Dynamical Mean Field Theory: Basic ideas and cluster extensions

A. J. Millis
Department of Physics
Columbia University

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Key people

***P. Werner**
Columbia->Fribourg

***E. Gull**
Columbia->Dresden

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The need for approximations

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Fermionic Many-Body Physics: the exponential wall

General Hamiltonian:

Choose some basis $\alpha = 1...M$

$$\mathbf{H} = \sum_{\alpha,\beta} E^{\alpha\beta}\psi^\dagger_\alpha\psi_\beta + \sum_{\alpha\beta\gamma\delta} I^{\alpha\beta\gamma\delta}\psi^\dagger_\alpha\psi^\dagger_\beta\psi_\gamma\psi_\delta + ...$$

$M = \infty$ for condensed matter

M finite for chemistry

Interest: ground state and excitations

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$$\mathbf{H} = \sum_{\alpha,\beta} E^{\alpha\beta}\psi^{\dagger}_{\alpha}\psi_{\beta} + \sum_{\alpha\beta\gamma\delta} I^{\alpha\beta\gamma\delta}\psi^{\dagger}_{\alpha}\psi^{\dagger}_{\beta}\psi_{\gamma}\psi_{\delta} + \ldots$$

Dimension of Hilbert space: 2^M

Direct diagonalization: exponentially difficult.

Present limit-- M~30.

(and wont get much bigger)

Direct diagonalization becomes impractical before size gets big enough,

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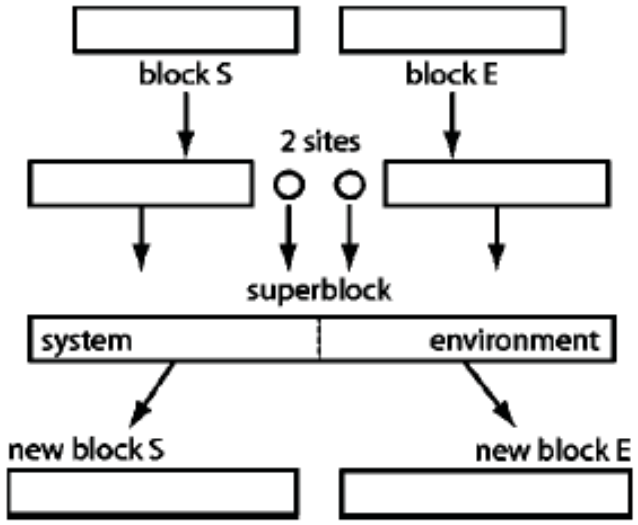
‘Optimized diagonalization’: density matrix renormalization group



U. Schollwoeck, RMP77 259

F. Verstraete et al. Adv. Phys. 57,143 (2008)

1d (provably), d>1 (probably): polynomial time method for finding ground state (at least for gapped systems).

Some excited state properties in d=1 (but is comprehensive description of excitations not possible in polynomial time)

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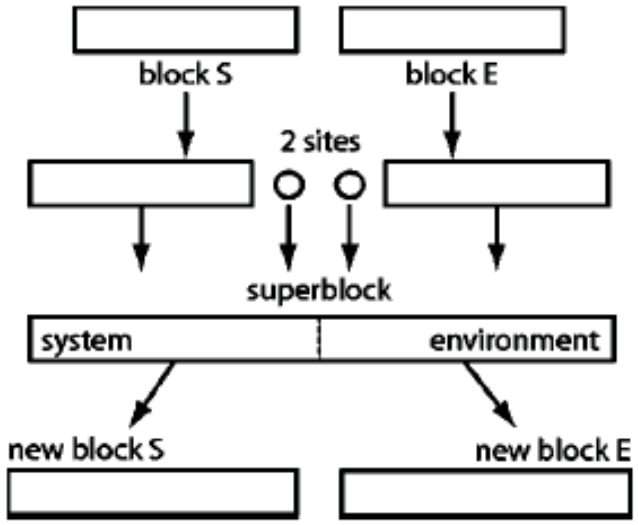
‘Optimized diagonalization’: density matrix renormalization group



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Method of choice for ground state properties of 1d model system problems

Becoming important tool in quantum chemistry

d>1 remains a big challenge

??Excitations??

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Standard method for exploring exponentially large configuration space:

Stochastic (Monte-Carlo) integration

Definition of expectation value

$$< A >_w = \frac{1}{Z_w} \int_{\mathcal{C}} dx \; A(x) w(x)$$

Z=partition function

x=some configuration

$$\mathbf{Z}_w = \int_{\mathcal{C}} dx \; w(x)$$

w(x): ``weight": contribution of x to partition function

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Stochastic part:

To estimate $$<A>_w = \frac{1}{Z_w}\int_C dx\ A(x)w(x)$$

Select M points x_i with probability $p(x_i)=w(x_i)/Z_w$ and compute $$<A>_{MC} = \frac{1}{M}\sum_{i-1}^{M} A(x_i)$$

for classical and unfrustrated boson problems: method of choice.

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BUT still not enough for fermions

Sign problem: antisymmetry of fermion wave function means that different configurations come with different signs. w(x) not always positive

Solution:

Sample using $\rho(x) = |w(x)|$ via

$$\mathbf{Z}_w = \int_{\mathcal{C}} dx\ w(x) = \int_{\mathcal{C}} dx\ sign(w(x))\rho(x)$$

$$\equiv Z_\rho < sign[w] >_\rho$$

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so

$$< A >_w = \frac{1}{Z_w} \int_{\mathcal{C}} dx \; A(x) w(x)$$

$$= \frac{\int_{\mathcal{C}} dx \; A(x) sign(w(x)) \rho(x)}{Z_\rho < sign(w) >_\rho}$$

$$= \frac{\langle A \; sign(w) \rangle_\rho}{< sign(w) >_\rho}$$

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Problem: <sign> exponentially small

(Assaad, 1991; Ceperly, 1996....)

$$< \mathrm{sign}[w] >_\rho = \frac{Z_w}{Z_\rho}$$

=> <sign> is ratio of two partition functions

Z_w: partition function of fermions $Z_w = \mathrm{Exp}\left[-\beta F_{ferm}\right]$

Z_p: partition function of sign-free (``boson") particles with same Hamiltonian. $Z_\rho = \mathrm{Exp}\left[-\beta F_{bos}\right]$

No antisym.=>fewer nodes for boson => $F_{bos} < F_{ferm}$

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Thus

$$< \mathrm{sign[w]} >_\rho = \frac{Z_w}{Z_\rho} = \mathrm{Exp}\left[- \left(\frac{F_{ferm} - F_{bos}}{T} \right) \right]$$

Free energy is extensive => <sign> vanishes exponentially as system size increases or temperature decreases

Direct fermion QMC becomes impractical before size gets big enough or T low enough

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Fermion calculations: exponential wall of computational complexity

Straightforward approaches: reach ‘wall’ before reach interesting system sizes, temperatures

Aim of dynamical mean field theory:
Maximize the information obtainable before reaching the ‘exponential wall’.
Side benefit: wall may be slightly ‘farther away’

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Dynamical Mean Field Theory: indirect approach

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Dynamical Mean Field Theory

Review articles

Antoine Georges, Gabriel Kotliar, Werner Krauth, and Marcelo J. Rozenberg, Rev. Mod. Phys. **68**, 13 (1996)

Thomas Maier, Mark Jarrell, Thomas Pruschke, and Matthias H. Hettler, Rev. Mod. Phys. **77**, 1027 (2005)

K. Held, II. A. Nekrasov, G. Keller, V. Eyert, N. Bluemer, A. K. McMahan, R. T Scalettar, T.h. Pruschke, V. I. Anisimov, and D. Vollhardt, D.; Phys. Status Solidi 243, 2599-2631 (2006)

G. Kotliar, S. Y. Savrasov, K. Haule, V. S. Oudovenko, O. Parcollet, and C. A. Marianetti, Rev. Mod. Phys. **78**, 865 (2006)

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Formalism: electron Green function

Define: **Exact eigenstates** $|\Psi^m_{N+1}(k)>$
of N+1 particle system
momentum k**, energy** E^m_k
relative to N-particle ground state $|GS>$

Define: **electron Green function** $G(k,\omega)$

$$= \int dt e^{-i\omega t} \mathcal{T} \left\langle GS \left| \left\{ \psi_k(t), \psi_k^\dagger(0) \right\} \right| GS \right\rangle$$

$\psi_k^\dagger$ **creates electron in state with wave function** $\sim e^{i\vec{k}\cdot\vec{r}}$

$\mathcal{T}$ is time ordering symbol

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Spectral representation

$$\mathbf{G}^R(k,\omega) = \int \frac{dx}{\pi} \frac{A(k,x)}{\omega - x - i\delta}$$

Spectral function $\mathbf{A}(k,\omega) = Im\left[G^R(k,\omega)\right]$

$$= \sum_m < GS|\psi_k|\Psi^m_{N+1} >< \Psi^m_{N+1}|\psi^\dagger_k|GS > \delta(\omega - E^m_{N+1})$$

$$+ \sum_m < GS|\psi^\dagger_k|\Psi^m_{N-1} >< \Psi^m_{N-1}|\psi_k|GS > \delta(\omega - E^m_{N-1})$$

Measures overlap of exact eigenstates with 'single-particle state created by $\psi^\dagger_k$

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Spectral representation II

Noninteracting system: $\psi_k^\dagger$ creates an exact eigenstate, say m=m$_1$

$$\psi_k^\dagger |GS> = |\Psi_{N+1}^m(k)> \delta_{m,m_1}$$

Spectral function is a delta function

$$\mathbf{A}(k,\omega) = \delta(\omega - E_k)$$

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Spectral representation III

General interacting system: state created by $\psi_k^\dagger$ does not closely resemble any eigenstate; has overlap with all

$$<\Psi_{N+1}^m(k)|\psi_k^\dagger|GS>= f(m)$$

Spectral function is a smooth function

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Spectral representation IV

Fermi liquid: as k-> k_F, the state created by $\psi_k^\dagger$ tends to have some overlap with one unique state, as well as with a continuum of others

$$<\Psi_{N+1}^m(k)|\psi_k^\dagger|GS>= Z_k\delta_{m,m_1} + f(m)$$

Spectral function tends to a delta function (quasiparticle peak) plus smooth ('incoherent part') background

Important concept: quasiparticle weight Z_k

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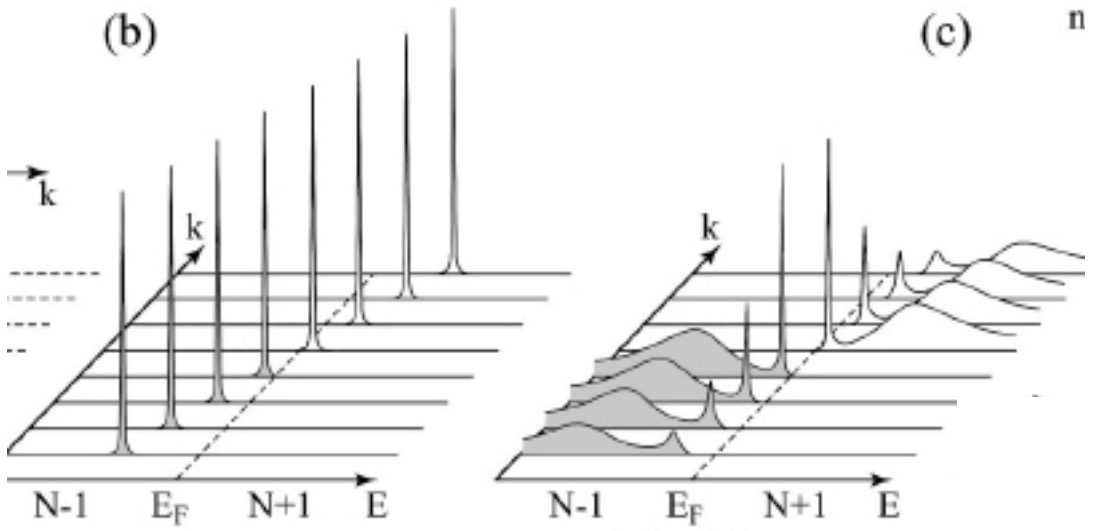
Angle-Resolved Photoemission (ARPES) measures (occupied state part of) **A** (up to matrix element)

Noninteracting Fermi liquid



Z: relative weight of near fermi surface peak

v*: peak dispersion

Im Sigma: peak width

Fig. 3, Damascelli, Hussain and Shen RMP 75 473 (2003)

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Spectral representation V

Alternative mathematical formulation: self energy

$$\mathbf{G}(k,\omega) = \frac{1}{\omega - \varepsilon_k - \Sigma(k,\omega)}$$

Self energy $\Sigma(k,\omega)$ **expresses difference between actual electron propagation and electron propagation in reference noninteracting system with dispersion** ε_k

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Spectral representation V

Self energy has real and imaginary parts. Spectral function

$$\mathbf{A}(k,\omega) = \frac{Im\Sigma(k,\omega)}{\left(\omega - \varepsilon_k - Re\Sigma(k,\omega)\right)^2 + Im\Sigma(k,\omega)^2}$$

Real part expresses renormalization of dispersion, overlap with exact eigenstate.
Imaginary part expresses quasiparticle lifetime

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Spectral representation VI

Fermi liquid: $Im\Sigma(k,\omega \to 0) \to 0$

Expand spectral function near w=0, fermi surface. Find

$$\mathbf{G(k,\omega) = \frac{Z}{\omega - v_k^*(|k| - k_F)}}$$

With

$$\mathbf{Z} = \left(1 - \frac{\partial Re\Sigma(k_F,\omega)}{\partial\omega}|_{\omega\to 0}\right)^{-1}$$

$$\mathbf{v_F^* = \frac{\partial_k \varepsilon_k + \partial_k Re\Sigma(k = k_F, \omega \to 0)}{1 - \frac{\partial Re\Sigma(k_F,\omega\to 0)}{\partial\omega}}}$$

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DMFT: indirect approach: express (some aspects of) solution of physical problem in terms of solution of auxiliary problem

Useful analogy: density functional theory

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Density Functional Theory

Theorem (Hohenberg and Kohn): $\exists$ functional Φ of electron density n(r): minimized at physical density; value at minimum gives ground state energy.

$$\Phi[\{n(r)\}] = \Phi_{univ}[\{n(r)\}] + \int (dr) V_{ion}(r) n(r)$$

Φ_{univ} depends only on electron mass, interelectron interaction

V_{ion} specifies material

Difficulties with this formulation:

- dont know Φ_{univ}
- cant do minimization

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Key insight (Kohn-Sham)

***Re-express minimization in terms of solution of auxiliary problem: single-particle Schroedinger equation with potential $V_{XC}[\{n(r)\}]$ determined by density**

***Recast problem of finding density functional as problem of approximating 'exchange-correlation' potential**

Result: broadly useful tool

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Dynamical Mean Field Theory

Many-body formalism: analogous to Hohenberg-Kohn

$$\mathbf{H} = \sum_{\alpha,\beta} E^{\alpha\beta}\psi^{\dagger}_{\alpha}\psi_{\beta} + \sum_{\alpha\beta\gamma\delta} I^{\alpha\beta\gamma\delta}\psi^{\dagger}_{\alpha}\psi^{\dagger}_{\beta}\psi_{\gamma}\psi_{\delta} + ...$$

=>Luttinger-Ward functional

$$\mathbf{F}[\{\mathbf{\Sigma}\}] = \mathbf{F_{univ}}[\{\mathbf{\Sigma}\}] - \mathbf{Trln}[\mathbf{G_0^{-1}} - \mathbf{\Sigma}]$$

G_0: Green function of noninteracting reference problem (contains atomic positions)

$\mathbf{F}_{univ}$**: determined (formally) from sum of diagrams. Depends only on interactions** $I^{\alpha\beta\gamma\delta}$

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Example

Second order term
Hubbard model

$\Phi_{LW}[\{\mathbf{G}\}]$ **defined as sum of all vacuum to vacuum diagrams (with symmetry factors)**

$\frac{1}{2}$

$$\frac{\delta \mathbf{\Phi}}{\delta \mathbf{G}} = \mathbf{\Sigma}$$

$$\mathbf{F_{univ}} = \mathbf{\Phi_{LW}}[\{\mathbf{G}\}] - \mathbf{Tr}\,[\mathbf{\Sigma G}]$$

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More formalities

$$\mathbf{F}[\{\boldsymbol{\Sigma}\}] = \mathbf{F}_{\mathbf{univ}}[\{\boldsymbol{\Sigma}\}] - \mathbf{Trln}[\mathbf{G}_{\mathbf{0}}^{-1} - \boldsymbol{\Sigma}]$$

Diagrammatic definition of F_{univ} =>

$$\frac{\delta \mathbf{F}_{\mathbf{univ}}}{\delta \boldsymbol{\Sigma}} = \mathbf{G}$$

Thus stationarity condition

$$\frac{\delta \mathbf{F}}{\delta \boldsymbol{\Sigma}} = \mathbf{0} => \mathbf{G} = \left(\mathbf{G}_{\mathbf{0}}^{-1} - \boldsymbol{\Sigma}\right)^{-1}$$

Difficulties with this formulation:
--dont know F_{univ} (exc. perturbatively)
--cant do extremization

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Key first step: infinite d limit
Metzner and Vollhardt, PRL 62 324 (1987)

1992 Breakthrough

Kotliar and Georges found analogue of Kohn-Sham steps: useful approximation for F and way to carry out minimization via auxiliary problem

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Analogy:

Density functional <=> ‘Luttinger Ward functional

Kohn-Sham equations <=> quantum impurity model

Particle density <=> electron Green function

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self energy is MxM matrix
[M(M+1)/2 indep fns of frequency]

$$\begin{bmatrix} \Sigma^{11} & \Sigma^{12} & \Sigma^{13} & . & . & . \\ \Sigma^{21} & \Sigma^{22} & . & . & . & . \\ . & . & \Sigma^{33} & . & . & . \\ . & . & . & \Sigma^{44} & . & . \\ . & . & . & . & . & . \\ . & . & . & . & . & . \end{bmatrix}$$

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Modern interpretation of Kotliar and Georges idea

Parametrize self energy in terms of small number N of functions of frequency

$$\Sigma^{\alpha\beta}(\omega) = \sum_{\mathbf{ab}} \mathbf{f}^{\alpha\beta}_{\mathbf{ab}} \; \Sigma^{\mathbf{ab}}_{\mathbf{DMFT}}(\omega)$$

$$\alpha = 1...\mathrm{M}; \; \mathbf{a} = 1...\mathrm{N} << \mathrm{M}$$

parametrization function f determines 'flavor' of DMFT (DFT analogue: LDA, GGA, B3LYP, ...)

Also must truncate interaction $\mathrm{I}^{\alpha\beta\gamma\delta}$ "appropriately"

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Approximation to self energy + truncated interactions imply approximation to F_{univ}

Approximated functional F^{approx}_{univ} is functional of finite (small) number of functions of frequency $\Sigma^{ab}(\omega)$, thus is the universal functional of some 0 (space) +1 (time) dimensional quantum field theory. Derivative gives Green function of this model:

$$\frac{\delta \mathbf{F}^{\mathbf{approx}}_{\mathbf{univ}}}{\delta \mathbf{\Sigma}^{\mathbf{ba}}(\omega)} = \mathbf{G}^{\mathbf{ab}}_{\mathbf{QI}}(\omega)$$

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Specifying the quantum impurity model

Need

--Interactions. These are the 'appropriate truncation' of the interactions in the original model

--a noninteracting ('bare') Green function $\mathcal{G}_0$

Then can compute the Green function and self energy

$$\mathbf{G_{QI}} = \left(\mathcal{G}_0^{-1} - \mathbf{\Sigma}\right)^{-1}$$

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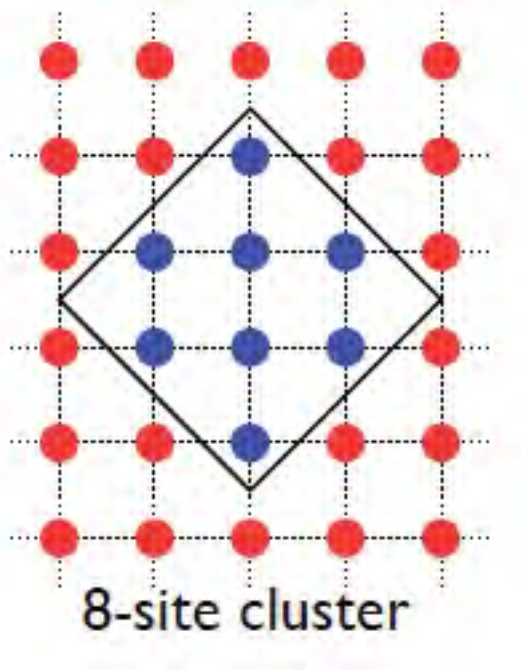
Useful to view auxiliary problem as 'quantum impurity model' (cluster of sites coupled to noninteracting bath)



Quantum impurity model is in principle nothing more than a machine for generating self energies (as Kohn-Sham eigenstates are artifice for generating electron density)

As with Kohn Sham eigenstates, it is tempting (and maybe reasonable) to ascribe physical signficance to it

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In Hamiltonian representation

$$\mathbf{H_{QI}} = \sum_{\mathbf{ab}} \mathbf{d_a^\dagger E_{QI}^{ab} d_b} + \mathbf{Interactions}$$

Impurity Hamiltonian

$$+ \sum_{\mathbf{p,ab}} \left(\mathbf{V_{ab}^p d_a^\dagger c_{pb}} + \mathbf{H.c} \right) . + \mathbf{H_{bath}}[\{\mathbf{c_{pa}^\dagger c_{pa}}\}]$$

Coupling to bath

Important part of bath: 'hybridization function'

$$\mathbf{\Delta^{ab}(z)} = \sum_{\mathbf{p}} \mathbf{V_{ac}^p} \left(\frac{1}{\mathbf{z} - \varepsilon_{\mathbf{p}}^{\mathbf{bath}}} \right) \mathbf{V_{cb}^{p,\dagger}}$$

$$\boxed{\mathcal{G}_0^{-1} = \omega - \mathbf{E_{QI}^{ab}} - \mathbf{\Delta^{ab}}(\omega)}$$

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Thus

$$\mathbf{F} \rightarrow \mathbf{F}^{\mathbf{approx}}_{\mathbf{univ}}[\{\mathbf{\Sigma}^{\mathbf{ab}}\}] - \mathbf{Trln}[\mathbf{G}_{\mathbf{0}}^{-1} - \sum_{\mathbf{ab}} \mathbf{f}^{\alpha\beta}_{\mathbf{ab}} \mathbf{\Sigma}^{\mathbf{ab}}]$$

and stationarity implies

$$\frac{\delta \mathbf{F}}{\delta \mathbf{\Sigma}^{\mathbf{ba}}} = \mathbf{G}^{\mathbf{ab}}_{\mathbf{QI}} - \mathbf{Tr}_{\alpha\beta} \mathbf{f}^{\alpha\beta}_{\mathbf{ab}} \left[\mathbf{G}_{\mathbf{0}}^{-1} - \sum_{\mathbf{cd}} \mathbf{f}^{\alpha\beta}_{\mathbf{cd}} \mathbf{\Sigma}^{\mathbf{cd}} \right]^{-1} = \mathbf{0}$$

or, using $\mathbf{G_{QI}} = \left(\mathcal{G}_{\mathbf{0}}^{-1} - \mathbf{\Sigma}^{\mathbf{ab}}\right)^{-1}$ **from 'impurity solver"**

$$\left(\mathcal{G}_{\mathbf{0}}^{-1}\right)^{\mathbf{ab}} = \mathbf{\Sigma}^{\mathbf{ab}} + \left(\mathbf{Tr}_{\alpha\beta} \mathbf{f}^{\alpha\beta}_{\mathbf{ab}} \left[\mathbf{G}_{\mathbf{0}}^{-1} - \sum_{\mathbf{cd}} \mathbf{f}^{\alpha\beta}_{\mathbf{cd}} \mathbf{\Sigma}^{\mathbf{cd}} \right]^{-1} \right)^{-1}_{\mathbf{ab}}$$

so $\mathcal{G}_{\mathbf{0}}$ **is fixed**

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In practice

Guess hybridization function

Solve QI model; find self energy

Use extremum condition to update hybridization function

Continue until convergence is reached.

