UCDAVIS

Metal-Insulator Transitions in Two Dimensions: Quantum Monte Carlo Studies

- Experimental and Theoretical Motivation
- The Hubbard Model
- Quantum Simulation Techniques
- 2D Superconductor – Insulator Transitions
- 2D Metal – Anderson Insulator Transitions
- 2D Metal – Mott Insulator Transitions
- Field – Tuned Transitions
- Conclusions

Collaborators

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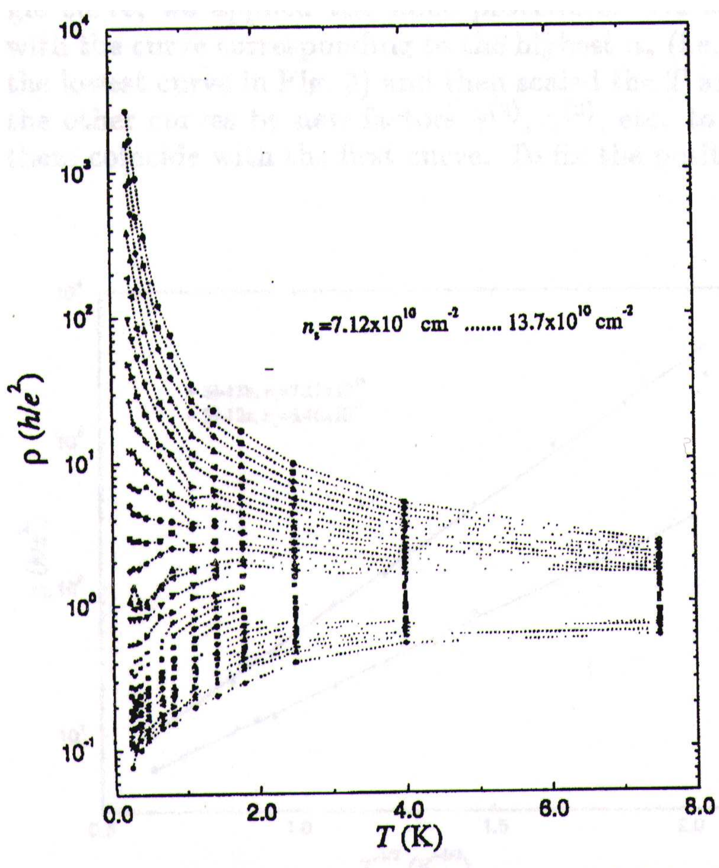
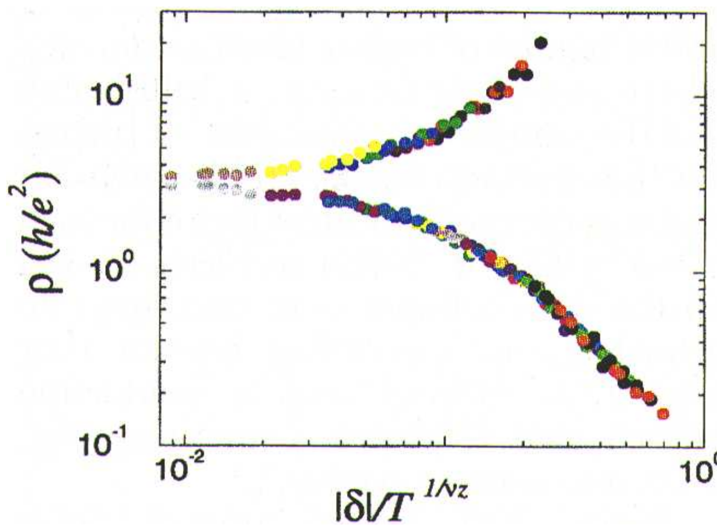
Experimental Motivation

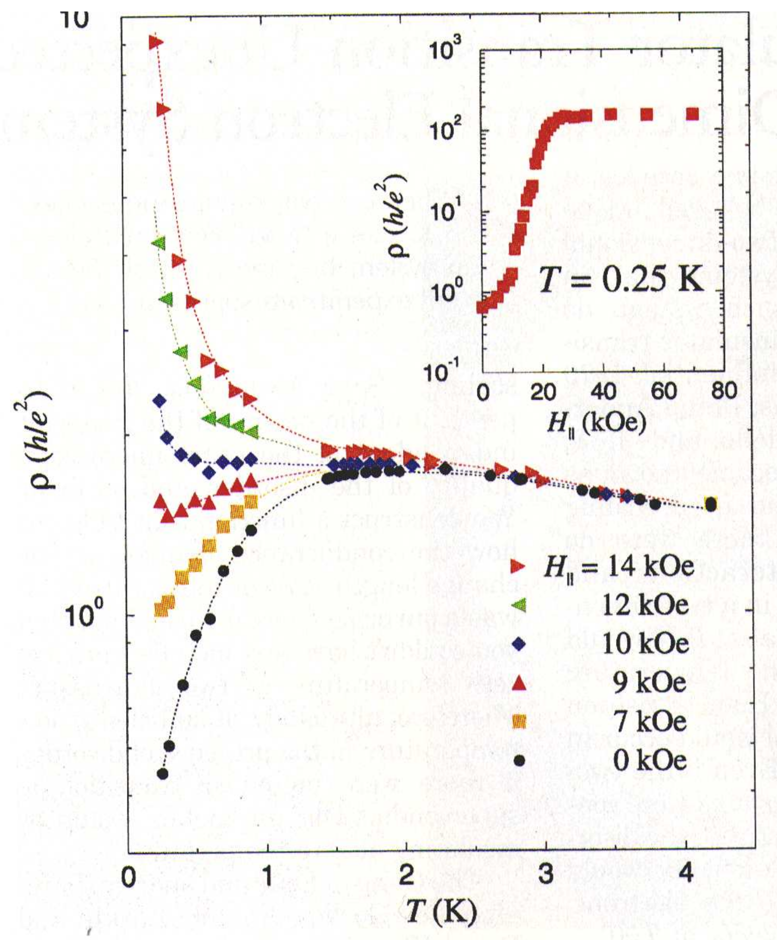
High mobility silicon MOSFETS show evidence for MIT.
Kravchenko *etal* (1994)





Scaling behavior strengthens case for separate metal/insulator phases.

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



Associated scaling plots again suggest MIT.

