

Unexpected metallic phases in models containing electron-phonon interactions

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Outline of talk

1. Motivation: electron-electron and electron-phonon interactions in complex materials
2. Model
3. Computational method
4. Results
5. Conclusion and outlook

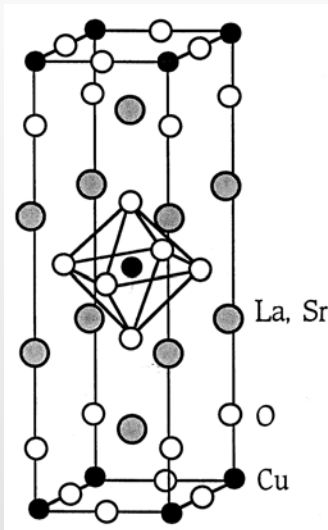
Challenge in strongly correlated electron materials: electron-electron and electron-phonon interactions typically give *insulating* states.

Once interactions are included, even the ground state problem is extremely challenging.

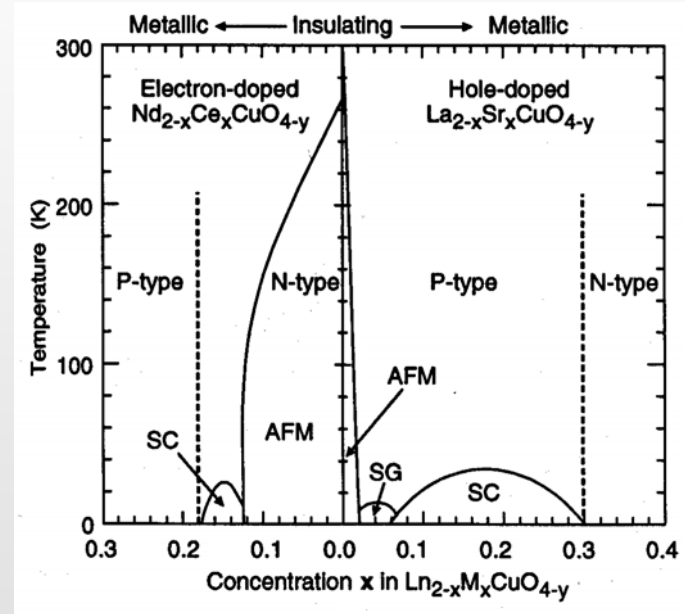
Here we show that in between the two insulating phases, a metallic phase can occur. This effect is not captured by mean-field theory.

High- T_c superconductors

Most famous “strongly correlated” material: high-temperature superconductivity (SC), discovered in 1986



All HTC have planes of Cu-O atoms

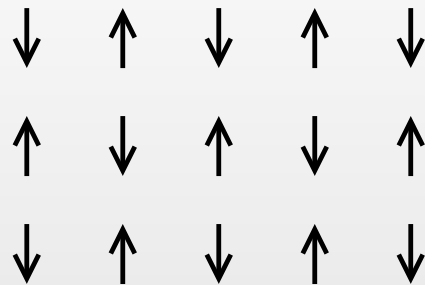


phase diagram, one class of HTC

Anti-ferromagnetism

Can we understand any of the phases in a simple physical picture?

Yes, for one, anti-ferromagnetism (AFM): spins on copper atoms are in a square lattice, aligned anti-parallel:



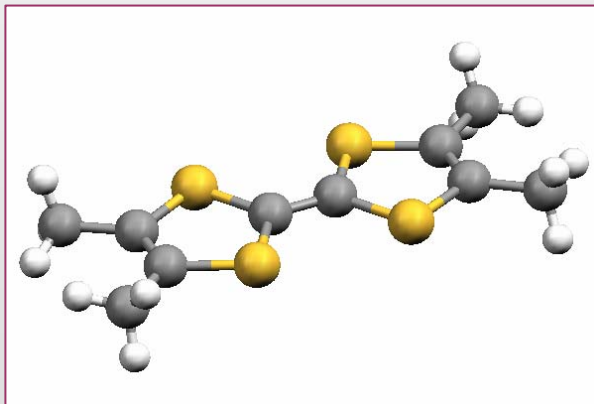
What kind of model can describe this state?

→ must have *interactions* between electrons, usually ignored in band theories of solids.

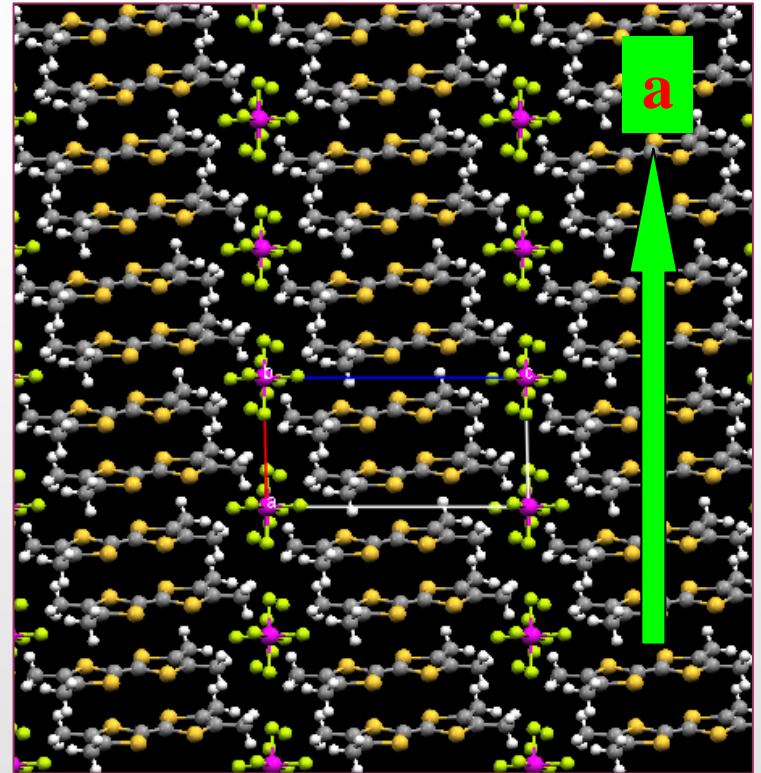
→ Hubbard model: two electrons occupy same orbital, energy U ; reduces to anti-ferromagnetic Heisenberg interaction for large U

Organic (molecular) Superconductors

- First organic SC ~ 1980, $(\text{TMTSF})_2\text{PF}_6$
- T_c 's order of magnitude lower than cuprates
- electron concentration different: anion PF_6 gives hole doping 1 hole/2 molecules.
- Other families: quasi-2D structure
- Many of current interest because of *triangular* lattice structures



TMTSF molecule



$(\text{TMTSF})_2\text{X}$ crystal. Highest conductivity axis (**a**) indicated.