This actually works

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Technical note

From your ‘impurity solver’ you need G at ‘all’ interesting frequencies. Solution ~uniformly accurate over whole relevant frequency range.

This is challenging

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advantages of method

***'Moving part'** $Tr_p\left[\phi_a(p) G_{lattice}(\Sigma^{approx})\right]$

some sort of spatial average over electron spectral function--but still a function of frequency

***Computational task: solve quantum impurity model: not necessarily easy, but do-able**

=>releases many-body physics from twin tyrannies of
--focus on coherent quasiparticles/expansion about well understood broken symmetry state
--emphasis on particle density and ground state properties

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In formal terms:

--Approximation to full M x M self energy matrix in terms of N(N+1)/2 functions determined from solution of auxiliary problem specified by self-consistency condition.

--Auxiliary problem: find (at all frequencies) Green functions of N-orbital quantum impurity model.

``Exponential wall'' remains:

Question (practical): for feasible N, can you get the physics information you want?

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Questions:

- **What kinds of impurity models (?possible f?)**
- **What can be solved**
  - **Where is the exponential wall (how large can N be?)**
  - **what kinds of interactions can be included**
  - **other issues**
- **What else (besides electron self energy) can be calculated**
- **Quality of approximation**
- **What has been done?**

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Technical challenge: "impurity solver"

<=>find local (d-d) green functions of

$$\mathbf{H_{QI}} = \sum_{\mathbf{ab}} \mathbf{d_a^\dagger E_{QI}^{ab} d_b} + \mathbf{Interactions}$$

$$+ \sum_{\mathbf{p,ab}} \left(\mathbf{V_{ab}^p d_a^\dagger c_{pb}} + \mathbf{H.c} \right) . + \mathbf{H_{bath}}[\{\mathbf{c_{pa}^\dagger c_{pa}}\}]$$

Two main methods:
--``exact" diagonalization
--(Continuous time) quantum Monte Carlo

Both methods: exponential wall
New ideas needed

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Exact diagonalization

--represent continuous (or at least large) Hilbert space of bath states by small number of (variationally chosen) levels with associated hybridization hybridization parameters
--diagonalize problem exactly (Lanczos)
--virtues: can treat 'arbitrary' interactions. formulated directly in real frequency

Difficulty: M bath levels per impurity level => dimension $4^{(M+1)N}$

Present methods: (M+1)N<17 **Minimizing M crucial**

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determining the bath parameters: more of an art than a science

Calculated quantities are a sum of poles

$$\mathbf{Im}\mathcal{G}_{\mathbf{0}}^{\mathbf{ED}}(\omega) = \sum_{\lambda} \mathbf{g}_{\lambda}^{\mathbf{0}} \delta(\omega - \omega_{\lambda})$$

$$\mathcal{G}_{\mathbf{0}}(\mathbf{i}\omega_{\mathbf{n}}) = \int \frac{\mathbf{dx}}{\pi} \frac{\mathbf{Im}\mathcal{G}_{\mathbf{0}}^{\mathbf{ED}}(\mathbf{x})}{\mathbf{i}\omega_{\mathbf{n}} - \mathbf{x}}$$

Typically fit bath params by minimizing

$$\sum_{\mathbf{n}} \frac{\left|\mathcal{G}_{\mathbf{0}}(\mathbf{i}\omega_{\mathbf{n}}) - \mathcal{G}_{\mathbf{0}}^{\mathbf{lattice}}(\mathbf{i}\omega_{\mathbf{n}})\right|^{\mathbf{2}}}{|\omega_{\mathbf{n}}|}$$

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Minimization not always stable

Trying to fit a nonlinear function

Problems particularly severe when G cannot be diagonalized at all frequencies

$$\left[\hat{\boldsymbol{\Delta}}(\omega_1), \hat{\boldsymbol{\Delta}}(\omega_2)\right] \neq \mathbf{0}$$

(Experience: best to fit diagonal components, then using this as guess, fit full matrix)

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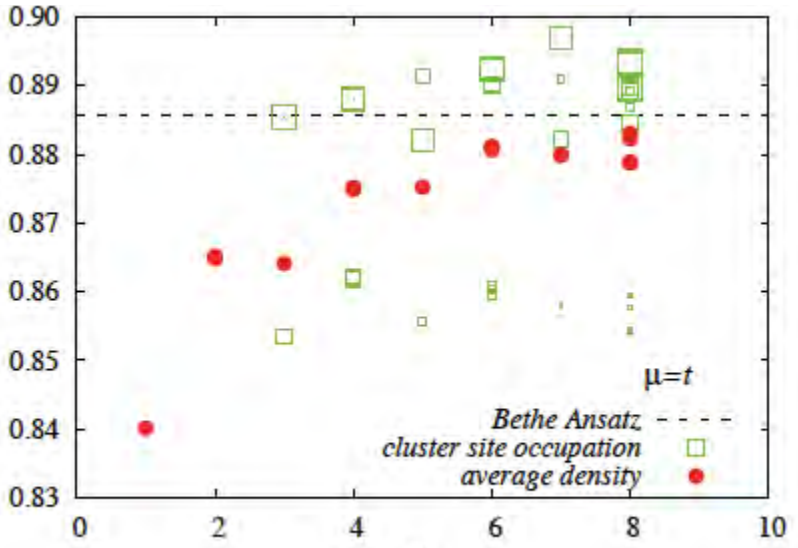
How many bath states do you need.

Capone et al (PRB 76 254116 (2007)): convergence with number of bath sites: M~8 or 9=> only model with N=1 practical

Koch et al (arXiv:0804.3320): need approx 6 bath sites per edge site

Liebsch (arXiv:1109.0158) shows reasonable (at least qualitatively) results for N=4, M=2 or 3.

Koch et al 1d Hubbard



Claim: need ~6/ edge site

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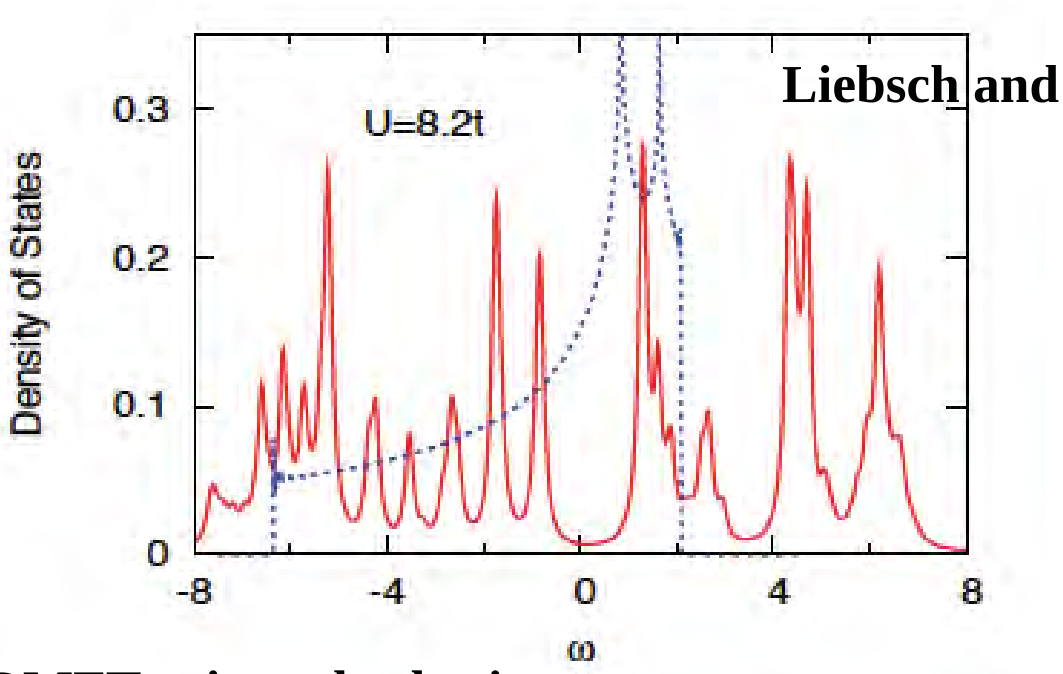
ED: Excitation spectrum discrete but not totally sparse.

Care needed in interpreting spectra



Liebsch and Tong:

3 site DMFT, triangular lattice.
4 bath sites per impurity

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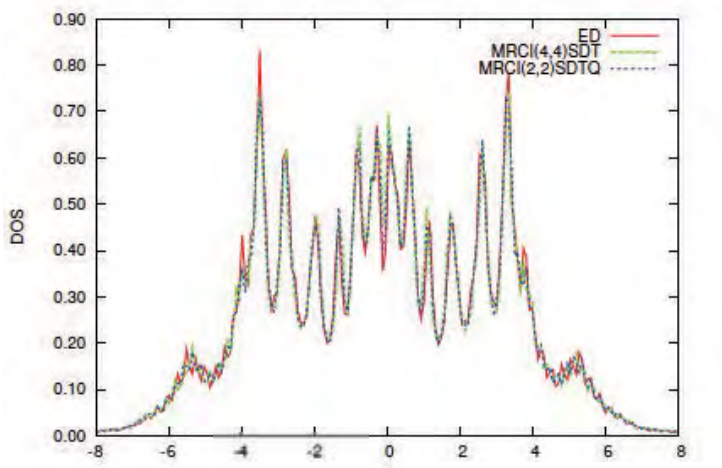
Open question

Quantum impurity models: interaction only a few sites=> interesting sparsity structure

=>maybe method ``smarter'' than Lanczos can reach larger systems.

G. Chan/D. Zgid: 'CI' based solver N=4, 6 bath sites



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Monte Carlo: imaginary time

Workhorse of 1980s, 1990s ('Hirsh-Fye' QMC). difficulties: --only Hubbard (local density-density) interaction. Fixed time discretization.

Breakthrough: continuous-time quantum Monte Carlo (CT-QMC)

***Rubtsov 05 Interaction expansion(CT-INT)**
***Werner/AJM 06 Hybridization expansion(CT-HYB)**
***Gull/Parcollet08 Auxiliary field (CT-AUX))**
***Rev Mod Phys 83 349 (2011).**

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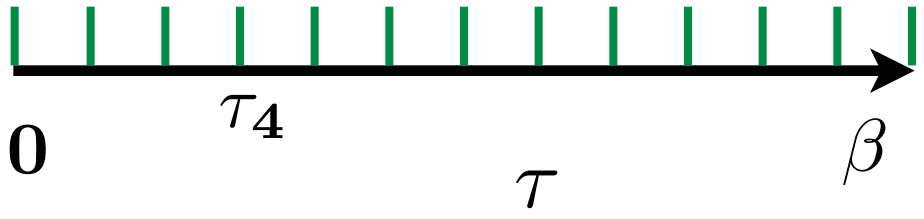
Hirsch-Fye for Hubbard model

Fixed time discretization $\Delta\tau \leq \mathrm{U}^{-1}$



Trotter decomposition: $\hat{\mathrm{K}} = \mathrm{e}^{-\Delta\tau\hat{\mathrm{H}}} \approx \mathrm{e}^{-\Delta\tau\hat{\mathrm{T}}}\mathrm{e}^{-\Delta\tau\mathrm{U}\mathrm{n}_\uparrow\mathrm{n}_\downarrow}$

At each τ_i and each site, discrete Hubbard-Stratonovich

$$e^{-\Delta\tau U\left(n_\uparrow n_\downarrow - \frac{n_\uparrow + n_\downarrow}{2}\right)} = \frac{1}{2}\sum_{s_i=\pm 1} e^{\lambda s_i (n_\uparrow - n_\downarrow)} \qquad \lambda = \operatorname{arcosh}\left[\exp\left(\frac{1}{2}\Delta\tau U\right)\right]$$

$$\mathrm{Z} = \sum_{\{\mathrm{s_i}\}} \mathrm{Exp}\left[\mathrm{TrlnG}(\{\mathrm{s_i}\})\right] \qquad \text{Matrix: dimension } \frac{\beta}{\Delta\tau} \times \mathrm{N_{sites}}$$

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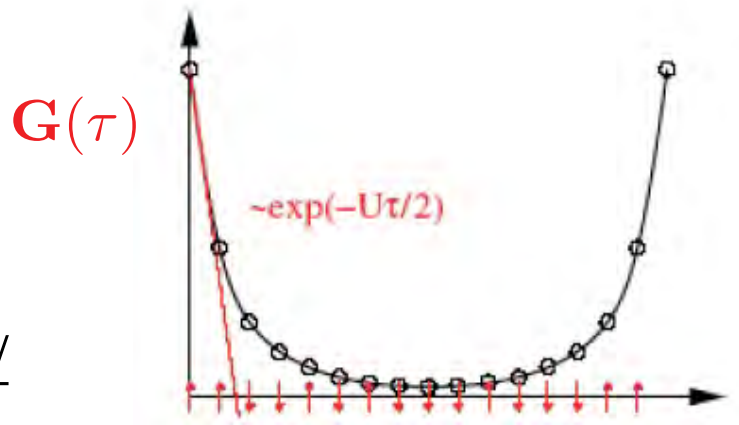
Notional scaling:

Operations with matrices
cost: ~cube of dimension

$$\text{cost: } \sim (\beta \mathbf{U} \mathbf{N}_{\text{sites}})^3$$

Issues:
--prefactor not small
--extrapolation in $\Delta\tau$ needed
(but see N. Bluemer thesis
http://komet337.physik.uni-mainz.de/Bluemer/thesis.en.shtml)
--longer range interactions: multiplicity of H-S fields, serious sign problem (Mikelsons)
--no good H-S for non-density ints



Sign problem for N>1

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Continuous time Monte Carlo:

$$\mathbf{H = H_a + H_b}$$

- **interaction representation with respect to H_b**

$$Z = \mathrm{Tr}\, T_\tau e^{-\beta H_a} \exp\left[-\int_0^\beta d\tau H_b(\tau)\right]$$

- **formal expansion in H_b**

$$= \sum_k (-1)^k \int_0^\beta d\tau_1 \ldots \int_{\tau_{k-1}}^\beta d\tau_k \times \mathrm{Tr}\left[e^{-\beta H_a} H_b(\tau_k) H_b(\tau_{k-1}) \ldots H_b(\tau_1)\right]$$

- **sample series stochastically**

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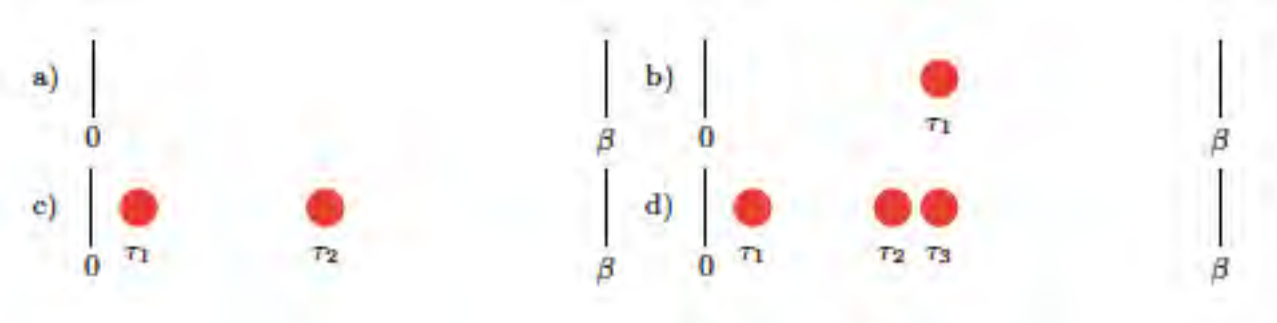
CT-QMC 2



Monte-Carlo: add or remove H_b vertex (if H_b has many terms, expand in each).
Connect vertices with H_a.

Tried in 1990s for continuum problems: worked poorly

Turns out: works VERY WELL for impurity problems

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Two principal `flavors’

H_b= hybridization (CT-HYB)

H_b=Interaction (CT-INT)

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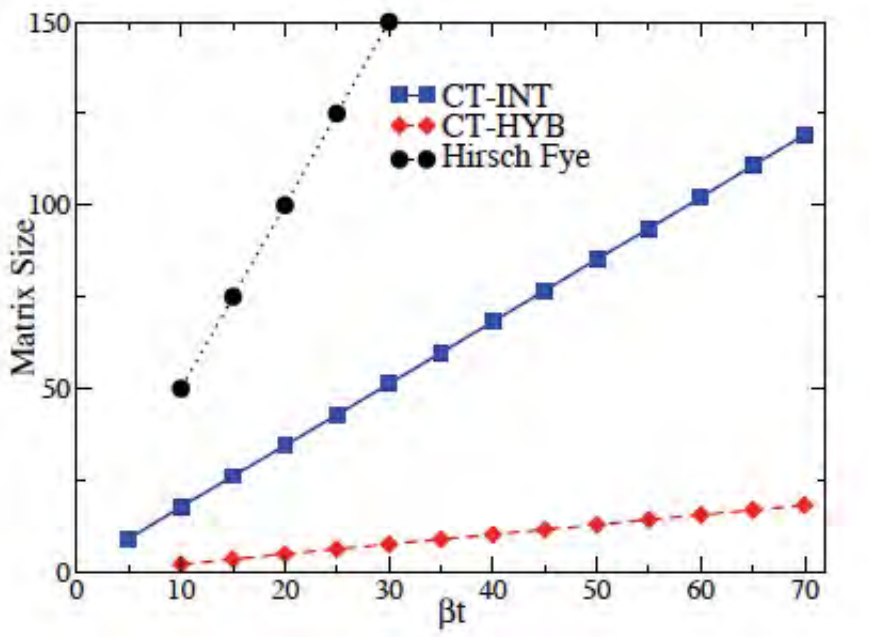
Continuous time: ‘many-body adaptive grid’

Puts time points where needed.

All methods involve manipulating matrices; cost ~cube of matrix size.

CT-QMC: much smaller matrix is needed



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‘Hybridization expansion’ CT-HYB

(P. Werner and AJM, PRL 97}, 076405 (2006))

$$H_{QI} = H_{loc}[\{d_a^\dagger, d_a\} + \sum_{p,a} \left(V_{pa} d_a^\dagger c_{pa} + H.c\right) . + H_{bath}[\{c_{pa}^\dagger c_{pa}\}]$$

- **interaction representation with respect to H_{loc}, H_{band}**

$$Z = Tr\left[T_\tau e^{\sum_{p,a}\left(V_{pa}^I d_a^\dagger(\tau) c_{pa}(\tau) + H.c.\right)}\right]$$

- **formal expansion in V**

$$= \sum_k \frac{1}{k!} \int_0^\beta d\tau_1 ... d\tau_k Tr\left[T_\tau \hat{\mathbf{V}}^{\mathbf{I}}(\tau_1) ... \hat{\mathbf{V}}^{\mathbf{I}}(\tau_k)\right]$$

- **sample series stochastically: add/remove V; accept or reject by usual importance sampling**

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CT-HYB

***General interactions can be treated**

But:

***Requires diagonalization of $H_{impurity}$**

***Computation of**

$$= \sum_k \frac{1}{k!} \int_0^\beta d\tau_1 ... d\tau_k Tr \left[T_\tau \hat{\mathbf{V}}^{\mathbf{I}}(\tau_1) ... \hat{\mathbf{V}}^{\mathbf{I}}(\tau_k) \right]$$

Requires manipulation of matrices of size of local Hilbert space

Restricted to ~5-7 orbitals at present

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Also

$$\mathbf{H_{QI}} = \sum_{\mathbf{ab}} \mathbf{d_a^\dagger E_{QI}^{ab} d_b} + \mathbf{Interactions}$$

$$+ \sum_{\mathbf{p,ab}} \left(\mathbf{V_{ab}^p d_a^\dagger c_{pb}} + \mathbf{H.c} \right) . + \mathbf{H_{bath}} [\{ \mathbf{c_{pa}^\dagger c_{pa}} \}]$$

Severe sign problem if

$$\left[\hat{\mathbf{\Delta}}, \hat{\mathbf{E}} \right] \neq \mathbf{0}$$

=>reasonably high symmetry desirable

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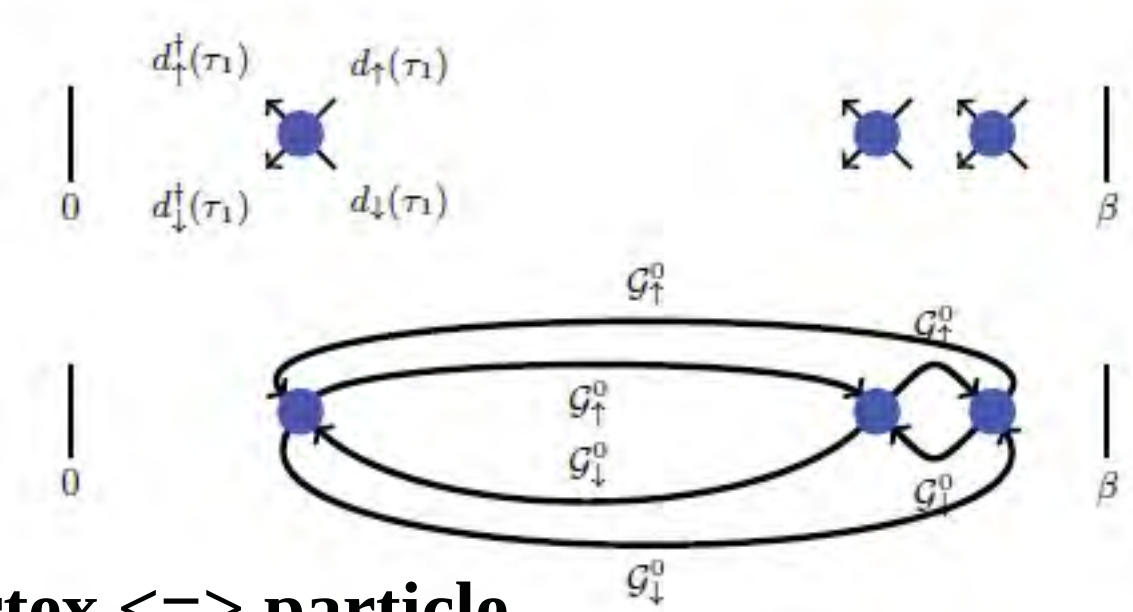
CT-INT: sample interaction perturbation diagram series stochastically



