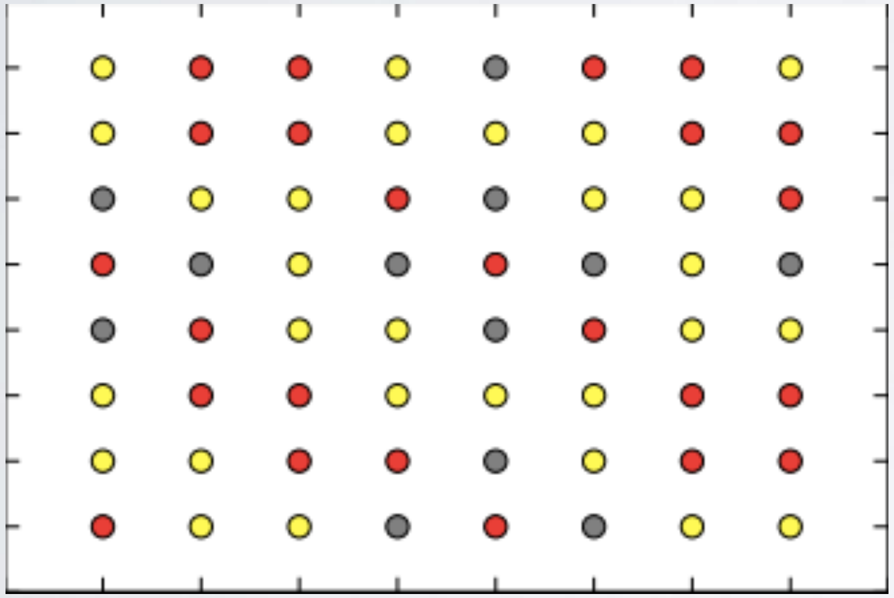
What should we look at?

Structure Factor

$$S_C(\mathbf{q}) = \frac{1}{L^2} \sum_{\mathbf{r}_i,\mathbf{r}_j} e^{i\mathbf{q}\cdot(\mathbf{r}_i-\mathbf{r}_j)} \left(\langle \hat{n}_i \hat{n}_j \rangle - \bar{n}^2 \right)$$



Density: quarter Filling



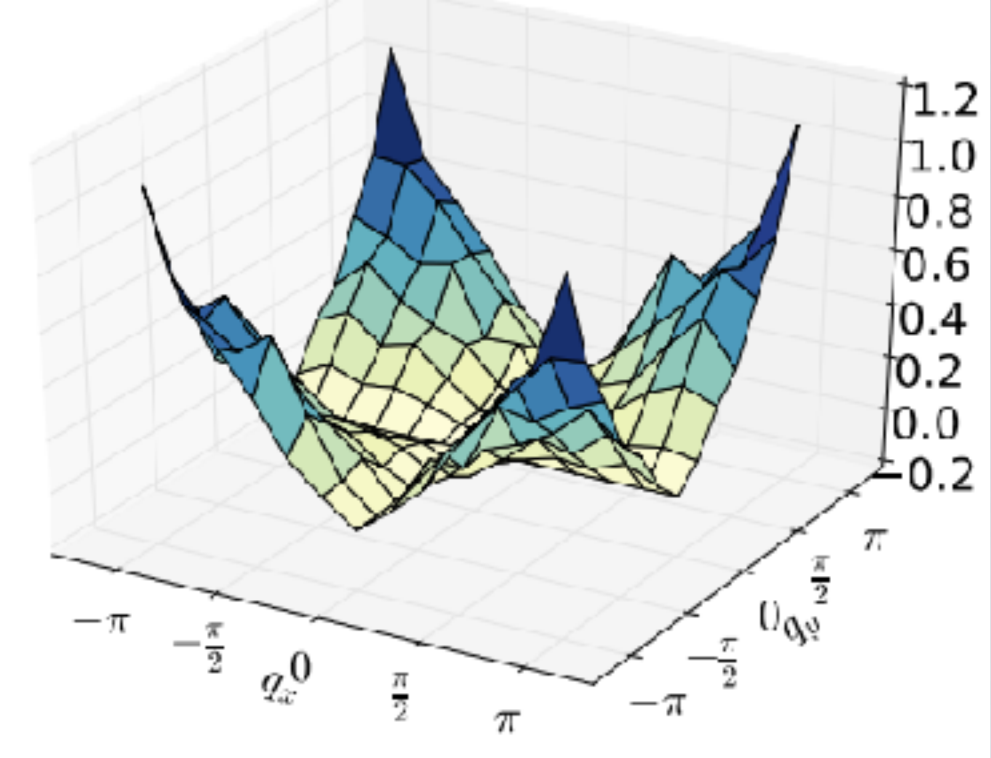
Does this have anything to do with the stripes present in superconducting materials?

