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UCDAVIS AGGIES

Quantum Monte Carlo Studies of Multiband Hubbard Models

- A. Ionic Hubbard Model
- B. Determinant Quantum Monte Carlo
- C. Band Insulator-Metal-Mott Insulator
- D. Future Directions/Handoff to Simone (3-band)

2 band: N. Paris, G. Batrouni, F. Hebert, K. Bouadim
3 band: S. Chiesa, J. Kunes, W. Pickett

Support: NSF, DOE (CMSN)

A. Ionic Hubbard Model

Simple Multiband Model,

$$H = -t \sum_{\langle lj \rangle \sigma} (c^{\dagger}_{l\sigma} c_{j\sigma} + c^{\dagger}_{j\sigma} c_{l\sigma}) + \Delta \sum_{l} (-1)^{l} \, n_l + U \sum_{l} n_{l\uparrow} n_{l\downarrow} \; .$$

At $U = 0$,

$$\begin{aligned} E_{\pm}(k) &= \pm\sqrt{\Delta^2 + \epsilon_k^2} \\ \epsilon(k) &= -2t(\cos k_x + \cos k_y) \end{aligned}$$

Two dimensional square lattice.
Band gap $E_g = 2\Delta$.

$\Delta = 0$, half-filling ($\rho = 1$), $T = 0$: AF insulator all U/t.

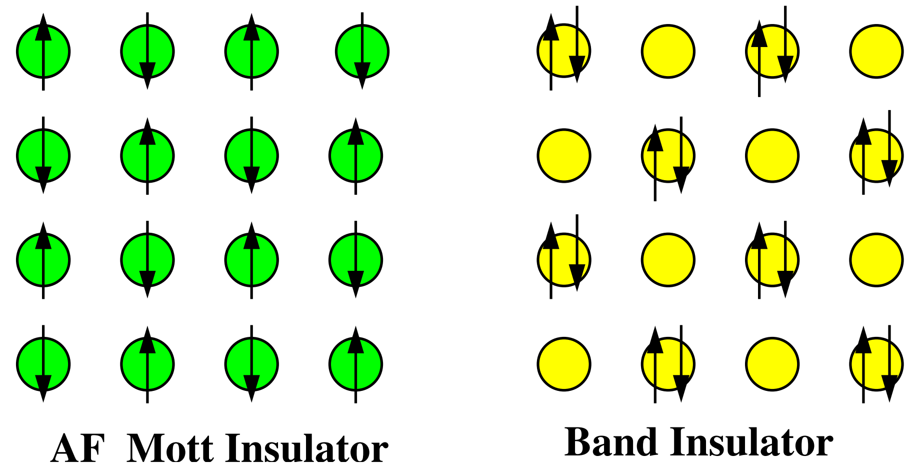
- Weak coupling: Slater gap (AF correlations).
- Strong coupling: Mott insulator.

How does U interplay with band insulating behavior?

Band insulator (BI) $\leftrightarrow$ Mott insulator (MI) at $t = 0$:

$E_{\rm AFMI} = 0$
$E_{\rm BI} = N(U/2 - \Delta)$

$U_c = 2\Delta$



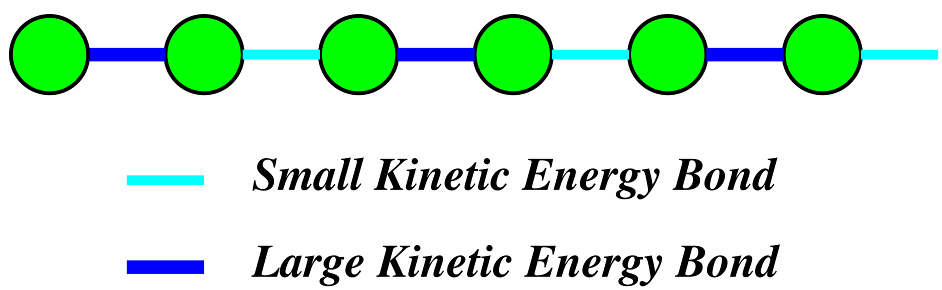
'CDW' correlations in BI not a broken symmetry.
Caused by external potential $\Delta(-1)^l$.

Analogies with extended Hubbard model $V \sum_{\langle lj \rangle} n_l n_j$.
CDW/SDW competition extensively studied in $d = 1$.
Strong coupling: First order SDW/CDW transition
Weak coupling: Second order SDW/CDW transition
Or: BOW intervenes

Physics in one dimension:

- Lanczos ($U_{\rm crit} = 2.27\Delta$), DMRG, QMC, Bosonization,...
  "General" consensus on weak coupling intermediate phase.
  But,...details: BOW or metal?
- Various applications, eg organic chains (polyacetylene)
  Static limit of Su-Schrieffer-Heeger type models

BOW Phase in d=1



Recent (2006) DMFT studies in two dimensions:

- Garg, Krishnamurthy, Randeria : single site DMFT
  $\Delta = 0$: Paramagnetic metal at weak coupling ($U <\approx 10t$).
  Metallic phase extends out to $\Delta \approx 0.04t$.
  Topology at variance with $t = 0$ BI/MI balance.
- Kancharia, Dagotto: Two site DMFT
  AF insulator along $\Delta = 0$ axis at weak coupling.
  BOW phase at $t = 0$ interface between BI/MI.