T-P Phase Diagram (Jerome)

Pressure applied physically or chemically by changing size of anion.

Many phases with unusual electronic and magnetic properties (broken symmetry phases).

Understanding phases requires both electron-electron and *electron-phonon* interactions:

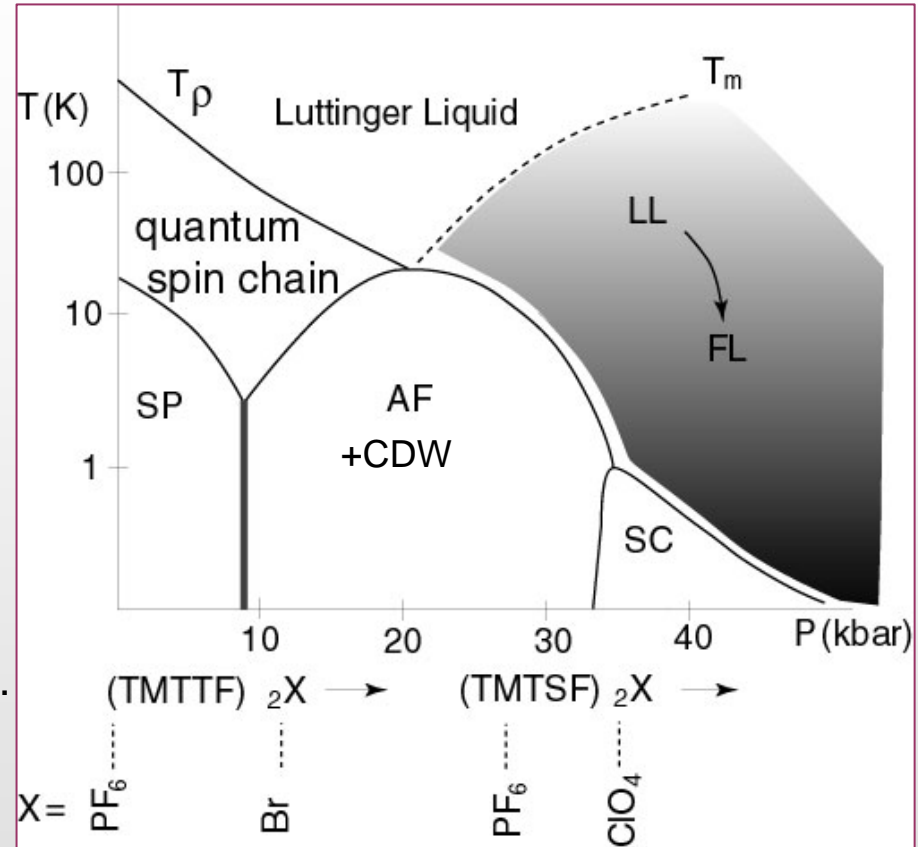
RTC, S Mazumdar, PRL **94**, 207206(2005)

RTC, SM, DK Campbell, PRB **67**, 115121 (2003).

RTC,SM,DKC,PRL **86**, 4084(2001).

SM, RTC, DKC, PRB **62**, 13400(2000).

SM *et al*, PRL**82**, 1522(1999).



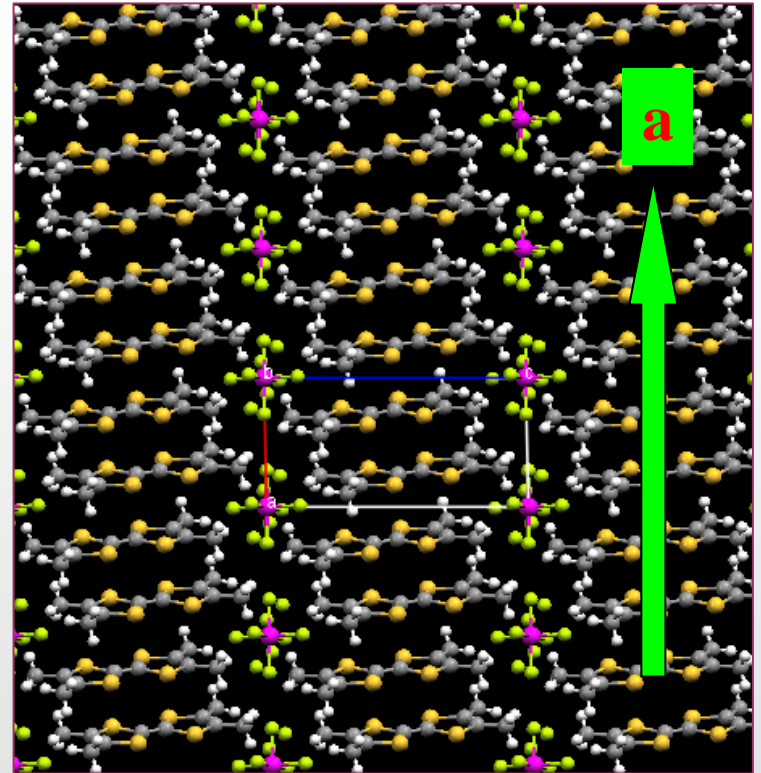
SP=spin-Peierls AF=antiferromagnetic
 SC=superconductivity LL=Luttinger Liq
 FL=Fermi Liquid CDW=charge density wave

Two kinds of phonons

Two basic kinds of phonon modes:

1. inter-molecular motion. Often modeled by Su-Shrieffer-Heeger (SSH) model, changing electron hopping *between* molecules.
2. intra-molecular motion. Internal vibrations of each organic molecule. Often modeled by Holstein model, changing *site energy* for electrons.