(another talk)

What should we look at?

Structure Factor

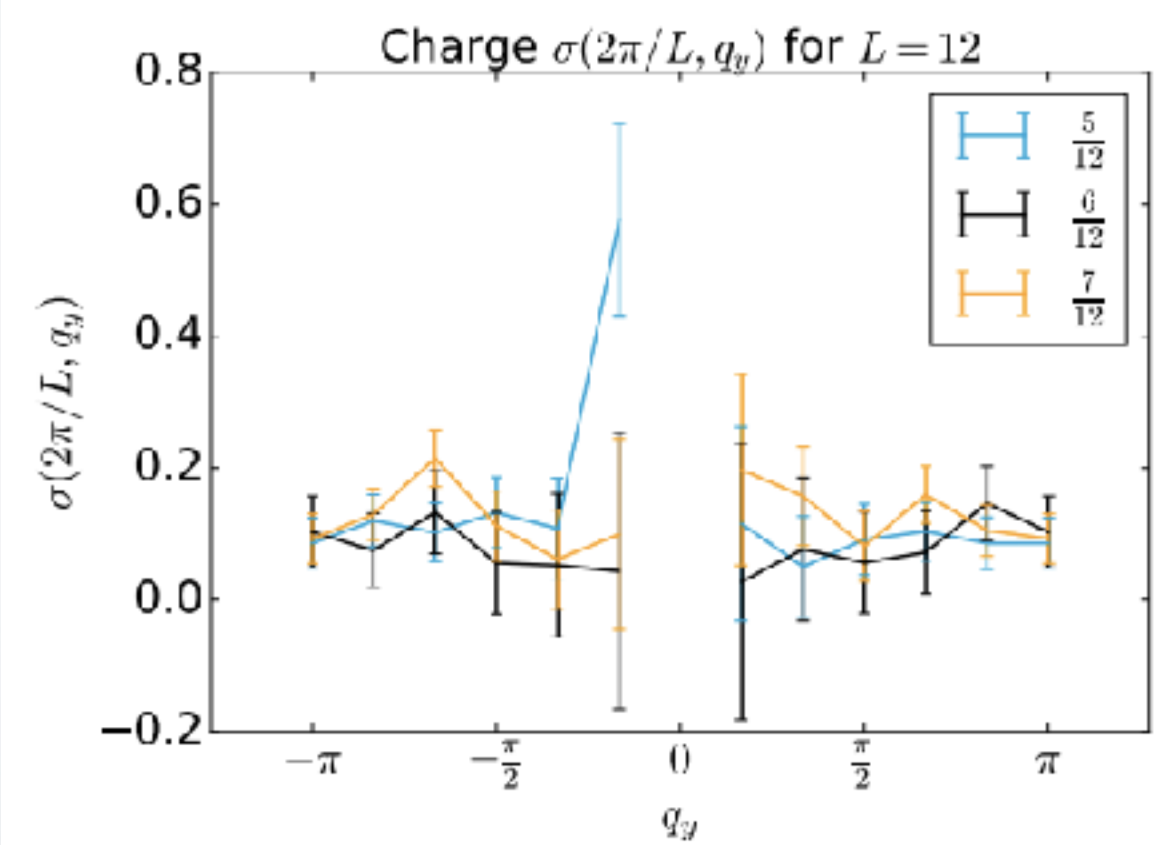
$$S_C(\mathbf{q}) = \frac{1}{L^2} \sum_{\mathbf{r}_i, \mathbf{r}_j} e^{i\mathbf{q}\cdot(\mathbf{r}_i - \mathbf{r}_j)} \left(\langle \hat{n}_i \hat{n}_j \rangle - \bar{n}^2 \right)$$



We would like to know if this conducts?