Related Problem?

Metal $\leftrightarrow$ Anderson Insulator transition ($d = 2$) Chakraborty

Random site energies

$\mu_l = \Delta(r - \frac{1}{2})$ instead of $\mu_l = \Delta(-1)^l$.

Anderson localization/insulator for $U = 0$ in $d = 2$.

Can $U \neq 0$ drive insulator $\longrightarrow$ metal transition?

Usual role of U decreases conduction (e.g. Mott).

Here: Band insulator $\longrightarrow$ metal due to U

Easier to study?

B. Determinant Quantum Monte Carlo

Goal: evaluate

$$\begin{aligned} \langle \hat{A} \rangle &= Z^{-1} \, \mathrm{Tr} \, [\hat{A} \, e^{-\beta \hat{H}}] \\ Z &= \mathrm{Tr} \, e^{-\beta \hat{H}} \end{aligned}$$

- $\hat{H}$ is the Hamiltonian expressed in terms of fermion creation and destruction operators $c^\dagger_{l\sigma}, c_{l\sigma}$.
- "Tr" is a trace over the 4^N dimensional Hilbert space.
- N is the number of sites.
- Each site $\quad | \cdot \rangle \quad | \uparrow \rangle \quad | \downarrow \rangle \quad | \uparrow\downarrow \rangle$.

Theorem for trace if $\hat{H}$ is *quadratic* in fermion operators:

$$\hat{H} = (\, c^\dagger_{1\sigma} \quad c^\dagger_{2\sigma} \quad . \quad . \,) \begin{pmatrix} h_{11} & h_{12} & . & . \\ h_{21} & h_{22} & . & . \\ . & . & . & . \\ . & . & . & . \end{pmatrix} \begin{pmatrix} c_{1\sigma} \\ c_{2\sigma} \\ . \\ . \end{pmatrix} .$$

Here h is an NxN matrix of numbers.

The identity is:

$$Z = \mathrm{Tr}\, e^{-\beta \hat{H}} = \det[I + e^{-\beta h}].$$

- “Tr” over a quantum mechanical 4^N dim Hilbert space.
- “det” is a usual determinant of NxN matrices.
- “I” is the N dimensional identity matrix
- “h” is the matrix of *numbers* entering $\hat{H}$.

More general identity: *set* of quadratic $\hat{H}(l)$, $l = 1, 2, \ldots L$:

$$Z = \mathrm{Tr}\,[e^{-\hat{H}(1)} \ldots e^{-\hat{H}(L)}] = \det[\, I + e^{-h(1)} \ldots e^{-h(L)}].$$

In addition, “Green’s function”,

$$\begin{aligned} G_{ij} = \langle c_{i\sigma} c_{j\sigma}^{\dagger} \rangle &= Z^{-1}\, \mathrm{Tr}\,[c_{\,i\sigma} c_{j\sigma}^{\dagger}\; e^{-\hat{H}(1)} \ldots e^{-\hat{H}(L)}\,] \\ &= [\, I + e^{-h(1)} \ldots e^{-h(L)}\,]_{ij}^{-1} \quad . \end{aligned}$$

Electron-electron interactions $U n_{i\uparrow} n_{i\downarrow} = U c^{\dagger}_{i\uparrow} c_{i\uparrow} c^{\dagger}_{i\downarrow} c_{i\downarrow}$
(Discrete) Hubbard–Stratonovich transformation,

$$e^{-U\Delta\tau(n_\uparrow - \frac{1}{2})(n_\downarrow - \frac{1}{2})} = \frac{1}{2} e^{-\frac{U\Delta\tau}{4}} \sum_S e^{\lambda S(n_\uparrow - n_\downarrow)}$$

$\cosh\lambda = e^{U\Delta\tau/2}$, and $S = \pm 1$.
Isolate interactions: divide $\beta = L\Delta\tau$
$\hat{H} = \hat{K} + \hat{V}$ where $\hat{K}$ quadratic (kinetic), $\hat{V}$ interactions.
Trotter decomposition:

$$Z = \mathrm{Tr}\, e^{-\beta\hat{H}} \approx \mathrm{Tr}\left[e^{-\Delta\tau\hat{K}} e^{-\Delta\tau\hat{V}} \ldots e^{-\Delta\tau\hat{K}} e^{-\Delta\tau\hat{V}} \right] .$$

$e^{-\Delta\tau\hat{K}}$ quadratic
Each $e^{-\Delta\tau\hat{V}}$: N Hubbard–Stratonovich variables, S_{il}

- space i, imaginary–time l.

