Quantum Simulations of Metal-Insulator and Superfluid-Insulator Transitions in the Disordered Hubbard Model

- Experimental and Theoretical Motivation
- The Clean Repulsive Hubbard Model
- Quantum Simulation Techniques
- Mott Insulator and Antiferromagnetic Transitions from QMC
- 2D Metal-Insulator Transitions (Disordered, Repulsive Hubbard)
- 2D Superconductor-Insulator Transitions (Disordered, Attractive Hubbard)
- Conclusions
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Experimental Motivation: Metal-Insulator Transitions

Similar experiments at fixed carrier density but varying magnetic field: Simonian *et al* (1997)

Associated scaling plots again suggest MIT.
Experimental Motivation: Superconductor-Insulator Transitions

Sheet Resistance of Bismuth Films
Thicknesses 4.36 Å (top curve) to 74.27 Å (bottom curve)

Tune with:
- Film Thickness
- O concentration
- Magnetic Field

High Disorder/Field: insulator \((dR/dT > 0)\)
Low Disorder/Field: supercond. \((dR/dT > 0)\)
Is resistance universal at transition?
Theoretical Motivation

Scaling theory of Localization (1979)
Enhanced backscattering from static impurities
No quantum diffusion in two dimensions
Assumes no electron-electron interactions

Later perturbative RG theories (1980’s)
Incorporate electron-electron interactions and disorder
Metallic phase possible
Interaction parameter scales to strong coupling

Quantum Monte Carlo
Incorporates electron-electron interactions and disorder exactly
Finite size lattices: several hundred $e^-$
Finite temperature $T > 0.02W$

Superconductor-Insulator Transitions
Actually, QMC first used to study SC – I rather than MIT
Well defined thermodynamic order parameter $\rho_s$
No restriction on temperature $T$ in simulations
The Hubbard Hamiltonian

\[ H = -t \sum_{\langle i,j \rangle \sigma} (c^\dagger_{i\sigma} c_{j\sigma} + c^\dagger_{j\sigma} c_{i\sigma}) + U \sum_i n_{i\uparrow} n_{i\downarrow} \]

Operators \( c^\dagger_{i\sigma} \) (\( c_{i\sigma} \)) create (destroy) an electron of spin \( \sigma \) on site \( i \).
Includes electron kinetic energy (\( t \)) and interaction energy (\( U \)).

Momentum space

\[ H = \sum_{k\sigma} \epsilon_k c^\dagger_{k\sigma} c_{k\sigma} + U \sum_{k,p,q} c^\dagger_{k+q \uparrow} c^\dagger_{p-q \downarrow} c_{k \uparrow} c_{p \downarrow} \]
\[ \epsilon_k = -2t (\cos k_x + \cos k_y) \]

In two dimensions, bandwidth \( W = 8t \).
on site repulsion \( U \approx 2t - 12t \approx \frac{1}{4} W - \frac{3}{2} W \).
\( \beta = t/T = 1/T = 10 \) means \( T \approx t/10 \approx W/80 \).
Mott Insulator and Antiferromagnetism

$U/t$ large and $\langle n \rangle = 1$.
All sites occupied by exactly one $e^−$.
Hopping causes double occupancy, costs $U$.
Two ways to destroy:
* decrease $U/t$
* dope: shift $\langle n \rangle \neq 1$

What is optimal spin arrangement?
Hopping of neighboring parallel spins forbidden by Pauli.
Antiparallel arrangement lower in second order perturbation theory.
In Hubbard model insulating behavior and antiferromagnetism go hand-in-hand.

$\Delta E^{(2)} = 0$
$\Delta E^{(2)} = -t^2/U = -J$
Classical Monte Carlo

Energy of set of degrees of freedom $x_i$:

$$E = \sum_{i}^{N} x_i \sum_{j \in \mathcal{N}(i)} \kappa_{ij} x_j$$

$E$ is often local: $x_i$ couples only to $x_j$ only in some neighborhood $\mathcal{N}(i)$.

Suggest change $x_i \rightarrow x'_i$.

Throw a random number $0 < r < 1$. If

$$r < e^{-\Delta E/T},$$

then accept the change.

If $\mathcal{N}(i)$ is independent of system size, so is time to update $x_i$. 
Quantum Monte Carlo

Classical Boltzmann weight, an exponential of a number, $E$, becomes the exponential of an operator, $\hat{H}$ which can be expressed as a path integral:

$$ e^{-\beta E} \rightarrow e^{-\beta \hat{H}} = e^{-\tau \hat{H}} e^{-\tau \hat{H}} e^{-\tau \hat{H}} \ldots e^{-\tau \hat{H}} $$

Extra “imaginary time” dimension of extent $\beta = 1/T$. If $\hat{H}$ is local, time is still linear in spatial lattice size. Cost is only extra dimension of lattice, a factor $\propto 1/T$.