Vertex <=> particle

Propagator <=> interparticle interaction

$$\textbf{Scaling} \sim (\mathbf{N_{site}} \beta \mathbf{U}))^{\mathbf{3}}$$

Like Hirsch-fye but prefactor much better

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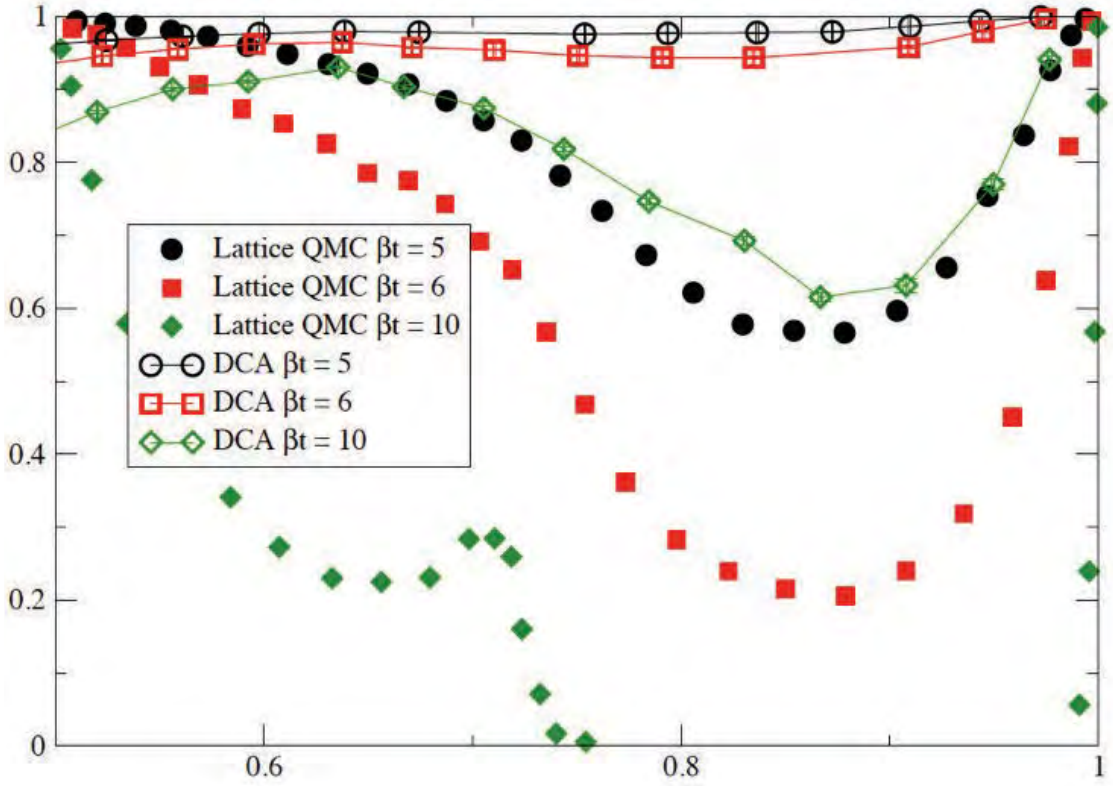
Empirical fact:

Coupling to bath=>

SIGN PROBLEM MUCH BETTER

2d Hubbard model, 36 sites

<sign>



Filling

F. Assaad (QMC)
E. Gull (DMFT)

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Technical remarks

Computations are trivially parallelizable:

Basic computation performed on a single core.

Initialization/thermalization time is very low

=>pays to distribute computation over ~10^4 cores

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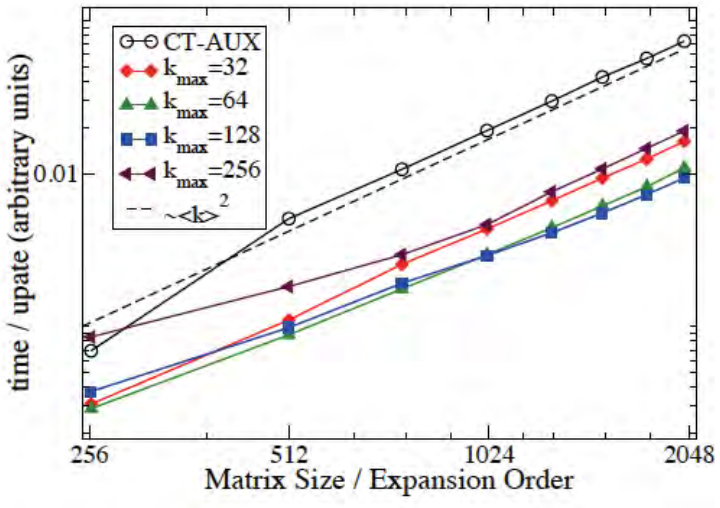
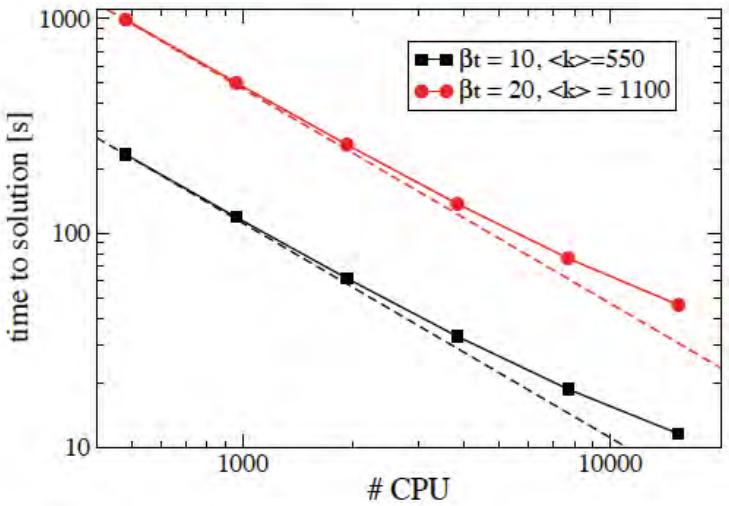
(sub)matrix updates
E. Gull et al PRB 83 075122

***Method deals with large matrices =>computational bottleneck is moving information from memory into cache**

=>Efficiency gain from arranging calculation to maximize # compute operations/memory call.





16 sites, U/t=8

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Typical computational costs (on 2-5 year old machines)

- **Single-site 1 orbital: minutes on a laptop**
- **Single-site, 2 orbital: 16 cores, 4 hours**
- **8 site Hubbard normal state (T=t/20): 64 cores, 8 hours**
- **8 site Hubbard superconducting state (T=t/60) 128 cores 8 hours**
- **8 site Hubbard, measurement for raman vertex (T=t/20), 4096 cores 8 hours (BNL Blue Gene)**

These times are 'reasonable'

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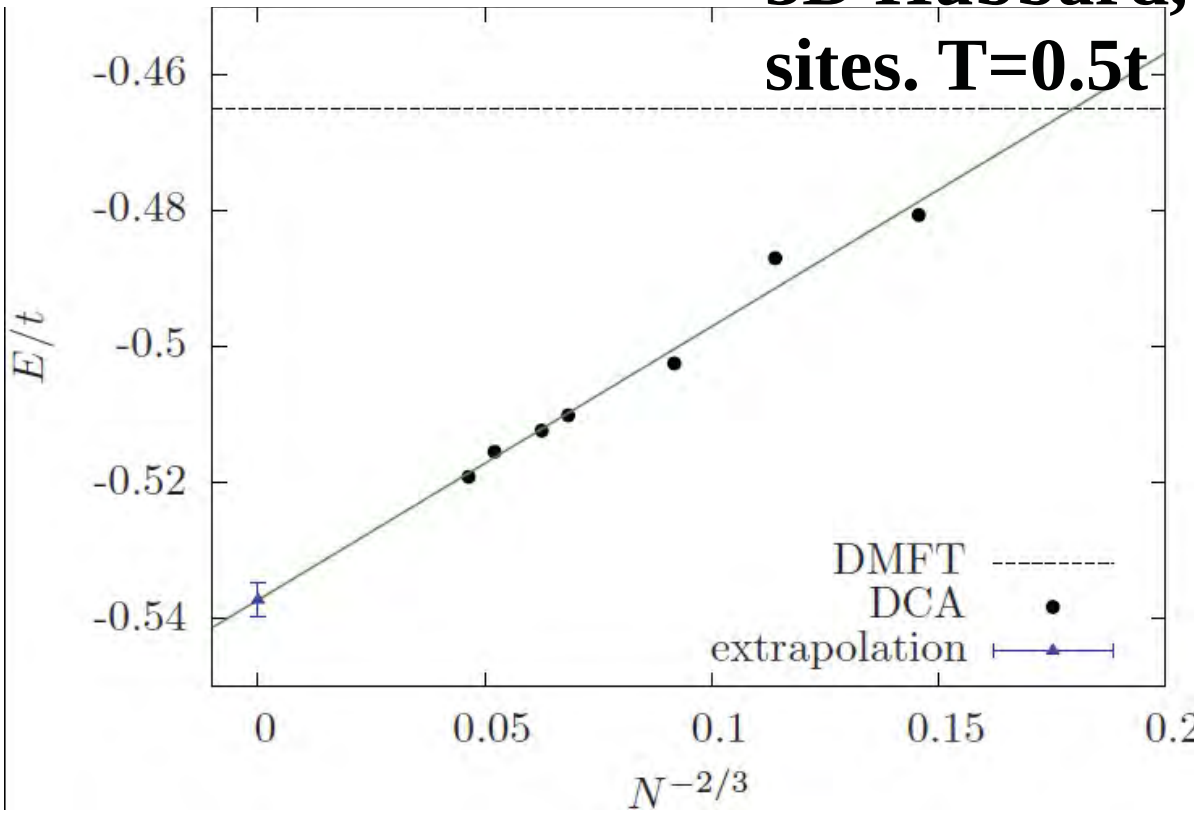
=>can treat large systems

3D Hubbard, up to 100 sites. T=0.5t



E. Gull and S. Fuchs

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BUT

Most efficient version relies on Hubbard-Stratonovich transformation (or something equivalent). Presently restricted to models with density-density (preferably on-site) interactions

$$\mathbf{H} = \varepsilon_{\mathbf{d}} \mathbf{d}^{\dagger}\mathbf{d} + \mathbf{U}\hat{\mathbf{N}}_{\mathbf{d}}^{\mathbf{2}} +$$

$$\varepsilon_{\mathbf{p}} \mathbf{p}_{\mathbf{p}}^{\dagger} + \mathbf{V}_{\mathbf{pd}} \mathbf{d}^{\dagger}\mathbf{p} + \mathbf{H.c}$$

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Summary: scaling

Naive scaling:

$$\begin{aligned}
\text{Hybridization algorithm} &\sim \beta^2\, e^{N_{site}} \\
\text{Interaction (Hubbard)} &\sim N_{site}^3 U^3 \beta^3 \\
\text{Interaction (General } U_{ijkl}) &\sim (N_{site} M_{int})^3 U^3 \beta^3
\end{aligned}$$

Sign problem

$$\left[\hat{E}, \hat{\Delta}\right] \neq 0 \text{ i.e. low symmetry or } N_{site} > 4$$

Or, clusters large enough to have loops

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What can be done in practice

realistic (exchange/pair-hopping) interactions:

At present can do 5 orbitals (dim 4^5 =1028) (=> single site dmft of transition metals, or actinides with truncation)

Hubbard (on-site, density-density interactions)

Complete solution at interesting temperatures may be within reach.

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Formulating the impurity model

What choices of $f_{ab}^{\alpha\beta}$ are

- mathematically consistent
- physically reasonable
- easiest to compute with

!!Choice of f includes choice of basis in both physical and impurity space!!

RMP 78 p. 875: formal dfn in terms of functional integral. But problem not fully understood.
=><u>room for new insights!</u>

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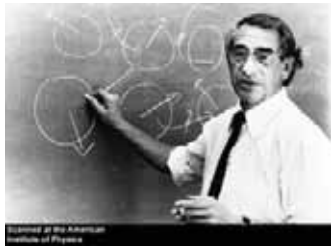

Example: Hubbard model

Hubbard model: periodic lattice of sites in d dimensions. One orbital per site. Position and momentum reps.

$$H_{Hub} = -\sum_{ij\sigma} t_{i-j} d^{\dagger}_{i\sigma} d_{j\sigma} + U \sum_{i} n_{i\uparrow} n_{i\downarrow}$$

$$H_{Hub} = -\sum_{k\sigma} \varepsilon_{k} d^{\dagger}_{i\sigma} d_{j\sigma} + U \sum_{k_1 k_2 q} d^{\dagger}_{k_1\uparrow} d^{\dagger}_{k_2\downarrow} d_{k_1+q\uparrow} d_{k_2-q\downarrow}$$

Real space: $\Sigma(i-j)$

Momentum space: $\Sigma(k)$

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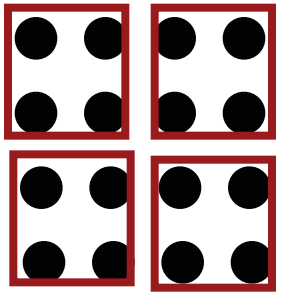
Real space representation: ``CDMFT"

G. Kotliar, S. Y. Savrasov, G. Palsson, and G. Biroli,
Phys. Rev. Lett. **87**, 186401 (2001).

Tile lattice with equal size cells, labelled by J.
Introduce label a for sites in a cell
Drop terms in $\sum$ which couple sites in different cells.



$$\Sigma(\mathbf{i}-\mathbf{j},\omega)=\Sigma^{\mathbf{a_i b_j}}(\omega)$$ If $\mathbf{i},\mathbf{j}\in\mathbf{J}$ and $\mathbf{a_i},\mathbf{b_j}$ are cluster sites corresponding to $\mathbf{i},\mathbf{j}$

$$\Sigma(\mathbf{i}-\mathbf{j},\omega)=0 \quad \text{otherwise}$$

Note: translation invariance broken If $N \neq 1$

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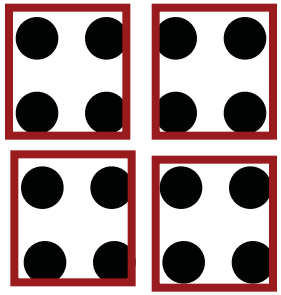
Easiest to express in supercell basis

Introduce spinor $\Psi_{\mathbf{J}}^{\dagger} = (\mathbf{d}_{\mathbf{J_1}}^{\dagger}, \ldots \mathbf{d}_{\mathbf{J_N}}^{\dagger})$

$$\mathbf{H_{Hub}} = \sum_{\mathbf{J}} \Psi_{\mathbf{J}\sigma}^{\dagger} \hat{\mathbf{E}} \Psi_{\mathbf{J}\sigma} + \mathbf{U} \sum_{\mathbf{a=1..N}} \mathbf{n_{J_a\uparrow} n_{J_a\downarrow}}$$

$$+ \frac{\mathbf{1}}{\mathbf{2}} \sum_{\mathbf{I \neq J}} \Psi_{\mathbf{I}\sigma}^{\dagger} \hat{\mathbf{T}}(\mathbf{I - J}) \Psi_{\mathbf{J}\sigma}$$



CDMFT function $\mathbf{f}_{ab}^{i,j} \rightarrow \delta_{I\,J} \hat{1}$

$$\hat{\mathbf{G}}(\mathbf{I - J}; \omega) = \left(\omega \hat{\mathbf{1}} - \hat{\mathbf{E}} \delta_{\mathbf{IJ}} - \hat{\mathbf{T}}(\mathbf{I - J}) - \hat{\mathbf{\Sigma}}(\omega) \delta_{\mathbf{I,J}} \right)^{-1}$$

$$\textbf{SCE: } \hat{\mathbf{G}}_{\mathbf{QI}}(\omega) = \hat{\mathbf{G}}(\mathbf{0}, \omega)$$

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Extremum condition:

$$\left(\omega\hat{\mathbf{1}} - \hat{\mathbf{E}}_{\mathbf{QI}} - \hat{\mathbf{\Delta}}(\omega) - \hat{\mathbf{\Sigma}}\right)^{-1} = \int' (\mathbf{dk}) \left[\omega\hat{\mathbf{1}} - \hat{\mathbf{E}} - \hat{\mathbf{T}}(\mathbf{k}) - \hat{\mathbf{\Sigma}}\right]^{-1}$$

(Here $\int'(dk)$ means integral over reduced zone of supercell with appropriate normalization

inverting and rearranging

$$-\hat{\mathbf{E}}_{\mathbf{QI}} + \hat{\mathbf{\Delta}} = -\omega + \mathbf{\Sigma} + \left[\int' (\mathbf{dk}) \left[\omega\hat{\mathbf{1}} - \hat{\mathbf{E}} - \hat{\mathbf{T}}(\mathbf{k}) - \hat{\mathbf{\Sigma}}\right]^{-1}\right]^{-1}$$

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Look at high frequency limit

$$\int' (\mathbf{dk}) \left[\omega \hat{\mathbf{1}} - \hat{\mathbf{E}} - \hat{\mathbf{T}}(\mathbf{k}) - \hat{\mathbf{\Sigma}}\right]^{-1} \rightarrow \frac{\mathbf{1}}{\omega}\left(\mathbf{1} + \frac{\hat{\mathbf{E}} + \hat{\mathbf{\Sigma}} + \int' (\mathbf{dk})\mathbf{T}(\mathbf{k})}{\omega}\right)$$

so the SCE becomes:

$$-\hat{\mathbf{E}}_{\mathbf{QI}} + \hat{\mathbf{\Delta}} = -\omega + \mathbf{\Sigma} + \omega - \hat{\mathbf{E}} - \hat{\mathbf{\Sigma}} - \int' (\mathbf{dk})\mathbf{T}(\mathbf{k})$$

So E_{QI}=E (integral of T vanishes because T is non-local) behavior at lower w fixes hybridization function

something like this occurs in all implementations

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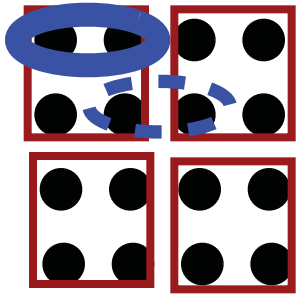
Special to CDMFT: `Periodization'

$$\Sigma(\mathbf{i}-\mathbf{j},\omega)=\Sigma^{\mathbf{a_i}\mathbf{b_j}}(\omega)$$

If $\mathbf{i},\mathbf{j}\in\mathbf{J}$ and $\mathbf{a_i},\mathbf{b_j}$ are cluster sites corresponding to $\mathbf{i},\mathbf{j}$



=>2 points of view on broken translation invariance:

- **Accept it: calculate only quantities not directly influenced by broken tranlational invariance (energy, local excitation spectra...)**

- **`Periodize': use results to reconstruct periodic function**

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Periodization

To estimate lattice quantity, Fourier transform cluster quantity over cluster sites (but for all momenta in zone)

$$\mathbf{f(\tilde{k}) = \frac{1}{N} \sum_{ij=1\ldots N} e^{i\tilde{k}\cdot(\tilde{r}_i - \tilde{r}_j)} f_{cl}(i,j)}$$

Key question: what quantity to use?

Civelli et al PRL 95 106402: self energy Σ

Stanescu et al PRB 74 125110:

cumulant $M = [\omega + \mu - \Sigma]^{-1}$

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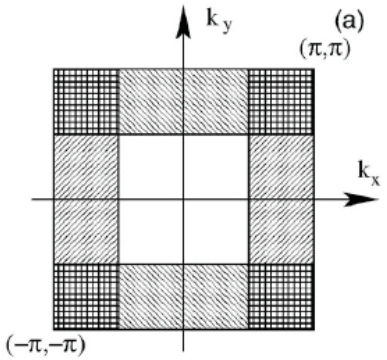
Self energy interpolation

Methods yield: $\Sigma(K,\omega)$ **at discrete momenta K**



e.g 4-site cluster

$\mathbf{K} = (0,0),\ (0,\pi),\ (\pi,\mathbf{0}),\ (\pi,\pi)$

Problem: zone diagonal $\Sigma\ ((\frac{\pi}{2},\frac{\pi}{2})$
made from $(0,0),(0,\pi),(\pi,0),(\pi,\pi)$

The physics of the points from which the interpolation is made may be very different from that of the point of interest. I prefer to avoid periodization

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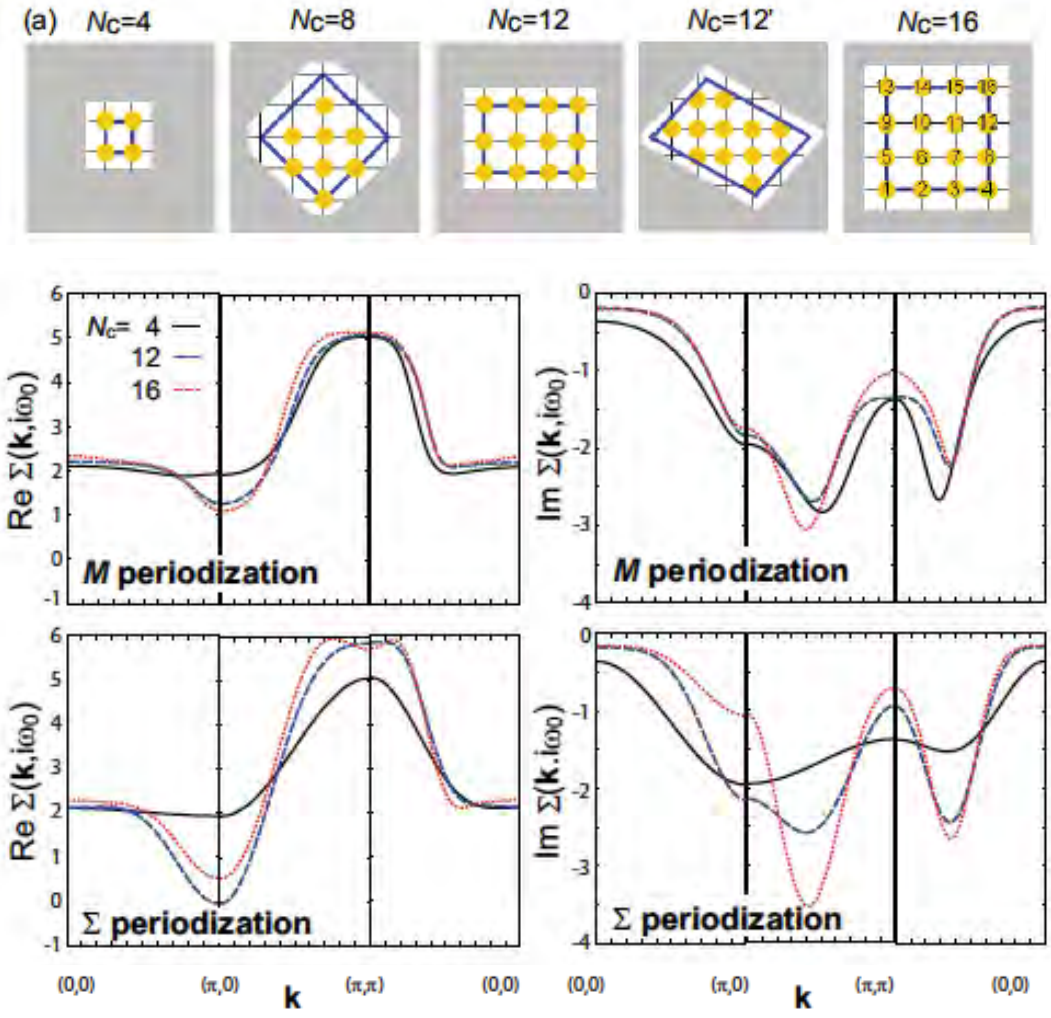
Very new results:
Sakai et al arXiv:1112.3227



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Longer ranged interactions

CDMFT: approx Luttinger Ward functional made of diagrams involving local (in supercell basis) Green function

$$\Phi[\{\mathbf{G}(I-J,\omega)\}] \rightarrow N_{sites}\Phi[\{\mathbf{G}(0,\omega)]\}$$

to do approx, set I=J

This is fine on level of Green functions: but what if interaction connects different sites??