In this work, focus on type #2, Holstein phonons.



$(\text{TMTSF})_2\text{X}$ crystal. Highest conductivity axis (**a**) indicated.

Hubbard-Holstein Hamiltonian

Interacting electrons ($c_{i\sigma}$) + dispersionless phonons (a_i) coupled to electron density

$$H = -t \sum_{i,\sigma} (c_{i+1,\sigma}^+ c_{i,\sigma} + h.c.) + U \sum_i n_{i,\uparrow} n_{i,\downarrow} \\ + \sum_i g (a_i^+ + a_i) n_i + \omega \sum_i a_i^+ a_i$$

Parameters:

- electron hopping t
- Coulomb onsite energy U
- electron-phonon coupling g and phonon frequency ω

focus on *half filling*, one electron per lattice site, and one dimension (1D).
Exactly solvable if only t and U (no phonon coupling).

A *hard* problem due to the size of the Hilbert space.

Computational Challenge

Basic problem: if we want to treat interactions between electrons,

→ matrix eigenvalue problem of size N_s that scales exponentially with N (number of orbitals).

What is N_s ? There are 4 possible electron configurations in each orbital:

(empty), \uparrow , \downarrow , $\uparrow\downarrow$ → $N_s \sim 4^N$

- H is a very sparse matrix, but this scaling quickly exhausts memory! And we really want $N \rightarrow \infty$!
- We also have an (in principle) *infinite* number of phonon states per oscillator, and the total number of states is the *product* of the two

Quantum Monte Carlo

Quantum Monte Carlo (QMC): a statistical method

- instead of summing over all states, *sample* from them.
- often (not always!) trivial to parallelize
- **BIG PROBLEM**: Fermion Sign problem

In QMC: a weight function $W(C_i)$, which gives the weight for configuration C_i . Then for the average of some property A :

$$\langle A \rangle = \frac{\sum_i A(C_i)W(C_i)}{\sum_i W(C_i)}$$

QMC

$$\langle A \rangle = \frac{\sum_i A(C_i)W(C_i)}{\sum_i W(C_i)}$$

To be a probability, $W(C_i)$ must be positive definite. But it isn't for most quantum systems!

Why not use the absolute value $|W_i|$? Define the sign, $S_i = \pm 1$

$$\langle A \rangle = \frac{\sum_i A(C_i)S(C_i)|W(C_i)|}{\sum_i |W(C_i)|} \times \frac{1}{\langle S \rangle} = \frac{\langle AS \rangle}{\langle S \rangle}$$

Unfortunately, for most systems of electrons $\langle S \rangle \cong 0$. This average is then very badly behaved, and usually gets *worse* for larger N .

But: no sign problem in some restricted cases (such as one dimension).

QMC

Recent incorporation of *loop* (cluster) updates have greatly increased power of QMC:

- first used for classical models (Ising)
- greatly reduces autocorrelation time of method

Stochastic Series Expansion (SSE) QMC

- in principle exact within statistical error
- based on expansion of partition function (finite temperature)
- easy to adapt for a variety of models (spins, Fermions, bosons)
- efficient loop updating
- limited by Fermion sign problem (not present in one dimension)
- here first application to Holstein phonons

Reference: Syljuåsen and Sandvik, *Phys. Rev. E* **66**, 046701 (2002)

Hubbard-Holstein physics

1. Hubbard U

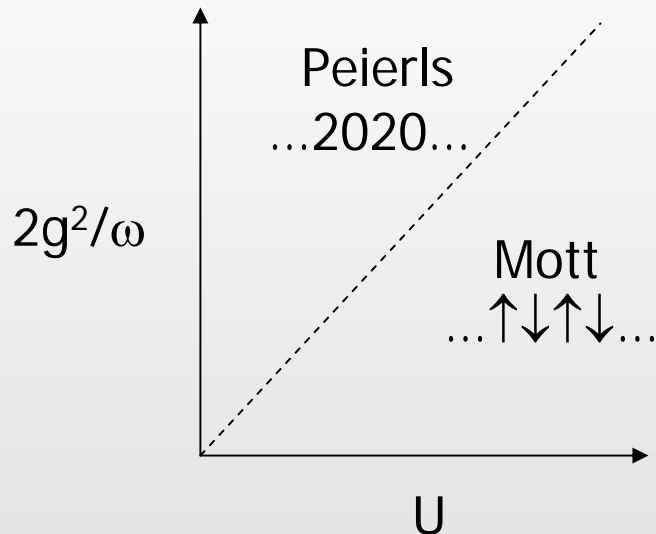
→ at $\frac{1}{2}$ -filling any positive U gives a charge gap (Mott-Hubbard insulator).
No spin gap.

2. Holstein coupling

→ Promotes Peierls charge-density wave (CDW) state with electron occupation ...2020... Both charge and spin gaps

→ in adiabatic (classical phonon) limit, $\omega \rightarrow 0$, CDW for any $g > 0$. Properties for *finite* ω are debated...

Mean field phase diagram



The *effective* U is $U_{\text{eff}} = U - 2g^2/\omega$

When

$U_{\text{eff}} < 0 \rightarrow$ Peierls state

$U_{\text{eff}} > 0 \rightarrow$ Mott state

both states are insulating

(brief) Holstein-Hubbard history

- Hirsch & Fradkin, PRB **27**, 4302(1983) :
 - for the spinless model, quantum fluctuations of phonon field destroy Peierls order. Need finite e-ph coupling for gap.
 - for model with spin, *any* finite e-ph coupling gives a gap (would agree with qualitatively with mean-field theory).
- Wu, Huang, Sun PRB **52**, 15683(1995) :
 - with spin, a *finite* e-ph coupling needed for a gap
- Jeckelmann, Zhang, White PRB **60**, 7950(1999) :
 - also find finite coupling numerically, but no check of size scaling
- Takada, Chatterjee PRB **67**, 081102R(2003) :
 - when U is present, predict a third *intermediate* phase between Peierls/Mott

Bottom line: no detailed numerical study for even 1D model!