Theoretical Motivation

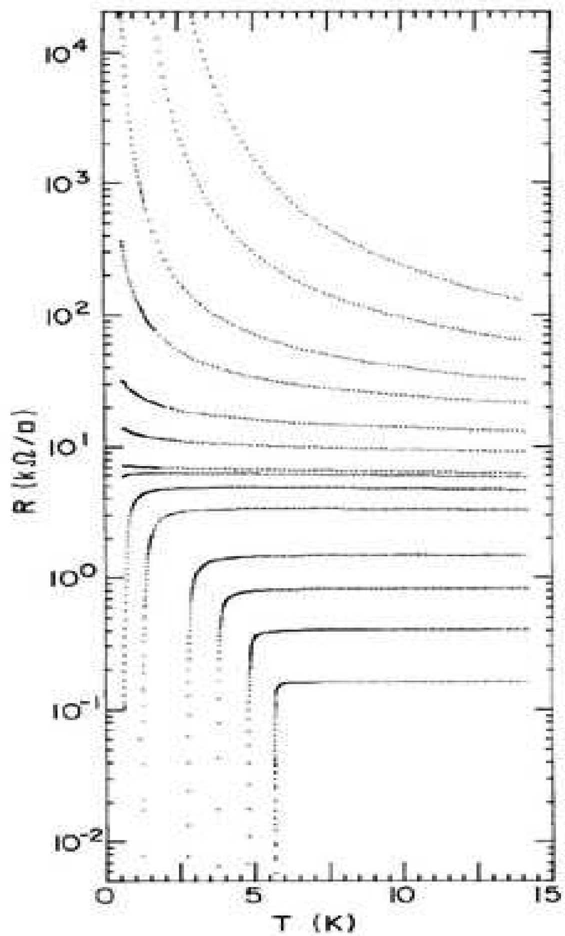
Scaling theory of Localization (1979)
Enhanced backscattering from static impurities
No quantum diffusion in two dimensions
Assumes no electron-electron interactions
Later perturbative RG theories (1980's)
Incorporate electron-electron interactions and disorder
Metallic phase possible
Interaction parameter 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 ρ_s
No restriction on temperature T in simulations

Sheet Resistance of Bismuth Films

Thicknesses 4.36 Å (top curve) to 74.27 Å (bottom curve)

Y. Liu *etal* (1991)



HUBBARD HAMILTONIAN

$$-\sum_{\langle \mathbf{i},\mathbf{j}\rangle\sigma} t_{\mathbf{ij}}\,(\,c^{\dagger}_{\mathbf{i}\sigma}c_{\mathbf{j}\sigma} + c^{\dagger}_{\mathbf{j}\sigma}c_{\mathbf{i}\sigma}\,)$$

Kinetic Energy $+1-\Delta_t \,<\, t_{\mathbf{ij}} \,<+1+\Delta_t$

$$+\sum_{\mathbf{i}} \epsilon_{\mathbf{i}}\,(\,n_{\mathbf{i}\uparrow} + n_{\mathbf{i}\downarrow}\,)$$

Chemical Potential $-\Delta_\mu \,<\, \epsilon_{\mathbf{i}} \,<+1+\Delta_\mu$

$$+U\sum_{\mathbf{i}}\,(\,n_{\mathbf{i}\uparrow}-\frac{1}{2}\,)\,(\,n_{\mathbf{i}\downarrow}-\frac{1}{2}\,)$$

Interaction Energy $U<0$: attractive $U>0$: repulsive

$$+B_{\parallel}\sum_{\mathbf{i}}(n_{\mathbf{i}\uparrow}-n_{\mathbf{i}\downarrow})$$

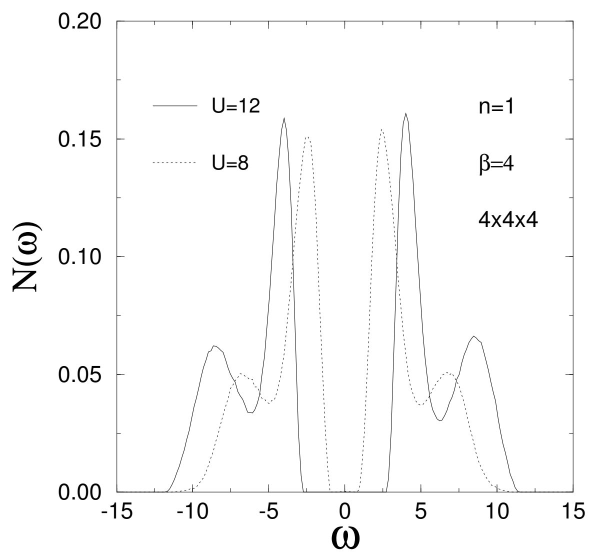
Zeeman Field

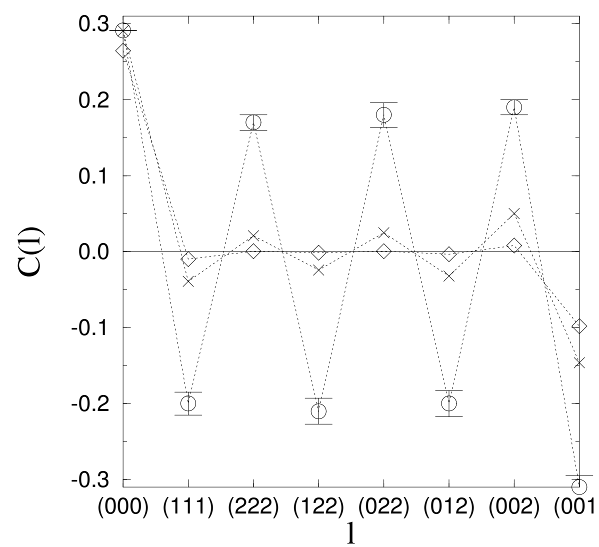
HUBBARD HAMILTONIAN- BASIC PHYSICS

(NO DISORDER OR ZEEMAN FIELD)

Mott Insulator at half-filling ($\rho = 1\ e^-$ per site)

Antiferromagnetic spin correlations





Away from half-filling: paramagnetic metal (d-wave superconductor?)
Stripes (charge inhomogeneities)?
U very large: ferromagnetic phases.

HUBBARD HAMILTONIAN- BASIC PHYSICS

WITH DISORDER (AND ZEEMAN FIELD)

?????

No interactions ($U = 0$)	With interactions ($U \neq 0$)
Anderson Insulator	Delocalize electrons

Zeeman field: Reduce U, return to insulator

DETERMINANT QUANTUM MONTE CARLO

Basic Features

Exact Treatment of interactions, disorder, ...

Can measure any finite T quantity $\langle c^{\dagger}_{\mathbf{i}\sigma_1} c^{\dagger}_{\mathbf{j}\sigma_2} \ldots c_{\mathbf{k}\sigma_3} c_{\mathbf{l}\sigma_4} \ldots \rangle$

Dynamics (real time) response more difficult (analytic continuation)

Systems of up to $\approx 4 \times 10^2$ electrons

In some models, down to zero T, in others $T > 0.02\ W$.

Technical Details

Path integral for partition function $Z = e^{-\beta H}$

Interaction terms decoupled with Hubbard-Stratonovich field $x(\mathbf{l}\tau)$

Non-interacting electrons moving in (classical) auxiliary field

Integrate out the electrons analytically

$Z = \int \mathcal{D}x(\mathbf{l}\tau)\ \mathrm{det}M_{\uparrow}(x)\ \mathrm{det}M_{\downarrow}(x)$

Monte Carlo sampling over this field

Eliminate 'Trotter error': $\beta = L\Delta\tau$ by taking $\Delta\tau \rightarrow 0$.

