The Hubbard Model

In Condensed Matter and AMO systems

- Transition Metal Oxides
- The Fermion Hubbard Model
- Transition Metal Oxides - The Whole Story
- High Temperature Superconductors
- Monte Carlo and Quantum Monte Carlo

∗ Disordered Superconductors

- The Boson Hubbard Model
- Conclusions

Purpose

Hulet's opening talk: Emphasized connections to CM (and beyond!).

Make those connections explicit in context of Hubbard Model physics.

Quantum Monte Carlo simulations

What they can tell us.

What they can't tell us ← Insight from trapped atom experiments?

Collaborators

S.R. White (UCI), R.L. Sugar, D.J. Scalapino (UCSB)
G. Batrouni, F. Hébert (INLN, Nice), G. Zimanyi (UCD)
M. Rigol (Georgetown), A. Muramatsu (Stuttgart)
P. Sengupta (LANL) V. Rousseau, P.J.H. Denteneer (Leiden)
M. Randeria, N. Trivedi (OSU)

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From Atoms to Solids

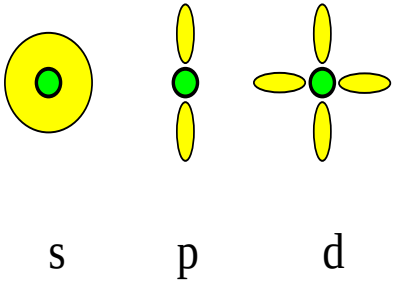
Individual atoms: discrete energy levels

Atoms far apart: electrons are localized on single atom

Atoms brought together (solid): degenerate level couple and broaden into a band.

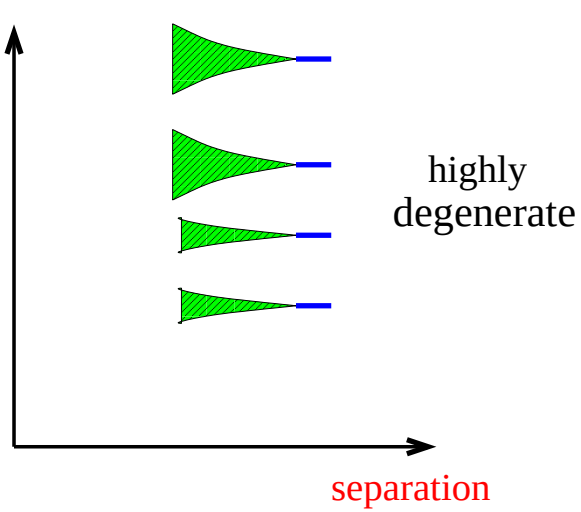
Eigenvectors are delocalized (plane/"Bloch" waves)

$$\begin{pmatrix} E_n & t \\ t & E_n \end{pmatrix} \qquad \text{Eigenvalues } \lambda = E_n \pm t \qquad \text{Eigenvectors } \psi = \frac{1}{\sqrt{2}} \begin{pmatrix} 1 \\ \pm 1 \end{pmatrix}$$



x e^{-r/a_0}

$-13.6 / n^2$



Band Insulators

Energy band completely filled: Insulator

Finite energy gap to next unoccupied level

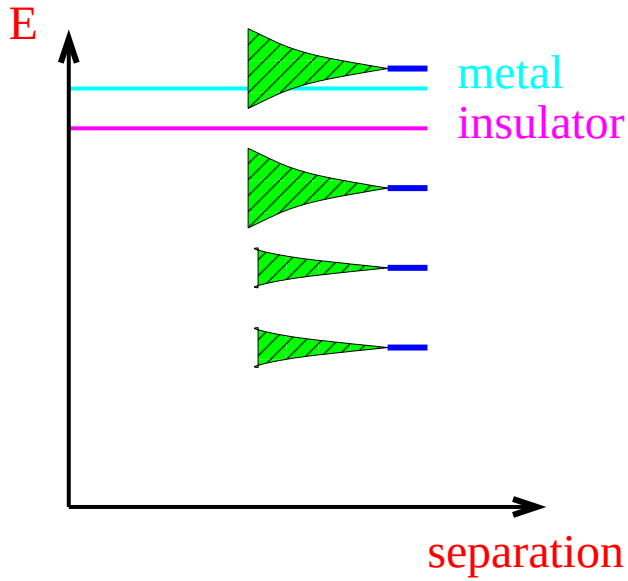
Simple counting arguments predict whether many solids are metallic or insulating!!

k eigenstate can be occupied by two electrons (spin $\uparrow, \downarrow$).

Solids with an odd number of electrons per unit cell must be metallic.

Alkalis (Li, Na, K): one valence e^- $(2s^1, 3s^1, 4s^1)$ per unit cell: Good metal.

Diamond, silicon, and germanium (C, Si, Ge): eight valence electrons per unit cell $(2s^2 2p^2, 3s^2 3p^2, 4s^2 4p^2)$: insulators.



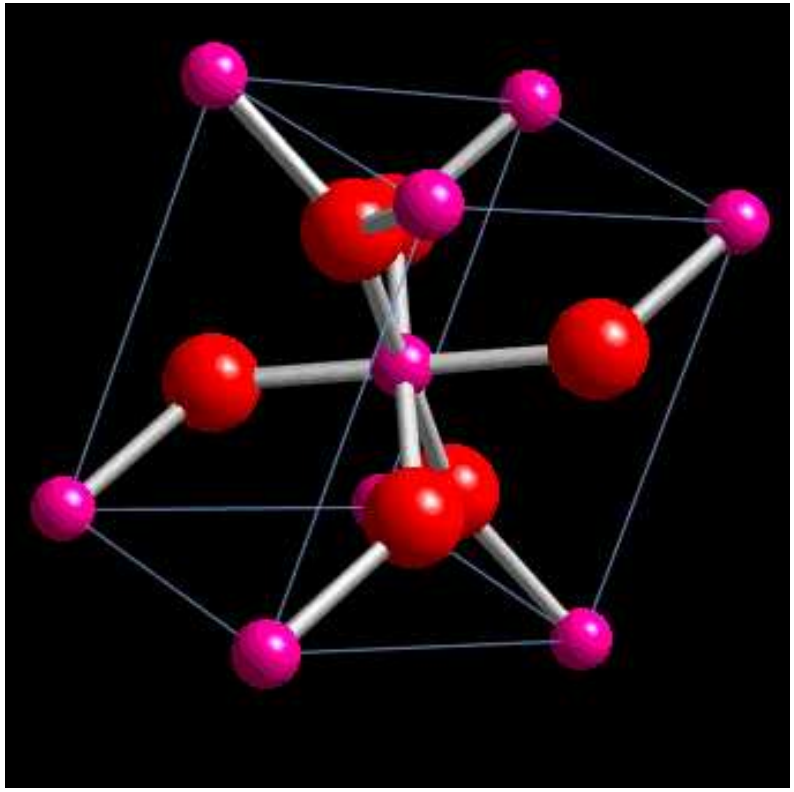
Transition Metal Monoxides (MnO, FeO, CoO)

Simplest band structure picture

- Mn^{2+} has $3d^5$ configuration
- half-filled band $\rightarrow$ metal

Experimentally

- $*$ insulating
- $*$ antiferromagnetic ($T_{\text{Neel}} = 122^{\circ}$ K)

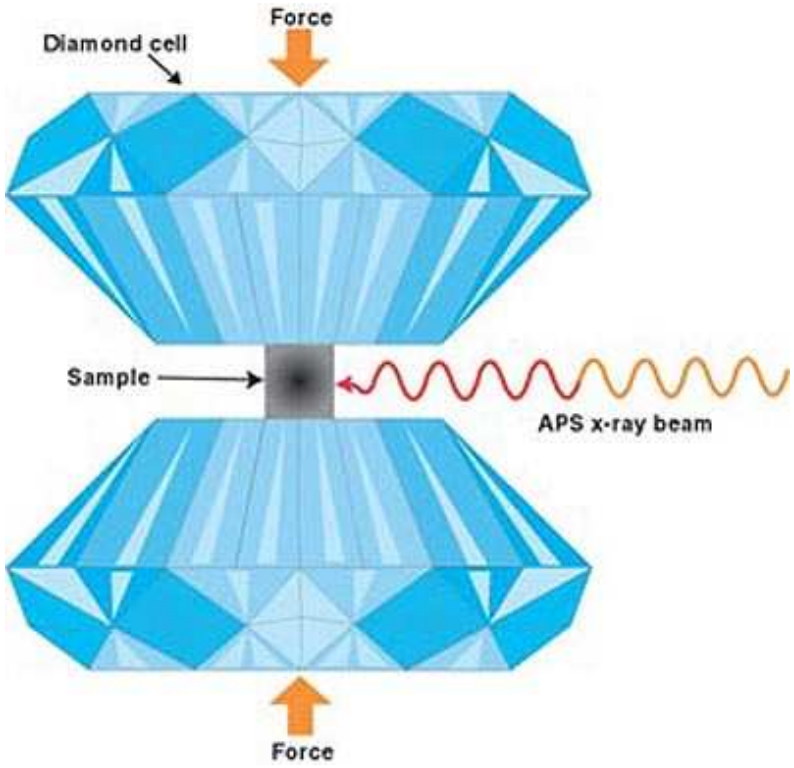


Can however make MnO have the expected metallic behavior...

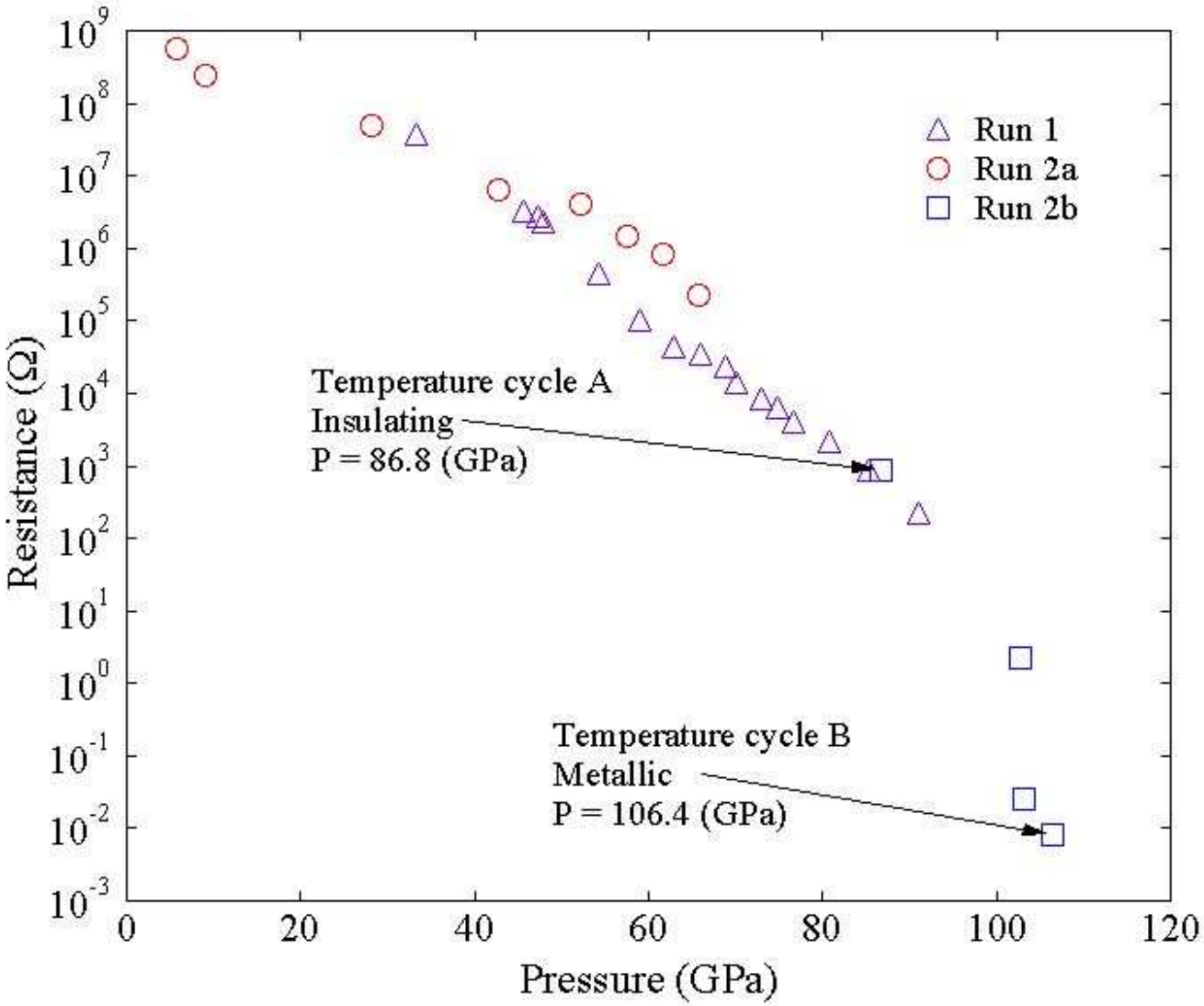
Diamond Anvil Cell

Apply pressure (and lots of it!) to push atoms closer.