This works for quantum spins and bosons (unfrustrated lattices).
But, “sign problem” for fermions.
If electron world lines exchange,
the contribution to partition
function is negative !!!

(Partial) solution: “Determinant” Quantum Monte Carlo.
Still have simulation in space and imaginary time,
Scales as cube of spatial size. Accessible systems $N_{el} \approx 200$. Lingering sign problem.
Within those limitations, provide exact solution of problem of disorder+interactions.

Peter Reynolds, QMC and sign problem for continuum models, eg nodes of He atom wavefunction [PRL 95, 110201 (2005)].

“Dynamical Mean Field Theory” (Kotliar)
Determinant Quantum Monte Carlo Results at half-filling $\langle n_{j\uparrow} + n_{j\downarrow} \rangle = 1$

Magnetic moment formation with $T$ and $U$

$$\langle m_z^2 \rangle = \langle (n_{j\uparrow} - n_{j\downarrow})^2 \rangle = 1 - 2 \langle n_{j\uparrow} n_{j\downarrow} \rangle .$$
Spin Correlations (8x8 lattice)

\[ \langle c(l) \rangle = \langle (n_{j+\uparrow} - n_{j+\downarrow})(n_{j\uparrow} - n_{j\downarrow}) \rangle \]

Local moment \( \langle m_z^2 \rangle \) is just \( c(l = 0) \).
Antiferromagnetic Structure factor

\[ S(Q) = \sum_l e^{iQl} \langle c(l) \rangle \]
Specific Heat

\[ U = 10 \]

- finite difference
- exponential fit
- \( t=0 \)
- Heisenberg Model

\[ C(T) \]

\[ T \]

0-14
Density of States

All of the preceding data at “half-filling” (one electron per lattice site).
This is a density where a special “particle-hole” symmetry of the Hubbard Hamiltonian prevents the sign problem.
$s^*$- and $d$-wave pairing vertices when doped away from half-filling
$\Gamma \to -1$ signals superconductivity.

* $d$-wave is dominant superconducting instability [Dagotto, $t-J$ models]
* But cannot reach low enough $T$ (sign problem) [But see Jarrell and Scalapino, DCA]

$N=8\times8$ lattice

$N=2\times2$ lattice

$\langle S \rangle \to 0$ exponentially with $N, 1/T$
Similar Results for Three Dimensional Hubbard Model

No disorder or Zeeman Field
Mott Insulator at half-filling
\((\rho = 1 \text{ } e^- \text{ per site})\)

Antiferromagnetic spin correlations

Kotliar: Three peak \(N(\omega)\) with AF splitting of central peak.
Now let’s consider effect of disorder on clean Hubbard model:

* How does disorder affect metallic phases away from half-filling?

Actually, we will rephrase this question:

Start with disordered model at $U = 0$:

* How do interactions affect Anderson insulating phases away from half-filling?

Separately, at half-filling:

* How does disorder affect AF Mott insulator at half-filling?
Effect of Interactions on the Anderson Insulator (quarter filling)

2-d hopping Hamiltonian with random bonds:

\[ H = - \sum_{\langle i,j \rangle, \sigma} t_{i,j} (c_{i\sigma}^\dagger c_{j\sigma} + c_{j\sigma}^\dagger c_{i\sigma}) \]

1 \(-\Delta t < t_{i,j} < 1 + \Delta t\)

What is the effect of turning on interactions

\[ H \rightarrow H + U \sum_i n_{i\uparrow} n_{i\downarrow} \]

\(\sigma_{dc}\) rises as \(T\) is lowered.

Metal-insulator transition (tuned by interaction strength?)

\(\Delta_t = 2\)
Effect of Increased Disorder on the Metal (quarter filling)

\[ H = - \sum_{\langle i,j \rangle_\sigma} t_{i,j} (c_{i\sigma}^\dagger c_{j\sigma} + c_{j\sigma}^\dagger c_{i\sigma}) \]

System returns to insulating.
Metal-insulator transition tuned by disorder strength?
Field-Tuned Metal-Insulator Transition

Hubbard Hamiltonian with a (Zeeman) magnetic field,

\[ H = - \sum_{\langle i,j \rangle \sigma} t_{i,j} (c_{i\sigma}^\dagger c_{j\sigma} + c_{j\sigma}^\dagger c_{i\sigma}) + U \sum_i n_{i\uparrow} n_{i\downarrow} + B_{||} \sum_i (n_{i\uparrow} - n_{i\downarrow}) \]

As \( B_{||} \) is turned on, metallic phase is destroyed.