OBSERVABLES

Kinetic Energy

$$\langle - \sum_{\langle \mathbf{i},\mathbf{j} \rangle \sigma} t_{\mathbf{i}\mathbf{j}} (c^{\dagger}_{\mathbf{i}\sigma} c_{\mathbf{j}\sigma} + c^{\dagger}_{\mathbf{j}\sigma} c_{\mathbf{i}\sigma}) \rangle$$

Potential Energy/Local moment

$$\langle \, (n_{\mathbf{i}\uparrow} - \frac{1}{2})(n_{\mathbf{i}\downarrow} - \frac{1}{2}) \, \rangle = \frac{1}{4} - \langle \, (n_{\mathbf{i}\uparrow} - n_{\mathbf{i}\downarrow})^2 \, \rangle$$

Compressibility

$$\kappa = \partial n / \partial \mu$$

Real space charge, spin, pairing correlations /structure factors

$$\langle n_{\mathbf{l}+\mathbf{j}} n_{\mathbf{l}} \rangle \qquad \langle m_{\mathbf{l}+\mathbf{j}} m_{\mathbf{l}} \rangle \qquad \langle \Delta^{s}_{\mathbf{l}+\mathbf{j}} \Delta^{s\,\dagger}_{\mathbf{l}} \rangle$$

$$n_{\mathbf{l}} = c^{\dagger}_{\mathbf{l}\uparrow} c^{\dagger}_{\mathbf{l}\uparrow} + c^{\dagger}_{\mathbf{l}\downarrow} c^{\dagger}_{\mathbf{l}\downarrow} \qquad m_{\mathbf{l}} = c^{\dagger}_{\mathbf{l}\uparrow} c_{\mathbf{l}\downarrow} \qquad \Delta^{s\,\dagger}_{\mathbf{l}} = c^{\dagger}_{\mathbf{l}\uparrow} c^{\dagger}_{\mathbf{l}\downarrow}$$

Current-current correlation function

$$\Lambda_{xx}(\mathbf{q}; i\omega_n) = \sum_{\mathbf{l}} \int_0^\beta d\tau \langle j_x(\mathbf{l}, \tau) j_x(0,0) \rangle e^{i\mathbf{q}\cdot\mathbf{l}} e^{-i\omega_n \tau}$$

$$j_x(\mathbf{l}\,\tau) = e^{H\tau} \left[it \sum_\sigma (c^\dagger_{\mathbf{l}+\hat{x},\sigma} c_{\mathbf{l},\sigma} - c^\dagger_{\mathbf{l},\sigma} c_{\mathbf{l}+\hat{x},\sigma}) \right] e^{-H\tau}$$

Conductivity

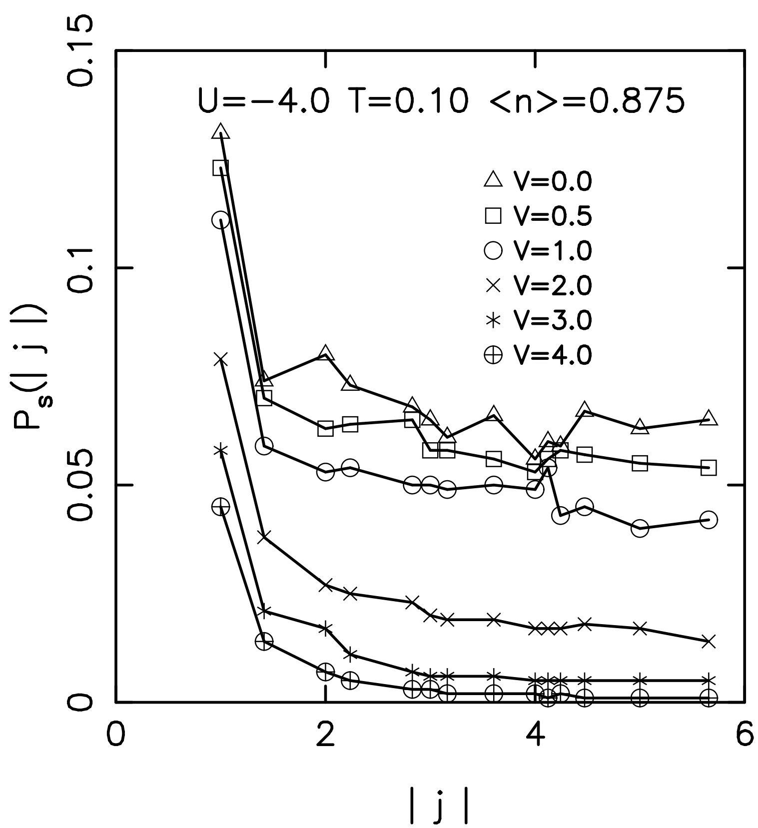
$$\sigma_{\mathrm{dc}} = \frac{\beta^2}{\pi} \Lambda(\tau = \beta/2)$$

EFFECT OF DISORDER ON PAIR CORRELATIONS IN THE ATTRACTIVE HUBBARD MODEL

Δ_μ=0: long range pair correlations (SC) at low T.

$$P^s_{\mathbf{j}} = \langle \Delta^s_{\mathbf{l}+\mathbf{j}} \Delta^{s\,\dagger}_{\mathbf{l}} \rangle$$
$$\Delta^{s\,\dagger}_{\mathbf{l}} = c^\dagger_{\mathbf{l}\uparrow} c^\dagger_{\mathbf{l}\downarrow}$$

$\Delta_\mu \neq 0$: Pair correlations are driven to zero.



Longitudinal Current-Current Correlation Function

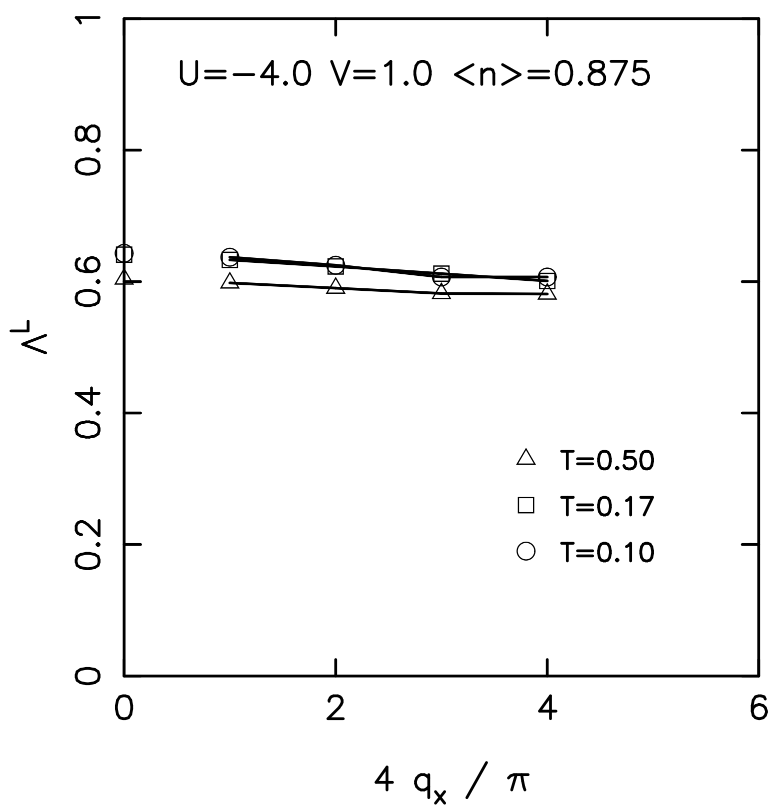
Current-current correlation function:

$$\Lambda_{xx} \quad (\quad \mathbf{q}; i\omega_n) = \sum_{\mathbf{l}} \int_0^\beta d\tau \langle j_x(\mathbf{l}, \tau) j_x(0,0) \rangle e^{i\mathbf{q}\cdot\mathbf{l}} e^{-i\omega_n \tau},$$

$$j_x \quad (\quad \mathbf{l}\,\tau) = e^{H\tau} \left[it \sum_\sigma (c^\dagger_{\mathbf{l}+\hat{x},\sigma} c_{\mathbf{l},\sigma} - c^\dagger_{\mathbf{l},\sigma} c_{\mathbf{l}+\hat{x},\sigma}) \right] e^{-H\tau}.$$