* Direct measurement of resistance
* Probe magnetic moments with synchotron radiation (APS at Argonne)

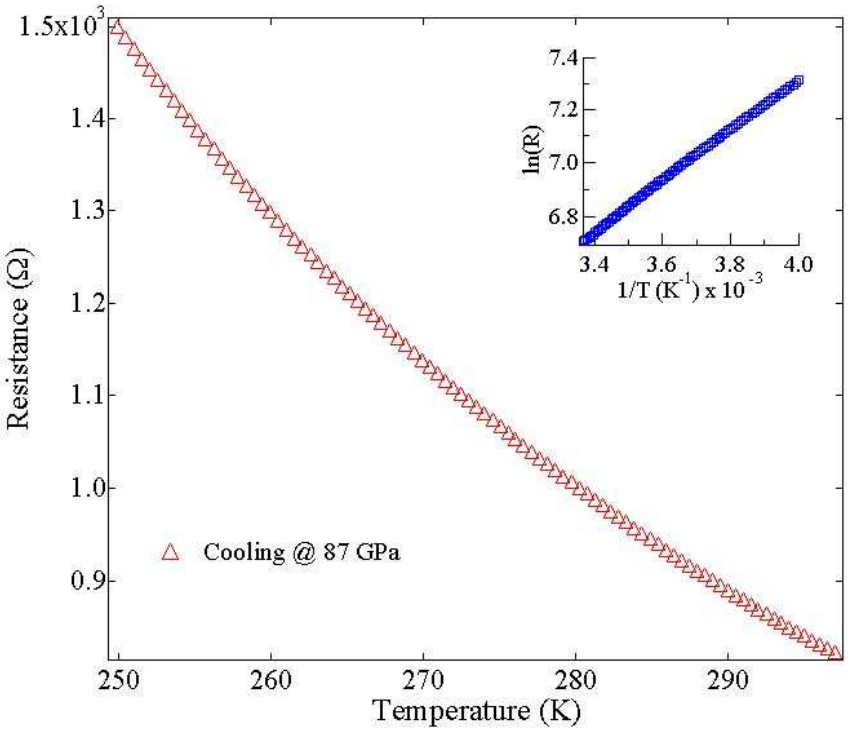


Resistance drops to typical metallic values at $P \approx 100$ GPa.

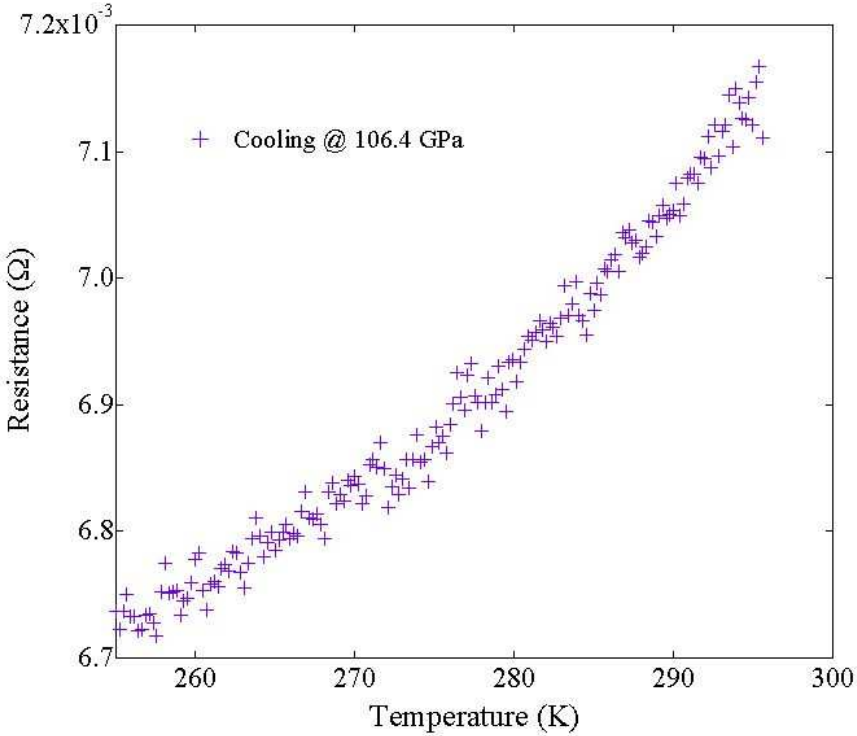


J.R. Patterson *etal.*, Phys. Rev. B69, 220101(R) (2004).

Temperature dependence changes:



insulating (gapped)
R increases as T lowered



metallic
R decreases as T lowered

RIXS: Energy of x-rays emitted when core (1s) hole created, and 3p e^- decays to fill it. Magnetic moment on 3d, if present, splits 3p level and induces secondary $K\beta'$ peak

RESULTS: $K\beta'$ intensity exhibits step-like structure.

- $0 < P < 30$ GPa: $I(K\beta')/I(K\beta) \approx 0.10$
- $60 < P < 105$ GPa: $I(K\beta')/I(K\beta) \approx 0.05$
- $105 < P < 130$ GPa: $I(K\beta')/I(K\beta) \approx 0.00$ → Moment destroyed

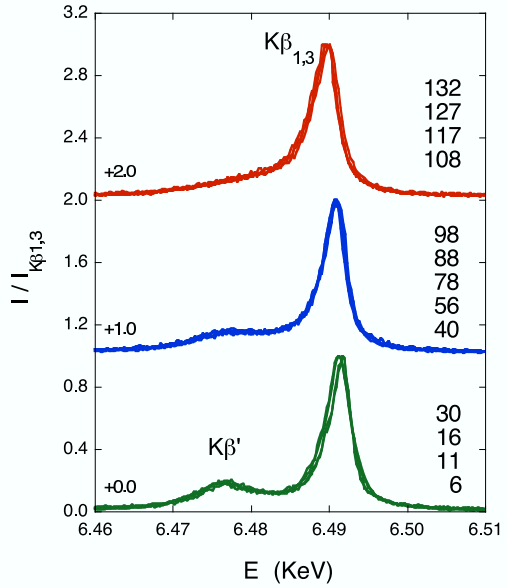


Fig 2

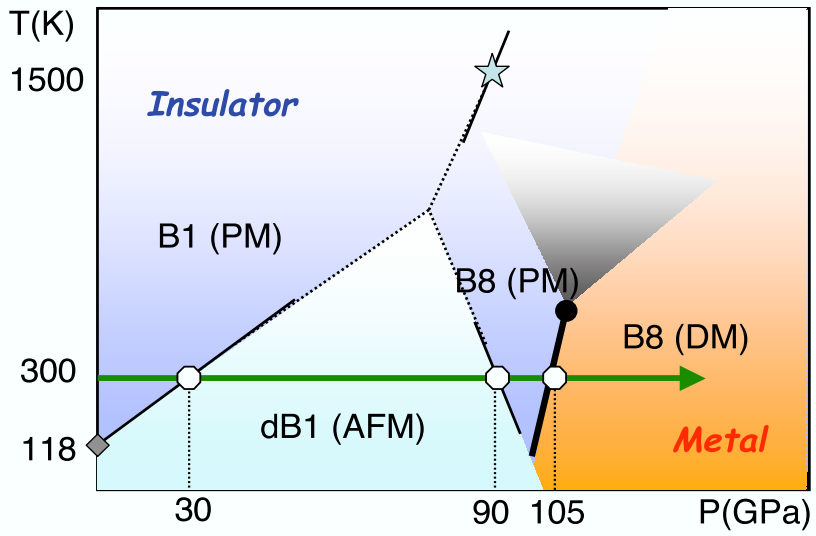


Fig. 1

Temperature-Pressure phase diagram (Yoo *etal.*, PRL, 2005)

[1] $P \approx 30$ GPa
Structural phase transition

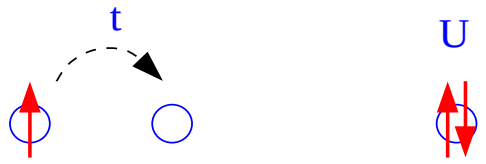
[2] $P \approx 90$ GPa
Antiferromagnetic to paramagnetic transition (moments disordered)

[3] $P \approx 105$ GPa
moments destroyed
Insulator to metal phase transition
Isostructural Volume Collapse ($\Delta V \approx 6.6\%$)

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 σ on site i.
Includes electron kinetic energy (t) and interaction energy (U).

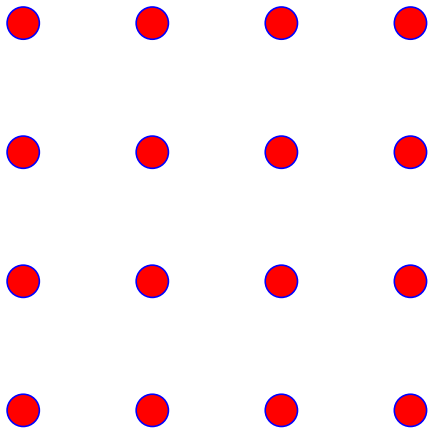


Momentum space

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

In two dimensions, bandwidth $W = 8t \approx 2\,eV$.
on site repulsion $U \approx 2 - 10\,eV$
$t = 1 \approx 0.25\,eV = 3000^\circ K$ is usual choice to set energy scale.
$\beta = t/T = 1/T = 10$ means $T \approx 300^\circ K$.

Mott Insulator



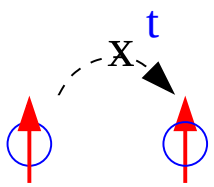
U/t large and $\langle n \rangle = 1$.

All sites occupied by exactly one e^-.

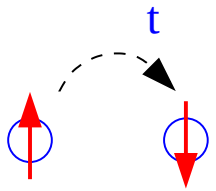
Hopping causes double occupancy, costs U.