$e^{-\Delta\tau V_l}$ now quadratic.
V_l: different Hubbard–Stratonovich variables for each l.

Summary:

$$Z = \sum_{S_{il}} \det M_\uparrow \, \det M_\downarrow .$$

- Determinant for each of the two spin species.
- *Classical* monte carlo problem.
- Sum over real, classical, variables S_{il}.
- "Boltzmann weight": product of two determinants.
  Possible "sign" problem.

Conductivity

$$\begin{aligned}\sigma_{\rm dc} &= \frac{\beta^2}{\pi}\Lambda_{xx}(\mathbf{q}=0,\tau=\beta/2)\ ,\\ \Lambda_{xx}(\mathbf{q},\tau) &= \langle\, j_x(\mathbf{q},\tau)\, j_x(-\mathbf{q},0)\,\rangle\\ j_x(\ell,\tau) &= i\sum_\sigma t_{\ell+\hat{x},\ell}\ e^{\tau H}(c^\dagger_{\ell+\hat{x},\sigma}c_{\ell\sigma}-c^\dagger_{\ell\sigma}c_{\ell+\hat{x},\sigma})e^{-\tau H}\ .\end{aligned}$$

AF Structure factor

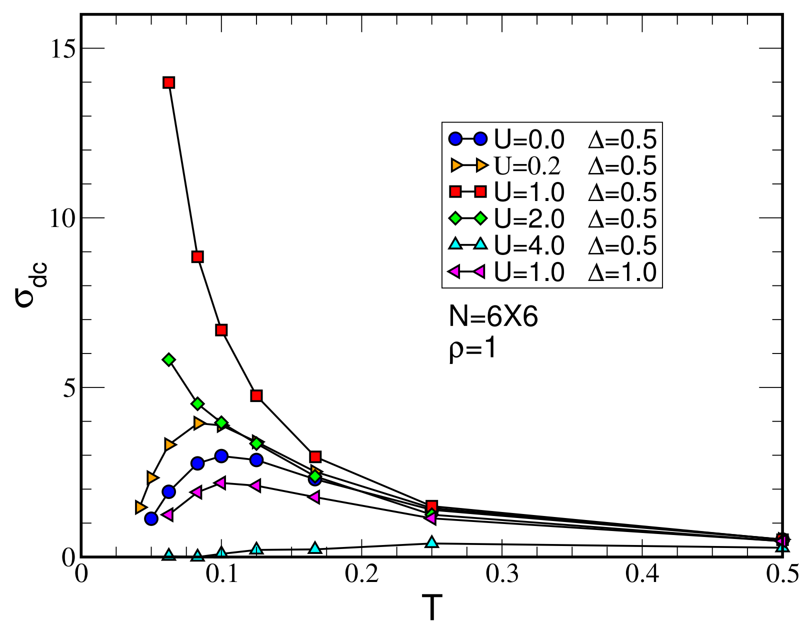
$$S(\pi,\pi)=\frac{1}{N}\sum_{lj}\langle\, S^-_{j+l}S^+_j\,\rangle=\frac{1}{N}\sum_{lj}\langle\, c^\dagger_{j+l\downarrow}c_{j+l\uparrow}\ c^\dagger_{j\uparrow}c_{j\downarrow}\,\rangle$$

Spectral function

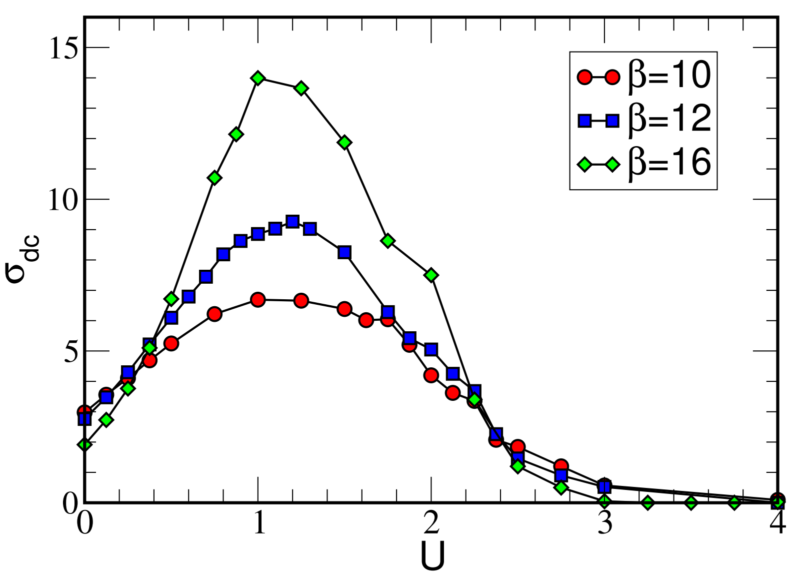
$$G(k,\tau)=\int d\omega\, A(k,\omega)\frac{e^{-\tau\omega}}{e^{-\beta\omega}+1}$$

Analytic continuation.