Finite critical coupling: KT transition

In *mean-field* theory, electron-phonon coupling usually leads to an insulating Peierls state for *any* 0^+ phonon coupling.

Now evidence for several phonon-coupled models that a Kosterlitz-Thouless (KT) type transition occurs, with *finite* critical e-ph coupling (zero-temperature transition).

Examples:

- 1D XY spin chain + dispersionless phonons: Caron, Moukouri PRL **76**, 4050 (1999)
- 1D Heisenberg mode + dispersionless phonons: Sandvik, Campbell PRL **83**, 195 (1999)
- 1D Peierls-Hubbard (dispersionless SSH phonons): Sengupta, Sandvik, Campbell PRB **67**, 245103 (2003).

Spin and Charge Stiffness ($U=0, \omega=1$)

Charge, spin stiffness: second derivative of energy

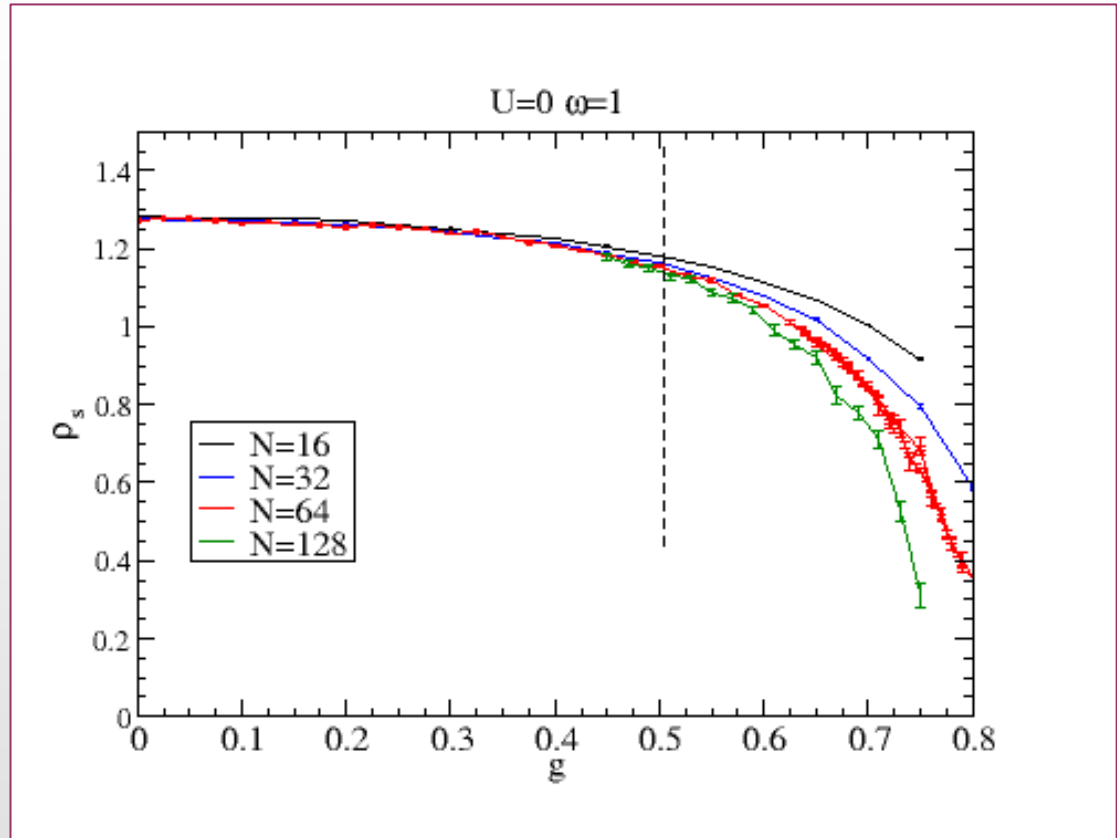
$$\rho = \frac{1}{N} \frac{\partial^2 E_0(\phi)}{\partial \phi^2}$$

Nonzero ρ : no gap

zero ρ : gapped

→ In KT transition, ρ jumps discontinuously to zero at $g=g_c$ ($N \rightarrow \infty$)

→ Finite N : stiffness scales logarithmically to finite value for $g < g_c$, scales to zero for $g > g_c$



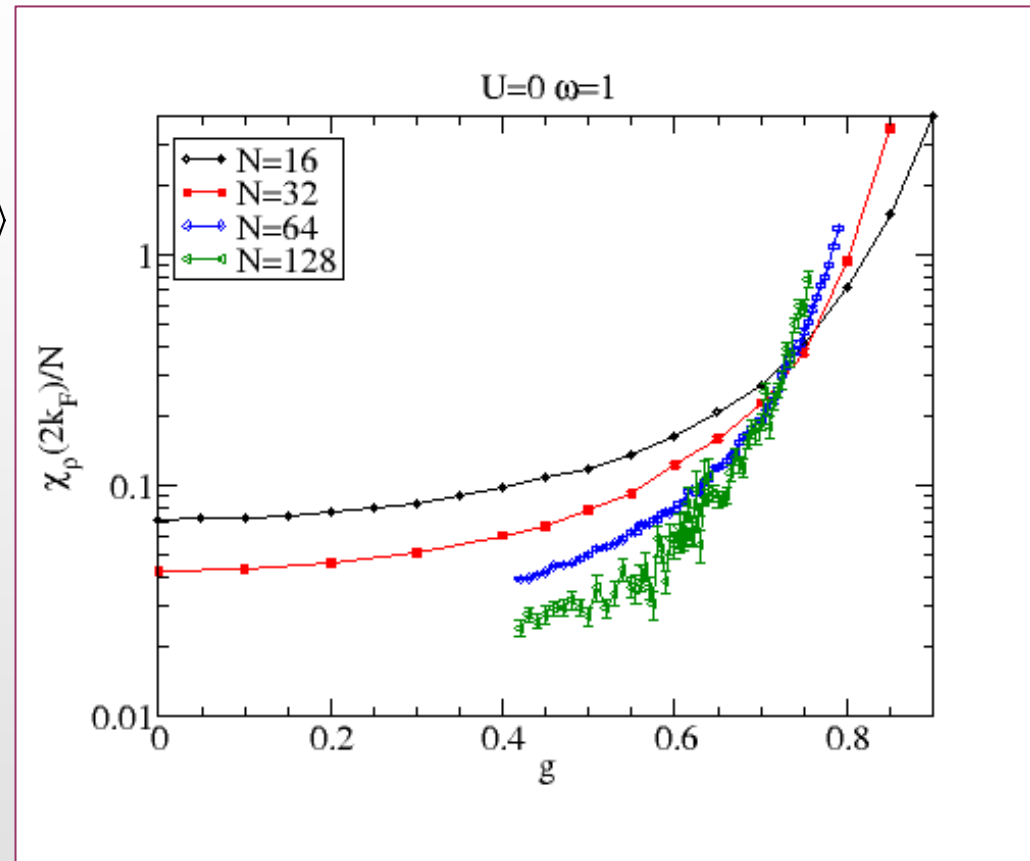
Charge susceptibility ($U=0, \omega=1$)