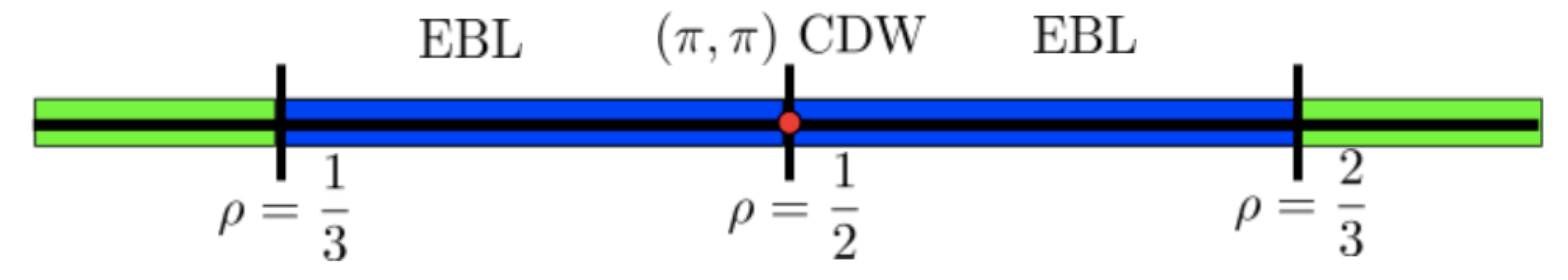
Check if $S(q)$ **linear as** $q \to 0$

$$\sigma(\mathbf{q}) = S_C(\mathbf{q})/4 \left|\sin(\tfrac{q_x}{2})\sin(\tfrac{q_y}{2})\right|$$



Density: 7/12 Filling

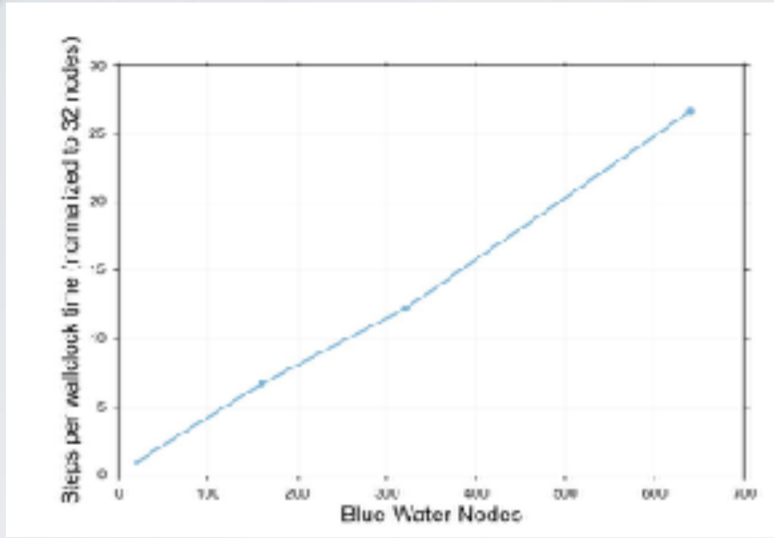
Exciton Bose Liquid?



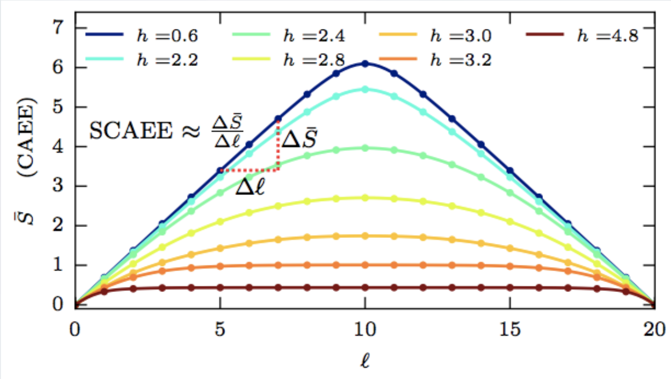
We have managed to connect, in a bulk 2D system, a microscopic H to a strange metal.