Spin polarization reduces effective interaction \( U \).
Location of Critical Point

Large $B_{||}$ and nonzero disorder: conductivity $\sigma_{dc}$ should vanish. (Effectively, no interactions).
Subtract large $U$ piece of $\sigma_{dc}$ to correct for finite $N$ and $T$.
$\delta\sigma_{dc} \to 0$ for $B_{||} \approx 0.4 \ t$.
Alternatively, look at crossing of $\rho$ vs. $B_{||}$. 

\begin{figure}
\centering
\includegraphics[width=\textwidth]{figure.png}
\caption{Graphs showing $\delta \sigma_{dc}$ and $\rho$ vs. $B_{||}$.}
\end{figure}
Resistivity Saturation Occurs Below Point of Full Spin Polarization

Examine $\Delta_t = 2.0 \, t$, (close to $\Delta_t(\text{crit}) = 2.4 \, t$ where bond disorder destroys metal). Zeeman field does not need to be very big to drive to insulator.

Get insulator well before full spin polarization.
Particle-Hole Symmetry One

Particle-hole mapping repulsive fermion Hubbard model (symmetry about half-filling)

\[ c_{i\sigma} \quad (-1)^i c_{i\sigma}^\dagger \]

\[ n_{i\sigma} \quad 1 - n_{i\sigma} \]

\[-t_{ij} (c_{j\downarrow}^\dagger c_{i\downarrow} + c_{i\downarrow}^\dagger c_{j\downarrow}) \quad -t_{ij} (c_{j\downarrow}^\dagger c_{i\downarrow} + c_{i\downarrow}^\dagger c_{j\downarrow}) \quad \text{(for bipartite lattice)}\]

\[ U(n_{i\uparrow} - \frac{1}{2})(n_{i\downarrow} - \frac{1}{2}) \quad U(n_{i\uparrow} - \frac{1}{2})(n_{i\downarrow} - \frac{1}{2}) \quad \text{(p-h symmetric)}\]

Hamiltonian unchanged except for chemical potential.

Physics at \( \rho \) and \( 1 - \rho \) (equivalently \( \mu \) and \( -\mu \)) identical!

What about disorder?

Bond and site disorder are fundamentally different!

* \( t_{ij} \) term doesn’t change sign.

* \( \mu_i \) term does.
Effect of Increased Disorder on the Mott Insulator (half filling)

We saw: Hubbard model at quarter filling (\( \rho = \frac{1}{2} \) electron/site): Interactions cause Anderson insulator to go metallic. Further increase of bond disorder converts back to insulator. Interactions and disorder compete. At half-filling, (\( \rho = 1 \) electron/site): Mott-Hubbard insulator. Electrons already localized to avoid \( U \). Effect of bond disorder?

Mott-Hubbard Insulator more robust. Conductivity turns downward more strongly as \( T \) is lowered.

Interactions and disorder cooperate. Bond disorder does destroy long-range antiferromagnetism.
Particle Hole Symmetry


Site disorder:

\[ \sum_i \mu_i (n_{i\uparrow} + n_{i\downarrow}) \quad -\Delta \mu < \mu_i < +\Delta \mu \]

Not particle-hole symmetric. Destroys the Mott-Hubbard insulator.

To test: ‘Random Zeeman fields’.

\[ \sum_i \mu_i (n_{i\uparrow} - n_{i\downarrow}) \quad -\Delta' \mu < \mu_i < +\Delta' \mu \]

Particle-hole symmetric.

Cooperate with Mott insulator.
Another View of Particle-Hole Symmetry

Examine the Mott-Hubbard gap by evaluating $\rho(\mu)$

Particle-hole symmetric disorder, $\Delta_t = 2t$ and $\Delta'_\mu = 2t$, Mott gap enlarges.