The longitudinal part must satisfy the equality,

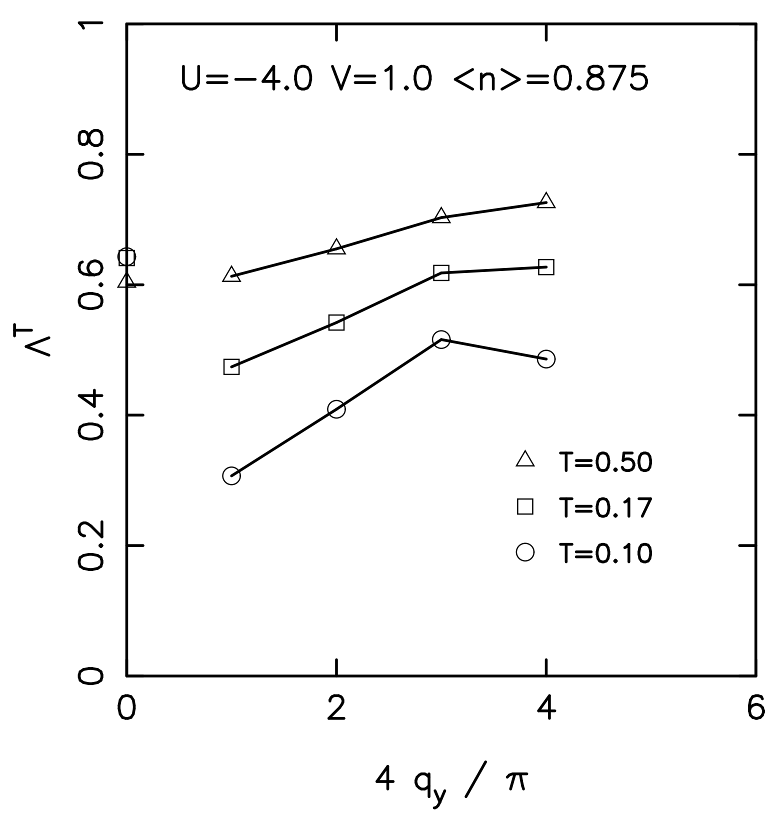
$$\Lambda^{\rm L} \equiv \lim_{q_x \to 0} \; \Lambda_{xx}(q_x, q_y = 0; i\omega_n = 0) = -K_x.$$

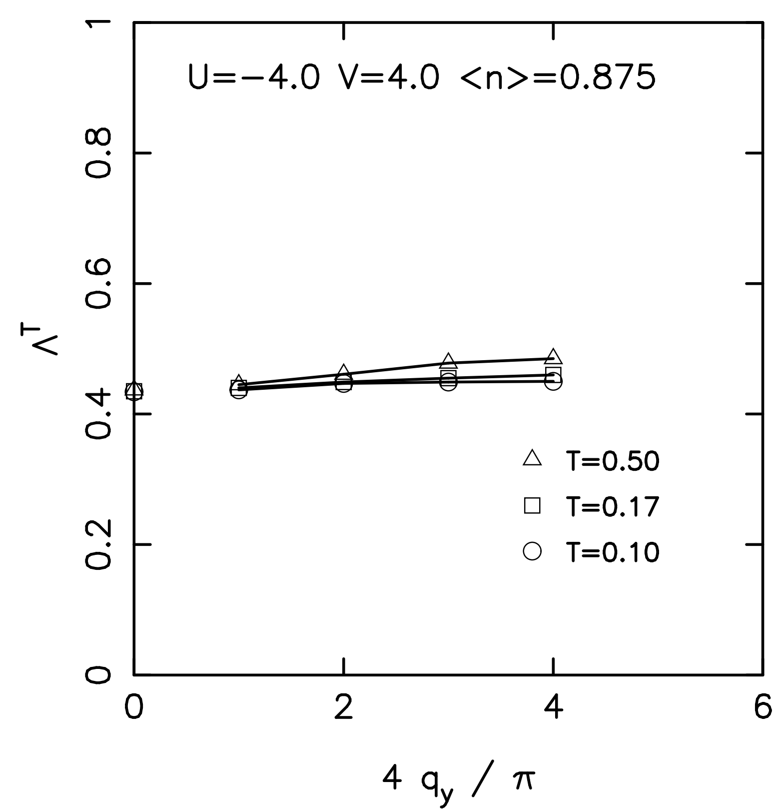


Transverse Current-Current Correlation Function

The transverse part measures the superfluid stiffness,

$$\begin{aligned} \Lambda^{\mathrm{T}} &\equiv \lim_{q_y \to 0} \Lambda_{xx}(q_x = 0, q_y; i\omega_n = 0) \\ \rho_s &= [\Lambda^{\mathrm{L}} - \Lambda^{\mathrm{T}}] = [K_x - \Lambda^{\mathrm{T}}]. \end{aligned}$$



