CONNECTING MICROSCOPICS TO EMERGENT PHENOMENA

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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....

\[ n \text{ things (electrons, spins, etc.)} \rightarrow \text{computational complexity: } 2^n \]

**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

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

Spin liquids do.

Topological

One vs. two ground states.

“No” symmetry breaking

Beyond Landau symmetry breaking paradigm

Still different phases.

Does break “chiral” symmetry

Edge modes

Long Range Entangled.

Spin liquids: Long quantum circuits to build spin liquid

Fractional Excitations

Bosons => exchange: +1
Fermions => exchange: -1
Anyons => phase (or unitary matrix)
Useful for building a quantum computer.
Question: What is my phase?

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.
Two smoking guns...

Chern Number

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

\[ B(\theta_1, \theta_2) = \text{Log} \left\{ \langle \psi(\theta_1, \theta_2) | \psi(\theta_1 + \delta\theta_1, \theta_2) \rangle \times \langle \psi(\theta_1 + \delta\theta_1, \theta_2) | \psi(\theta_1 + \delta\theta_1 + \delta\theta_2, \theta_2) \rangle \times \langle \psi(\theta_1 + \delta\theta_1, \theta_2 + \delta\theta_2) | \psi(\theta_1, \theta_2 + \delta\theta_2) \rangle \times \langle \psi(\theta_1, \theta_2 + \delta\theta_2) | \psi(\theta_1, \theta_2) \rangle \right\} \]

A new chiral spin liquid!

Modular S-Matrix

Build minimally entangled states

\[ \Psi_{\text{MES}} = \alpha_1 \Psi_1 + \alpha_2 \Psi_2 \]

\[ S = \frac{1}{\sqrt{2}} \begin{pmatrix} 1 & 1 \\ 1 & -1 \end{pmatrix}, \quad U = e^{i \frac{2\pi}{3}} \begin{pmatrix} 1 & 0 \\ 0 & i \end{pmatrix} \]

\[ S = \begin{pmatrix} 0.705 & 0.694 \\ 0.694 & -0.736 e^{-i0.088} \end{pmatrix}, \quad U = e^{i \frac{2\pi}{3}} \begin{pmatrix} 1.000 & 0.000 \\ 0.000 & i e^{0.053i} \end{pmatrix} \]
Cost on Blue Waters for exact-diagonalization

400 points.
Each point is $\sim 150$ node hours per block
$\sim 30$ blocks (embarrassingly parallel)
Matrix size: 377 million x 377 million

**Goal:** Get a single point, in wall-clock time of a few hours
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: $3 \times 10^{-5}$
100 sites: $7 \times 10^{-30}$

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

SIMPS data: $W=10$, $L=30$

ED data: $W=0.8$, $L=16$

$\langle \psi_E | S^Z_6 | \psi_E \rangle$

Energy

$S^T_z = -3$, $S^T_z = -1$, $S^T_z = -2$, $S^T_z = 0$
Pseudogap and Strange metal are not understood - even qualitatively.

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

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

\[ \hat{H} = K \sum_r c_r^\dagger c_r + \hat{\mathbf{x}}_r^\dagger c_r^\dagger \hat{\mathbf{x}}_r + \hat{\mathbf{y}}_r^\dagger c_r^\dagger \hat{\mathbf{y}}_r + \uparrow \leftrightarrow \downarrow + \text{h.c.} \]

- Electrons live on 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.

$$\langle \Psi_T | c \rangle$$

$$\langle \Psi_T | \exp[-\tau H] | c \rangle$$

$$\langle \Psi_T | \exp[-2\tau H] | c \rangle$$

$$\langle \Psi_T | \exp[-3\tau H] | c \rangle$$

8000 steps

$10^4$ to $10^6$ samples from a possible $2^{228}$ possibilities,
What should we look at?

Structure Factor

\[ S_C(q) = \frac{1}{L^2} \sum_{r_i, r_j} e^{i q \cdot (r_i - r_j)} (\langle \hat{n}_i \hat{n}_j \rangle - \bar{n}^2) \]

Peaks in the structure factor <=> charge density wave

Density: Half Filling

Does not extrapolate to zero.
What should we look at?

Structure Factor

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

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**

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

We would like to know if this conducts?

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

\[
\sigma(q) = S_C(q) / 4 \left| \sin \left( \frac{q x}{2} \right) \sin \left( \frac{q y}{2} \right) \right|
\]

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

Strange Metal in superconducting materials

Many Body Localization

Chiral Spin Liquid