Canonical site disorder has little effect, for $\Delta_\mu = 2t$. 
Particle-Hole Symmetry Two

“Attractive” \((-|U|)\) fermion Hubbard model

Allows interpolation (with \(|U|\)) between

- Large \(|U|\): Short coherence length/bosons/BEC
- Small \(|U|\): Large coherence length/fermions/BCS

Particle-hole mapping between attractive and repulsive fermion Hubbard model

\[
\begin{align*}
\text{\(c_i\downarrow\)} & \quad \text{\((-1)^i c_i^\dagger\)} & \quad \text{for \(\downarrow\) only!} \\
\text{\(n_i\downarrow\)} & \quad \text{\(1 - n_i\downarrow\)} \\
-t_{ij} \left( c_{j\downarrow}^\dagger c_{i\downarrow} + c_{i\downarrow}^\dagger c_{j\downarrow} \right) & \quad -t_{ij} \left( c_{j\downarrow}^\dagger c_{i\downarrow} + c_{i\downarrow}^\dagger c_{j\downarrow} \right) & \quad \text{(for bipartite lattice)} \\
U(n_{i\uparrow} - \frac{1}{2})(n_{i\downarrow} - \frac{1}{2}) & \quad -U(n_{i\uparrow} - \frac{1}{2})(n_{i\downarrow} - \frac{1}{2}) & \quad \text{(p-h symmetric)} \\
S_j^+ = c_{j\uparrow}^\dagger c_{j\downarrow} & \quad \Delta_j^\dagger = (-1)^j c_{j\uparrow}^\dagger c_{j\downarrow}^\dagger & \quad \text{SC correlations} \\
S_j^z = n_{j\uparrow} - n_{j\downarrow} & \quad n_j = n_{j\uparrow} + n_{j\downarrow} & \quad \text{CDW correlations}
\end{align*}
\]
Site disorder term in Hamiltonian

\[ \sum_i v_i n_i \quad -\frac{V}{2} < v_i < +\frac{V}{2} \]

Below: \( V = 0, 0.5, 1, 2, 3, 4. \)

(s-wave) pair correlations \( P_s(l) = \langle \Delta_{j+l} \Delta_j^\dagger \rangle \) driven to zero.

As are Drude-weight \( D \) and superfluid stiffness \( D_s \).

Resistivity $\rho(T)$ also signals the transition

Value of resistance at separatrices is non-universal? $V_c$ from resistivity separatrix consistent with value from vanishing of $D$ and $D_s$.

Units: $e^2 = \hbar = 1$ so $\rho_Q = \hbar/4e^2 = \pi/2$. 
Crossing plots $\rho(V)$ locate critical point more precisely.

Again, intersection point $\rho_c$ appears to be non-universal.
CONCLUSIONS

Quantum Monte Carlo shows evidence for M-I Transition in the disordered repulsive Hubbard model
* As a function of interaction strength $U$
* As a function of degree of disorder
* As a function of magnetic field
* Field-driven MIT occurs prior to full spin polarization
* Particle–Hole symmetry appears to play an important role

Quantum Monte Carlo shows evidence for SC-I Transition in the disordered attractive Hubbard model
* Static disorder can destroy SC if strong enough.

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Simple “Stoner” Picture of Magnetic Order

Interaction energy lowered by polarizing the spins:

$$\delta PE = U(N + \delta N)(N - \delta N) - UN^2 = -U(\delta N)^2 = -UN(E_F)\delta N\delta E$$

Kinetic energy raised by polarizing the spins:

$$\delta KE = +\delta N\delta E$$

Total Energy change:

$$\delta E = \delta KE + \delta PE = [1 - UN(E_F)]\delta N\delta E$$

Stoner Criterion: $UN(E_F) > 1 \rightarrow$ magnetism!

Density of states

$$N(E_F) = \delta N/\delta E \propto 1/t$$
Many analytic treatments.

One example: Mean-field theory.

\[ U n_{i\uparrow} n_{i\downarrow} \rightarrow U \left[ n_{i\uparrow} \langle n_{i\downarrow} \rangle + \langle n_{i\uparrow} \rangle n_{i\downarrow} - \langle n_{i\uparrow} \rangle \langle n_{i\downarrow} \rangle \right] \]

Equivalent to Random Phase Approximation

\[ \chi(q, \omega) = \frac{\chi_0(q, \omega)}{1 - U \chi_0(q, \omega)} \]

\[ \chi_0(q, \omega) = \sum_p \frac{f(\epsilon_k) - f(\epsilon_{k+q})}{\omega - (\epsilon_k - \epsilon_{k+q})} \]

Fermi function: \[ f(\epsilon_k) = \left[ e^{-\beta(\epsilon_k - \mu)} + 1 \right]^{-1} \].

Important failure:

\[ T_{\text{Neel}} \propto U \text{ at large } U. \]

Instead, \[ T_{\text{Neel}} \propto J = t^2/U \text{ at large } U. \]

MFT confuses temperature scales:

- Moment-formation \( U \).
- Moment-ordering \( J = t^2/U \).