Charge susceptibility:

$$\chi_\rho(q) = \frac{1}{N} \sum_{k,l} e^{iq(k-l)} \int_0^\beta d\tau \langle n_k(\tau) n_l(0) \rangle$$

measure $q=\pi$ (staggered)
correlations:

1. In Peierls phase ($g > g_c$):
 $\chi_\rho(\pi)/N$ diverges
2. In undistorted phase ($g < g_c$):
 $\chi_\rho(\pi)/N$ converges to zero



Finite-size scaling ($U=0, \omega=1$)

Charge susceptibility: $\chi_\rho(q)$

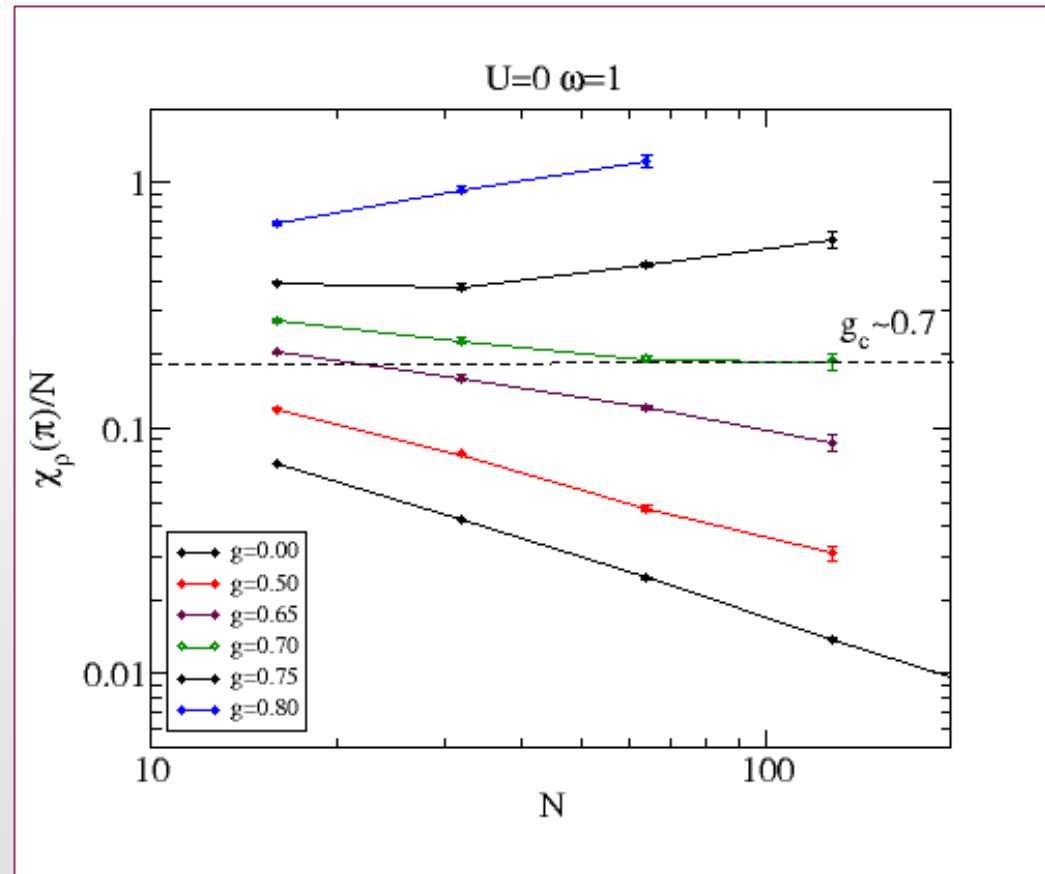
3. At critical coupling g_c :

$\chi_\rho(\pi)$ diverges *linearly* with N ,
log corrections vanish.

Our results consistent with KT-
type transition at $g_c \sim 0.7$

similar result in a spin system:

AW Sandvik and DK Campbell, PRL
83, 195 (1999)



Charge Structure factor slope ($U=0, \omega=1$)