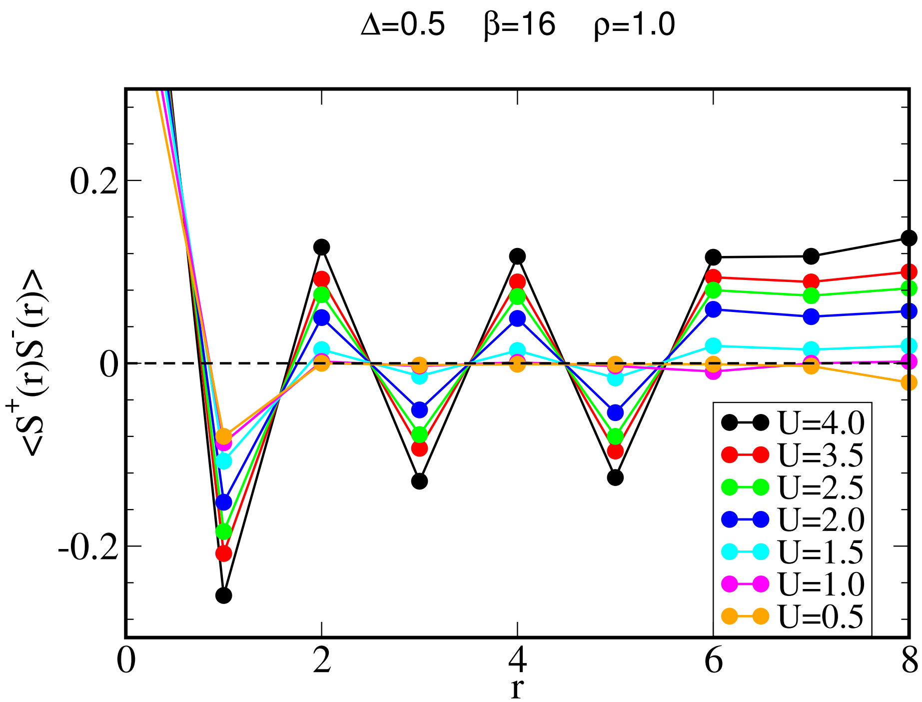
C. Band Insulator - Metal - Mott Insulator



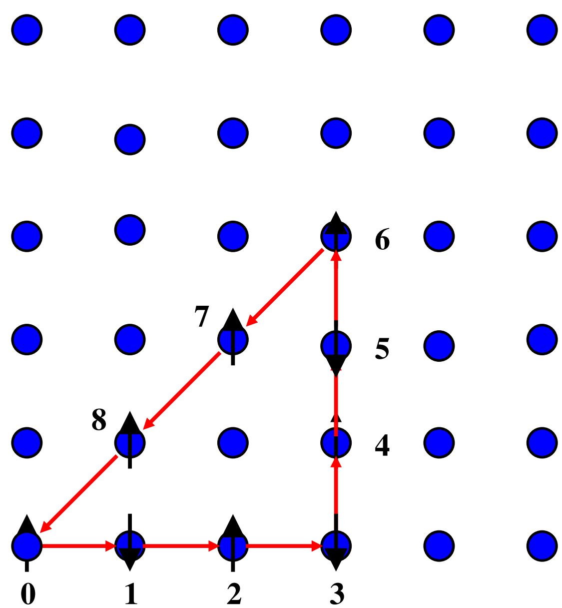
$U \neq 0$ drives BI metallic. Low temperature sign of $d\sigma_{\rm dc}/dT$ reversed.

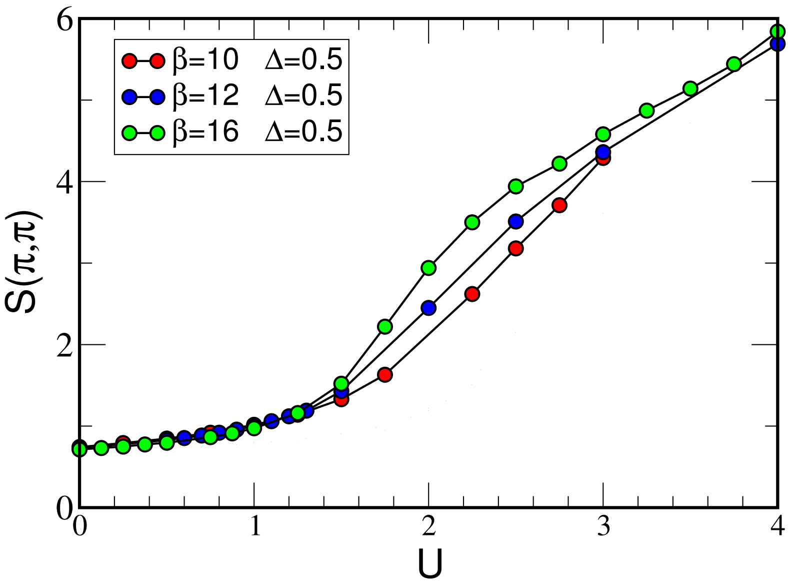


Crossings indicate rough
U_{c1} (BI-metal)
U_{c2} (metal-MI).