Answer: truncate interactions

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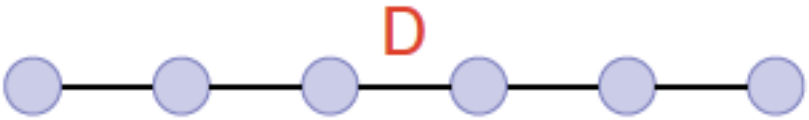
Instructive example: H_n

N. Lin, C. Marianetti, A. J. Millis and D. Reichman PRL 106 096402



Set of n hydrogen atoms

Atoms far apart: strong coupling problem

--what we did: on each atom, keep only 1s state (STO-6G basis)

–Compute matrix elements of $H = \sum_i \frac{-\nabla_i^2}{2m} + \frac{1}{2}\sum_{i\neq j} \frac{e^2}{|r_i - r_j|}$ between these orbitals

$$H^{\text{elec}} = \sum_{ij\sigma}(t_{ij} - \delta_{ij}\mu)c^\dagger_{i\sigma}c_{j\sigma} + \frac{1}{2}\sum_{ijkl\sigma\sigma'} V_{ijkl}c^\dagger_{i\sigma}c^\dagger_{j\sigma'}c_{k\sigma'}c_{l\sigma}$$

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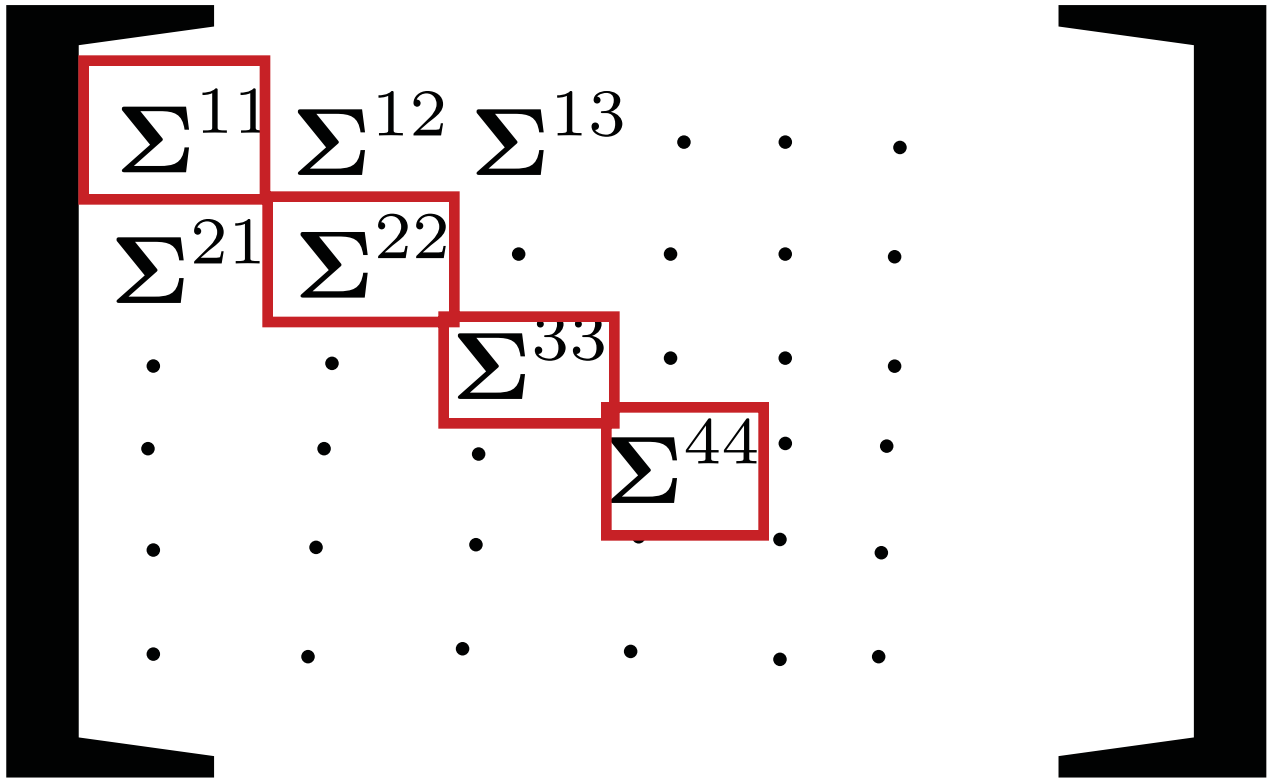
CDMFT: isolate blocks in self energy



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treat orbitals outside 'active blocks' via Hartree-Fock

$$\mathbf{\Sigma^{ab}}(\omega) \rightarrow \mathbf{\Sigma^{ab}_{HF}} + \delta_{\mathbf{ab}} \left(\mathbf{\Sigma_a}(\omega) - \mathbf{\Sigma^{aa}_{HF}} \right)$$

Similarly treat in-block interactions exactly; other interactions by Hartree-Fock

$$\mathbf{I}^{abcd} \rightarrow I_{HF} + (I^{aaaa} - I^{aaaa}_{HF})$$

Keep V12, V34 in DMFT; treat V23 by hartree-fock

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treat orbitals outside 'active blocks' via Hartree-Fock

$$\mathbf{\Sigma^{ab}}(\omega) \rightarrow \mathbf{\Sigma^{ab}_{HF}} + \delta_{\mathbf{ab}} \left(\mathbf{\Sigma_a}(\omega) - \mathbf{\Sigma^{aa}_{HF}} \right)$$

Similarly treat in-block interactions exactly; other interactions by Hartree-Fock

$$\mathbf{I}^{abcd} \rightarrow I_{HF} + (I^{aaaa} - I^{aaaa}_{HF})$$

Note 'double-counting' correction

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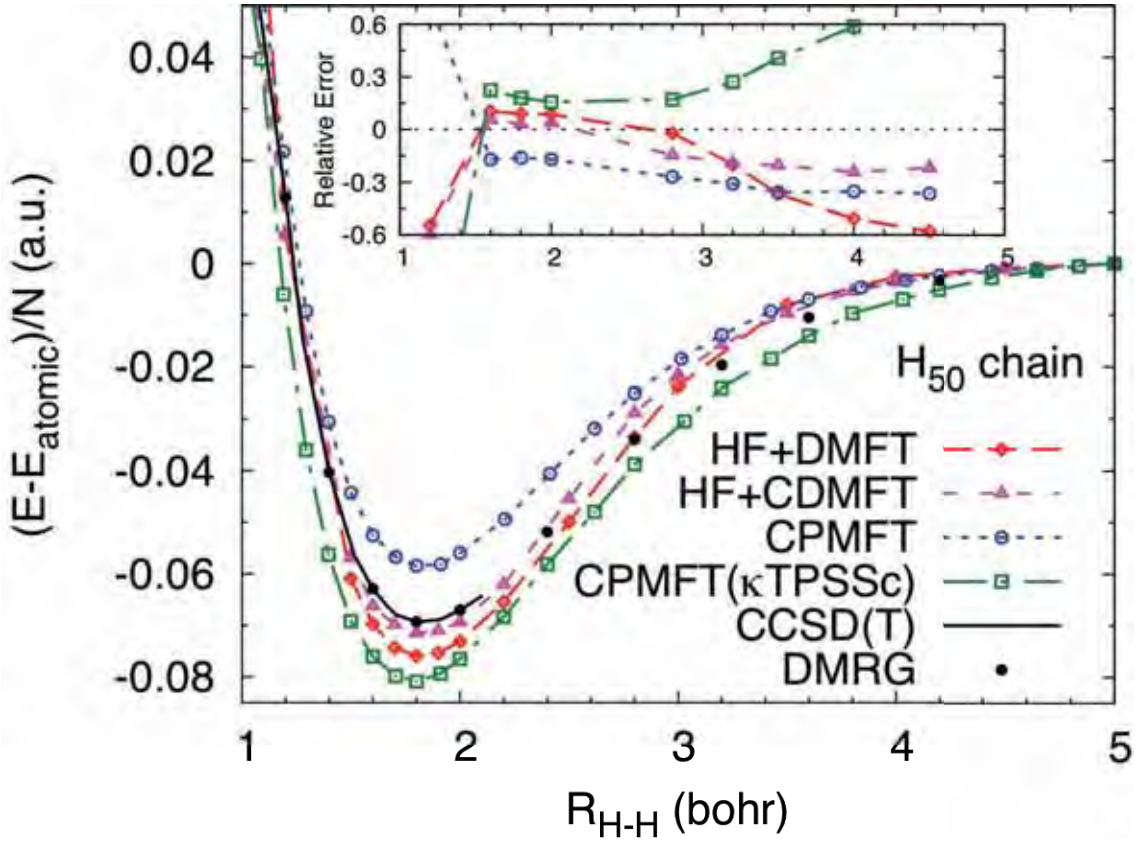
Results: energy



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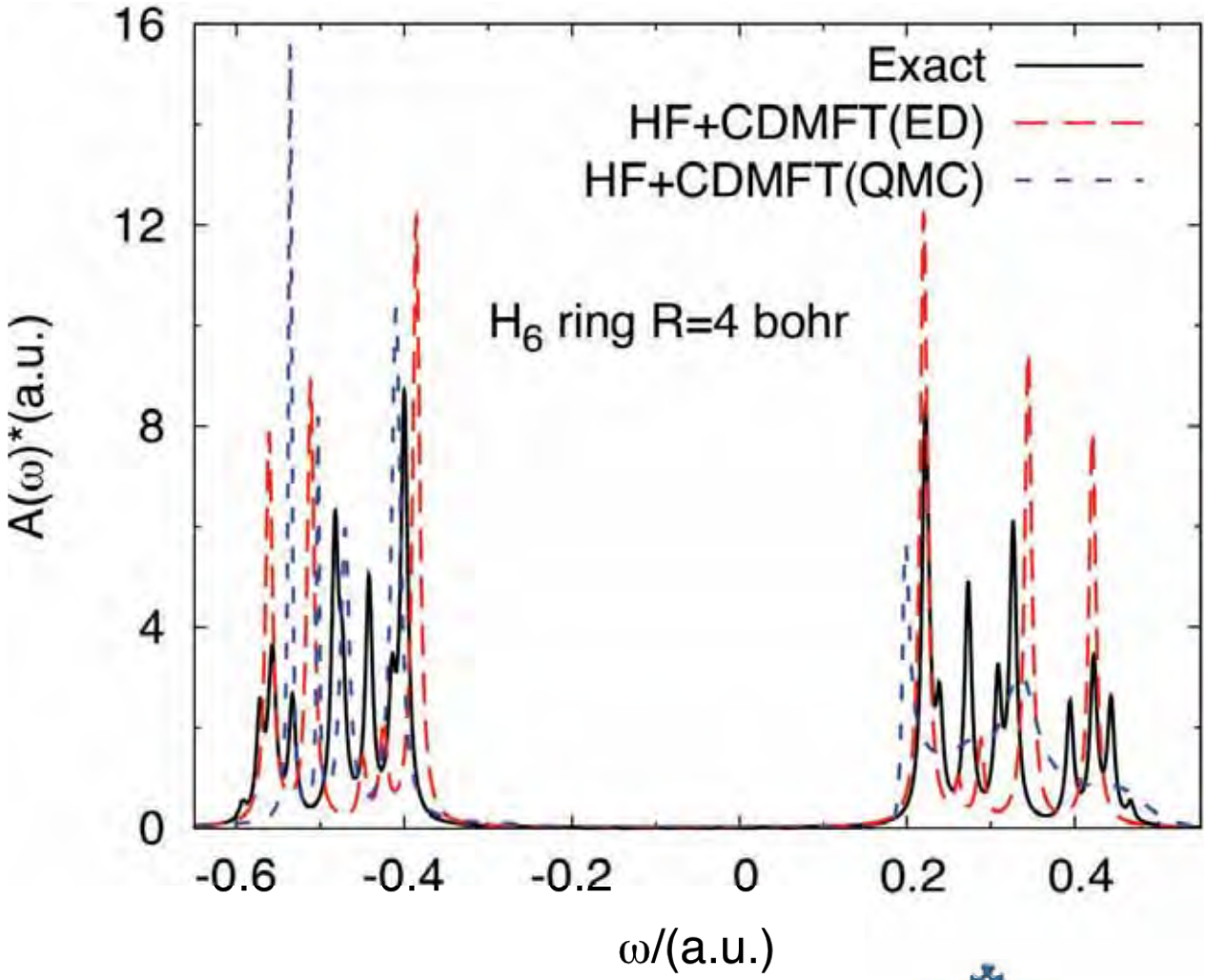
Results: excitation



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Implication

Single-site DMFT not adequate

CDMFT approximation is somehow ‘smart’: errors produced by asymmetrical treatment of interactions get compensated....

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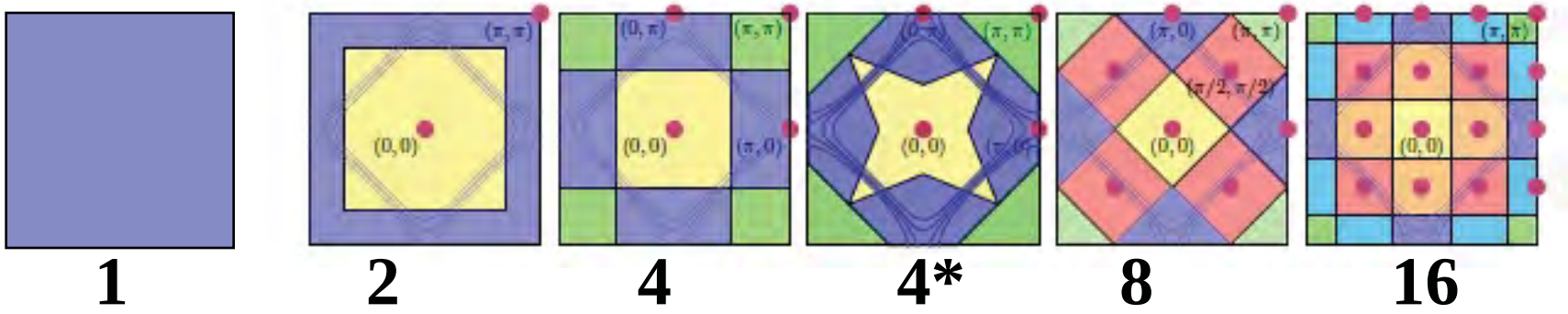
Momentum space representation: DCA

M. H. Hettler, M. Mukherjee, M. Jarrell, and H. R. Krishnamurthy
Phys. Rev. B **61**, 12739 (2000)

tile Brillouin zone: choose N momenta K_a, draw an equal area patch around each one



$$\Sigma_{\mathbf{p}}(\omega) \rightarrow \Sigma_{\mathbf{p}}^{\mathbf{approx}}(\omega) = \sum_{\mathbf{a}} \phi_{\mathbf{a}}(\mathbf{p}) \Sigma_{\mathbf{a}}(\omega)$$

$\phi_{\mathbf{a}}(\mathbf{p}) = 1$ if p is in the patch containing K_a and is 0 otherwise

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Coarse-grain interaction in k space

Evaluate interation at discrete k-points:

$$\mathbf{V}(\mathbf{k_1}, \mathbf{k_2}, \mathbf{k_3}, \mathbf{k_4}) \rightarrow \mathbf{V}(\mathbf{K_1}, \mathbf{K_2}, \mathbf{K_3}, \mathbf{K_4})$$

=> defines quantum impurity model

Then

$$\mathbf{F} \rightarrow \mathbf{F}^{\mathbf{approx}}_{\mathbf{univ}}[\{\mathbf{\Sigma_a}\}] - \mathbf{Trln}[\mathbf{G_0^{-1}} - \sum_{\mathbf{a}} \phi_{\mathbf{a}}(\mathbf{k})\mathbf{\Sigma_a}(\omega)]$$

So:

$$\mathbf{G}^{\mathbf{a}}_{\mathbf{QI}} = \mathcal{A}_{\mathbf{patch}} \int (\mathbf{dk})\phi_{\mathbf{a}}(\mathbf{k}) \left(\mathbf{G_0^{-1}} - \sum_{\mathbf{a}} \phi_{\mathbf{a}}(\mathbf{k})\mathbf{\Sigma_a}(\omega) \right)^{-1}$$

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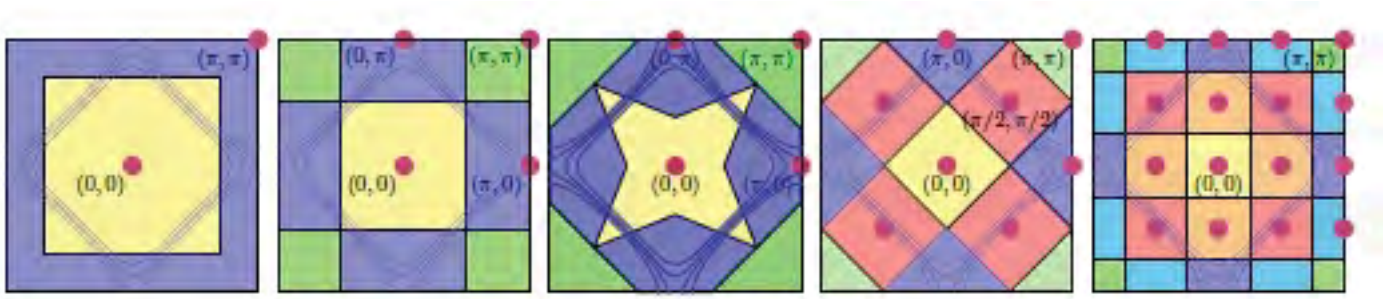
Comments



- Patches need to have equal area
- Patches do not need to have any particular shape
- (as long as they tile the Brillouin zone)
- Patching does not have to respect point group symmetry
- Translational invariance respected (in fact, required) but self energy piecewise continuous

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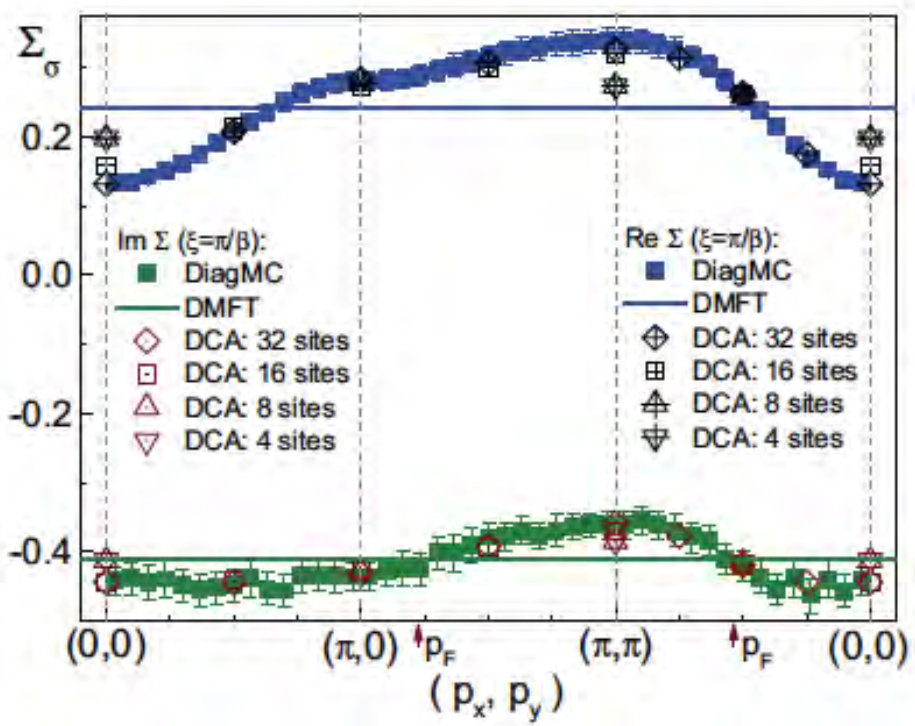
Status of the approximation

Favorable cases: (moderate correlations, simple interactions) --direct comparison to numerically exact results available



Kozik, Houcke, Gull, Pollett, Prokof'ev, Svistunov, Troyer EPL 90 10004 (2010)

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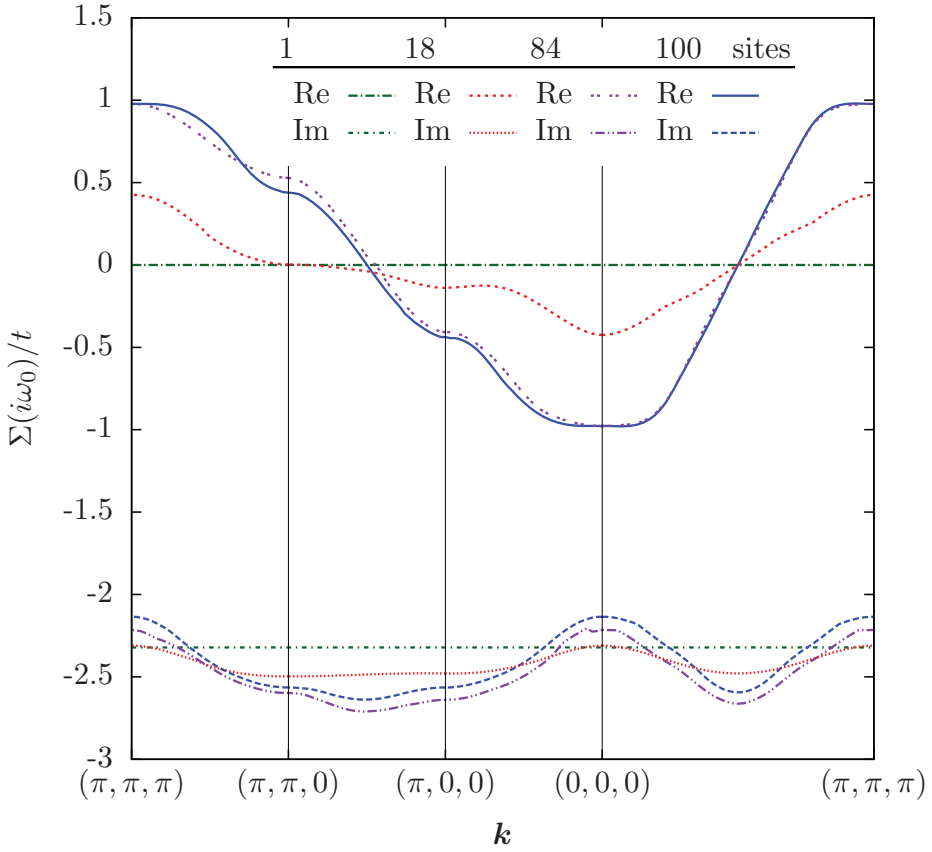
3 dimensional Hubbard model