Two ways to destroy:

* decrease U/t
* dope: shift $\langle n \rangle \neq 1$



$\Delta E^{(2)} = 0$



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

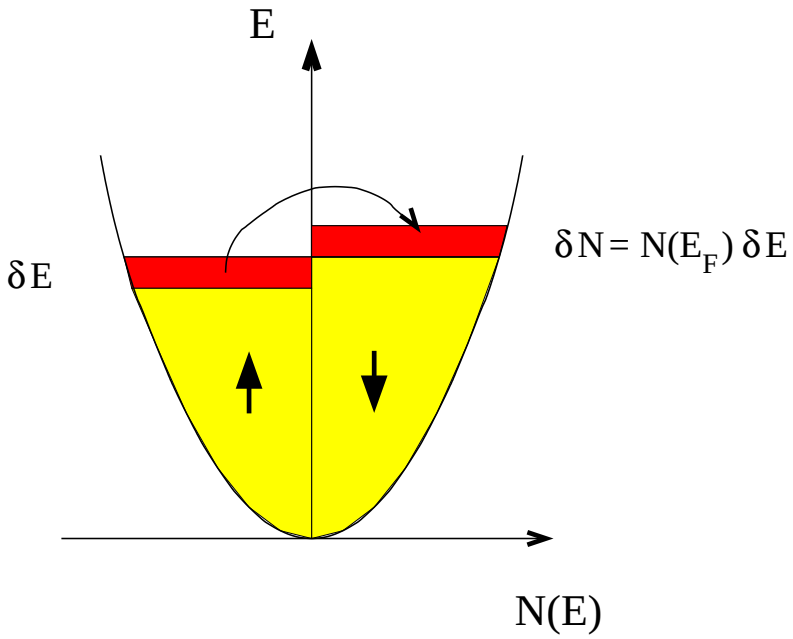
What is optimal spin arrangement?

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.

Simple "Stoner" Picture of Magnetic Order



Density of states

$N(E_F) = \delta N/\delta E \propto 1/t$

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:

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

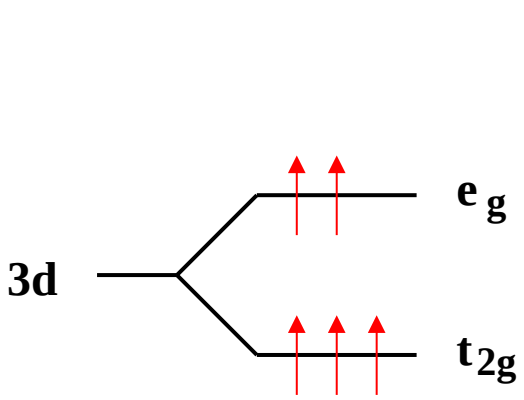
Total Energy change:

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

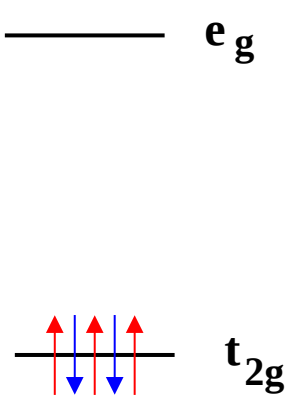
Stoner Criterion: $UN(E_F) > 1 \rightarrow$ magnetism!

Transition Metal Monoxides - The Whole Story ?

Kinetic Energy	$3d$ bandwidth	t_d
Correlation Energy	On-site Coulomb	U_d
Multiple orbitals	Hund's rule (exchange)	J_H
Both Mn and O atoms	Charge transfer energy	$E_{3d} - E_{2p}$
Mn in cubic environment	Crystal field splitting	$E_{e_g} - E_{t_{2g}}$



Exchange splitting
>
crystal field

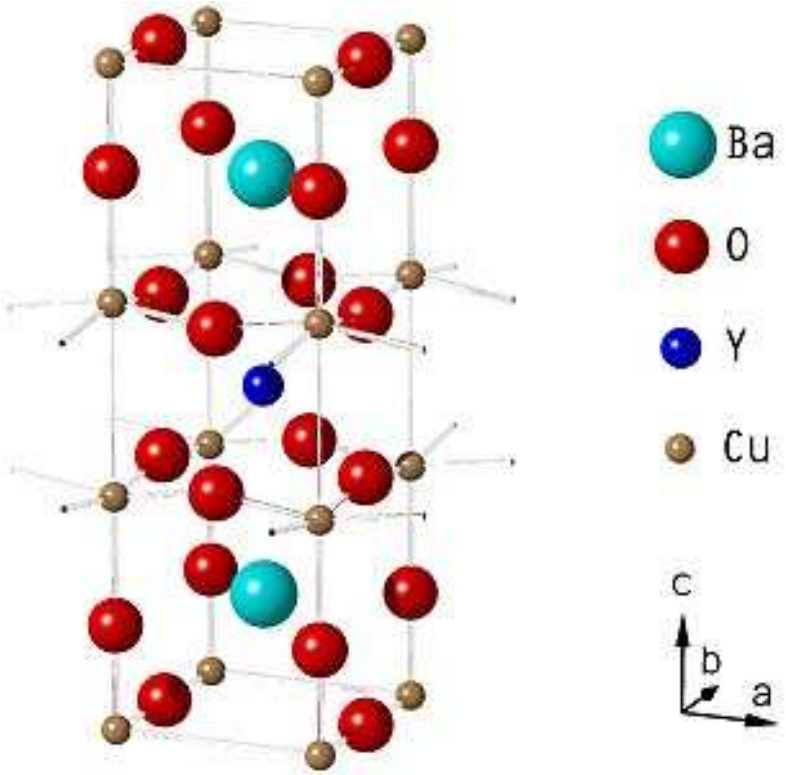


crystal field
>
Exchange splitting

Loss of moment transition actually a "high-spin to low spin transition"?
Crystal field splitting decreases below exchange splitting as pressure applied.

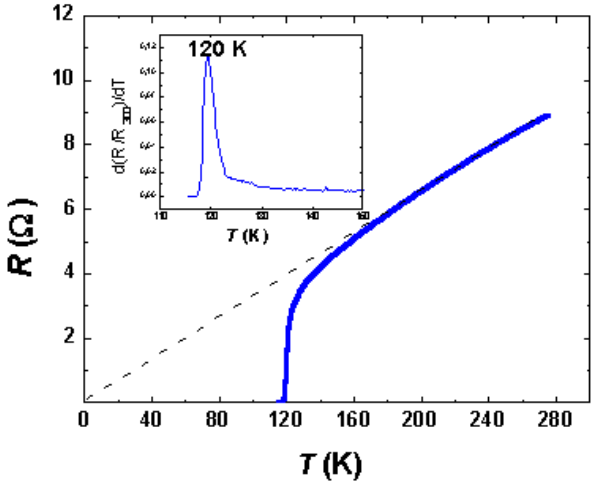
High Temperature Superconductor $YBa_2Cu_3O_{7-\delta}$

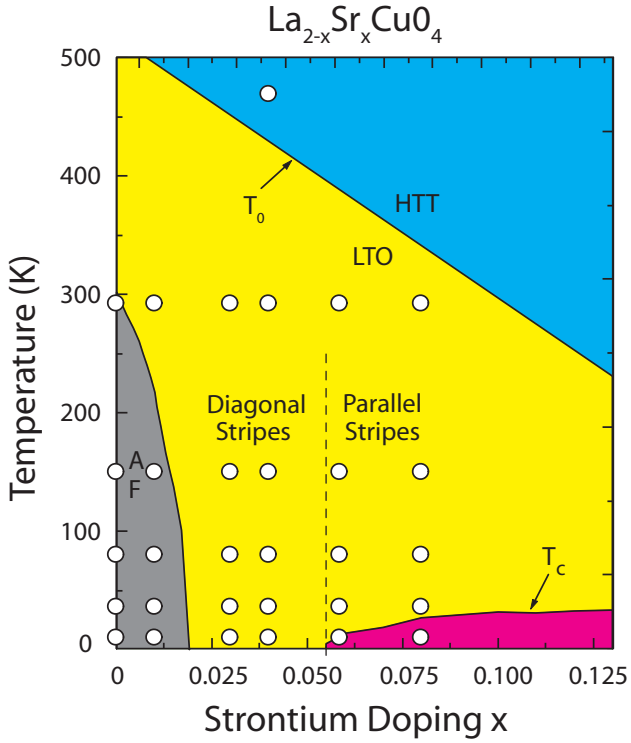
Control Mott insulator and antiferromagnetism with δ (electron density).



Antiferromagnetic when one hole per copper. Neél temperature goes to zero when doped.

Superconductivity when doped and temperature lowered (Hg compound shown)

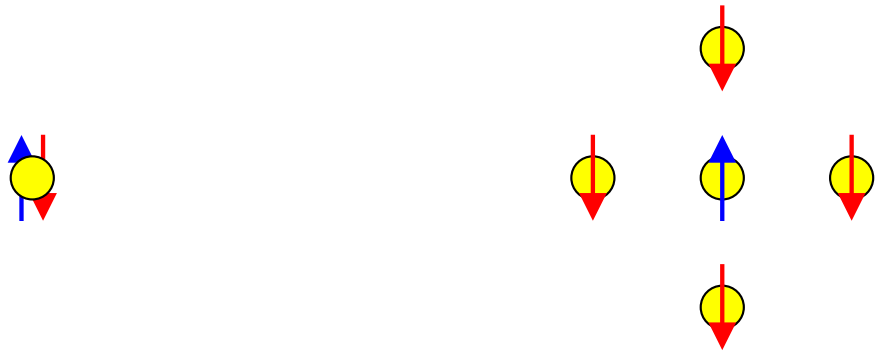




As expected from Hubbard: At 1 hole/Cu: antiferromagnetic and insulating

Unexpected from Hubbard?

- Superconductivity and, in particular, d-wave symmetry
- Charge inhomogeneities



s−wave **s*−wave (phases uniform)**

d−wave (phases alternate)

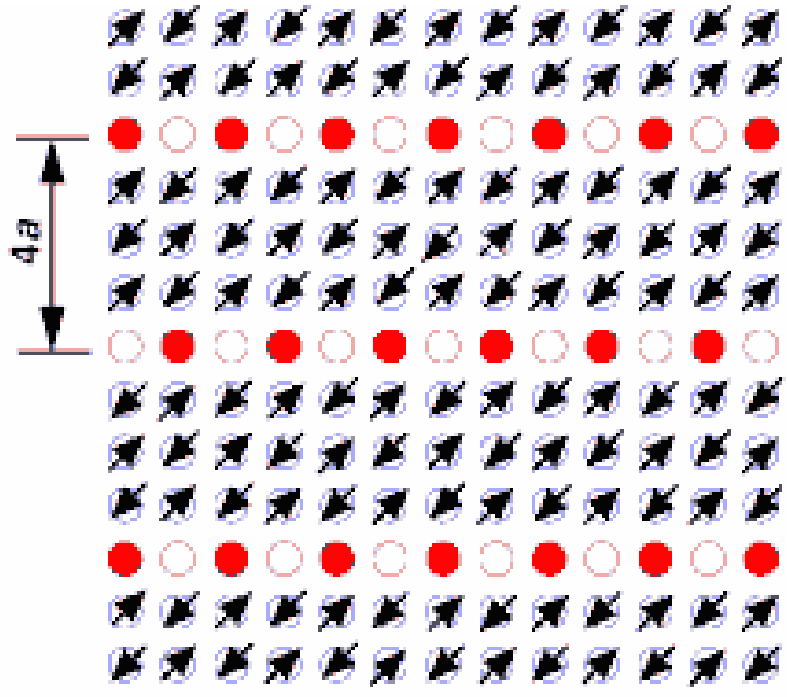
$$
\begin{aligned}
\Delta_s^\dagger &= c_{j\uparrow}^\dagger c_{j\downarrow}^\dagger \\
\Delta_{s*}^\dagger &= c_{j\uparrow}^\dagger \left[c_{j+x\downarrow}^\dagger + c_{j+y\downarrow}^\dagger + c_{j-x\downarrow}^\dagger + c_{j-y\downarrow}^\dagger \right] \\
\Delta_d^\dagger &= c_{j\uparrow}^\dagger \left[c_{j+x\downarrow}^\dagger - c_{j+y\downarrow}^\dagger + c_{j-x\downarrow}^\dagger - c_{j-y\downarrow}^\dagger \right]
\end{aligned}
$$

Actually, d-wave pairing had been suggested in the Hubbard model before high-T_c in context of heavy fermion systems.