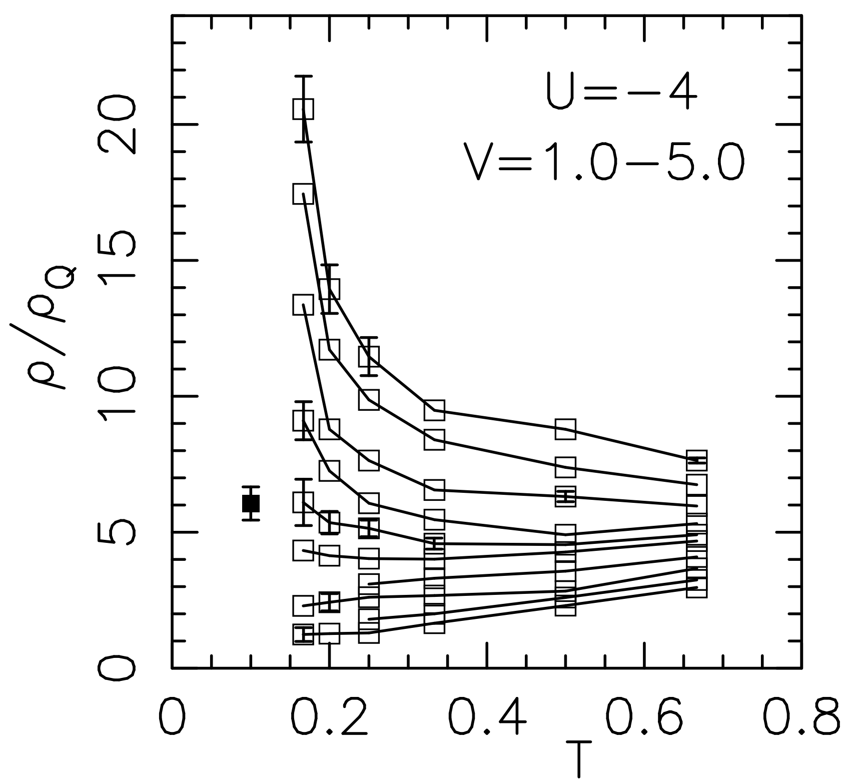


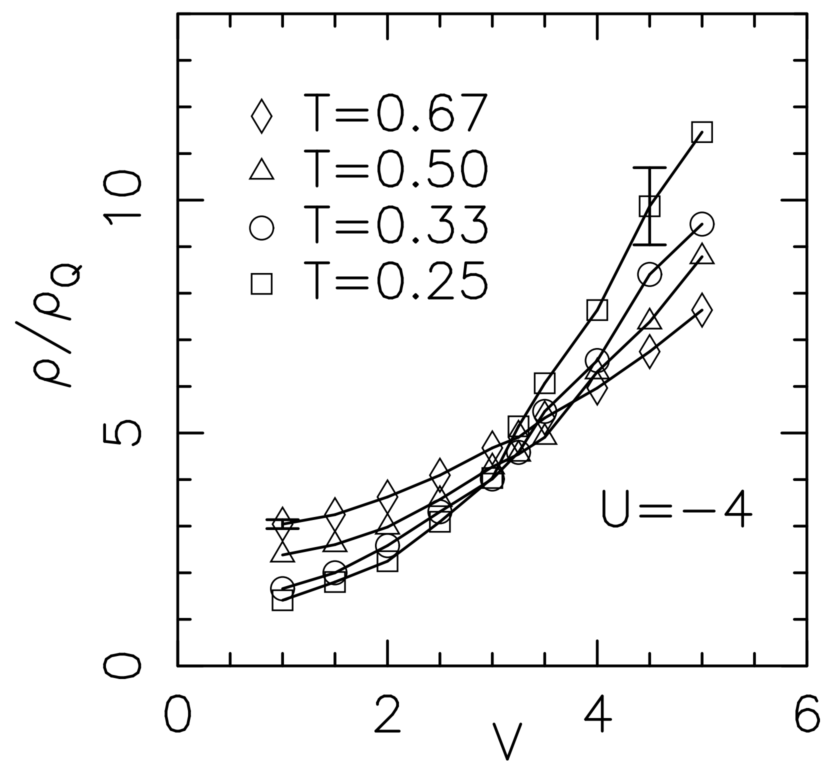
Transport Evidence for the Superconductor-Insulator Phase Transition

$$\Lambda(\tau) = \int_{-\infty}^{+\infty} \frac{d\omega}{\pi} \frac{\exp(-\omega\tau)}{[1 - \exp(-\beta\omega)]} \mathrm{Im}\Lambda(\omega)$$

In the normal state, $\mathrm{Im}\Lambda(\omega) \sim \omega\sigma_{\mathrm{dc}}$ at low frequencies,

$$\sigma_{\mathrm{dc}} = \beta^2/\pi \quad \Lambda(\tau = \beta/2).$$



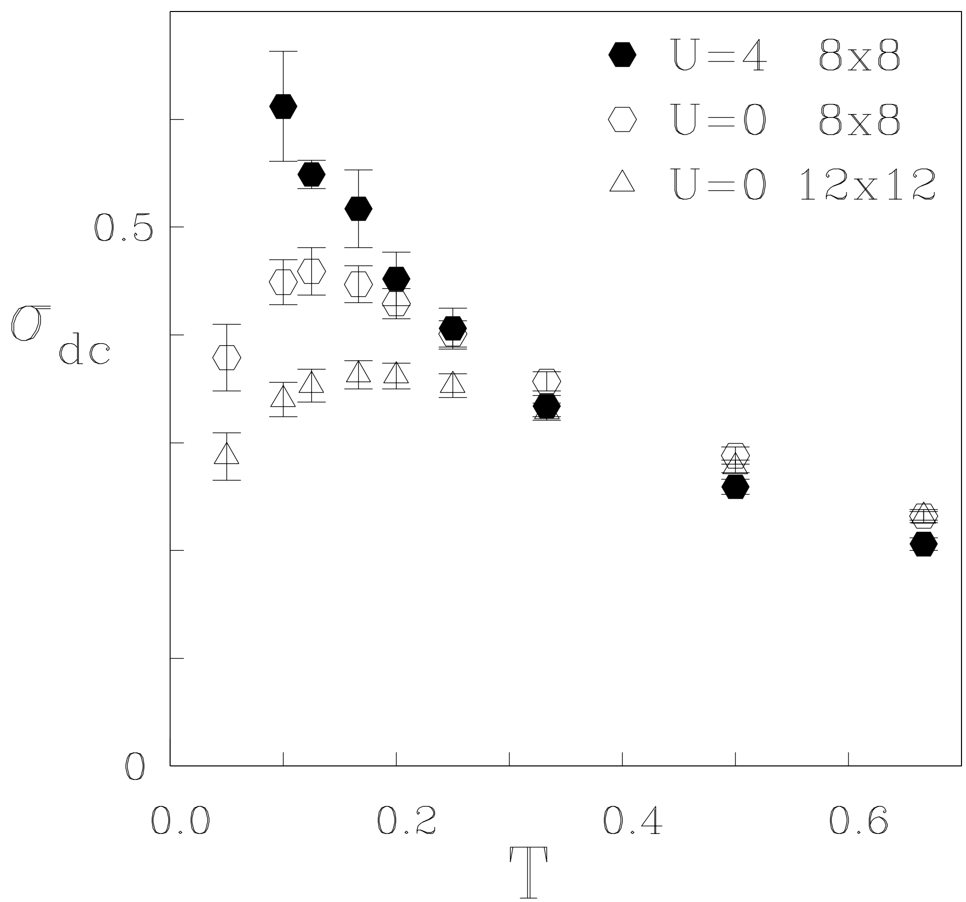


REPULSIVE HUBBARD MODEL

Effect of Interactions on the Anderson Insulator

$$H = -\sum_{\langle \mathbf{i},\mathbf{j}\rangle\sigma} t_{\mathbf{i},\mathbf{j}} (c^{\dagger}_{\mathbf{i}\sigma} c_{\mathbf{j}\sigma} + c^{\dagger}_{\mathbf{j}\sigma} c_{\mathbf{i}\sigma}) \qquad 1 - \Delta_t < t_{\mathbf{i},\mathbf{j}} < 1 + \Delta_t$$

When U is turned on, conductivity rises as T is lowered.



$\Delta_t = 2$

$\rho = 1/2$

Effect of Increased Disorder on the Metal

Increase disorder strength in metallic phase.