S. Fuchs, E. Gull, L. Pollett et al PRL 106 030401 (2011)

U=8t cluster sizes up to 100 sites high-ish T=t/2



Controlled extrapolation to thermodynamic limit now possible at high T

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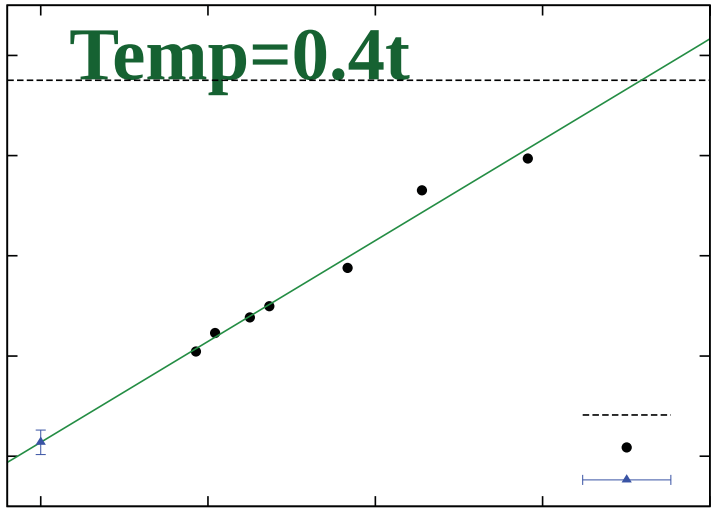
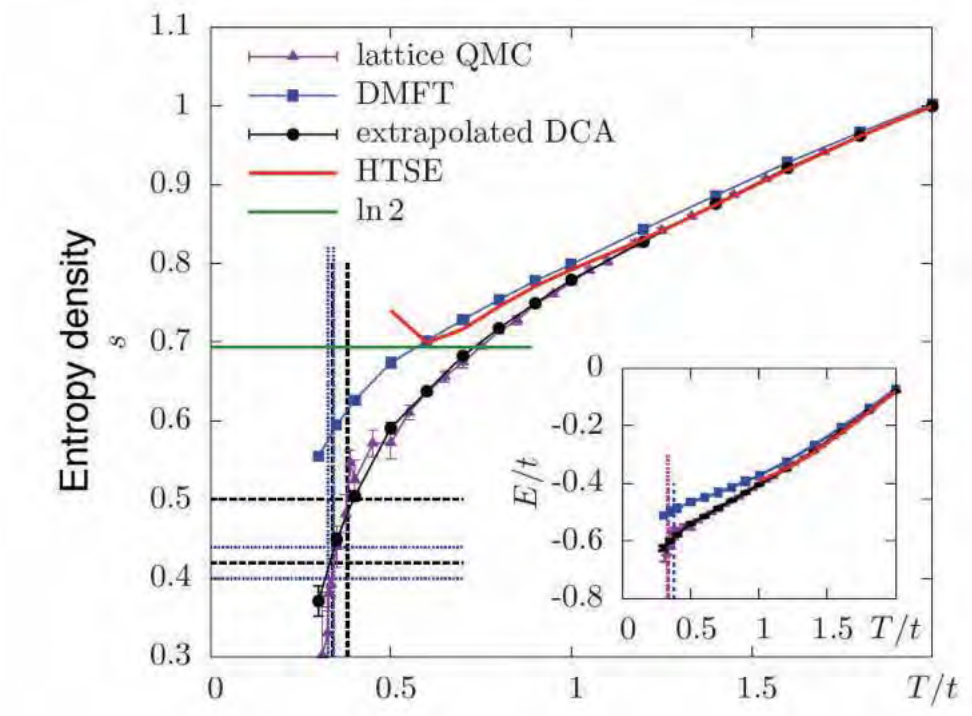
3 dimensional Hubbard model

S. Fuchs, E. Gull, L. Pollett et al PRL 106 030401 (2011)

DCA: cluster sizes up to 100 sites. U=8t





Controlled extrapolation to thermodynamic limit now possible

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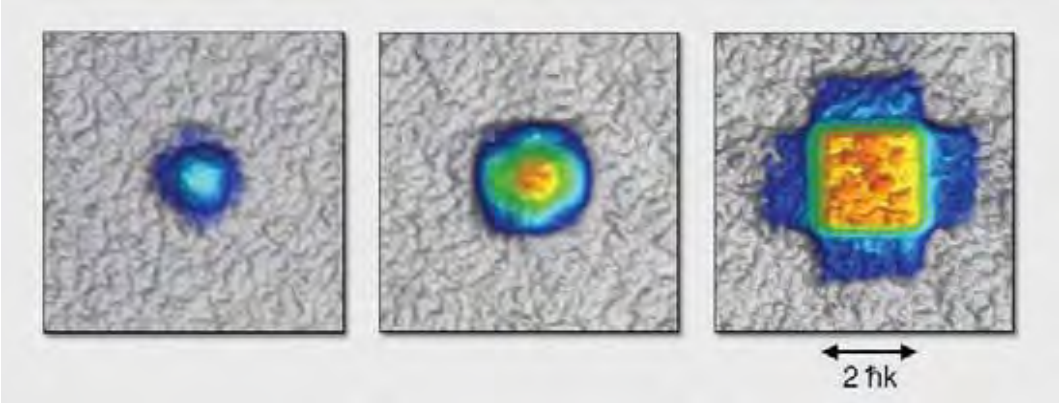
‘Optical emulator’: cold atomic gasses as analogue computers for model systems of condensed matter physics



fermion density distribution

T. Esslinger, Ann. Rev. CMP 129 (2010)

Very promising, but present experiments cannot reach low enough T; also validation needed

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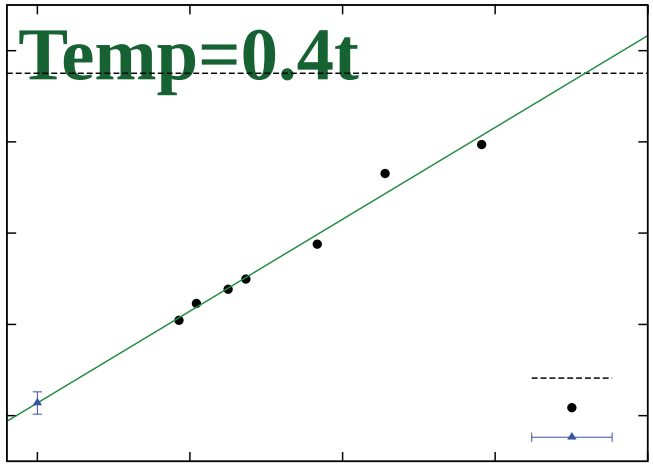
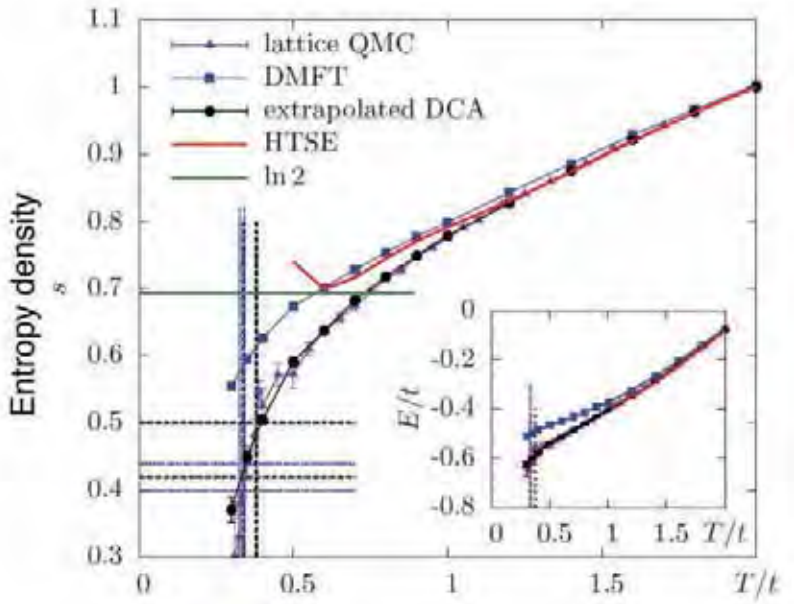
3 dimensional Hubbard model

S. Fuchs, E. Gull, L. Pollett et al PRL 106 030401 (2011)

DCA: cluster sizes up to 100 sites. U=8t





Controlled extrapolation to thermodynamic limit now possible (at lower T than experiment)

DMFT: Optical emulator emulator

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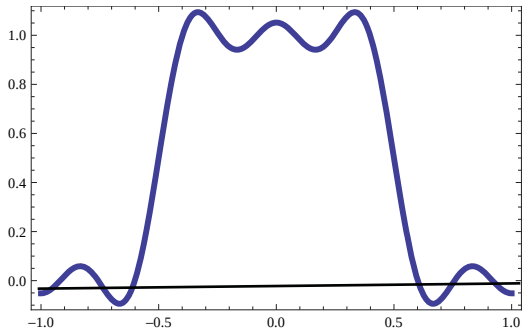
Other formulations

$$\Sigma^{\alpha\beta}(\omega) = \sum_{\mathbf{ab}} \mathbf{f}^{\alpha\beta}_{\mathbf{ab}} \; \Sigma^{\mathbf{ab}}_{\mathbf{DMFT}}(\omega)$$

Conditions on f not known

Considerations:

$\mathbf{Causality:\ Im\Sigma^{aa}(\omega + i\delta) > 0;}$
$\mathbf{want\ Im\Sigma^{\alpha\alpha}(\omega + i\delta) \geq 0\ also}$



$\mathbf{Orthogonal\ function\ expansion}$
$\mathbf{\Sigma(k,\omega) = \Sigma_0(\omega) + \Sigma_1(\omega)\ cos(k_x) +}$
$\mathbf{rings:\ can\ find\ region\ where} Im\Sigma(k,\omega) < 0$

see e.g. Phys. Rev. B68 195121/1-8 (2003)

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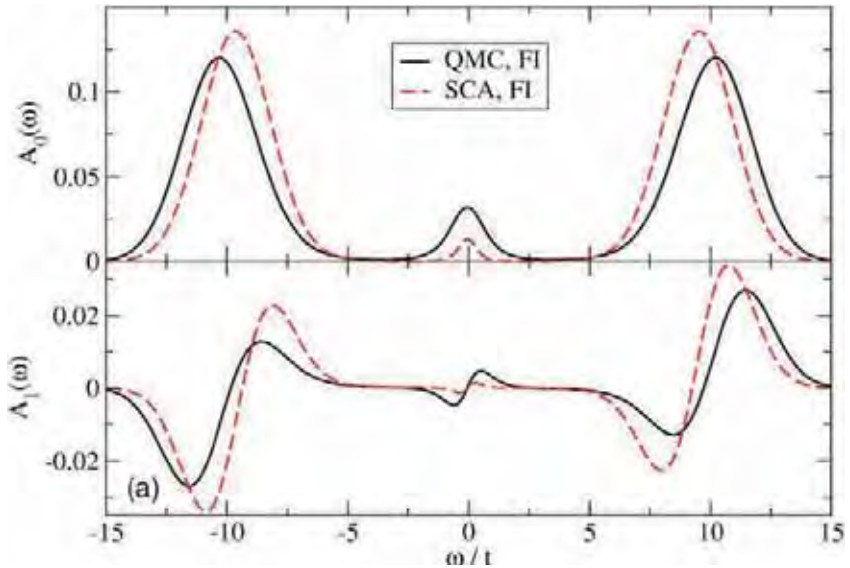
More subtle: pole structure in correlated insulator

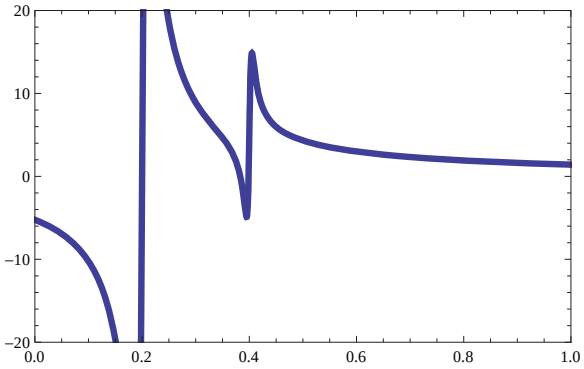
In Mott insulator $\Sigma^{\alpha\alpha}$ $\frac{1}{\omega - \Omega_\alpha}$

In impurity model Σ^{aa} $\frac{1}{\omega - \Omega_a}$

$f_{aa}^{\alpha\alpha}$ must couple only one a to each α

If not, states in the gap





see Phys. Rev. B75, 205118 (2007)

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Applications of cluster DMFT

Main application so far: to high-Tc cuprates

(modelled by Hubbard model, for which you can reach large systems)

But it is likely the physics is more generally important.

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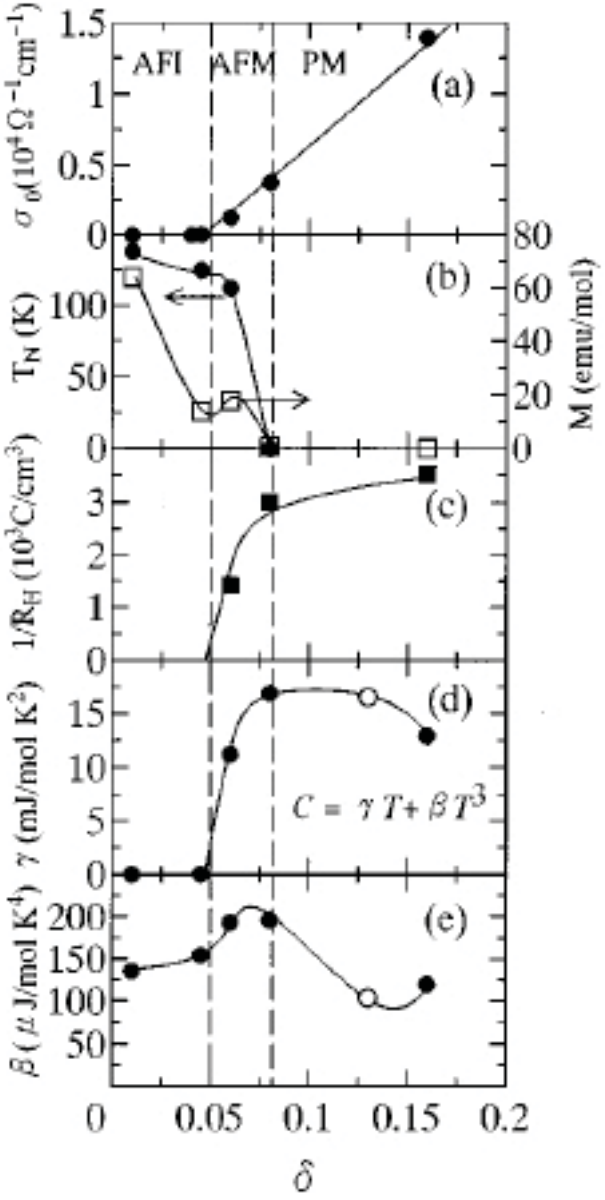
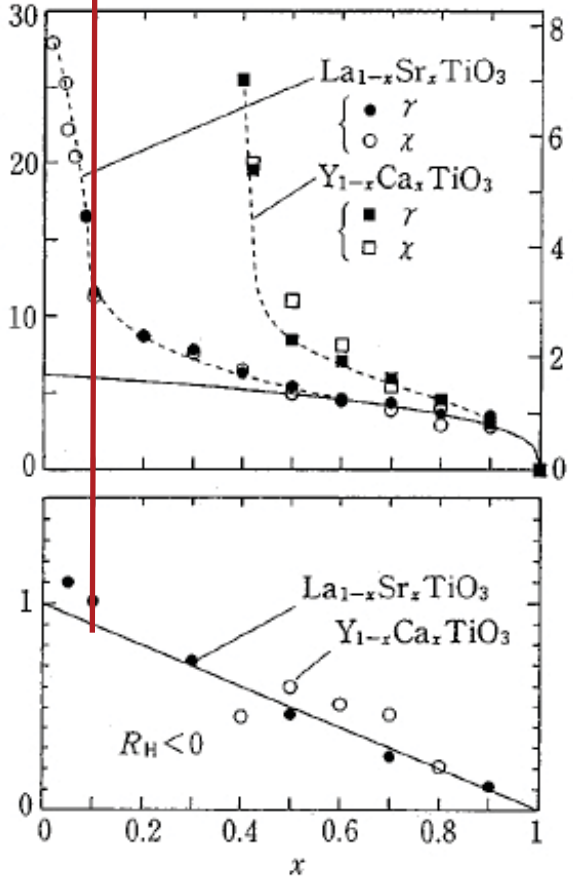
$ReTiO_3$

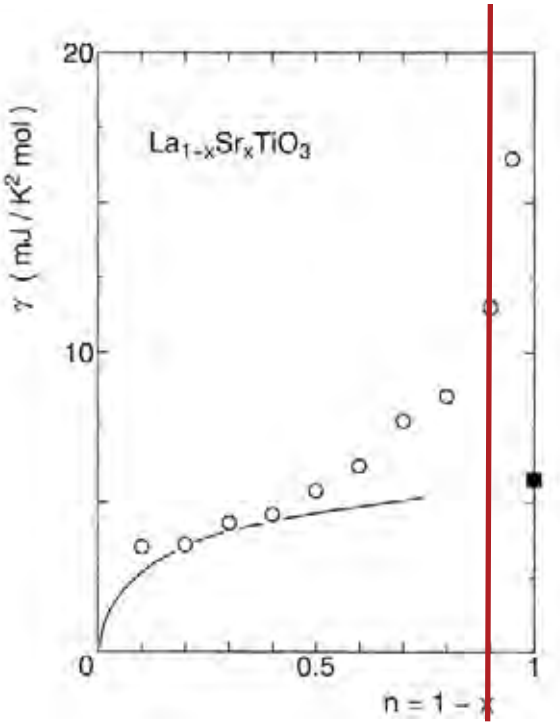
from Taguchi PRB59 7917



from Imada RMP



from Kumagai PRB48 7636



Kumagai says oxygen doping is less than 0.01. Taguchi says that oxygen doping in the Kumagai samples is 0.04

Mott divergence not tied to n=1?

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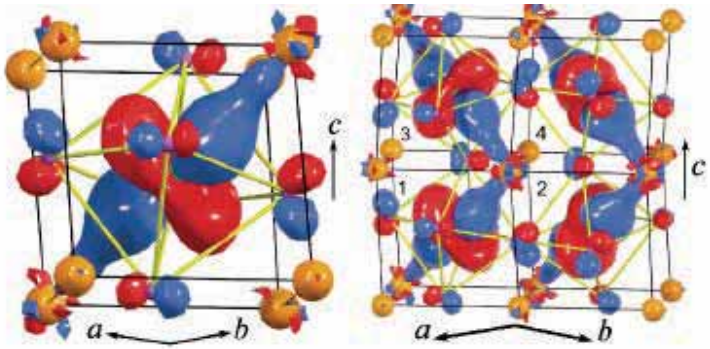
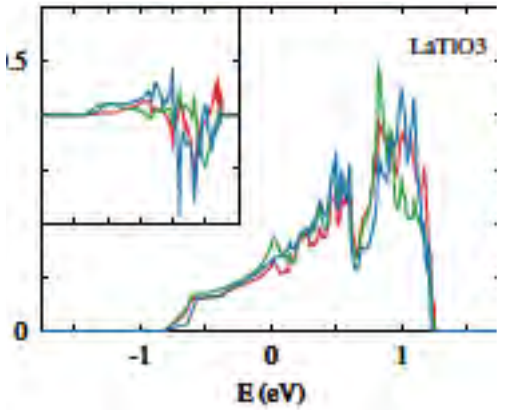
Orbital order (?fluctuations?) important

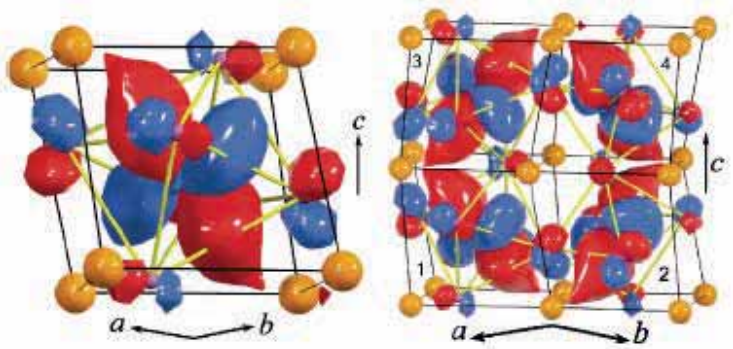
Pavarini et al PRL 92 176403: importance of $GdFeO_3$ (octahedral rotation) distortion

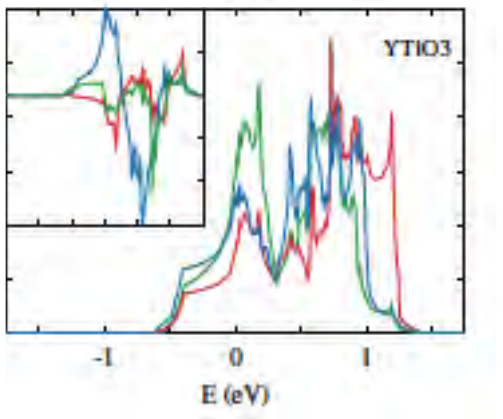
$LaTiO_3$





$YTiO_3$





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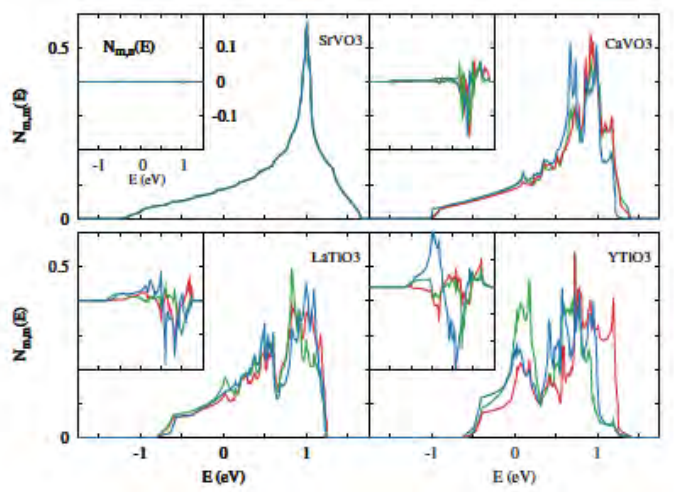
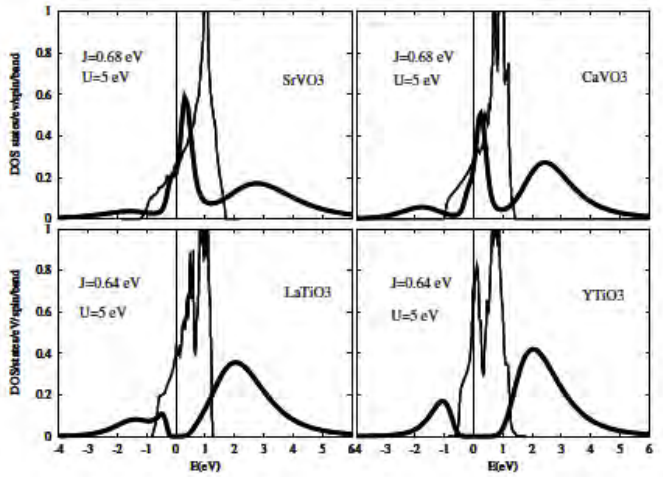
Orbital order (?fluctuations?) important