Mechanism of conventional superconductivity:
Attractive interaction between e^- mediated by exchange of phonons (lattice vibrations).

Possible mechanism of (un)conventional superconductivity:
Attractive interaction between e^- mediated by exchange of magnons (vibrations of lattice of antiferromagnetically aligned spins).

"Stripes": Doped holes are not uniformly distributed.



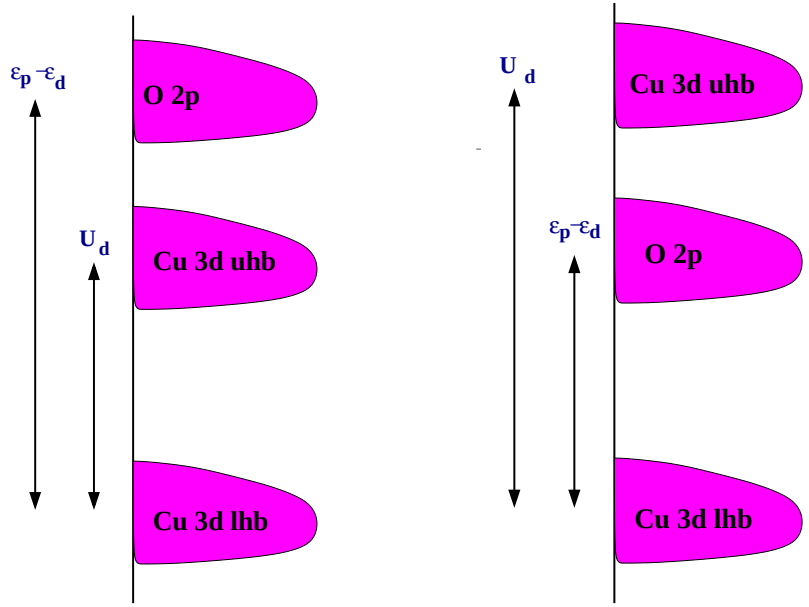
Are stripes in the Hubbard Hamiltonian?!

Yes! Inhomogeneous Hartree-Fock (Zaanen); Density Matrix Renormalization Group (White).

Again, many 'real life' complications

Like TMOs: Oxygen orbitals. 3-band ('Emery') model.

Charge transfer versus Mott-Hubbard Insulator



Role of number of layers and interlayer atoms

$La_{1-x}Sr_xCuO_2$: $T_c \approx 35^\circ K$.

$Y_1Ba_2Cu_3O_{7-\delta}$: $T_c \approx 90^\circ K$.

Hubbard Hamiltonian 'particle-hole' symmetry.

Cuprate superconductors: electron doped $\neq$ hole doped.

Role of phonons

Classical Monte Carlo

Energy of set of degrees of freedom x_i:

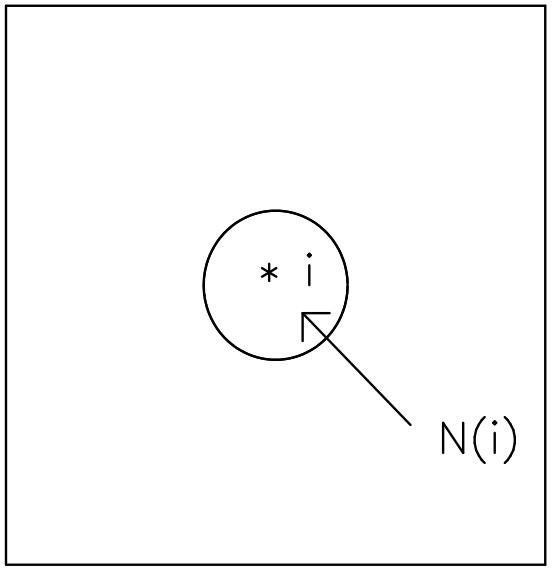
$$E = \sum_{i}^{N} x_i \sum_{j \in \mathcal{N}(i)} \kappa_{ij}\, x_j$$

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

Suggest change $x_i \to x_i'$.
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:

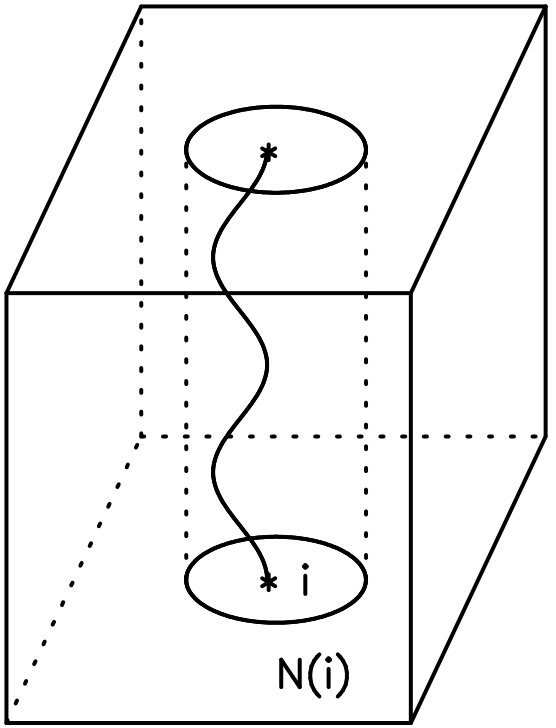
$$e^{-\beta E} \rightarrow e^{-\beta \hat{H}} = e^{-\tau \hat{H}} e^{-\tau \hat{H}} e^{-\tau \hat{H}} \ldots e^{-\tau \hat{H}}$$

Extra "imaginary time" dimension of extent $\beta = 1/T$.

If $\hat{H}$ is local, time is still linear in spatial lattice size.

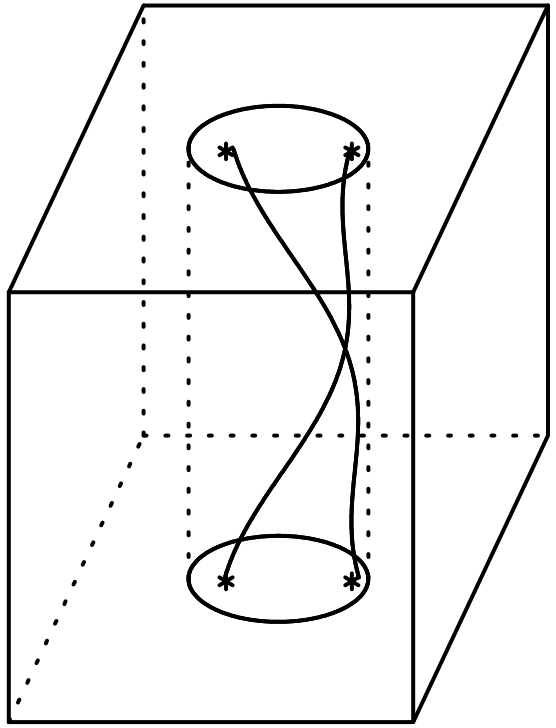
Cost is only extra dimension of lattice, a factor $\propto 1/T$.

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 !!!



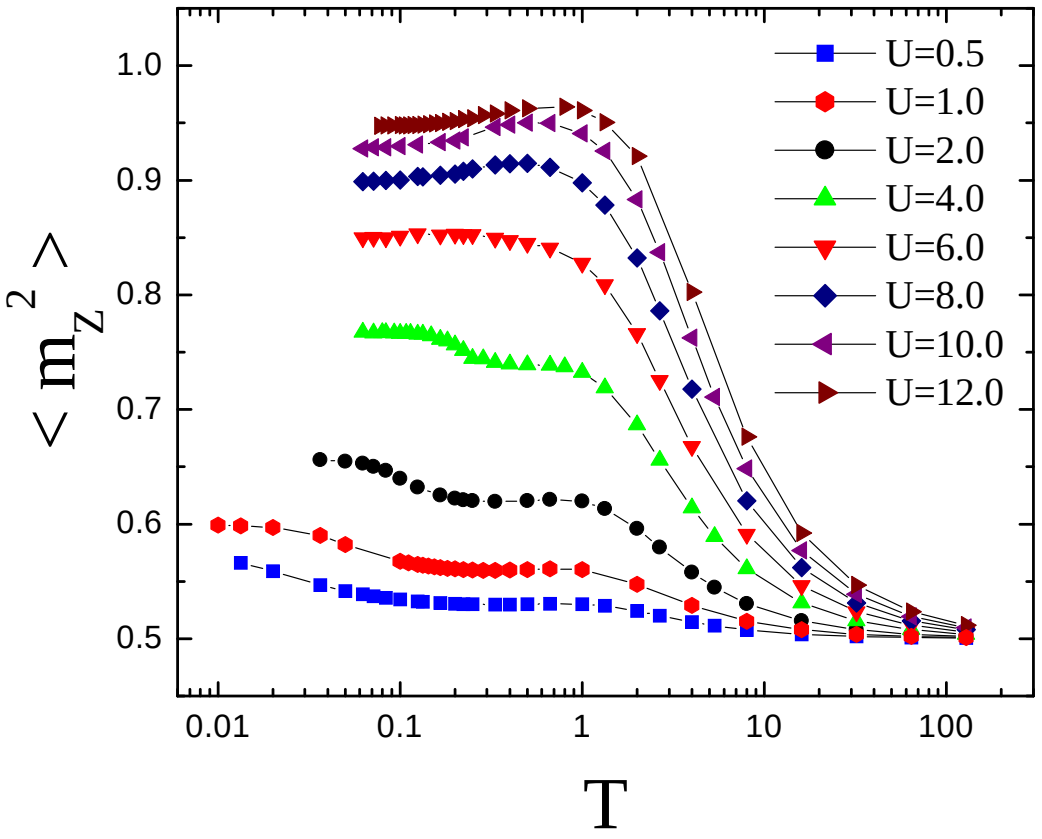
(Partial) solution: "Determinant" Quantum Monte Carlo.
Still have simulation in space and imaginary time,
but algorithm scales as cube of spatial size. Worse: Lingering sign problem.