Another observable to detect gap:
structure factor

$$S_\rho(q) = \frac{1}{N} \sum_{k,l} e^{iq(k-l)} \langle n_k n_l \rangle$$

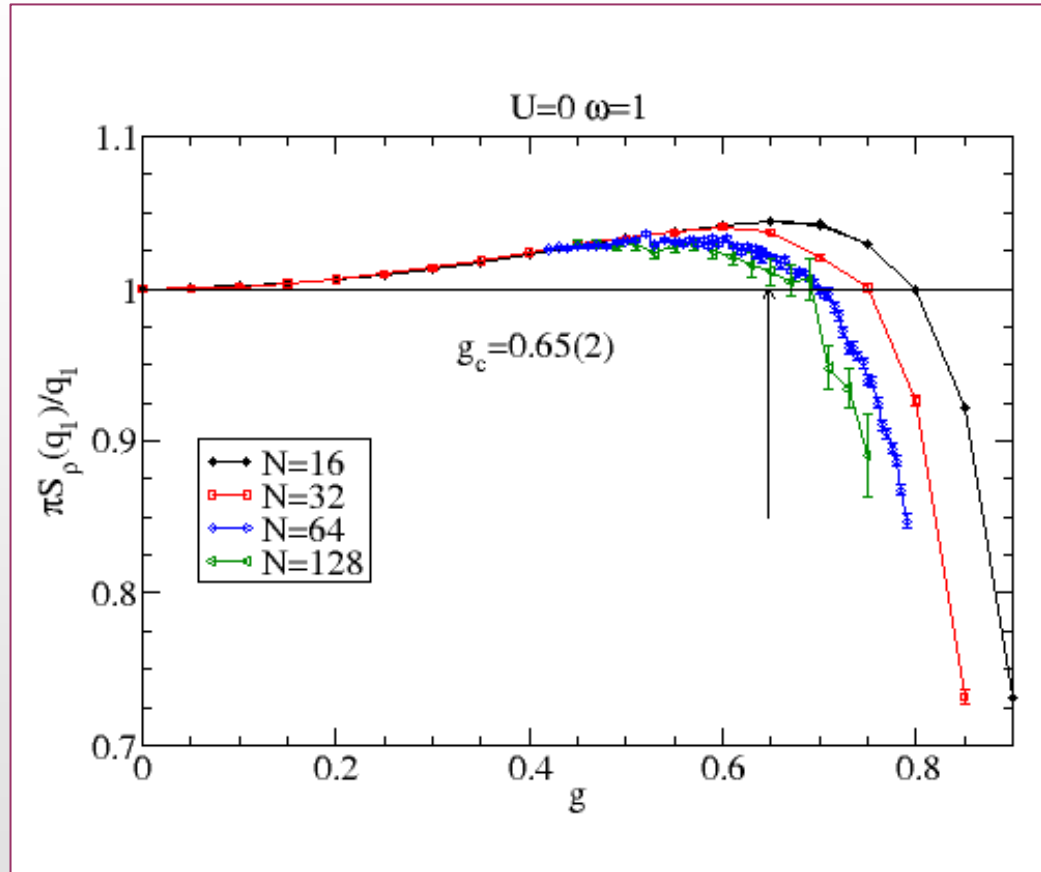
Compute the *slope* of the structure factor vs. q , as $q \rightarrow 0$

slope $> \pi$: no gap

slope $< \pi$: gap

Can detect very small gap, statistics are better than for susceptibility.

This is essentially a measure of the *Luttinger Liquid* exponent K_ρ



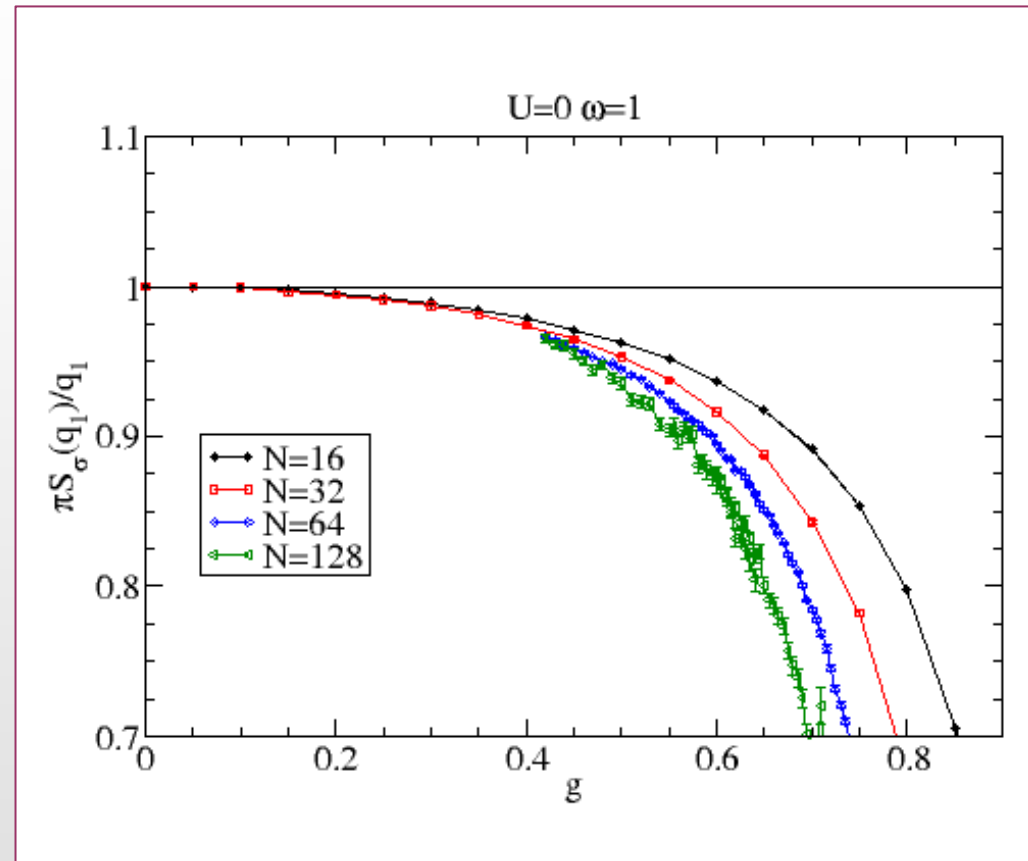
Spin gap ($U=0, \omega=1$)

What happens to the *spin* degrees of freedom?

→ there is a *spin gap* for any e-ph coupling $g>0$

Summary, $U=0, 1/2$ filling:

- a KT-type transition occurs at finite e-ph coupling g_c
- $g>g_c$: Peierls spin, chg gap
- $g<g_c$: spin gap but no chg gap. Identical to $U<0$ Hubbard model, CDW and singlet SC correlations are *degenerate*.