Pavarini et al PRL 92 176403: importance of $GdFeO_3$ (octahedral rotation) distortion





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Short ranged correlations: other systems

CMR: `Colossal' magneto- resistance

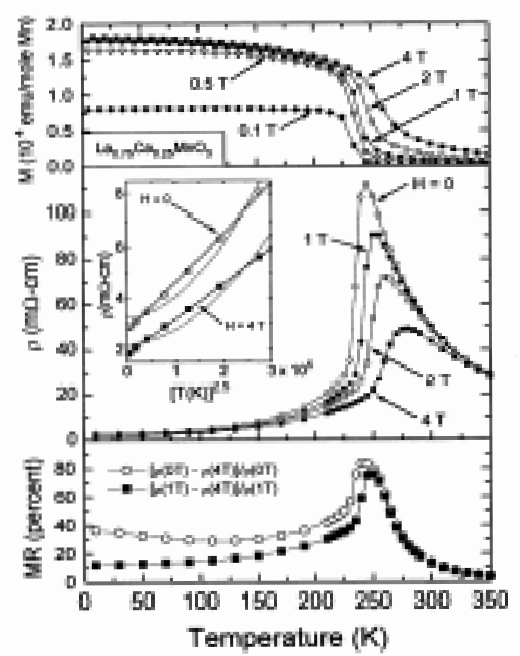
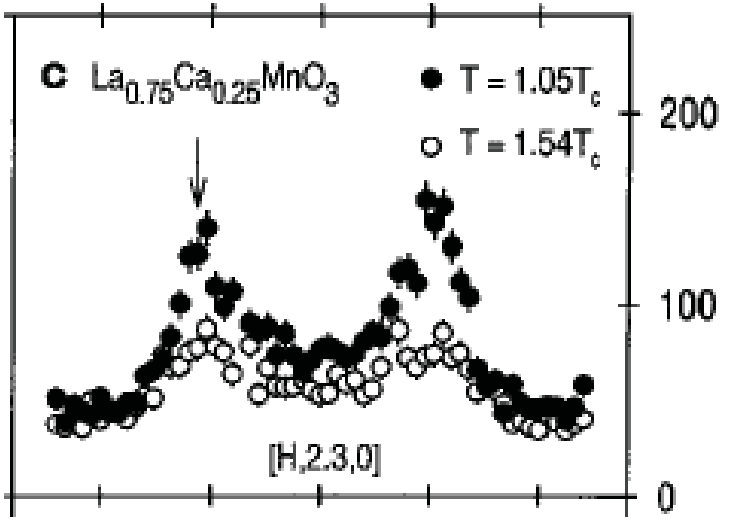


FIG. 2. The magnetization, resistivity, and magnetoresistance of $La_{0.75}Ca_{0.25}MnO_3$ as a function of temperature at various fields. The inset shows ρ at low temperatures; the lines are fits to the data as described in the text.

High T phase: insulating behavior associated with short ranged order



Wavevector: (1/4,0,0)

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These + many other results:

=>motivation to go beyond single-site DMFT

This has only been systematically done for 2d Hubbard model (main application: high Tc)

Remainder of lectures: overview of published results, mainly aimed at high Tc. Illustrate strengths and limits of method.

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Characteristic features of high-Tc superconductivity

1. Superconductivity created by adding carriers to nontrivial insulator
2. Characteristic scaling with doping: optical conductivity strongly doping dependent; carrier mass much less so
3. `Pseudogap' for hole doped materials
4. Precursor: scattering rate anisotropy

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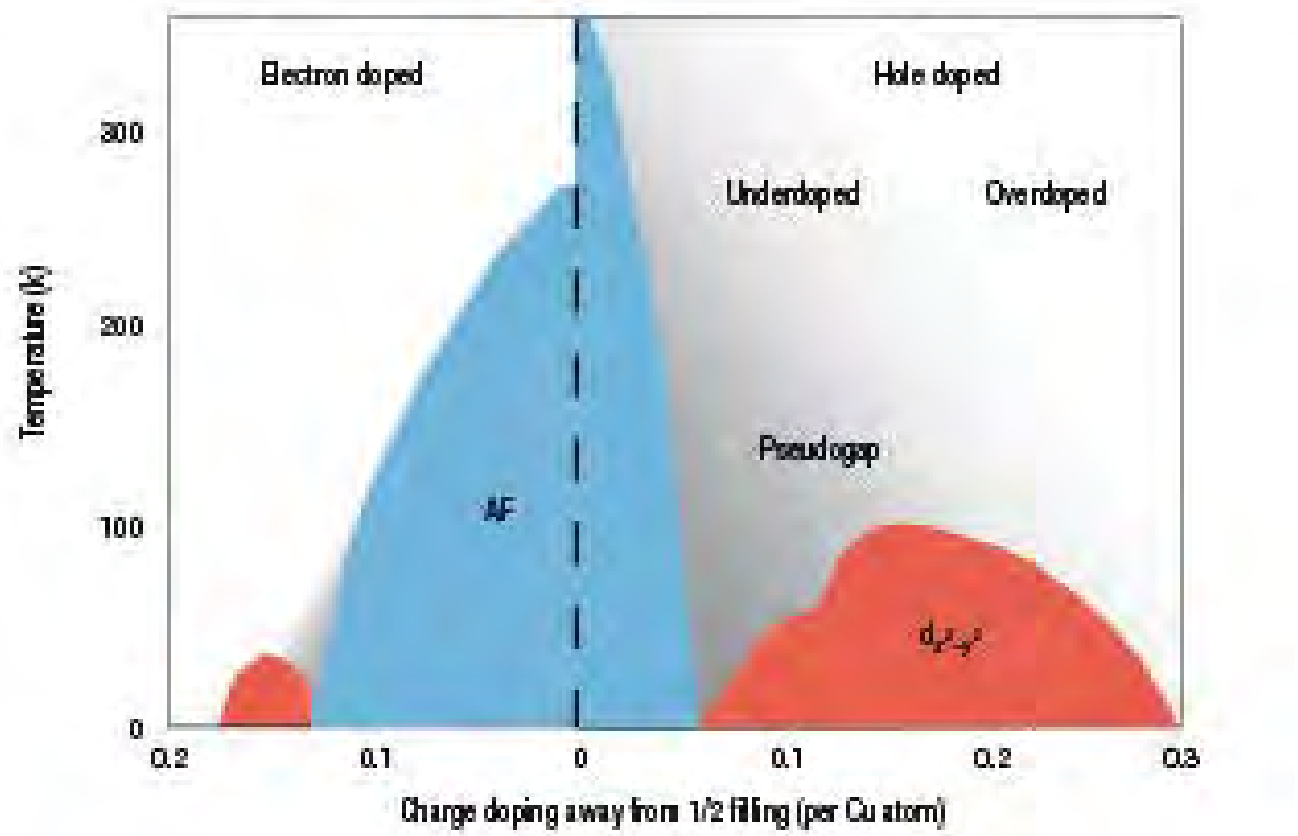
Phase diagram



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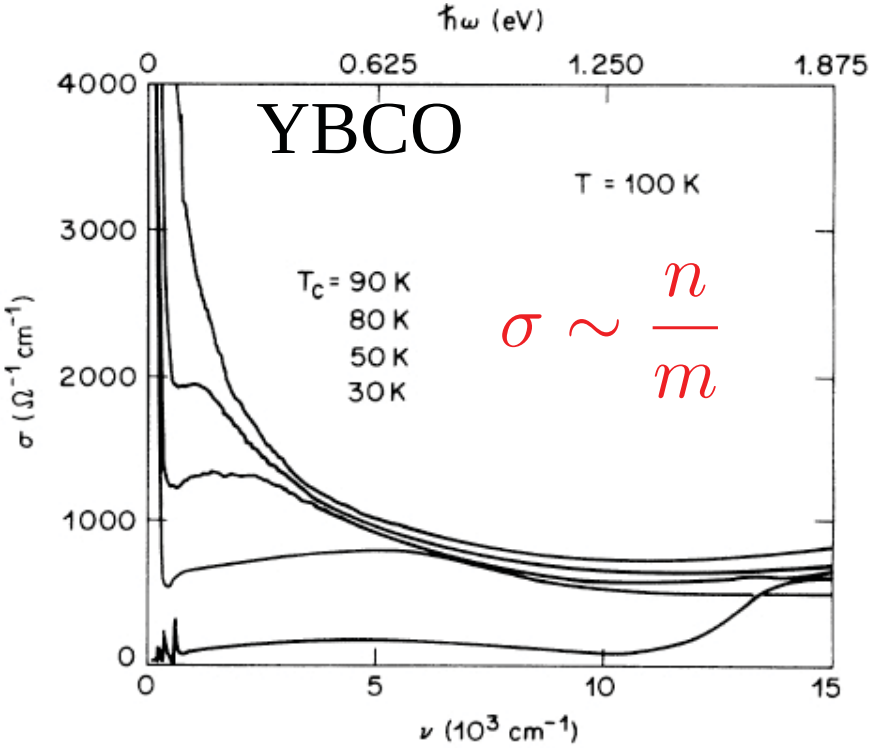
Probes of carrier motion

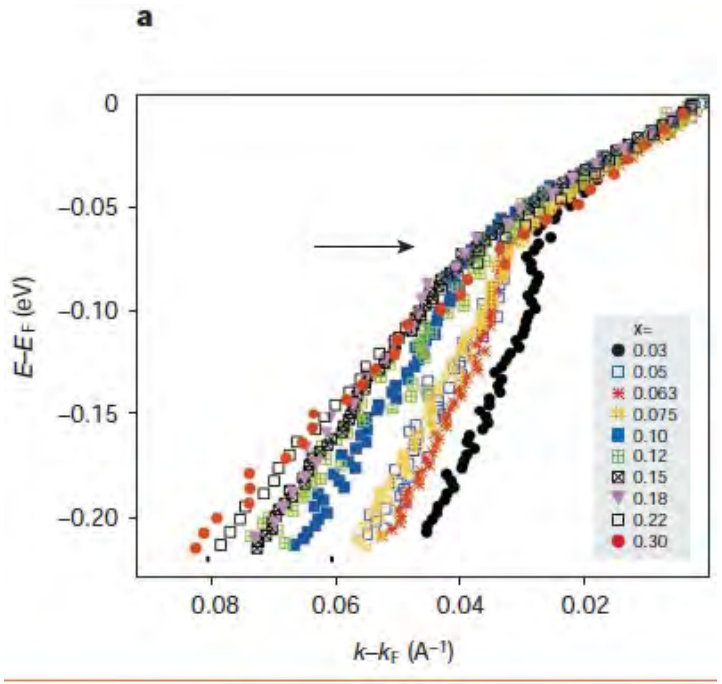
Optical conductivity:



Orenstein, Thomas, Millis et. al,
Physical Review B42, 6342-62 (1990).

n/m: strongly doping dep.

Photoemission:



carrier velocity: weakly doping dependent

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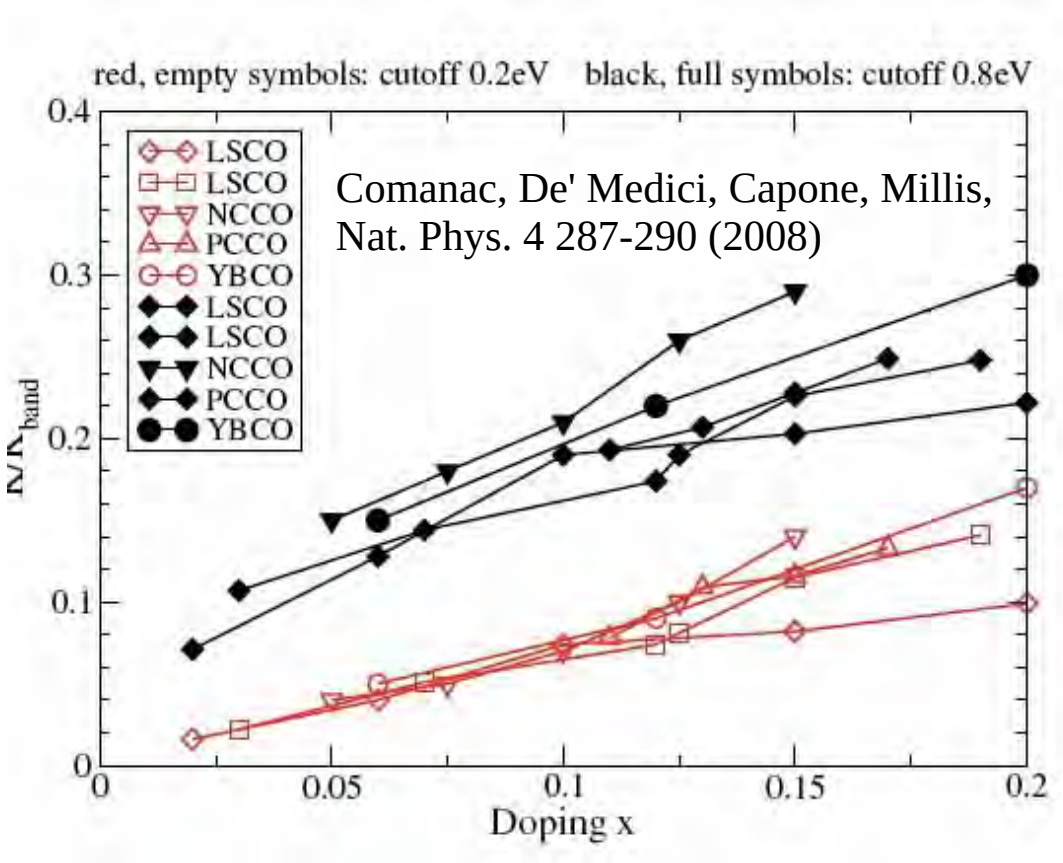
Characterize by ‘spectral weight’



$$= \frac{\hbar d_c}{e^2} \int_0^{\Omega} \frac{2d\omega}{\pi} \sigma(\omega)$$

$\Omega = 0.2eV$:
$K \sim x$

$\Omega = 0.8eV$:
$K \sim x + 0.1$

Low freq conductivity ~x but quasiparticle velocity is not

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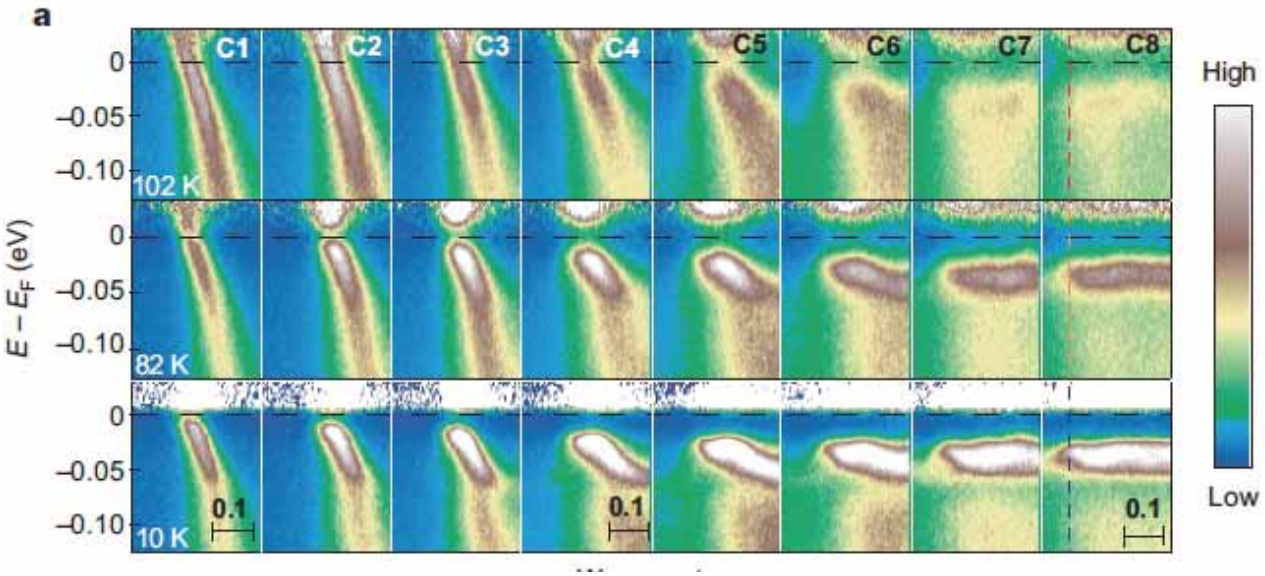
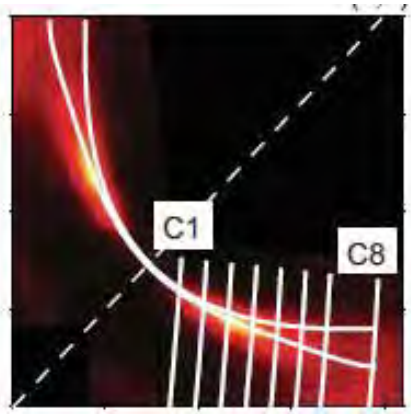
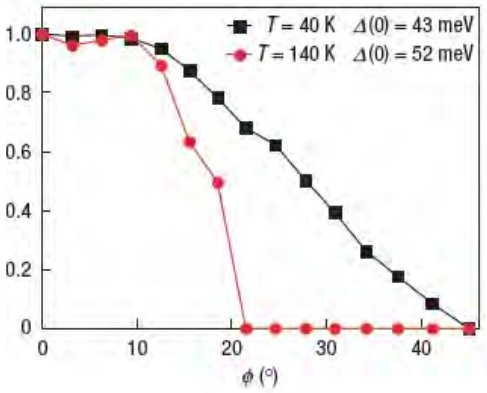
`Pseudogap'

Suppression of density of states in zone corner

Angle-resolved photoemission sample w/ 90K T_c:







S. Lee et al, Nature 450, p. 81 (2007)

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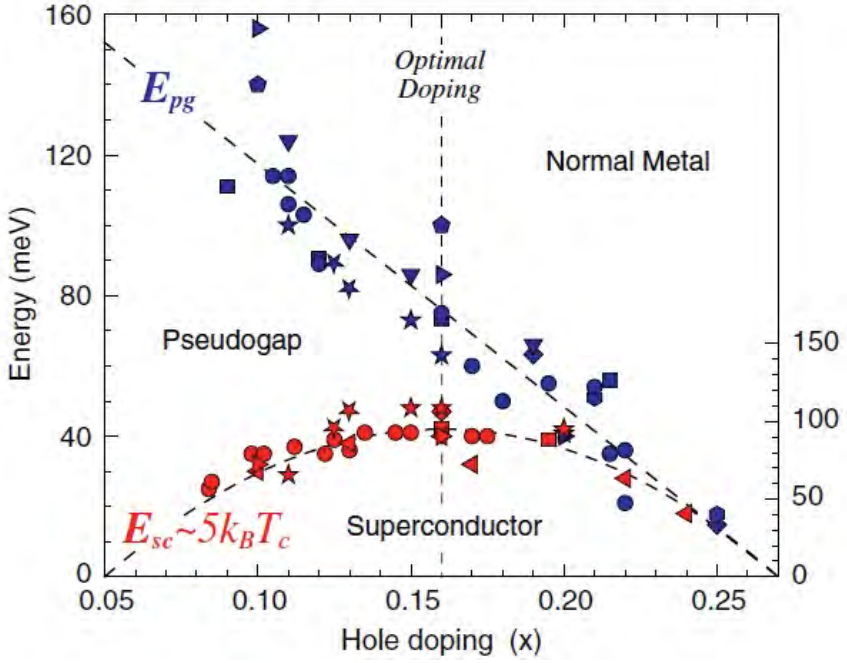
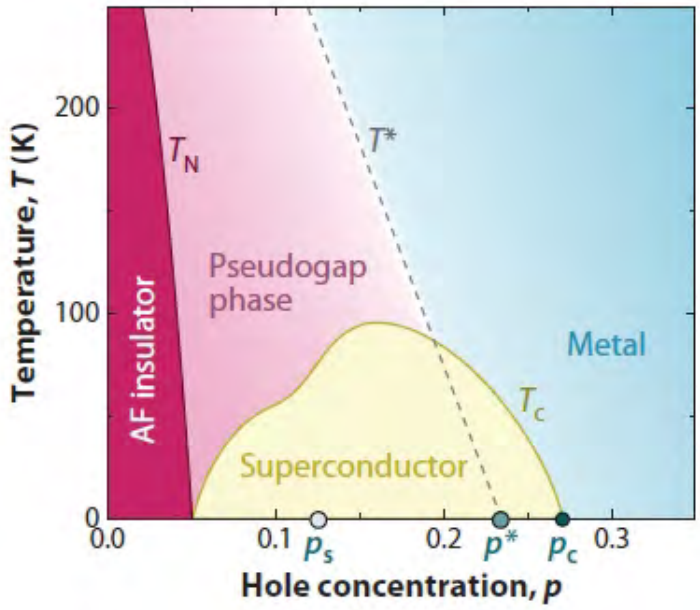
`Pseudogap'

Magnitude increases as doping decreases

Onset temp. increases as doping decreases





Huefner et al Rep. Prog. Phys. 71 062501 (2008)

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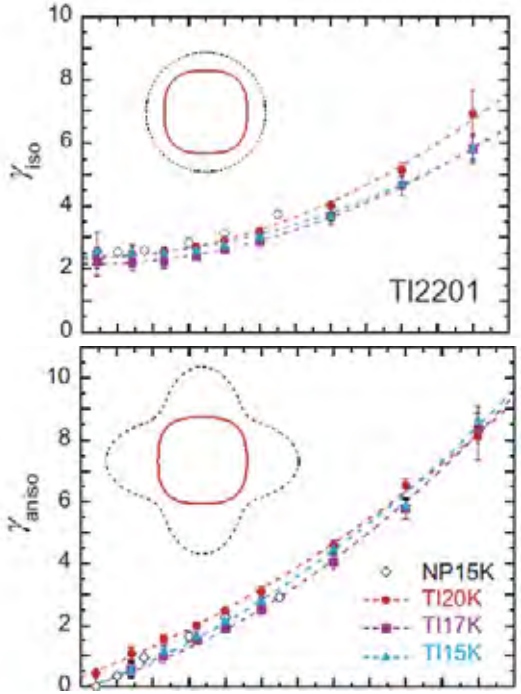
Precursor of pseudogap in momentum-space dependent scattering rate



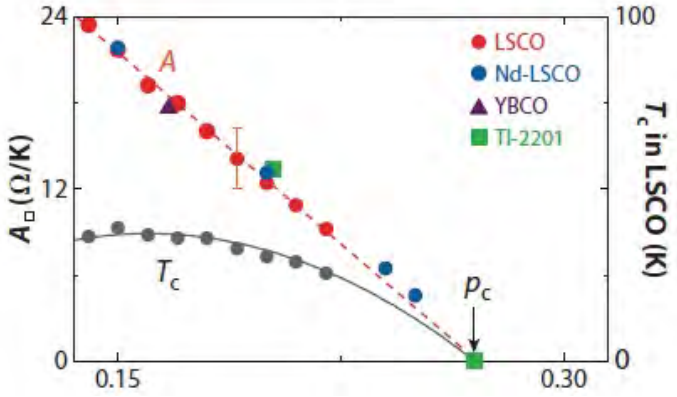
Temperature

M. J. French et al., N. J. Phys.

11 055057 (2009)

Idea: from anisotropy of magnetoresistance, can tease out variation of electronic scattering rate around fermi surface.