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

Determinant Quantum Monte Carlo

Magnetic moment formation with T and U

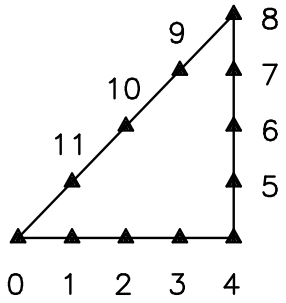
$$\langle m_z^2 \rangle = \langle (n_{j\uparrow} - n_{j\downarrow})^2 \rangle$$

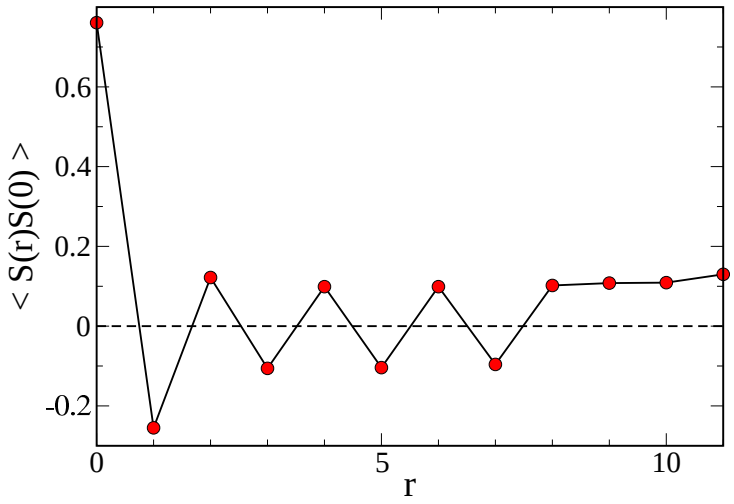


Spin Correlations (8x8 lattice)

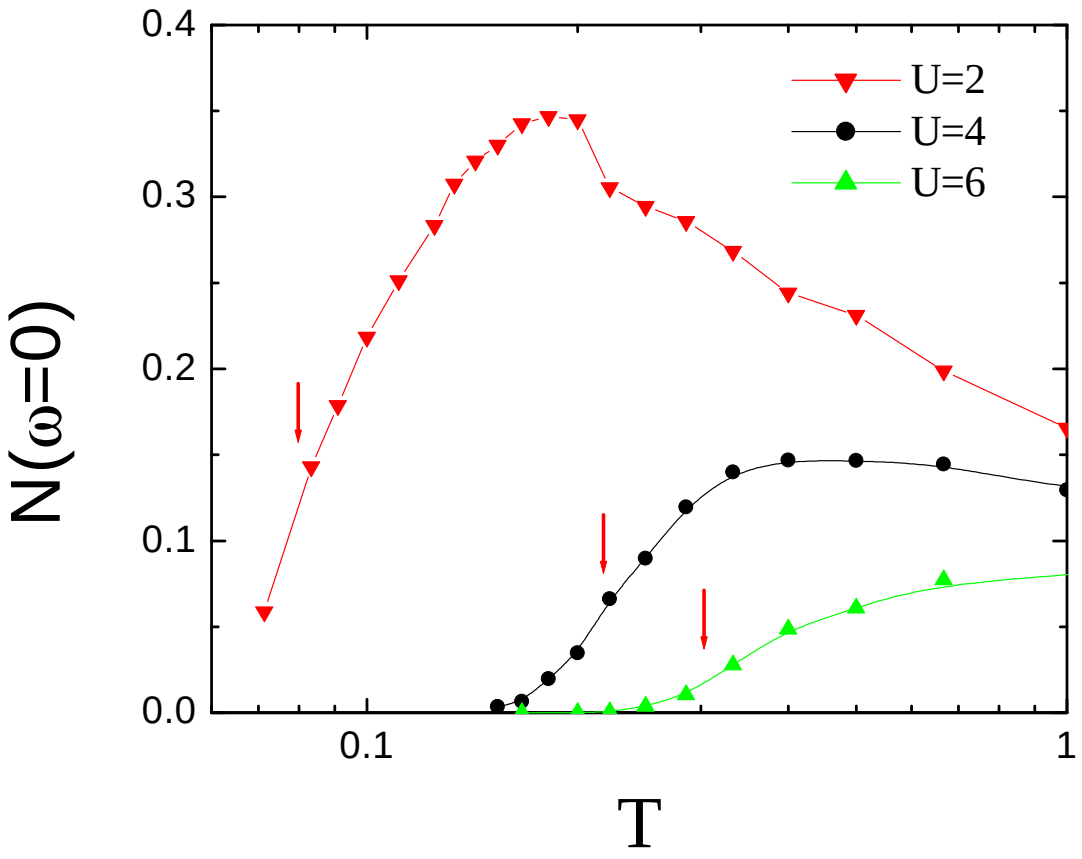
$$\langle\, c(l)\,\rangle \quad = \quad \langle\, (n_{j+l\uparrow} - n_{j+l\downarrow})(n_{j\uparrow} - n_{j\downarrow})\,\rangle$$

Local moment $\langle\, m_z^2\,\rangle$ is just $c(l=0)$.





Density of States



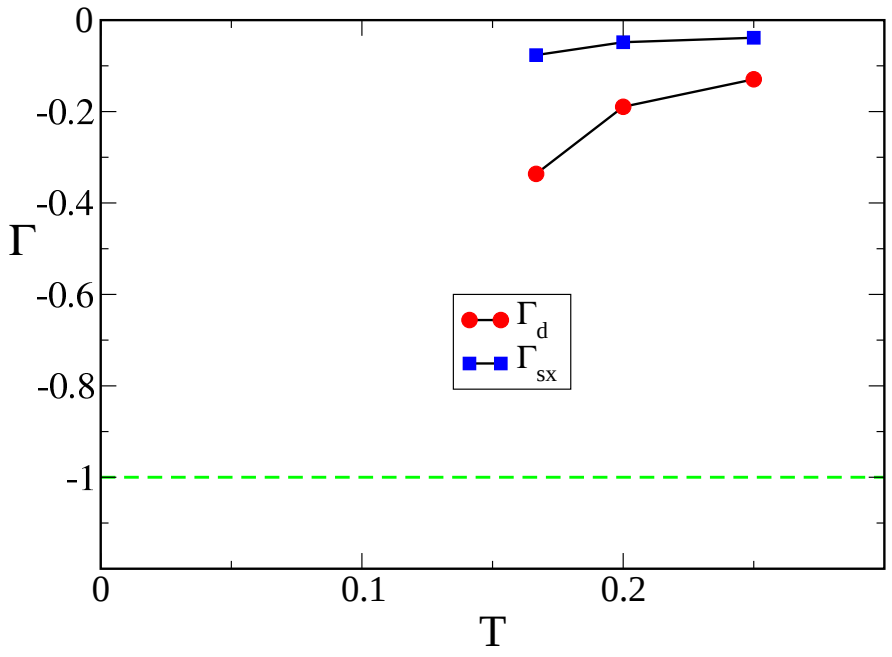
All of the preceding data at "half-filling" (one electron per lattice site).

This is a density where a special "particle-hole" symmetry of the Hubbard Hamiltonian prevents the sign problem.

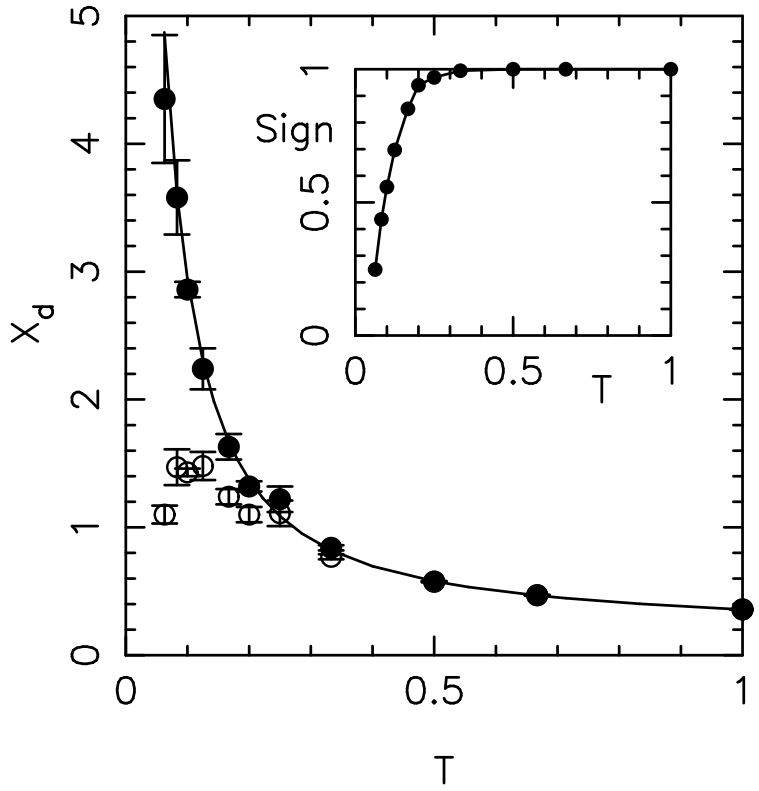
$s*$- and d-wave pairing vertices when doped away from half-filling

$\Gamma \to -1$ signals superconductivity.

- $*$ d-wave is dominant superconducting instability
- $*$ But cannot reach low enough T (sign problem)



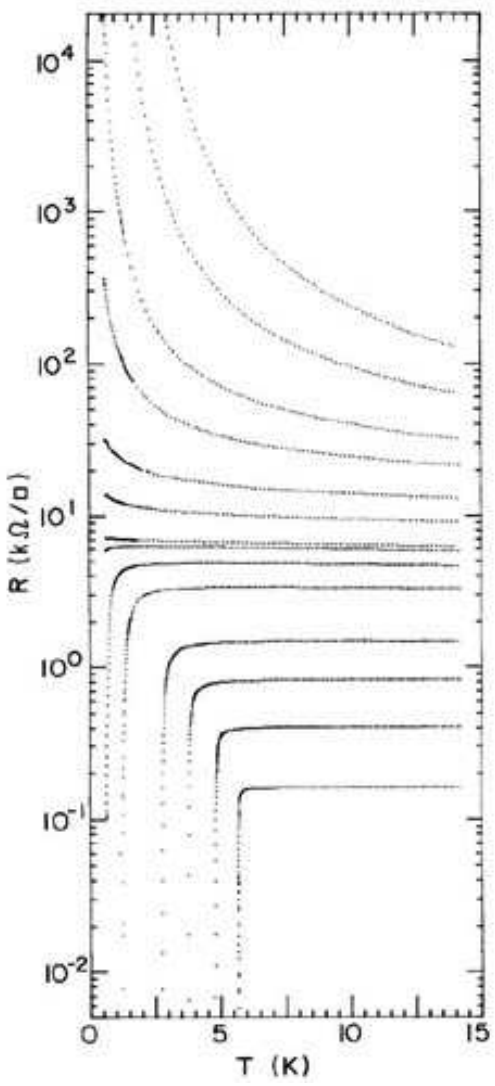
N=8x8 lattice



N=2x2 lattice

$< S > \to 0$ exponentially with $N, 1/T$

Disordered Superconductors



Bi, Pb, Sn, $In_{1-x}O_x$ films

Superconductor-Insulator Transition

Tune with:

- Film thickness
- O concentration
- Magnetic field strength

High disorder/field: metal $dR/dT > 0$

Low disorder/field: superconductor $dR/dT < 0$

Is resistance universal at transition??

Mechanism?

Complex superconducting order parameter $\Delta_j = |\Delta_j| e^{i\phi_j}$

- Magnitude of pairing gap vanishes: $|\Delta_j| \to 0$.
- Phase fluctuations: ϕ_j uncorrelated.