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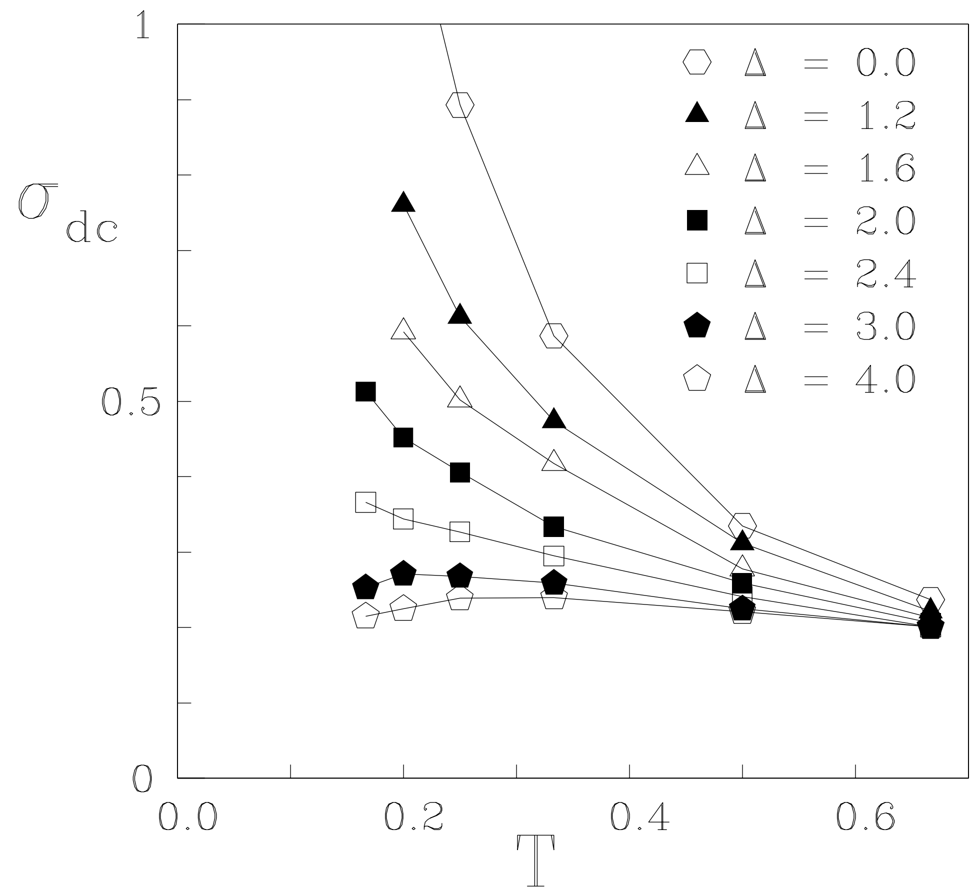
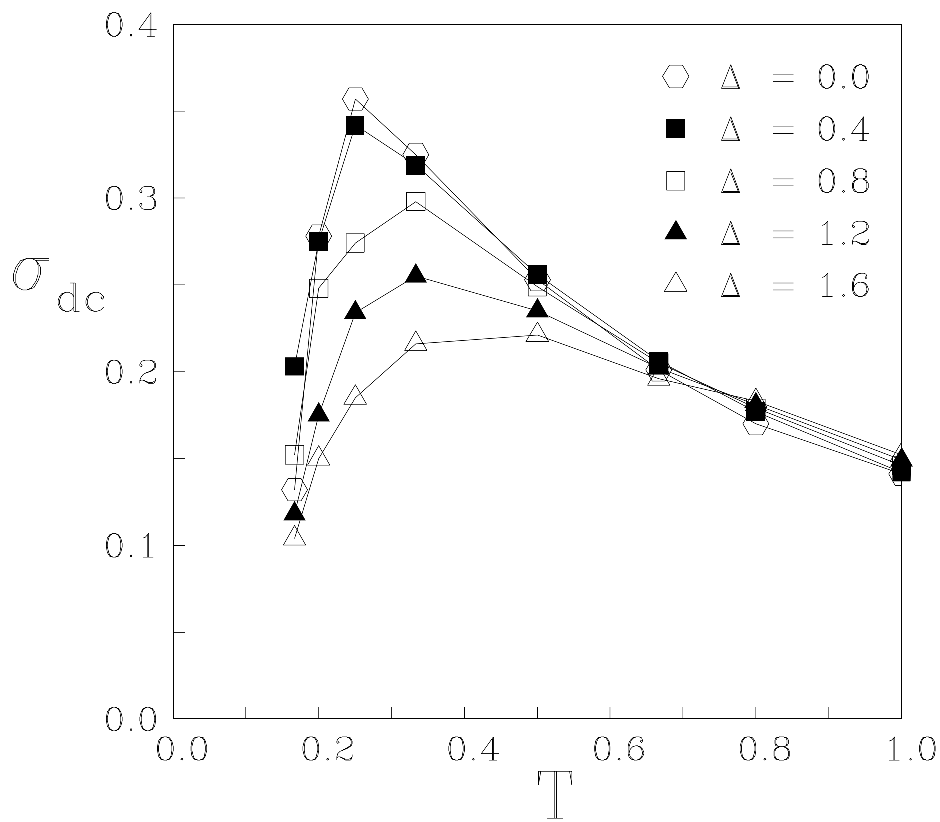
$$H = - \sum_{\langle \mathbf{i},\mathbf{j} \rangle \sigma} t_{\mathbf{i},\mathbf{j}} \, (\, c^{\dagger}_{\mathbf{i}\sigma} c_{\mathbf{j}\sigma} + c^{\dagger}_{\mathbf{j}\sigma} c_{\mathbf{i}\sigma} \,)$$

System returns to insulating. MIT (tuned by disorder strength).



Disordered Mott-Hubbard Insulator

We just showed: Hubbard model at quarter filling ($\rho = 1/2$):
Interactions cause Anderson insulator to go metallic.
Further increase of bond disorder converts back to insulator.
Interactions and disorder compete.
At half-filling, (($\rho = 1$) Mott-Hubbard insulator.
Electrons localize to avoid double occupation. Effect of bond disorder?



Bond disorder makes the 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

Bond disorder: particle-hole symmetric.

Bond disorder strengthens Mott-Hubbard insulator.

Site disorder

$$\sum_{\mathbf{i}} \mu_{\mathbf{i}}(n_{\mathbf{i}\uparrow} + n_{\mathbf{i}\downarrow}) \qquad -\Delta_\mu < \mu_{\mathbf{i}} < +\Delta_\mu$$