Result: unconventional term (rate ~T not T^2) associated with (0,pi) turns on as doping is decreased.



L. Taillefer Ann. Rev. Condens.Matter Phys. 2010. 1:51–70

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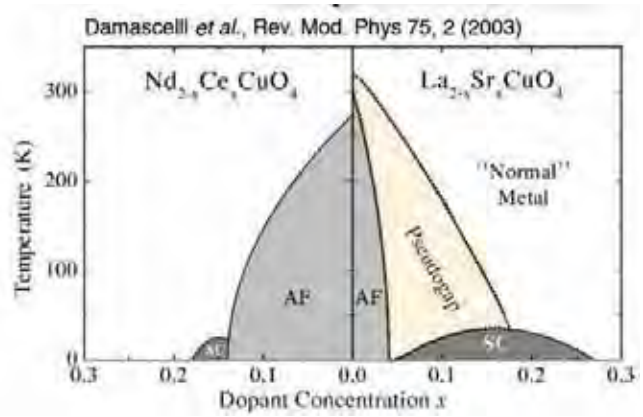
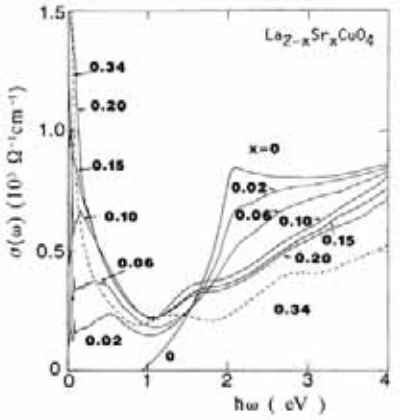
Are these phenomena properties of a theoretical model?

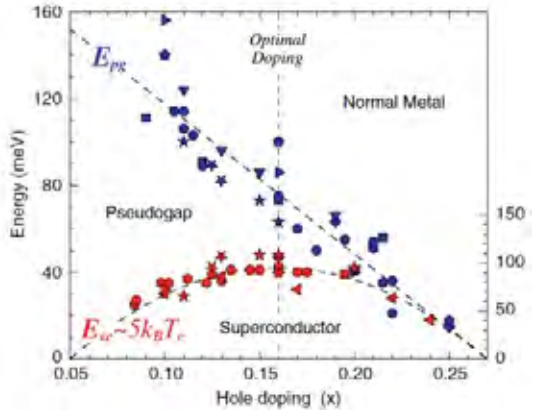
Phase diagram



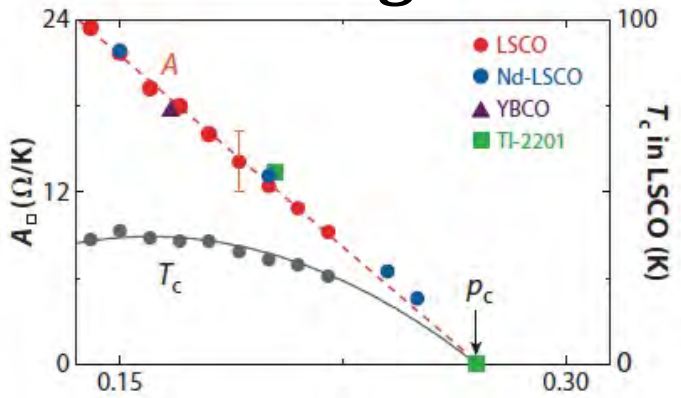
Conductivity



Pseudogap



Scattering rate



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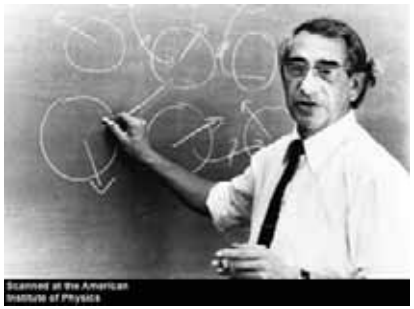
www.picsearch.com

Main theoretical idea: interesting phenomena related to Mott transition in Hubbard model:



http://theor.jinr.ru/~kuzemsky/jhbio.html

One (spin degenerate) orbital per lattice site.
hopping t short ranged.

$$\mathbf{H} = -\sum_{ij} t_{i-j} c^{\dagger}_{i\sigma} c_{j\sigma} + U \sum_{i} n_{i\uparrow} n_{i\downarrow}$$

Important parameters:

--relative interaction strength U/t

--electron density n

Hopping parameters from band theory

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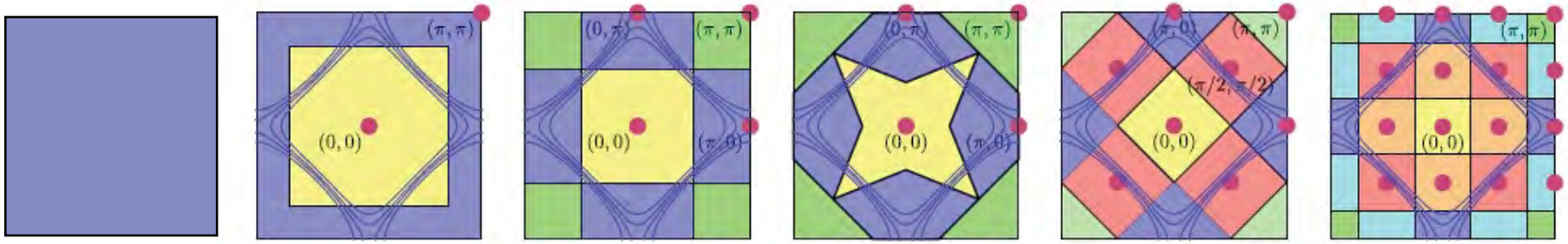
1,2,4,8,16 site cluster DMFT



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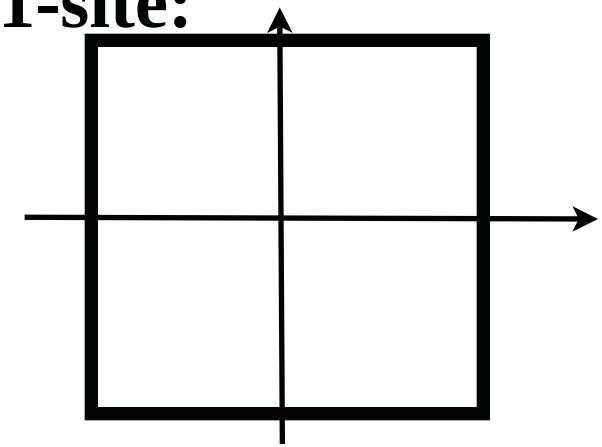
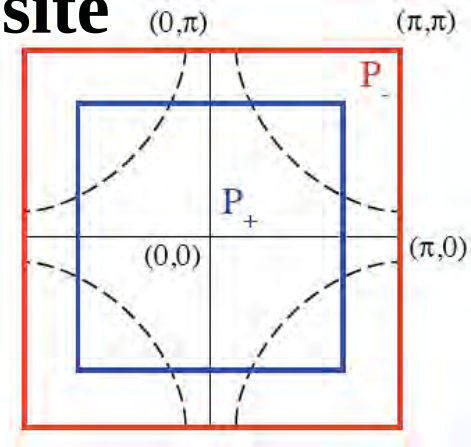
Clusters: trade off momentum resolution<=>computability

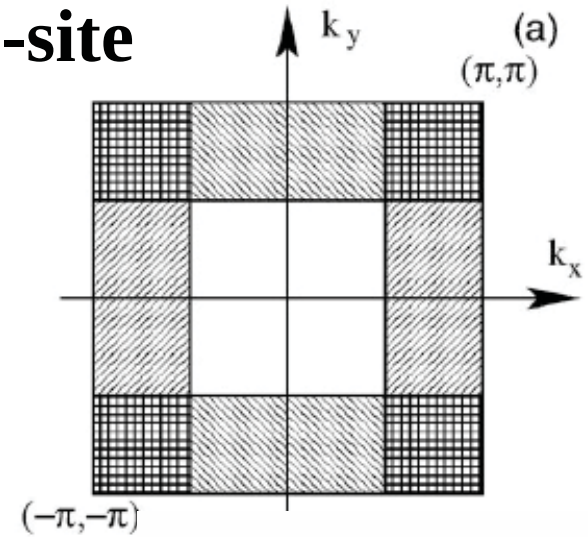
1-site:



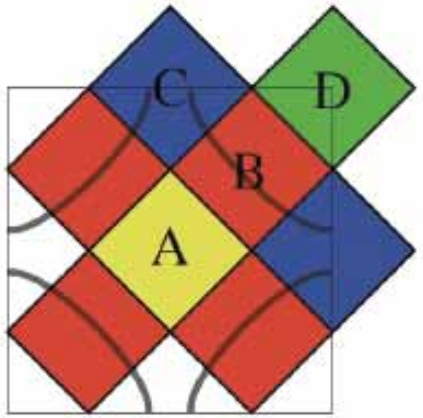
2-site



4-site



8-site



Ferrero et al EPL89 57009

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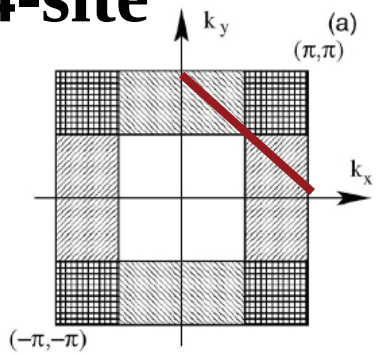
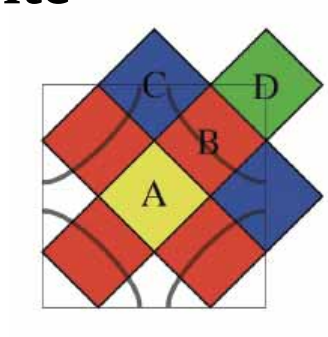
Cluster notes

4-site



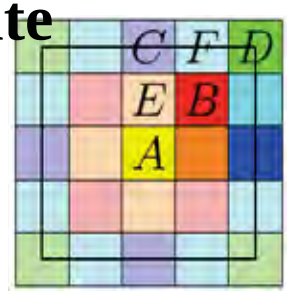
4-site: amenable to CT-HYB ('expand in V')=> much info available. Near half filling, fermi surface almost entirely in (0,Pi) sector

8-site



8-site: only CT-AUX. Systematic studies down to T=t/60 feasible. Direct (coarse-grained) access to nodal and antinodal Fermi surface regions

16-site



16-site: only CT-AUX. Systematic studies down to T=t/10 feasible. At one parameter: t/40 (if sign)

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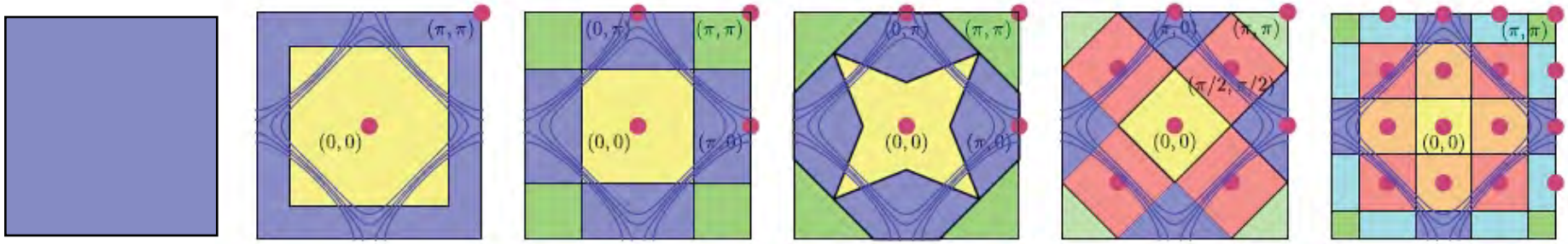
1,2,4,8,16 site cluster DMFT



Quantitative extrapolation to infinite cluster limit not possible with present 'technology'. Focus on qualitative physics: quantities for which all clusters give (qualitatively) the same answers.

Look at metal insulator transition

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=>Fundamental interest of
(correlation-driven) Metal-Insulator transition

breakdown of fermi liquid at strong interactions

$$\mathbf{A}(k,\omega) = \frac{Im\Sigma(k,\omega)}{\left(\omega - \varepsilon_k - Re\Sigma(k,\omega)\right)^2 + Im\Sigma(k,\omega)^2}$$

Insulator: Gap in electronic spectrum => $\mathbf{Im\Sigma(k,\omega) = 0;\ |\omega| < \Delta}$

<u>and</u> no solution to $\omega - \varepsilon_{\mathbf{k}} - \mathbf{Re\Sigma(k,\omega) = 0}$

for any k at $|\omega| < \mathbf{\Delta}$

Real part of self energy must be very large at low freq.

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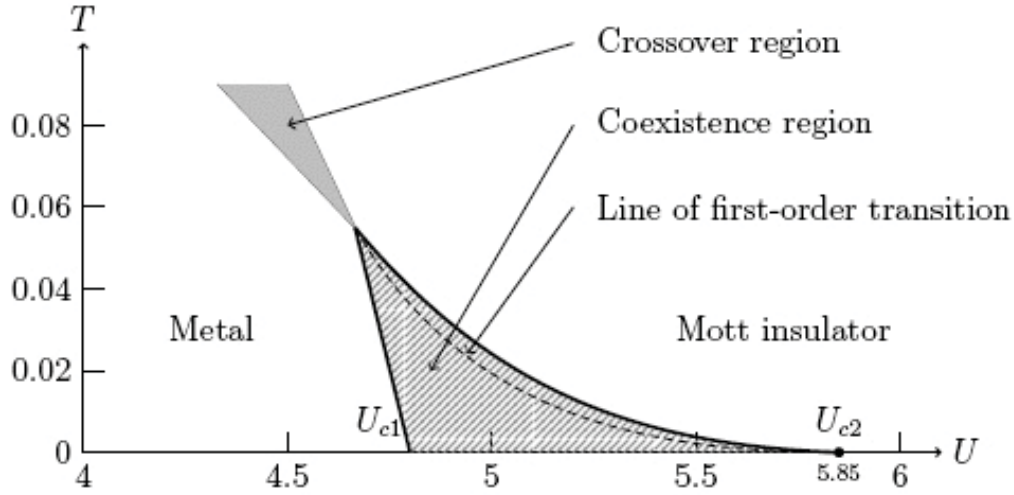
Intuitive idea: 'Mott' if insulating in absence of intersite correlations (i.e. from purely local physics)

Implementation: 1-site DMFT (no spatial correlations)

Bethe lattice.
bandwidth =4

density n=1



T=0 correlation-driven metal insulator transition at $U=U_{c2}$

Gives precise theoretical meaning to 'Mott transition'.

Note! Insulator: ground state degeneracy

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Characterize Insulator

Choose zero of energy to be chemical potential

Metal if "quasiparticle equation"

$$G^{-1}(k,\omega) = \omega - \varepsilon_k - Re\Sigma(k,\omega) = 0$$

is satisfied for some k near w=0

To kill the metal: make "renormalized chemical potential" $\mathrm{Re}\Sigma$ **larger than max** $|\varepsilon_{\mathbf{k}}|$

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Consider particle-hole symmetric situation

$$\mathbf{Re\Sigma}(\omega) = \int \frac{\mathbf{dx}}{\pi} \frac{\mathbf{Im\Sigma(x)}}{\omega - \mathbf{x}} \qquad Im\ \Sigma(\omega)\ \mathbf{even} \rightarrow Re\ \Sigma(\omega)\ \mathbf{odd}$$

If gap, $Im\ \Sigma(\omega) = 0$ **at low energies**

If $Re\ \Sigma(\omega) \rightarrow 0$ **at** $\omega = 0$**then quasiparticle equation satisfied** $\rightarrow$ **states in gap**

Self energy must have pole at w=0 (in p-h symm)

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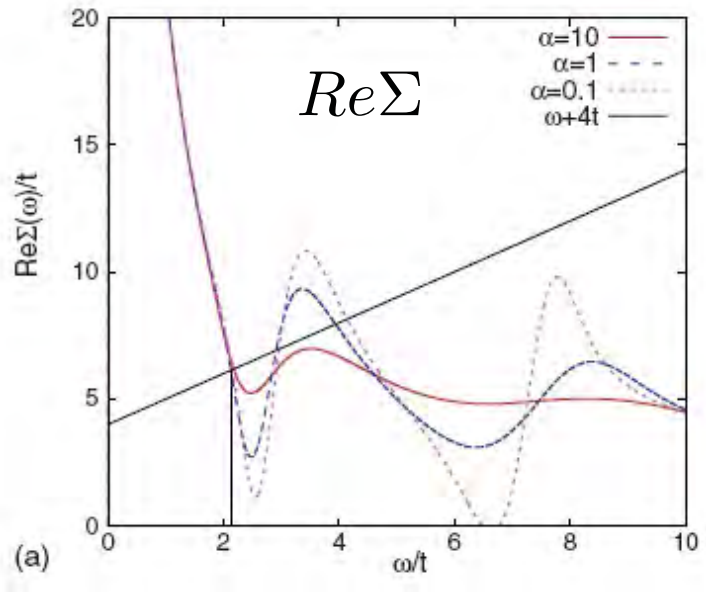
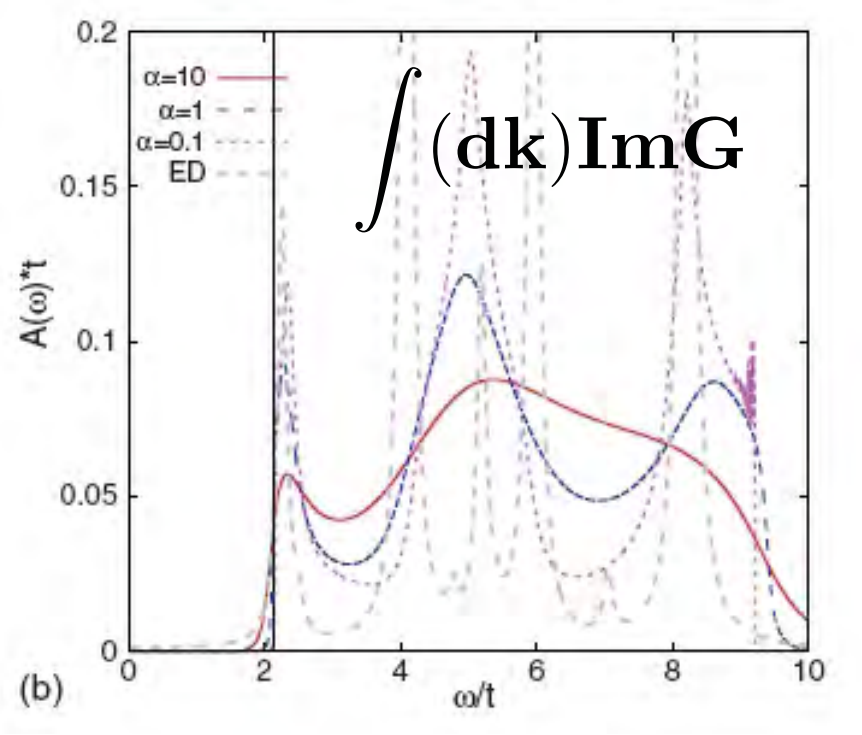
Single site DMFT: insulating state pole in sigma splits the band

$$\Sigma(z) = \frac{\Delta^2}{z - \omega_0}$$





Xin Wang Phys. Rev.B80, 045101 (2009)

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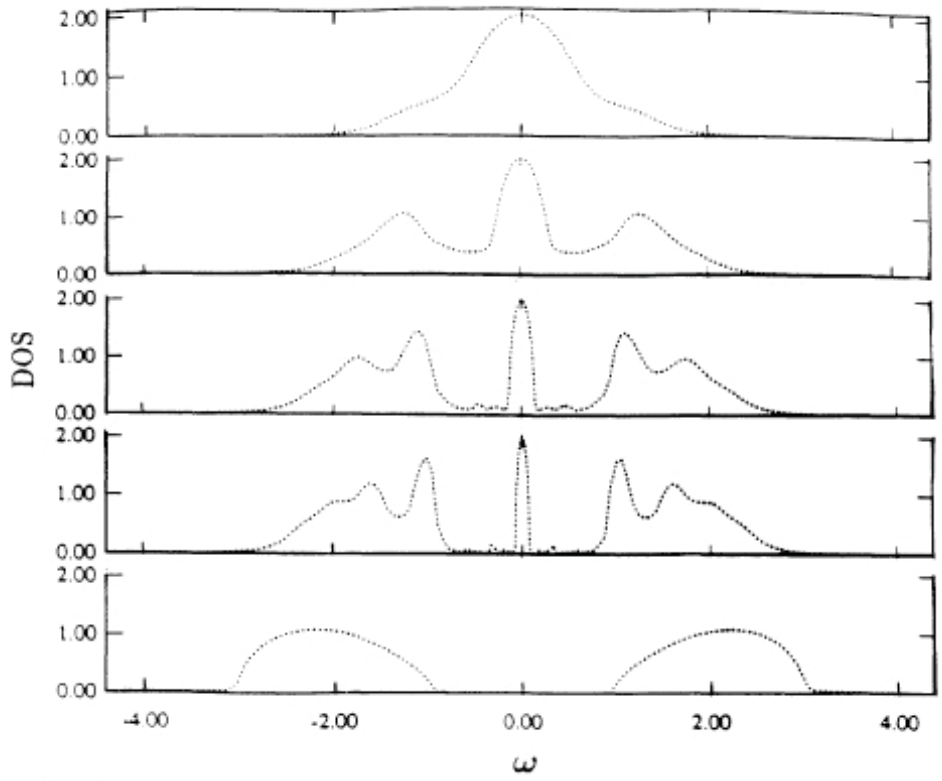
Characterize approach to insulator as interaction is increased at half filling



Side bands: localized (atomic-like) states

Central peak: coherent, strongly renormalized fermions
Central peak is fragile. As raise T it goes away.