Comparison: 1D Hubbard (no phonons)

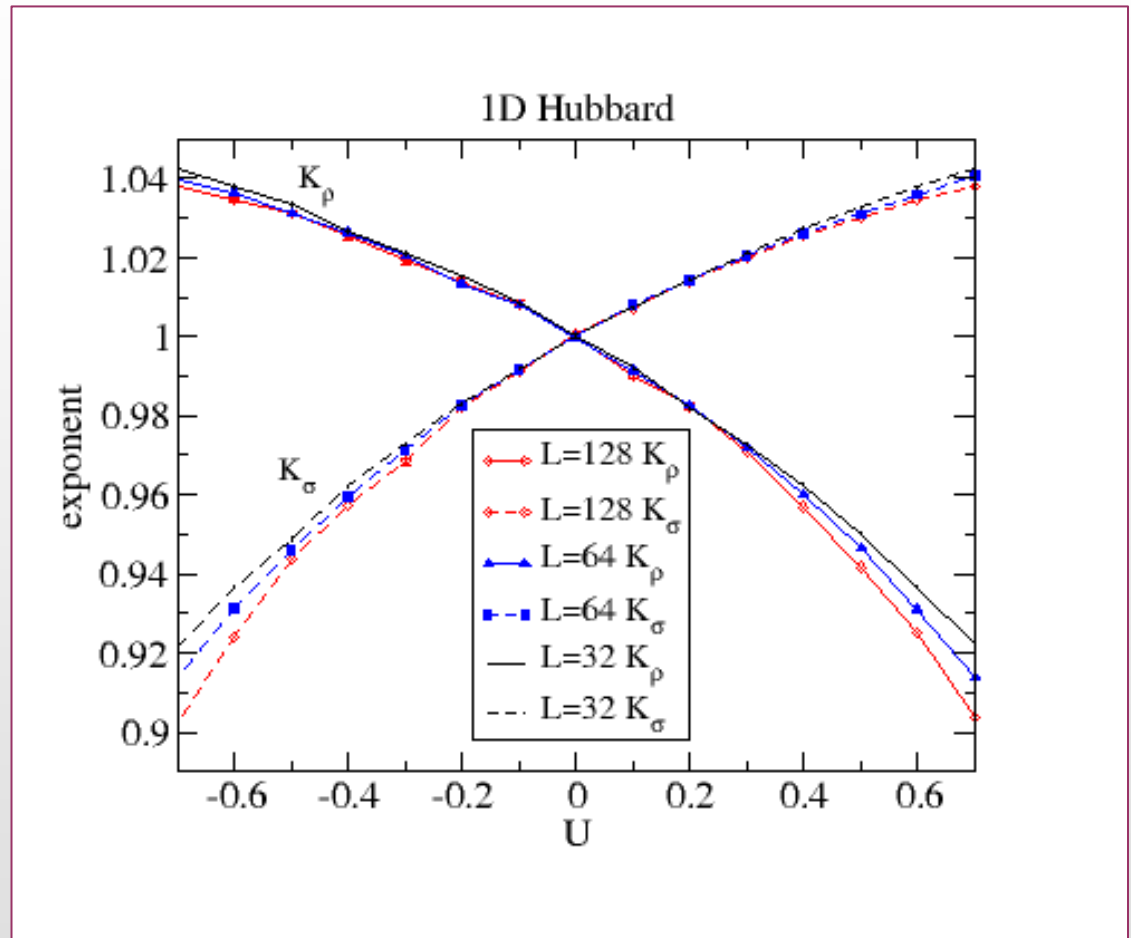
Note that scaling of exponents to 1 with lattice size is very slow (logarithmic), either for:

A. $U < 0$:

charge exponent $K_\rho = 1$

A. $U > 0$:

spin exponent $K_\sigma = 1$



Finite U

What happens when $U > 0$?

→ now a third phase is possible. If U is large enough, we get a Mott-Hubbard insulator.

Mott-Hubbard state: charge gap, but no spin gap

Cartoon picture: anti-ferromagnetic correlations: ... $\uparrow\downarrow\uparrow\downarrow\uparrow\downarrow$...

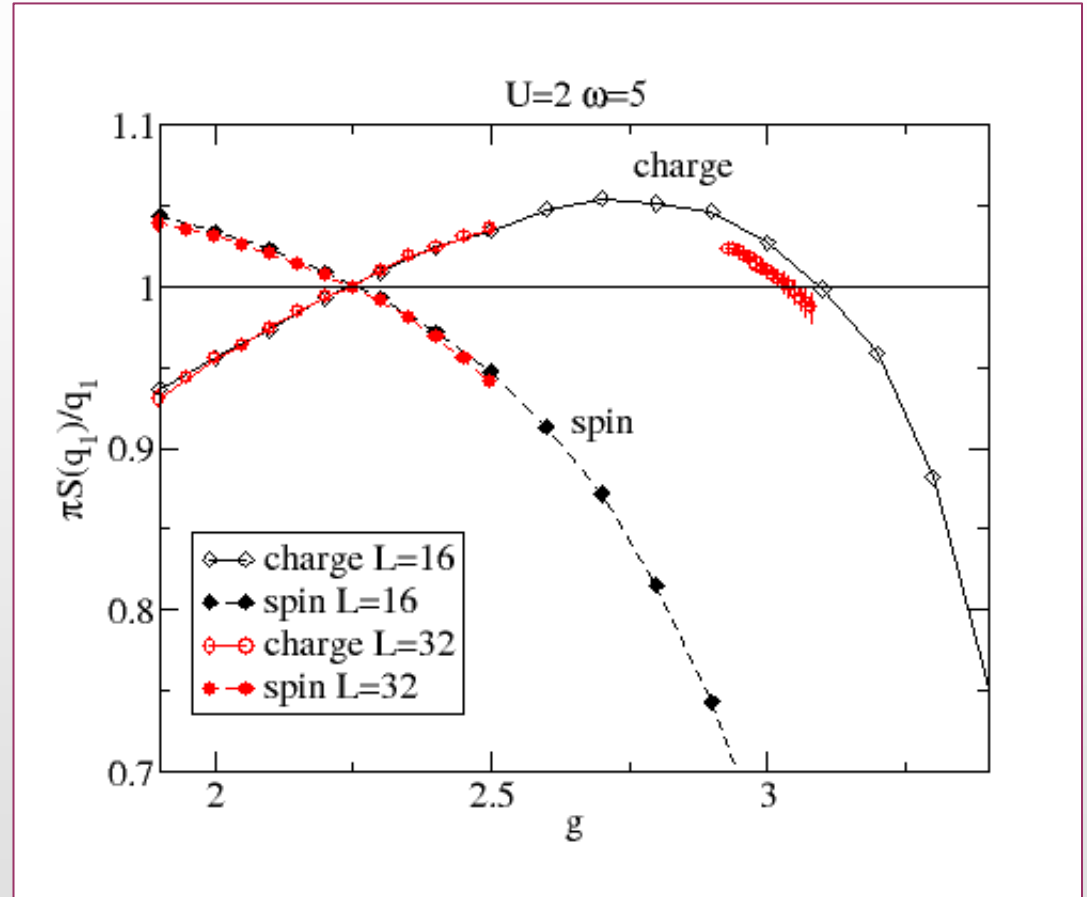
Finite U (U=2, ω=5)