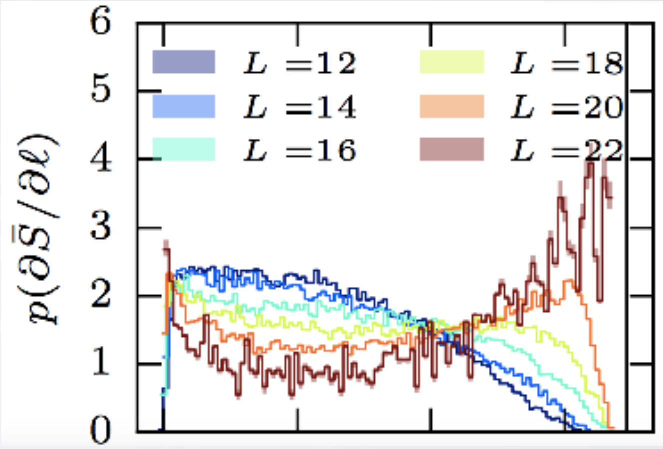
(We've looked here at the charge degrees of freedom but there is also an interesting story about what the spin degrees of freedom are doing).

Conclusions

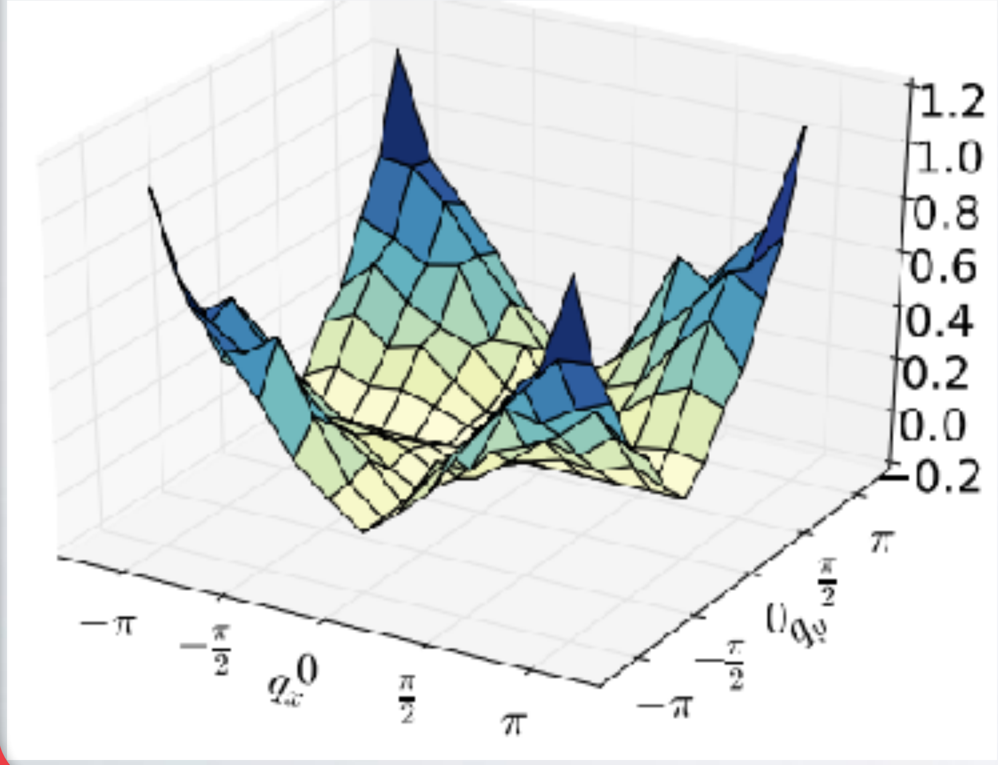


Many Body Localization





Strange Metal in superconducting materials



Chiral Spin Liquid