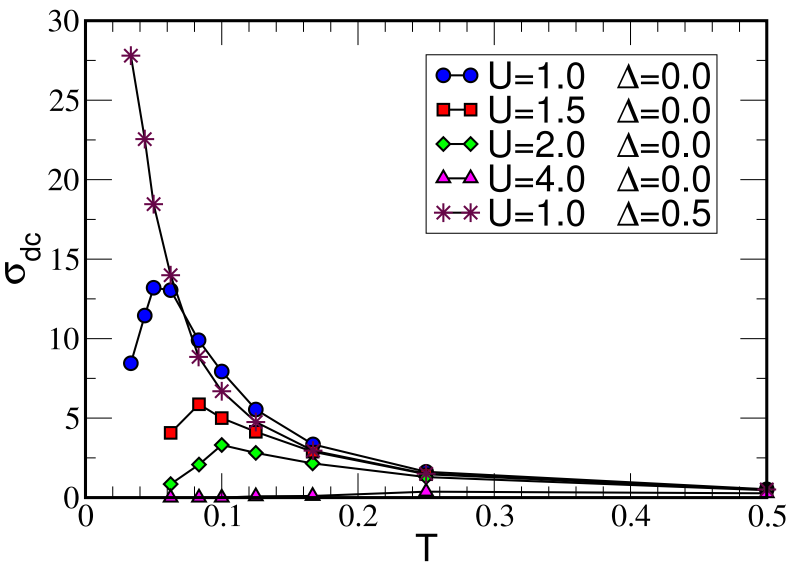


Spin-Spin correlations

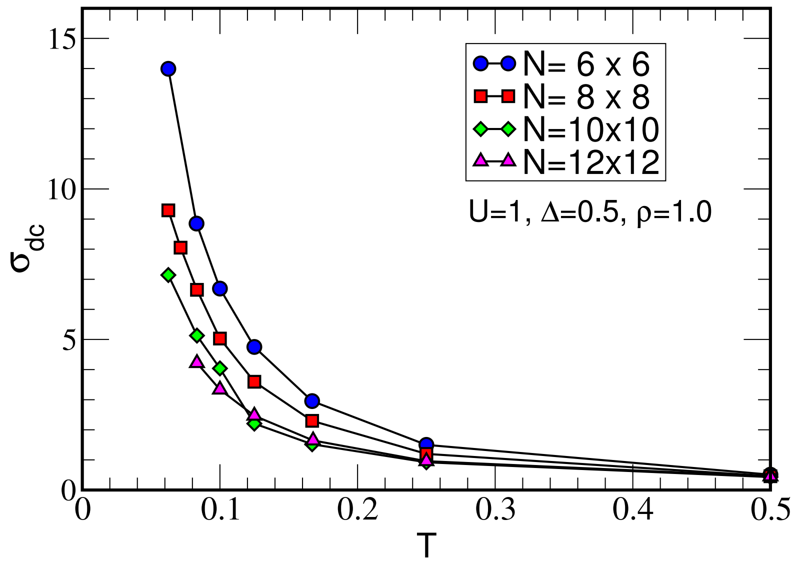




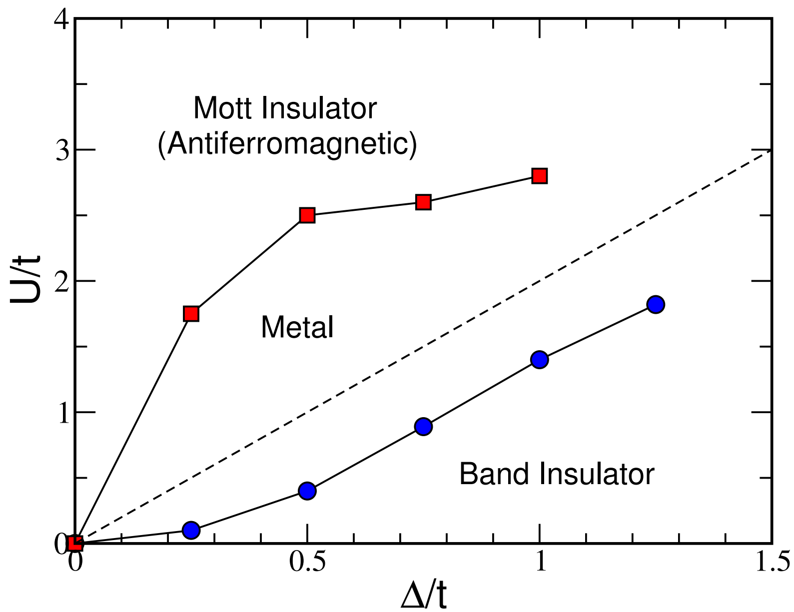
AF correlations ($S(\pi,\pi)$) build up as U increases.