M.P.A. Fisher *etal* suggest bosonic Hubbard model

Alternately, "attractive" $(-|U|)$ fermion Hubbard model

Allows interpolation (with $|U|$) between

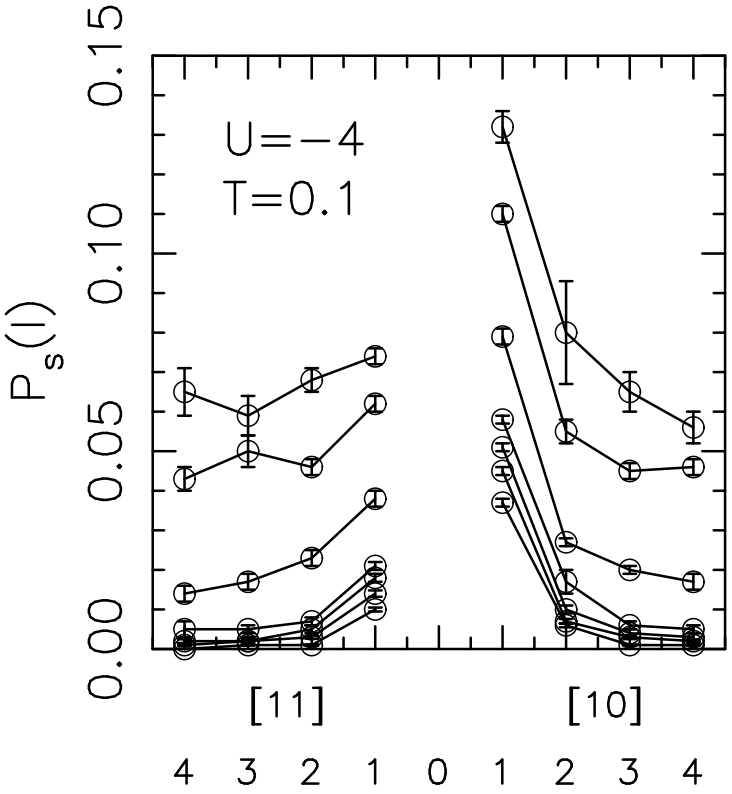
- Large $|U|$: Short coherence length/bosons/BEC
- Small $|U|$: Large coherence length/fermions/BCS

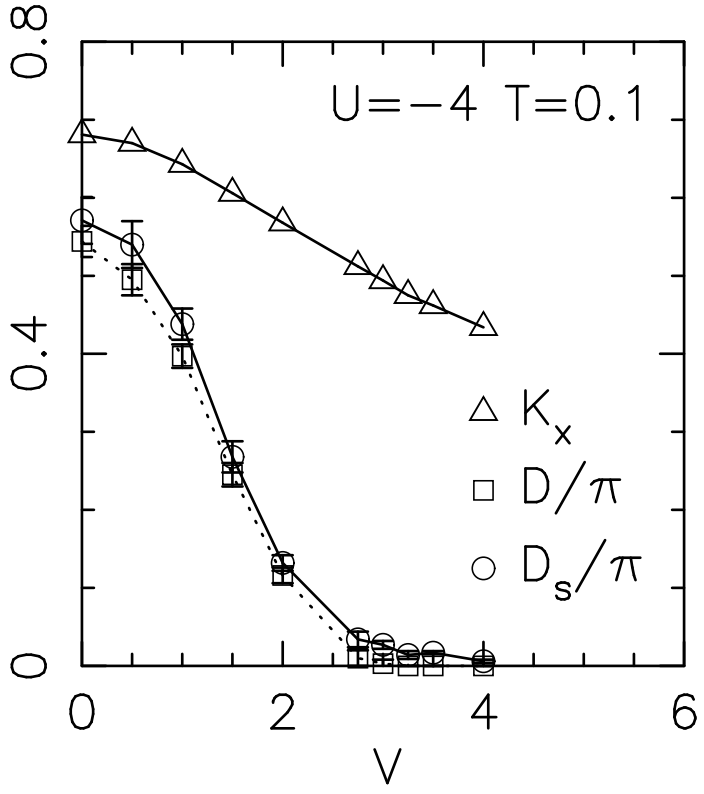
Particle-hole mapping between attractive and repulsive fermion Hubbard model

$c_{i\downarrow}$	$(-1)^i c^\dagger_{i\downarrow}$	
$-t\,(\,c^\dagger_{j\downarrow} c_{i\downarrow} + c^\dagger_{i\downarrow} c_{j\downarrow}\,)$	$-t\,(\,c^\dagger_{j\downarrow} c_{i\downarrow} + c^\dagger_{i\downarrow} c_{j\downarrow}\,)$	(for bipartite lattice)
$U(n_{i\uparrow} - \frac{1}{2})(n_{i\downarrow} - \frac{1}{2})$	$-U(n_{i\uparrow} - \frac{1}{2})(n_{i\downarrow} - \frac{1}{2})$	(p-h symmetric)
$S^+_j = c^\dagger_{j\uparrow} c_{j\downarrow}$	$\Delta^\dagger_j = (-1)^j c^\dagger_{j\uparrow} c^\dagger_{j\downarrow}$	SC correlations
$S^z_j = n_{j\uparrow} - n_{j\downarrow}$	$n_j = n_{j\uparrow} + n_{j\downarrow}$	CDW correlations

Site disorder term in Hamiltonian

$$\sum_i v_i n_i \qquad -\frac{V}{2} < v_i < +\frac{V}{2}.$$



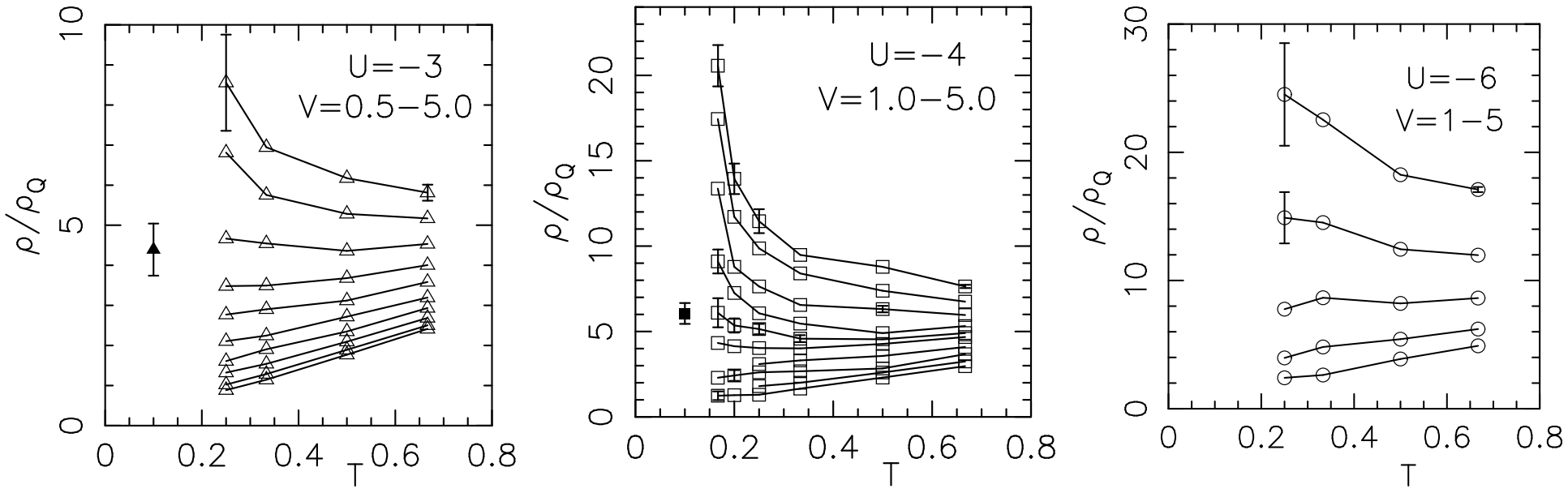


(s-wave) pair correlations $P_s(l) = \langle \Delta_{j+l} \Delta_j^\dagger \rangle$ driven to zero.

As are Drude-weight D and superfluid stiffness D_s.

N. Trivedi *etal*, PRB 54, 3756 (1996).

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



Value of resistance at separatrices is non-universal?

ρ is difficult to obtain from QMC (real time dynamics).

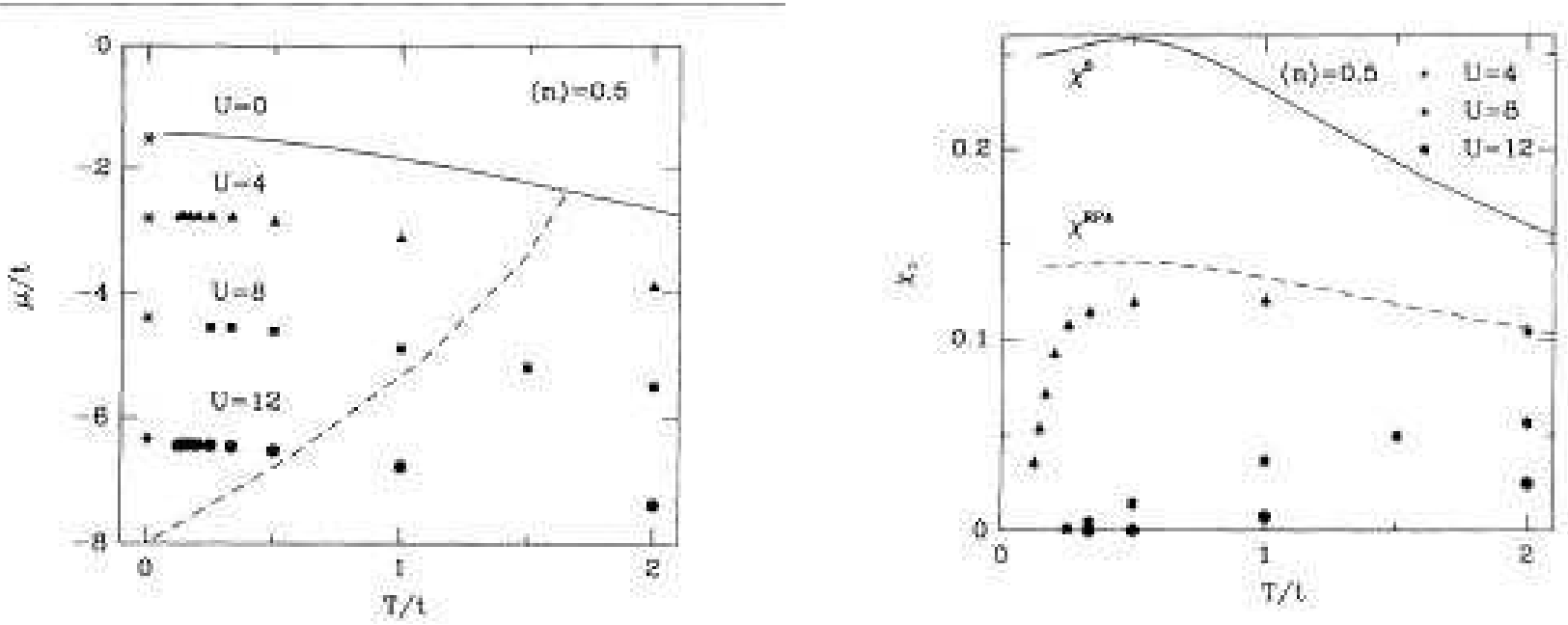
Application of (non-disordered) attractive Hubbard Model to cuprates.

Cuprates exhibit "spin gap":

Preformed Cooper pairs (bosons) exist above T_c

Spin up and down cancel: magnetic susceptibility χ suppressed

Sharp Fermi surface remains.



Left panel: $\mu(U,T)$ indicates system is degenerate. μ is much higher than T from the bottom of the band $(-4t)$ including Hartree shift.

$$\mu(T,U) + 4t + \langle n \rangle U/2) > T$$

Right panel: Yet spin susceptibility χ is sharply suppressed.