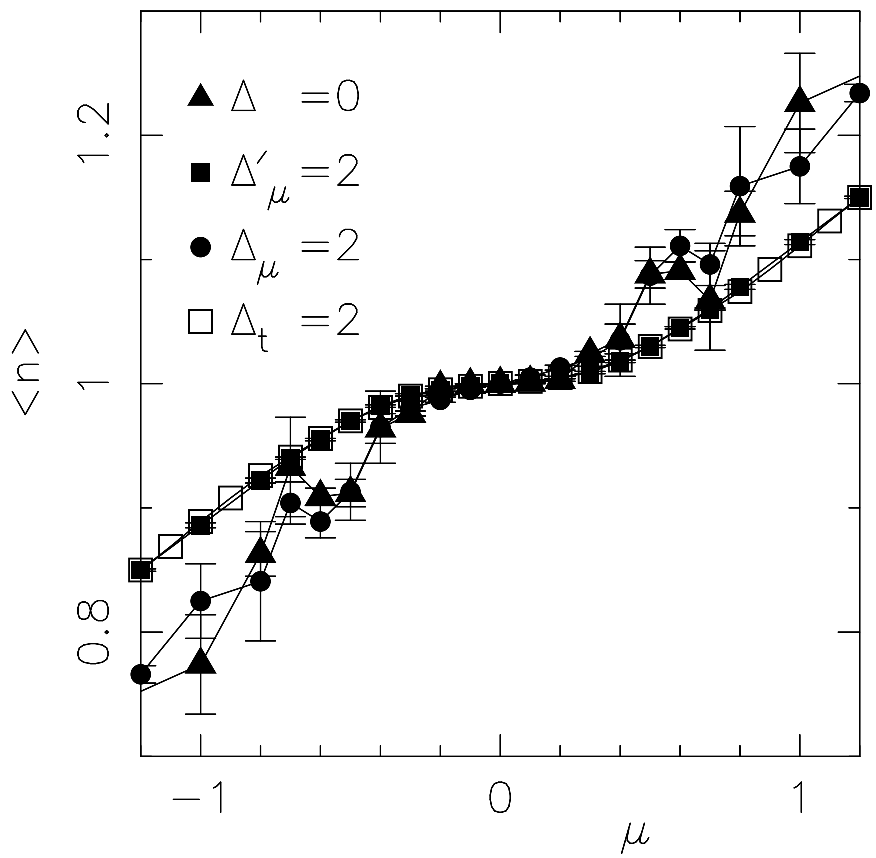
not particle-hole symmetric. It destroys the Mott-Hubbard insulator.

Another View of Particle-Hole Symmetry

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

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

Canonical site disorder has little effect, for $\Delta_\mu = 2t = U/2$.



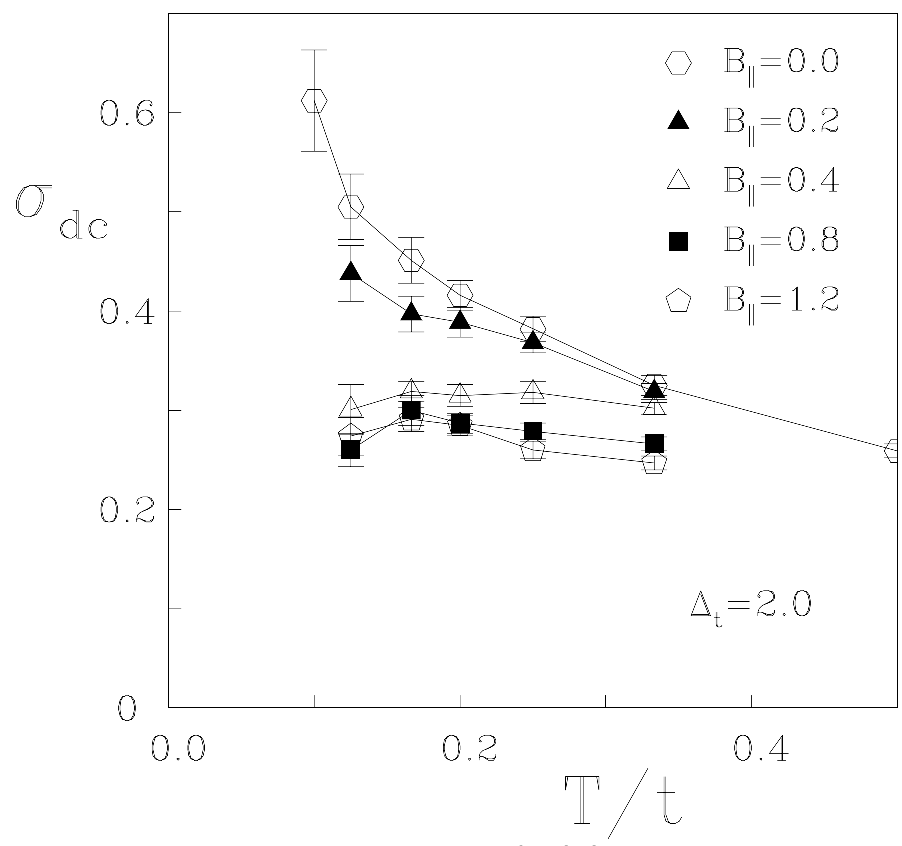
Field Tuned Metal Insulator Transition

Hubbard Hamiltonian with a (Zeeman) magnetic field,

$$H = -\sum_{\langle \mathbf{i},\mathbf{j}\rangle\sigma} t_{\mathbf{i},\mathbf{j}}(c^{\dagger}_{\mathbf{i}\sigma}c_{\mathbf{j}\sigma} + c^{\dagger}_{\mathbf{j}\sigma}c_{\mathbf{i}\sigma}) + U\sum_{\mathbf{i}} n_{\mathbf{i}\uparrow}n_{\mathbf{i},\downarrow} + B_{\parallel}\sum_{\mathbf{i}}(n_{\mathbf{i}\uparrow} - n_{\mathbf{i}\downarrow})$$

As $B_{\parallel}$ is turned on, the metallic phase is destroyed.

Simple picture: spin polarization reduces effective interaction U.