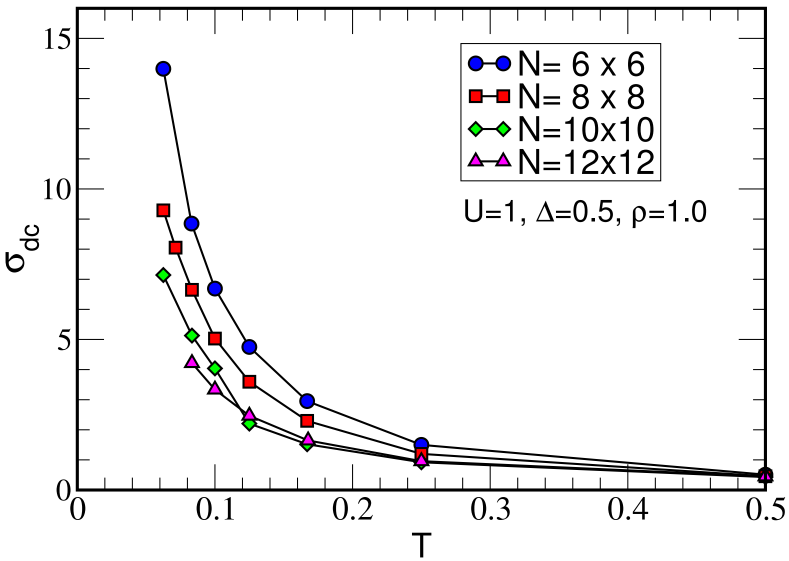
Check: For $\Delta = 0$ always insulating. Weak/strong coupling different.



Larger lattices:
$d\sigma_{\rm dc}/dT$ remains
negative (metallic).
Finite size scaling?



Phase diagram.
Dashed line: $t = 0$.



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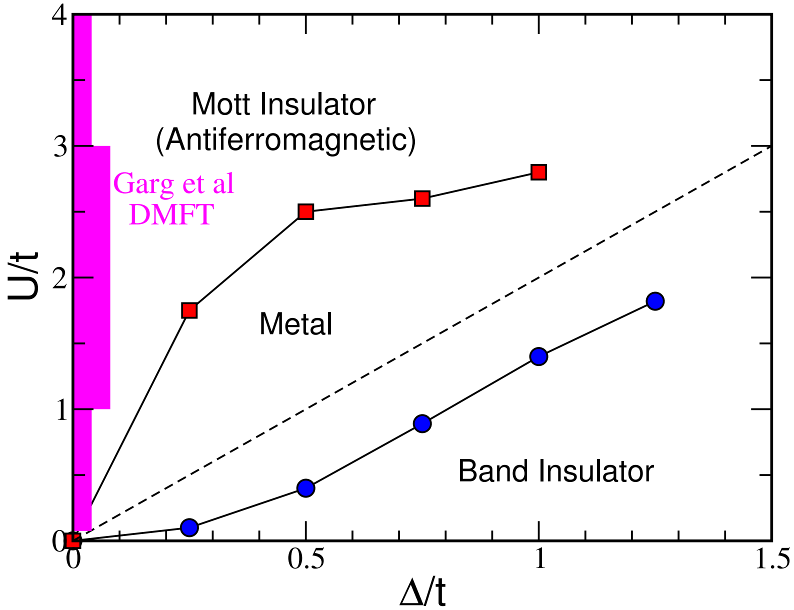

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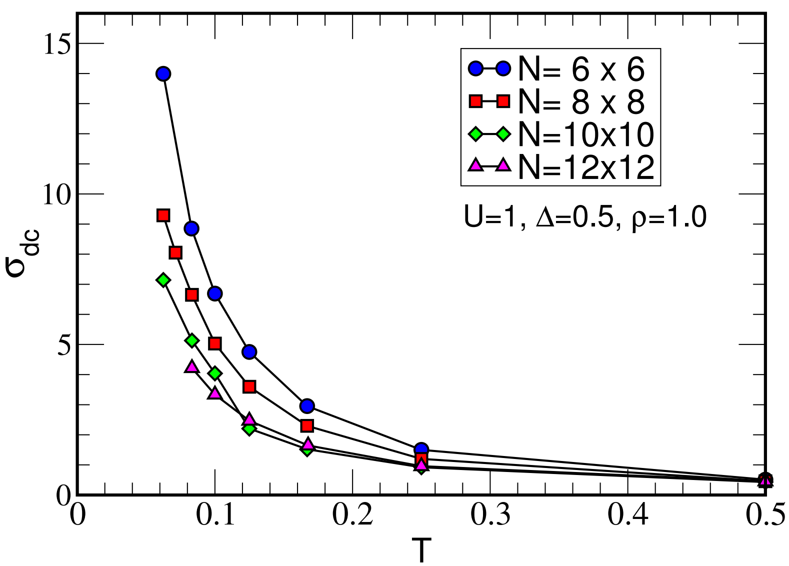