The bosonic Hubbard model

$$H = -J \sum_{\langle i,j \rangle} (b_i^\dagger b_j + b_j^\dagger b_i) + U \sum_i \hat{n}_i (\hat{n}_i - 1)$$

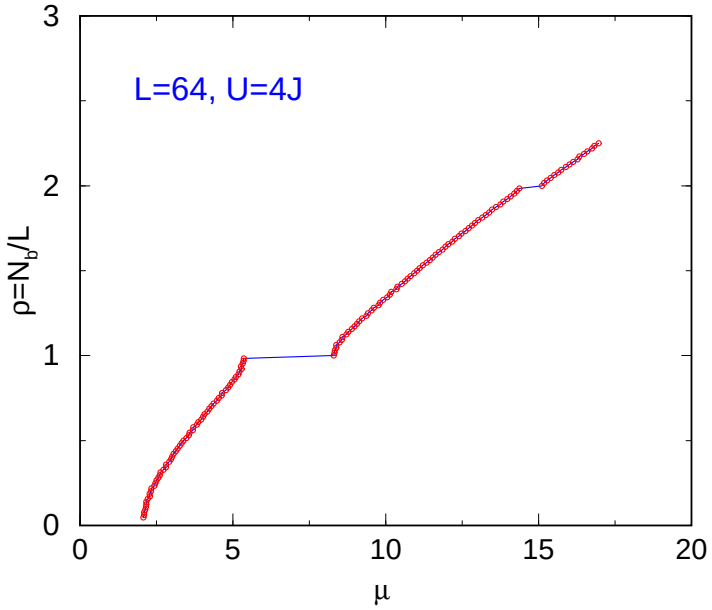
Again, disordered site energies:

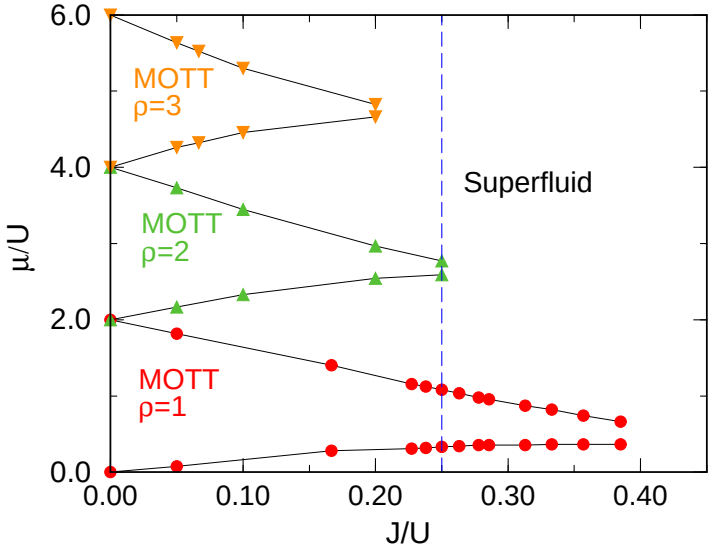
$$+ \sum_i v_i n_i \qquad\qquad -\frac{V}{2} < v_i < +\frac{V}{2}.$$

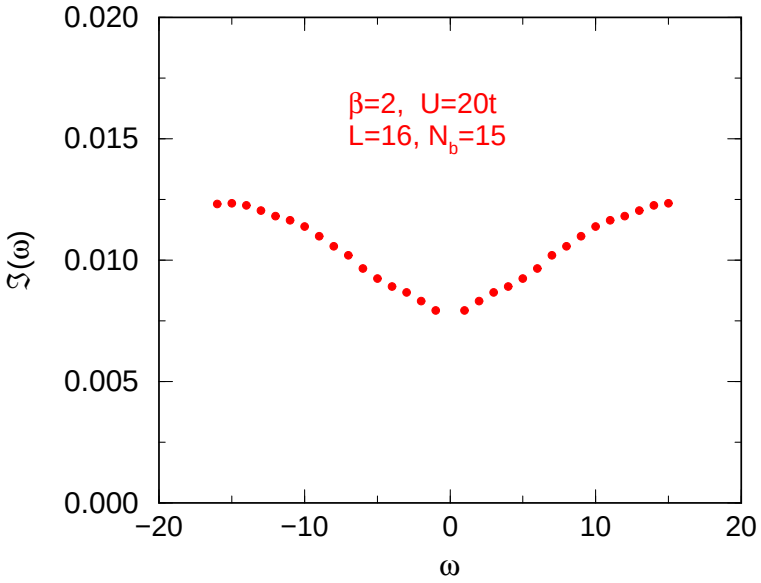
Extreme limit of attractive fermion Hubbard model.
M.P.A. Fisher *etal*, PRB40, 546 (1989).
or with a confining potential:

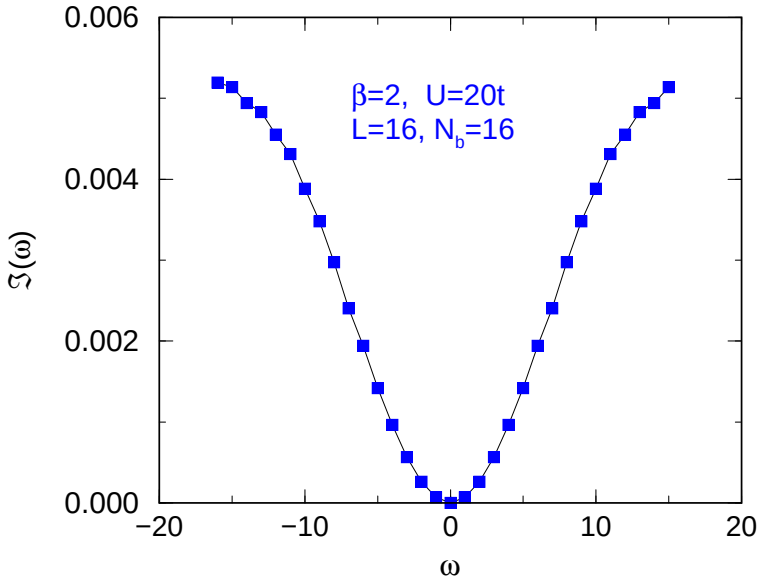
$$+ \sum_i v_i n_i \qquad\qquad v_i = V i^2$$

Phase diagram: Translationally Invariant Case









G.G. Batrouni *etal*, PRL 65, 1765 (1990).

Quantum Phase Transition

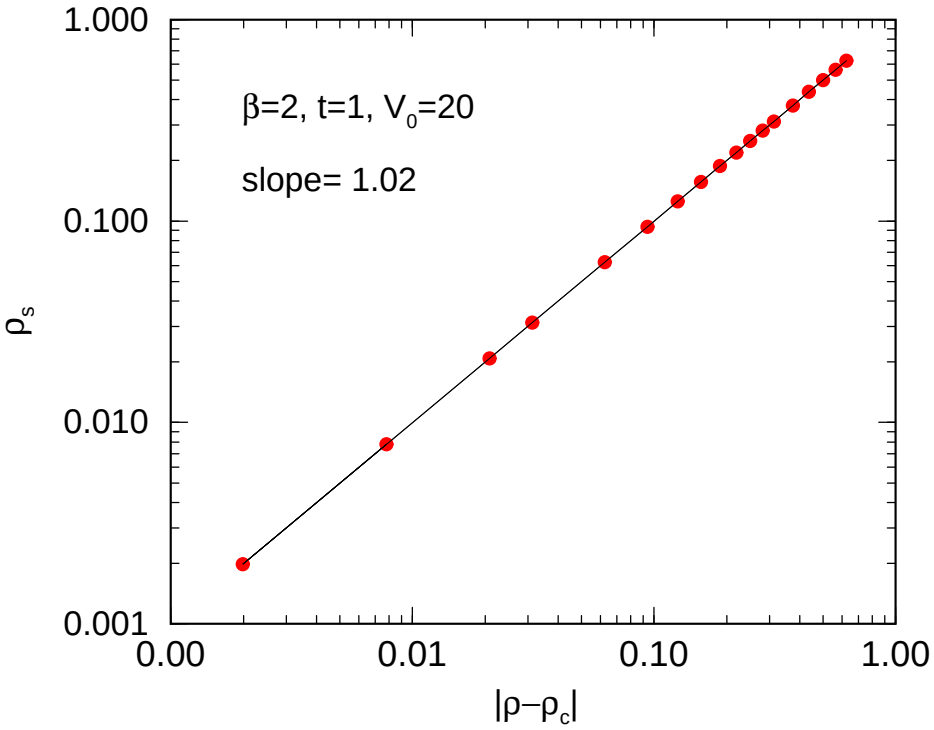
$$\kappa = \frac{\partial \rho}{\partial \mu} \rightarrow |\mu - \mu_c|^{-\nu/2} \text{ as } \mu \rightarrow \mu_c \qquad \rho_s \sim |\rho - \rho_{Mott}|^{z-d}$$

System sizes ranging from

$L = 16$ to $L = 256$

Quantum phase transition!

$z = 2, \quad \nu = 1$



(1)

Turn on disorder

New bose glass phase!

$\rho_s = 0$ but no Mott gap (incommensurate density).

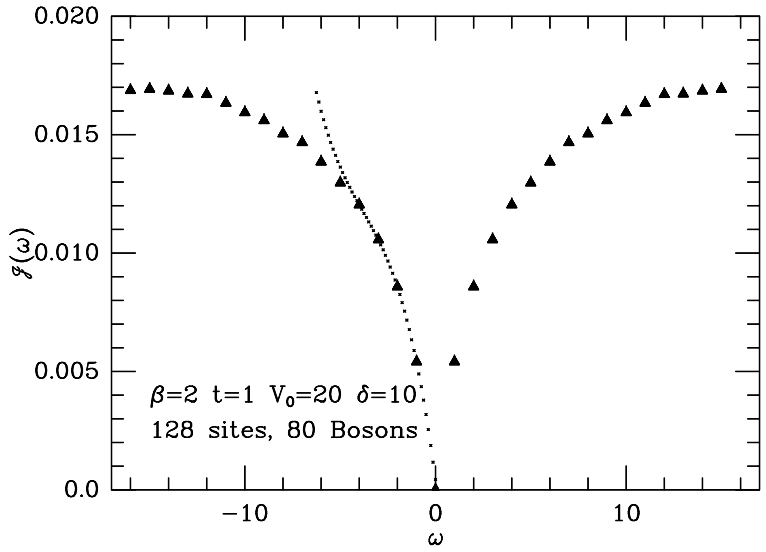


Figure 7

G.G. Batrouni and R.T. Scalettar

"World Line Simulations of the Bosonic Hubbard Model in the Ground State"