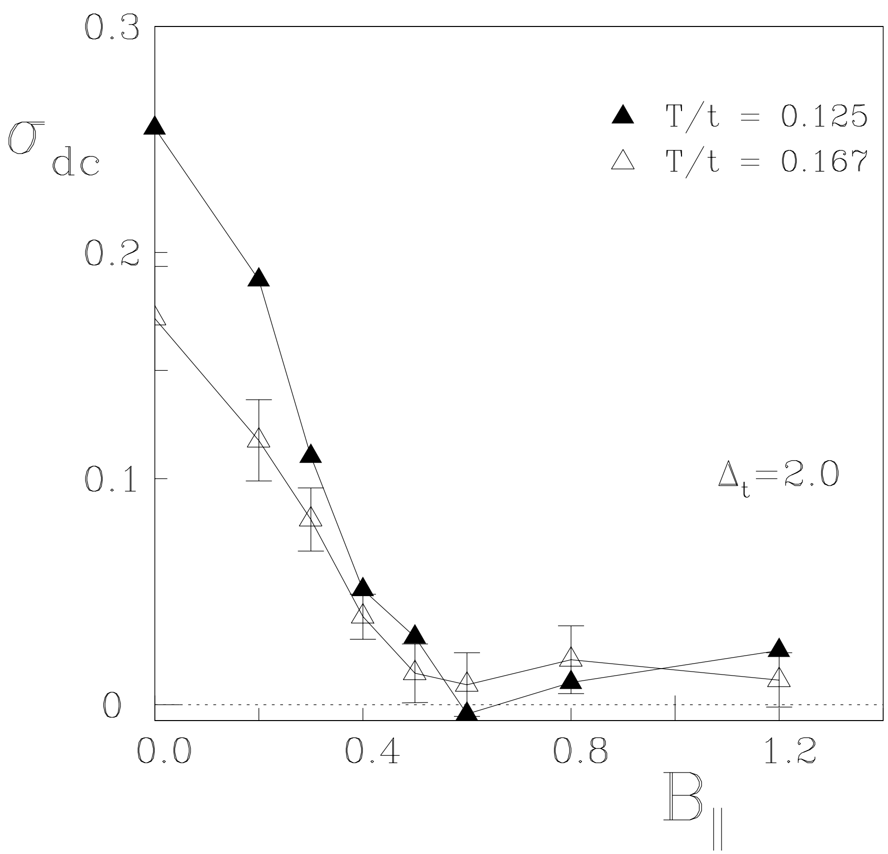
Location of Critical Point

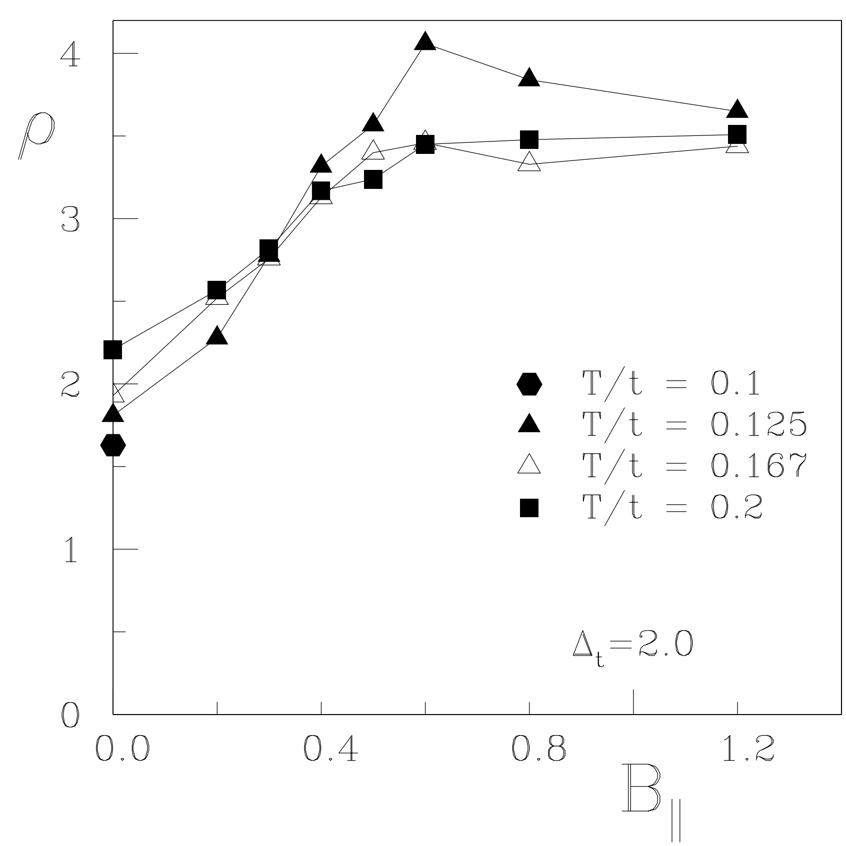
Large $B_{\|}$ and nonzero disorder: conductivitity $\sigma_{\rm dc}$ should vanish. (Effectively, no interactions).

Subtract large U piece of $\sigma_{\rm dc}$ to correct for finite N and T.

$\delta\sigma_{\rm dc} \rightarrow 0$ for $B_{\|} \approx 0.4\ t$.

Alternatively, look at crossing of ρ vs. $B_{\|}$.



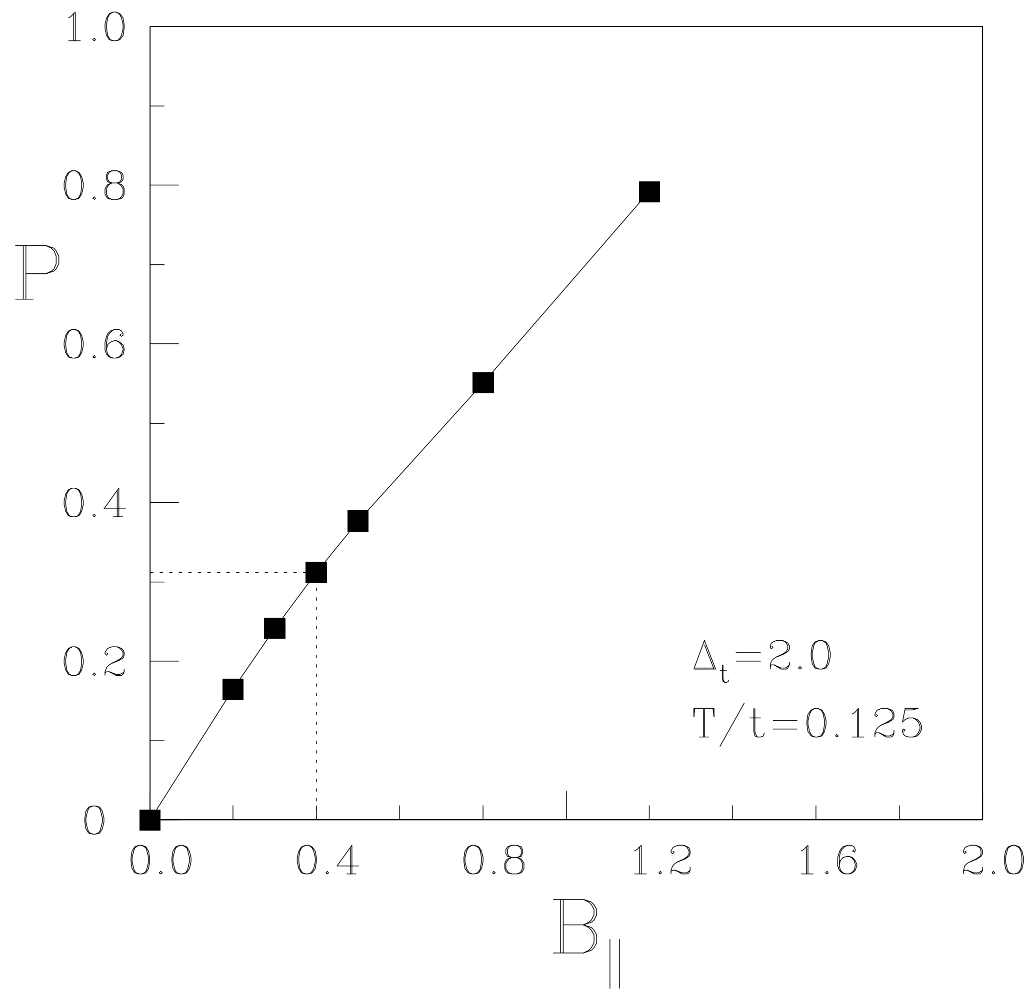


Resistivity Saturation occurs below point of full spin polarization.

$\Delta_t = 2.0\ t$ is fairly close to critical value $\Delta_t(\text{crit}) = 2.4\ t$ where bond disorder destroys metallic phase.

Zeeman field does not need to be very big to drive to insulator.

In particular, get insulator well before full spin polarization.



Conclusions

QMC shows clear evidence for MIT in the disordered 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