Now 3 phases:

1. Mott-Hubbard: no spin gap, but charge gap.
2. Intermediate: spin gap, no charge gap.
3. Peierls: spin and charge gaps.

The Mott/Int. transition is very close to the mean-field value:

$$\frac{2g^2}{\omega} = U$$



Phase diagram

For large enough U , the Intermediate region vanishes.

Also at large U : the Mott/Peierls transition becomes strongly first order, numerically difficult to study.

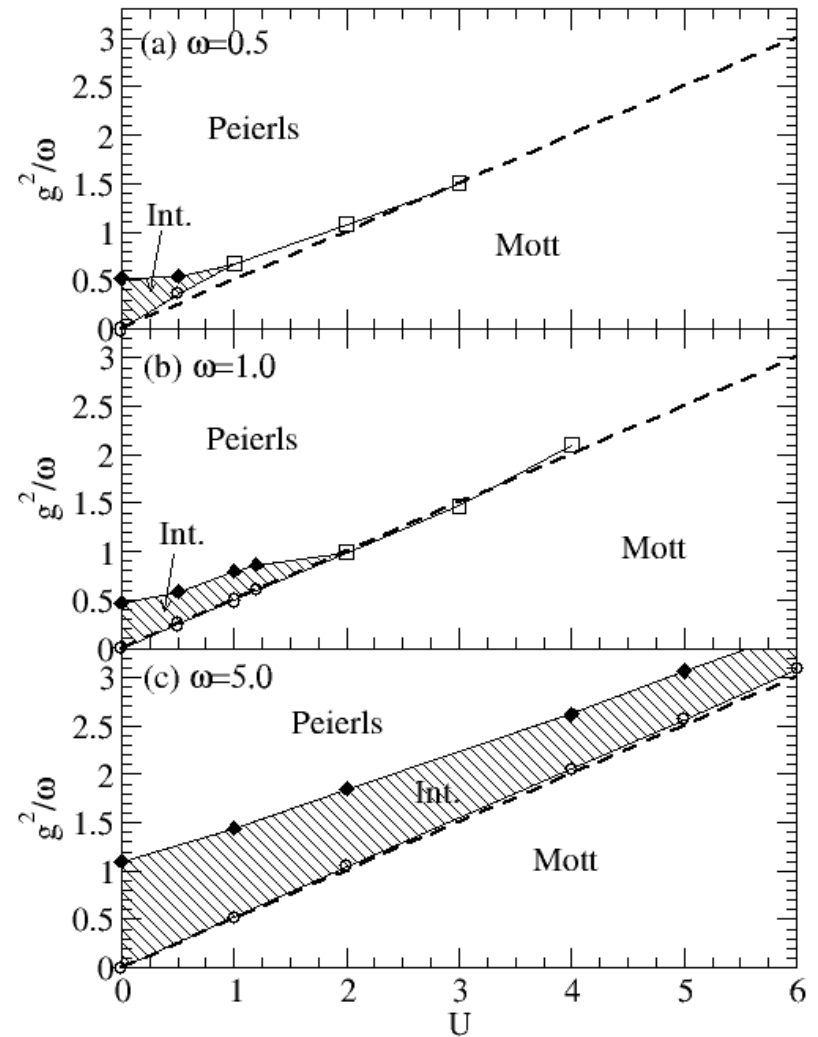
Uncertain if small int. region remains even for large U . Similar to 1D extended Hubbard model "Nakamura" phase?

see:

M. Nakamura, JPSJ **68**, 3123 (1999)

P. Sengupta *et al*, PRB **65**, 155113(2002)

+ several recent articles



Conclusions

- with Holstein (dispersionless) phonons, a KT transition exists at finite e-ph coupling to get the Peierls state.
- below the critical coupling, a spin-gapped metallic state similar to the negative-U Hubbard model. SC and CDW should be degenerate in this state.
- At finite U behavior depends on U and ω :
 - small U and ω : three phases, Mott, Intermediate, and Peierls
 - as U increases in comparison to ω , the Intermediate state shrinks
 - some indications of a narrow intermediate state at large U, as found in the $\frac{1}{2}$ -filled extended Hubbard model

Outlook

What are the implications for more realistic models/materials?

1. Other fillings? Most organic SC's are not $\frac{1}{2}$ -filled, but $\frac{1}{4}$ -filled. Preliminary results show same effect happening at $\frac{1}{4}$ -filling.
2. Higher dimensions? Is it possible to get SC dominating in the I region? Calculations on a ladder confirm this: M. Tezuka *et al*, PRL **95**, 226401 (2005).
3. Organic SC's also have *bond*-coupled phonons. Their effect is to create CDW states that are *extended*, i.e., not a single-site CDW as at $\frac{1}{2}$ -filling. Could this then lead to *realistic* (extended) SC pairing?
4. our paper:
R.T. Clay and R.P. Hardikar, PRL **95**, 096401 (2005)