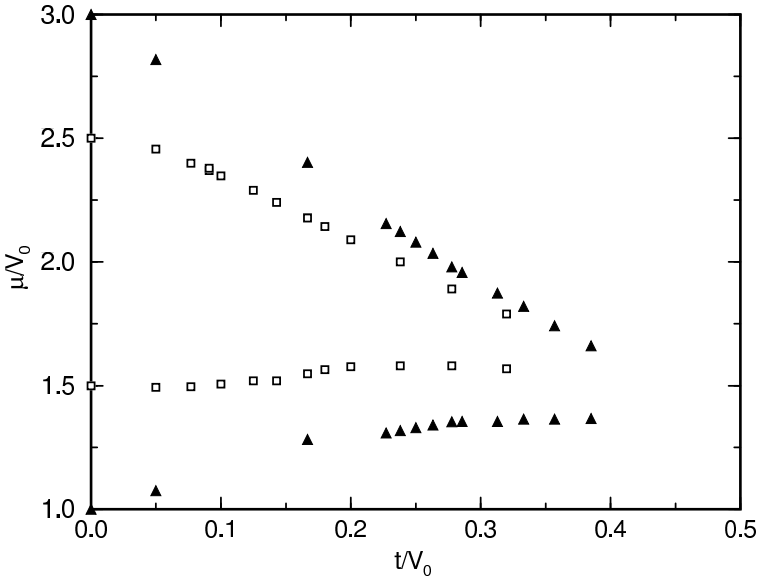


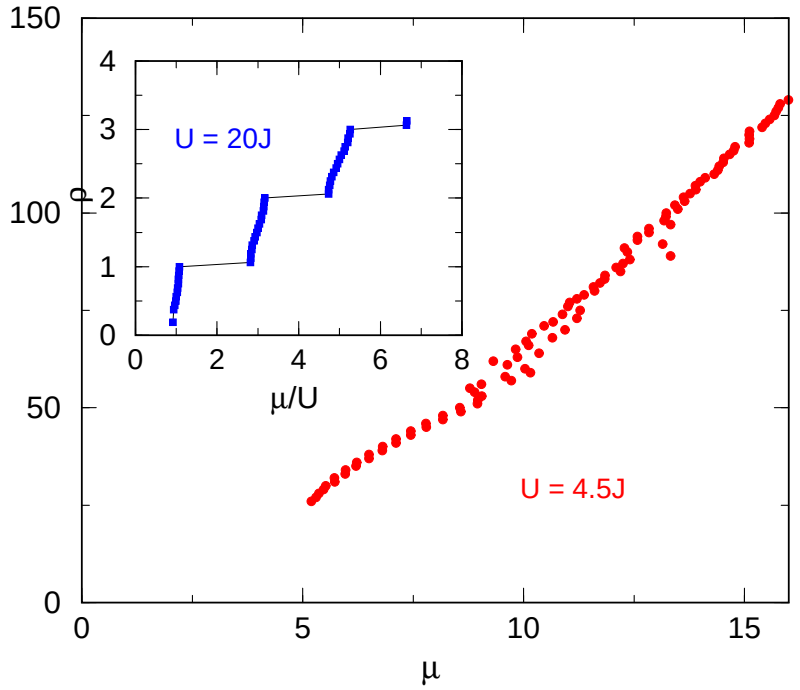
Figure 10

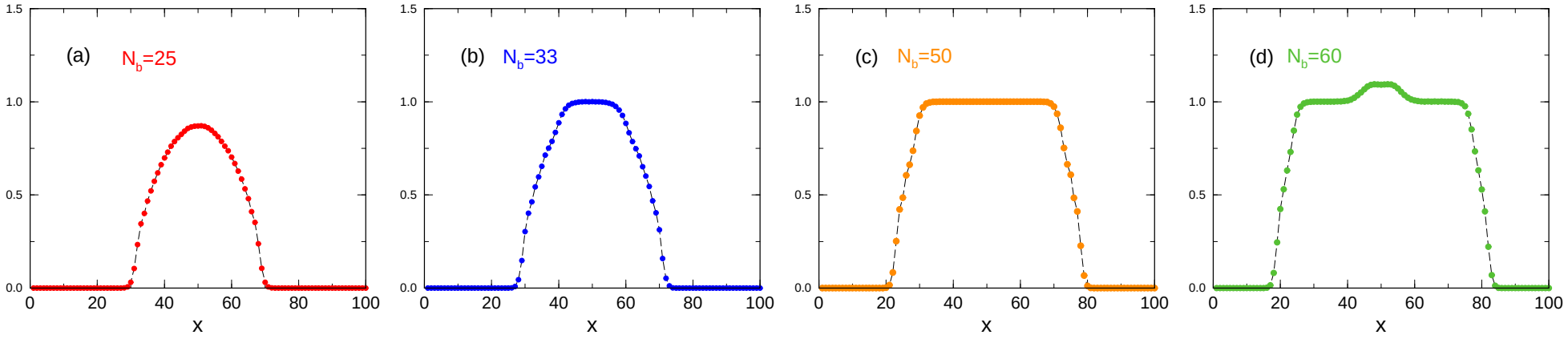
G.G. Batrouni

"Quantum Monte Carlo on a Lattice: The World Line Algorithm"

One dimensional trapped Boson Hubbard model

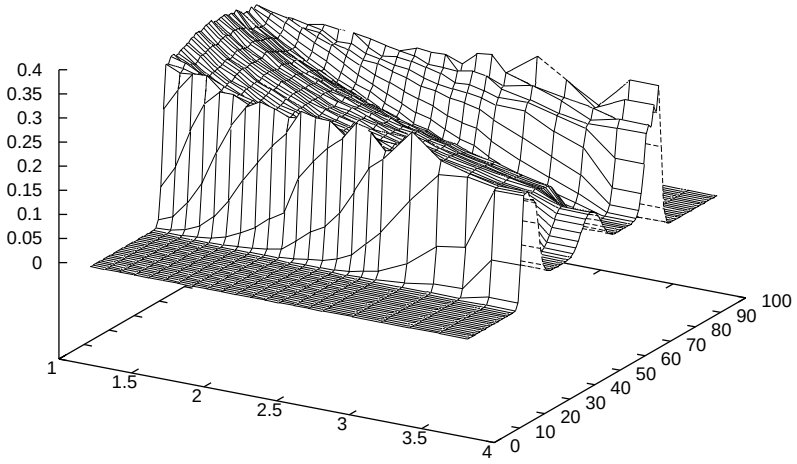
No globally incompressible Mott plateau in the trapped system! As a whole, the system is always compressible.

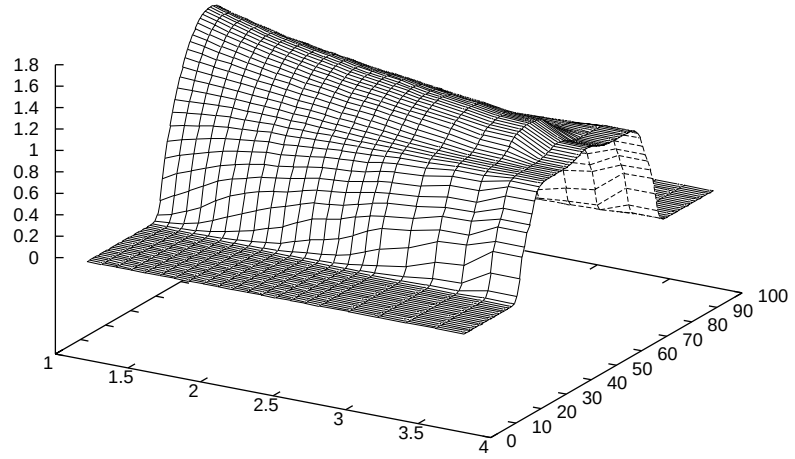




G. G. Batrouni *et al*, Phys. Rev. Lett. **89** 117203 (2002).

ρ and κ profiles: Fixed $N_b = 50$

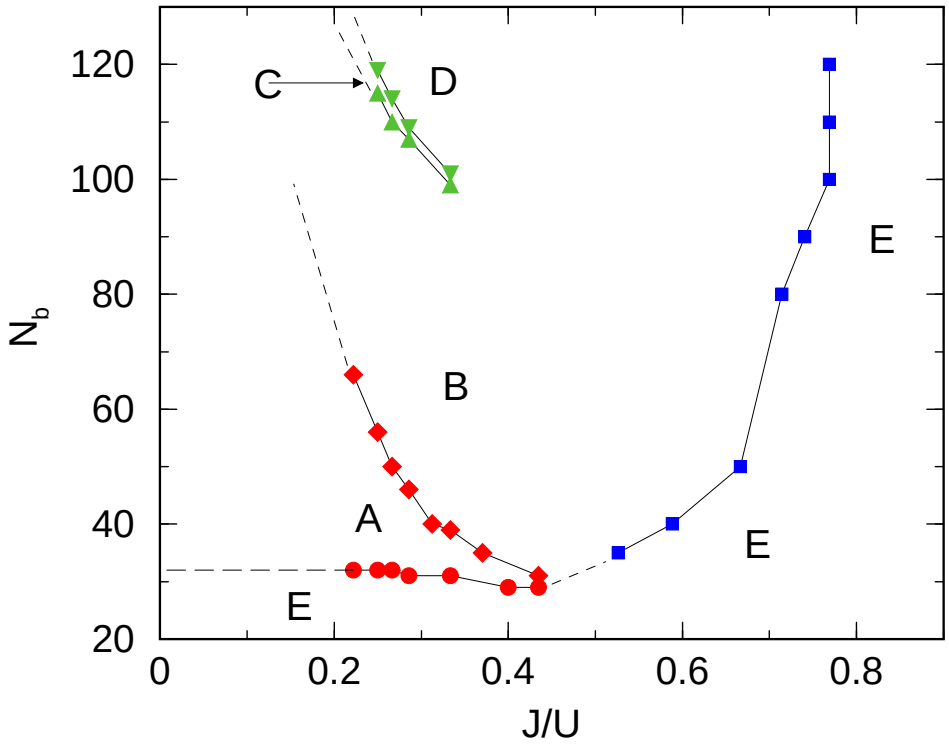


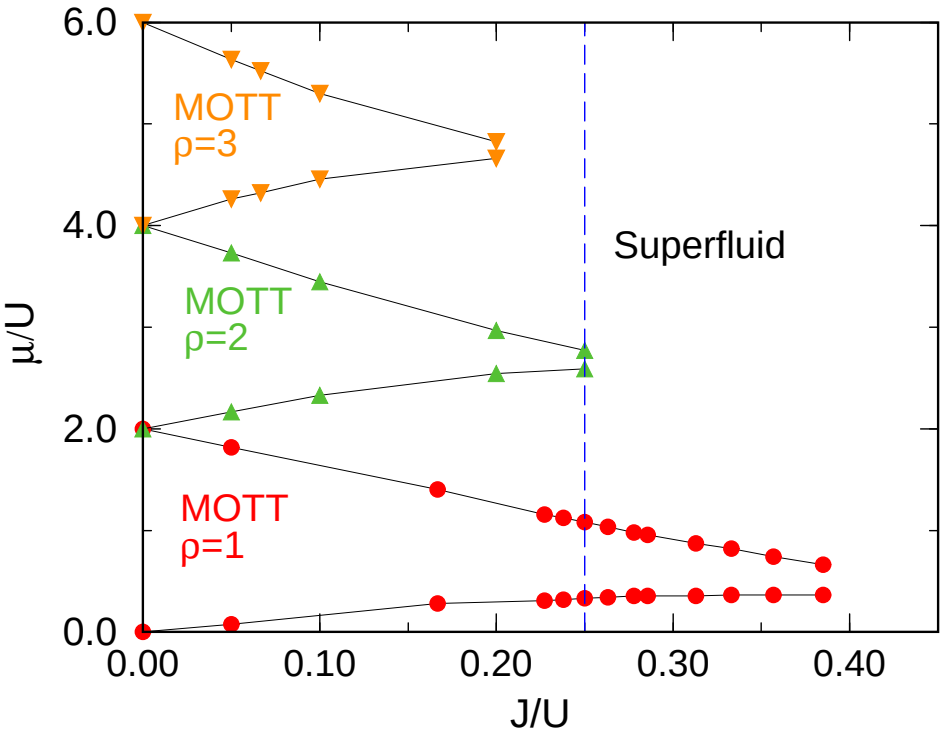


As U is increased, the system **gradually** crosses over to Mott:

No quantum phase transition.

State diagram





A: $\rho = 1$ Mott

B: SF in center + $\rho = 1$ Mott

C: $\rho = 2$ Mott + SF + $\rho = 1$ Mott

D: SF in center + $\rho = 2$ Mott + SF + $\rho = 1$ Mott

E: SF

The trapped one dimensional bosonic Hubbard model does not exhibit quantum critical behavior like the uniform system.

CONCLUSIONS

Hubbard Model provides (quite amazing) insight into qualitative physics of strongly interacting solids

- Metal-Insulator Transitions
- Magnetism
- d-wave Superconductivity
- Charge inhomogeneities

No real solid is precisely represented by the Hubbard model.

In general, you can't solve the fermion Hubbard model with QMC

- Boson Hubbard model is okay
- Fermion Hubbard model at half-filling is okay
- Fermion Hubbard model with $U < 0$ is okay

Challenge/Opportunity for AMO community

- Provide precise realization of Hubbard Model!
- Solve it!