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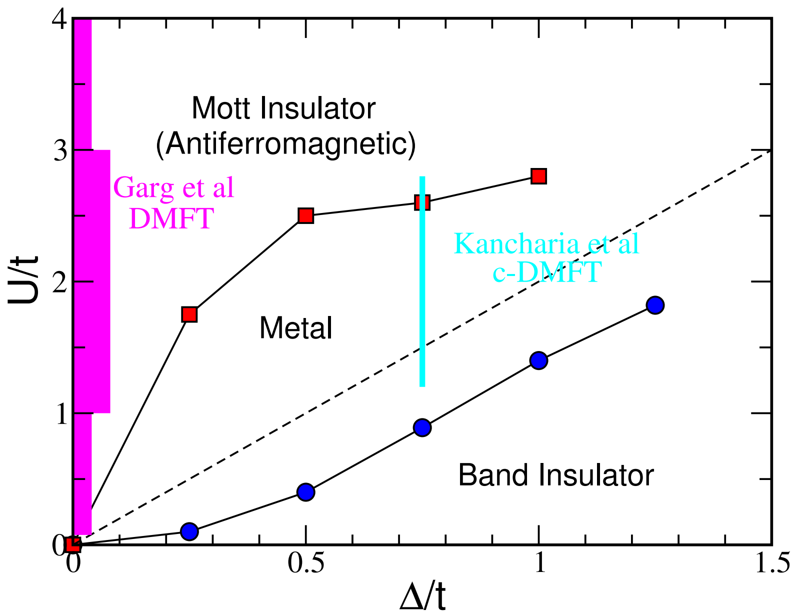

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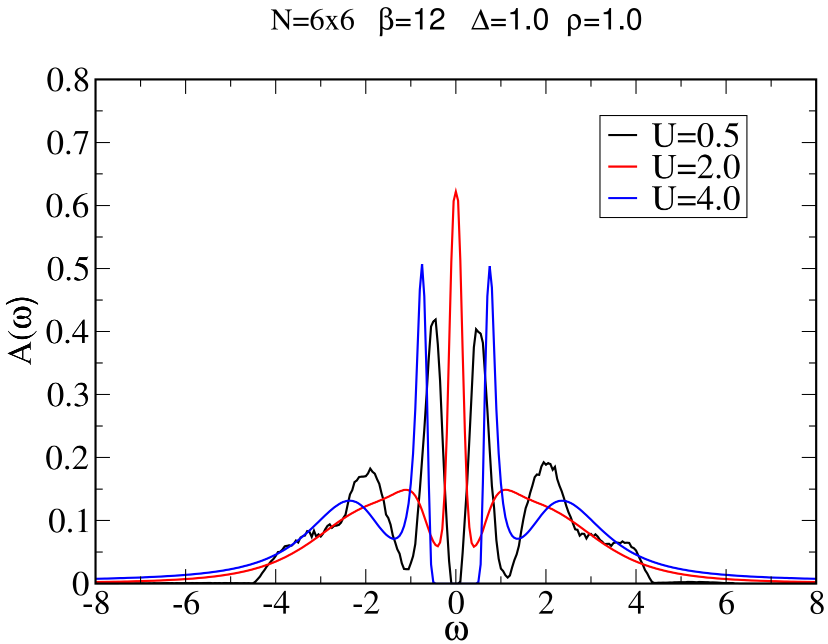
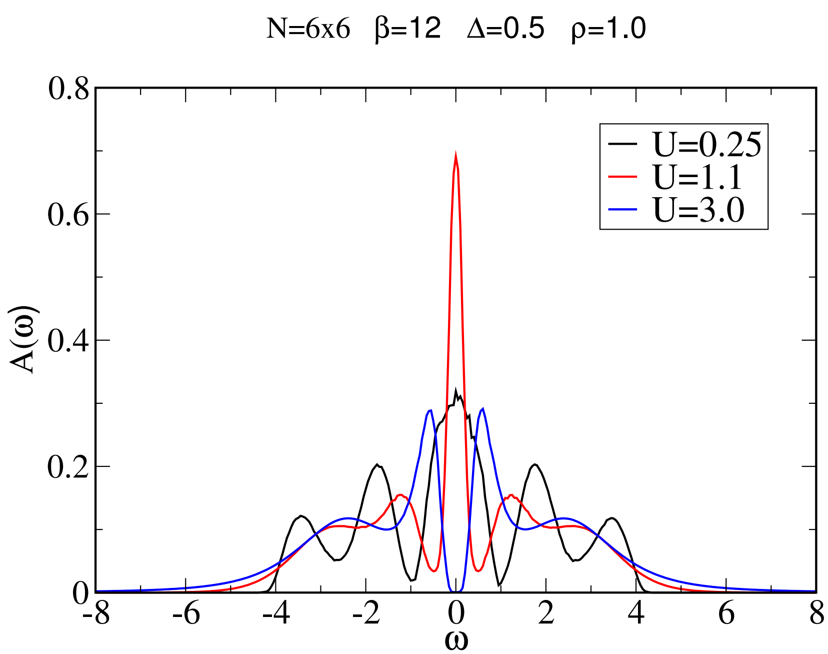


Spectral function $A(\omega)$

$U = 0.5$: $A(\omega = 0) = 0$: BI

$U = 2$: $A(\omega = 0) \neq 0$: Metal

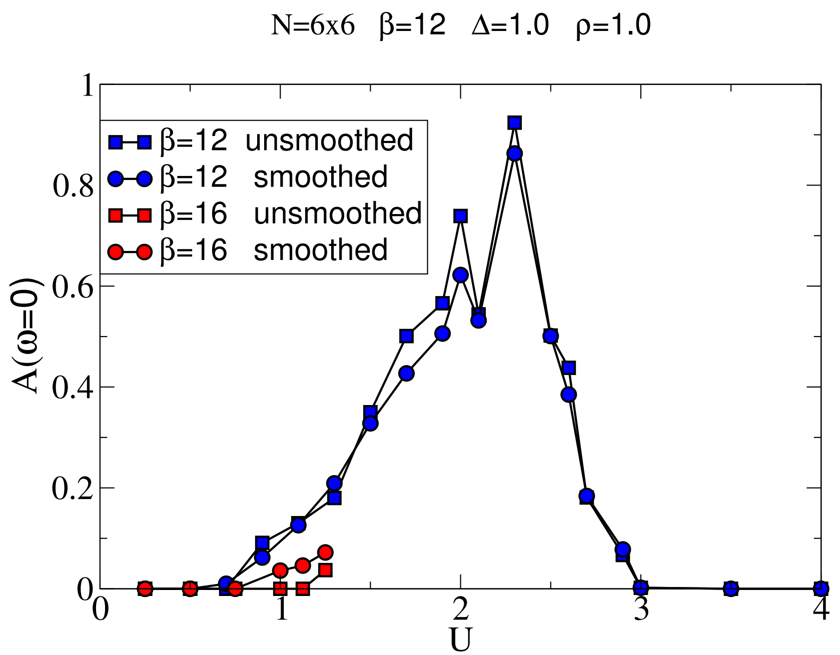
$U = 4$: $A(\omega = 0) = 0$: MI



$\Delta = 0.5$

Cannot resolve BI.

U Dependence of Spectral Weight at Fermi Surface.



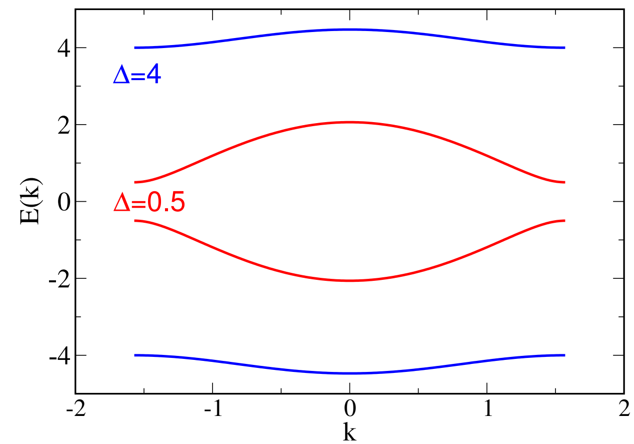
From conductivity $\sigma_{\rm dc}$:

- $U_{c1} \approx 1.4t$. (BI $\leftrightarrow$ Metal.)
- $U_{c2} \approx 2.8t$. (Metal $\leftrightarrow$ MI.)

D. Concluding Remarks/Future Work

Further work on Ionic Hubbard model

- Large Δ limit:
  Mott at quarter-filling: $\rho = 0.5$
- BOW correlations
- Finite size scaling: *Really* a metal?



General Multiband Hubbard Models

- Band Insulator/Charge Transfer Insulator
- Three band (Emery) model CuO_2 sheets
  Hanke (DQMC); Maier, Jarrell (DCA)
- Chiesa, Kunes, Pickett: $A(\omega)$ Lanczos/DMFT