X. Y. Zhang, M. J. Rozenberg, and G. Kotliar
Phys. Rev. Lett. **70**, 1666 (1993

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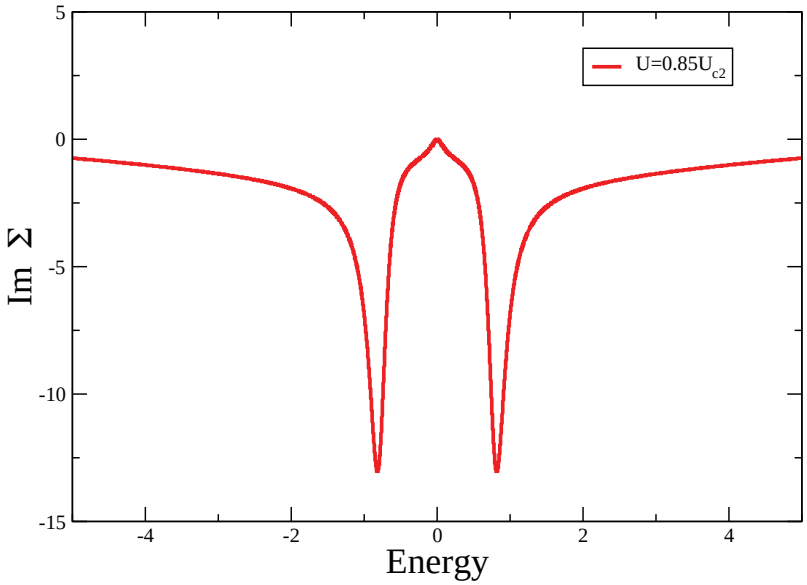
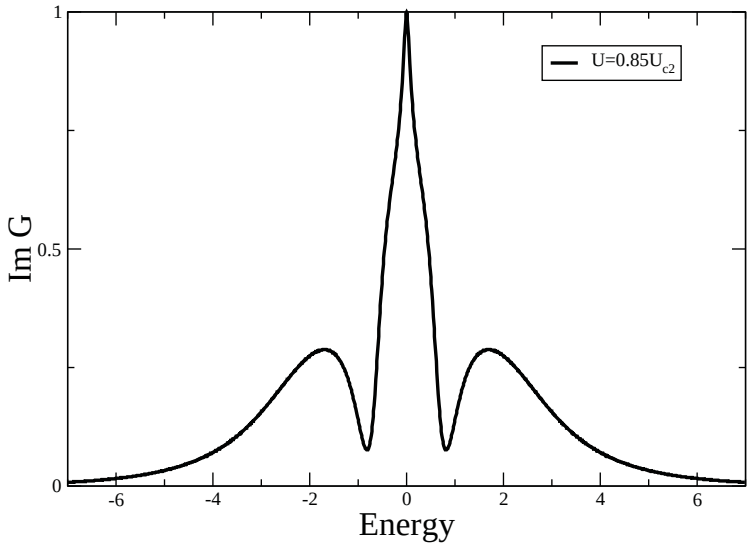
interaction driven MIT via pole splitting





Self energy has two poles, which converge as U->U_{c2}

P. Cornaglia data
U=0.85 U_{c2}

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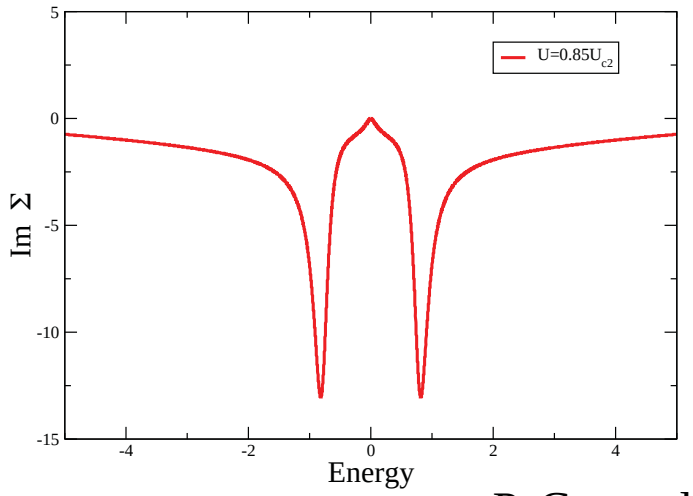
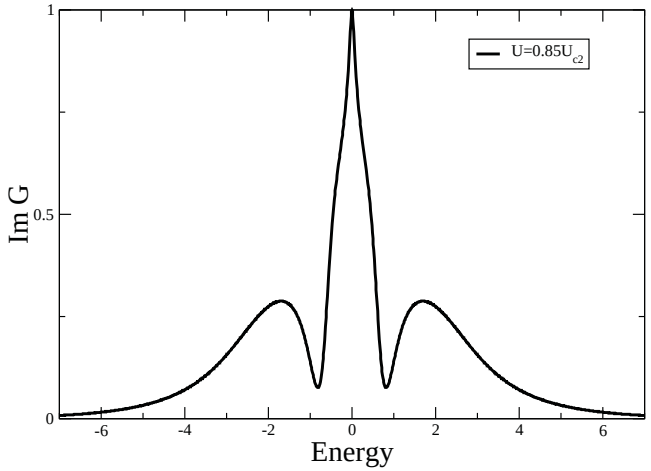
interaction driven MIT via pole splitting

$$\Sigma(z) \approx \frac{\Delta_1^2}{z-\omega_1} + \frac{\Delta_2^2}{z-\omega_2} \qquad \omega_{1,2} \to 0 \text{ as } U \to U_{c2}$$





P. Cornaglia data
U=0.85 U_{c2}

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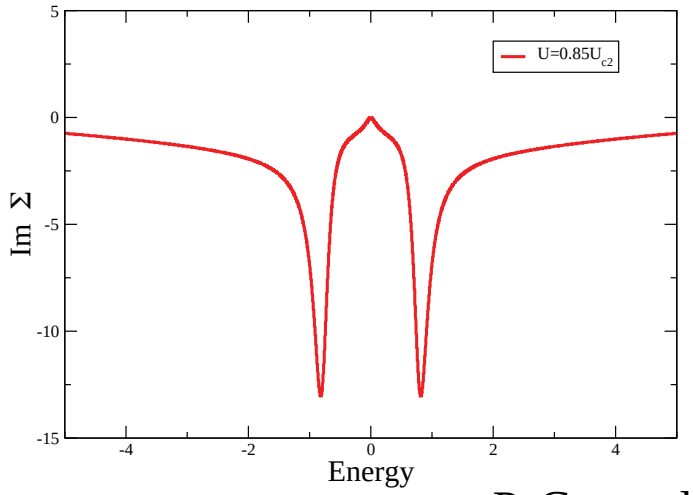
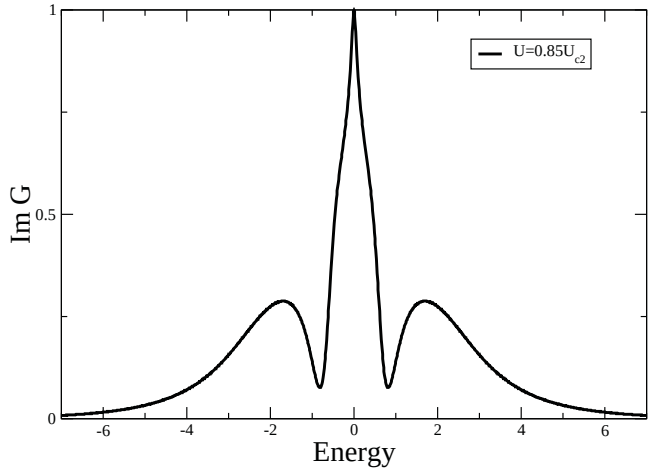
interaction driven MIT via pole splitting

$$\Sigma(z) \approx \frac{\Delta_1^2}{z-\omega_1} + \frac{\Delta_2^2}{z-\omega_2} \qquad \omega_{1,2} \to 0 \text{ as } U \to U_{c2}$$

$$\Sigma(z \to 0) = -\frac{\Delta_1^2\omega_2 + \Delta_2^2\omega_1}{\omega_1\omega_2} - z\frac{\Delta_1^2\omega_2^2 + \Delta_2^2\omega_1^2}{\omega_1^2\omega_2^2}$$





P. Cornaglia data
U=0.85 U_{c2}

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interaction driven MIT via pole splitting

$$\Sigma(z) \approx \frac{\Delta_1^2}{z-\omega_1} + \frac{\Delta_2^2}{z-\omega_2} \qquad \omega_{1,2} \to 0 \text{ as } U \to U_{c2}$$

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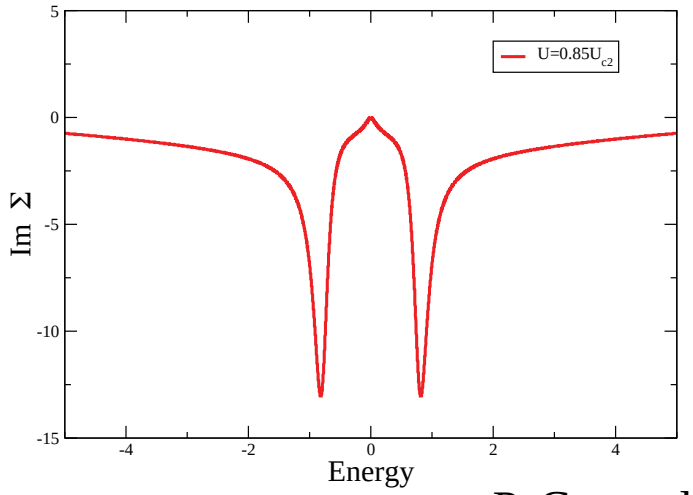
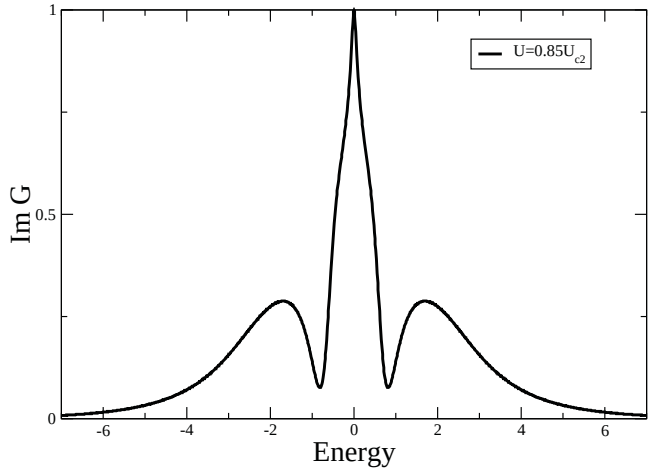
μ renormalization

0 if p-h symmetry





P. Cornaglia data

U=0.85 U_{c2}

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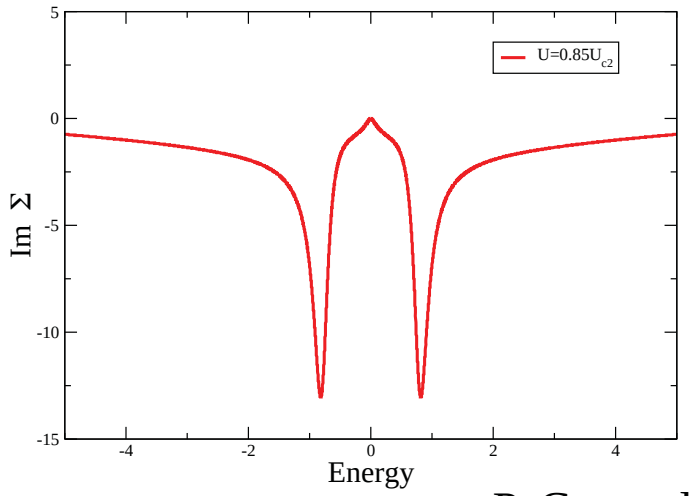
interaction driven MIT via pole splitting

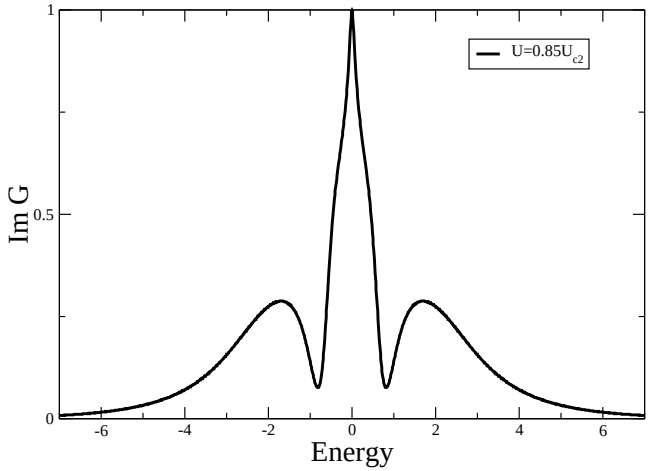
$$\Sigma(z) \approx \frac{\Delta_1^2}{z-\omega_1} + \frac{\Delta_2^2}{z-\omega_2} \qquad \omega_{1,2} \to 0 \text{ as } U \to U_{c2}$$

$$\Sigma(z \to 0) = -\frac{\Delta_1^2\omega_2 + \Delta_2^2\omega_1}{\omega_1\omega_2} - z\frac{\Delta_1^2\omega_2^2 + \Delta_2^2\omega_1^2}{\omega_1^2\omega_2^2}$$

μ renormalization
0 if p-h symmetry

'mass' renormalization
diverges as approach insulato





P. Cornaglia data
U=0.85 U_{c2}

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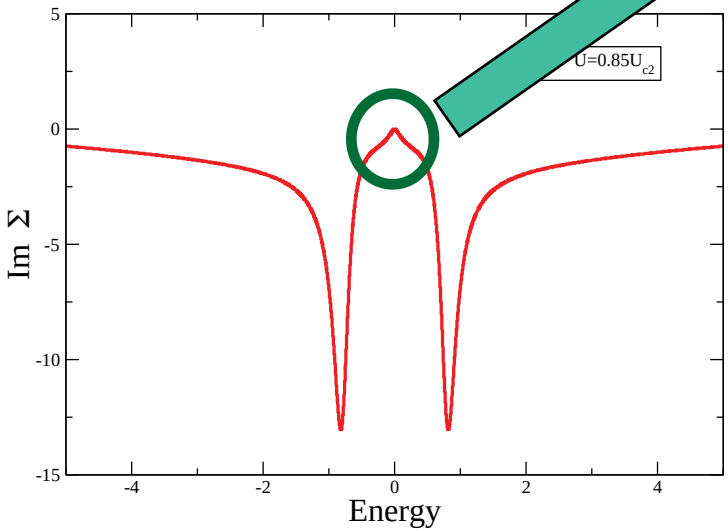
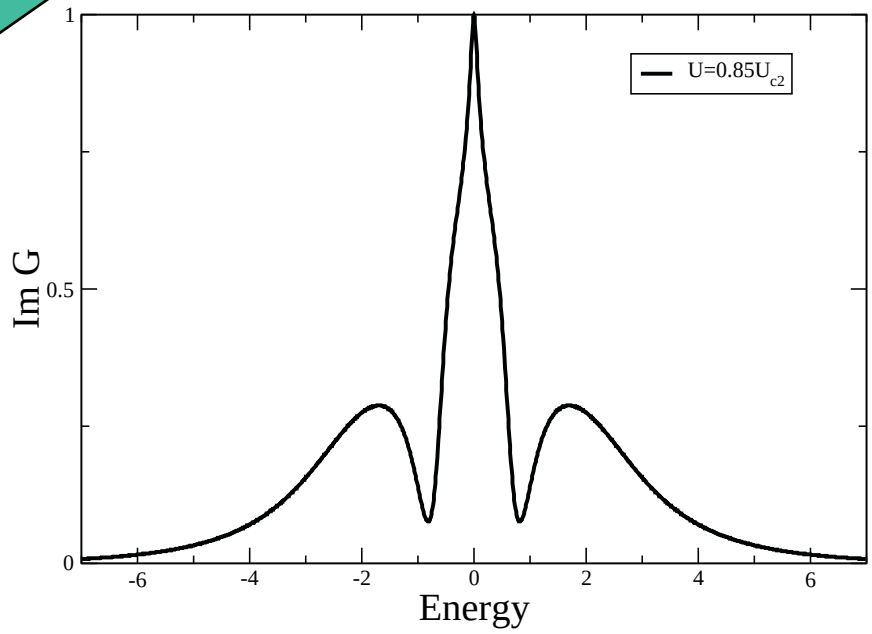
interaction driven MIT via pole splitting

$$\Sigma(z) \approx \frac{\Delta_1^2}{z-\omega_1} + \frac{\Delta_2^2}{z-\omega_2}$$

Subtle low frequency behavior: not just poles

P. Cornaglia data
U=0.85 U_{c2}





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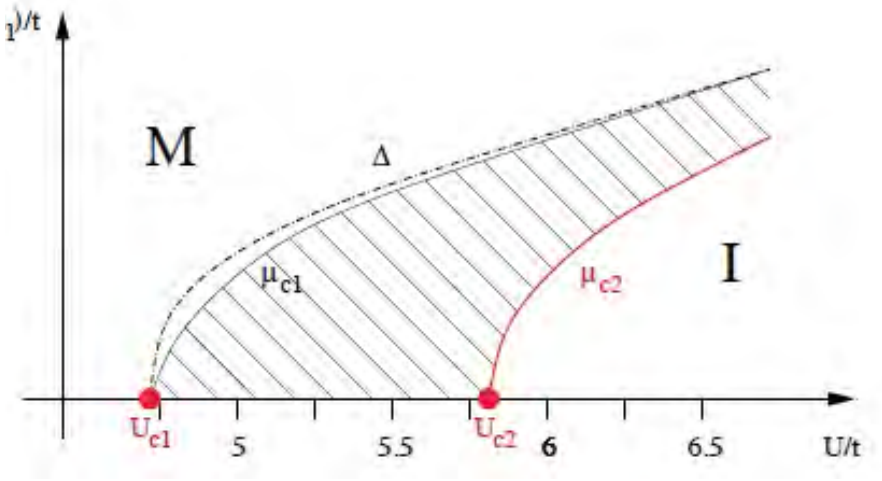
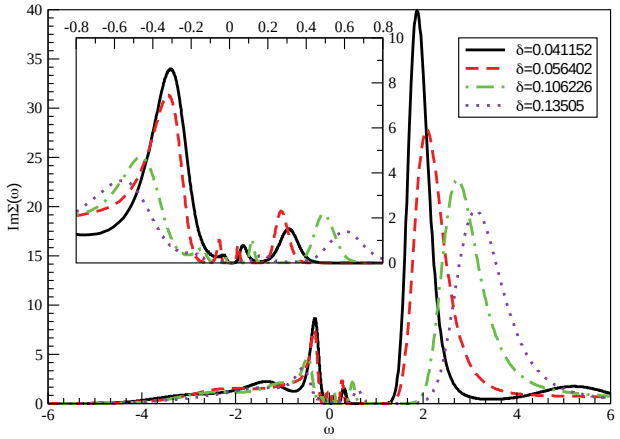
doping driven transition: also coexistence regime; 2 pole structure





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Single-site DMFT neglects spatial correlations. How much of this structure is artifact of this neglect??

In 2d: almost all is artifact.
In 3d: not yet known

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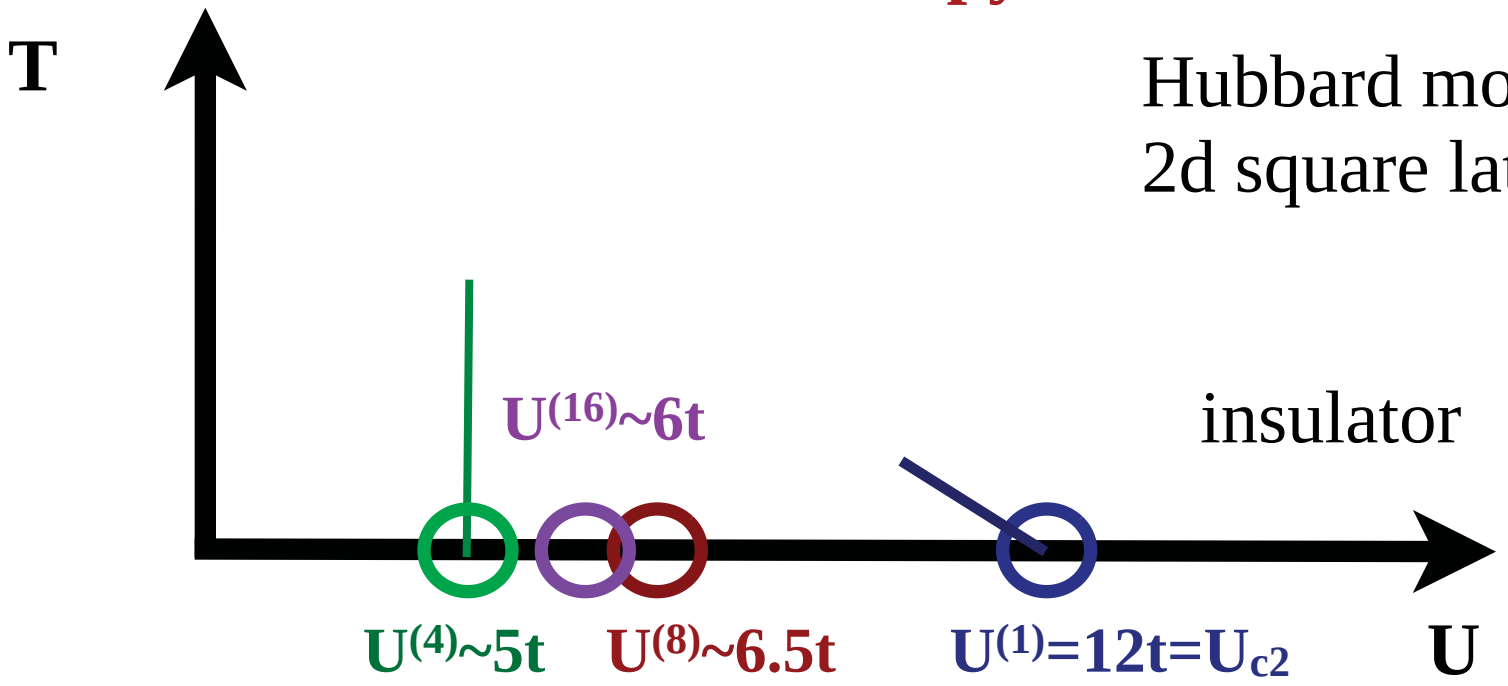
2d: Larger clusters

Paramagnetic insulator stabilized at lower U

Insulator has lower entropy than metal



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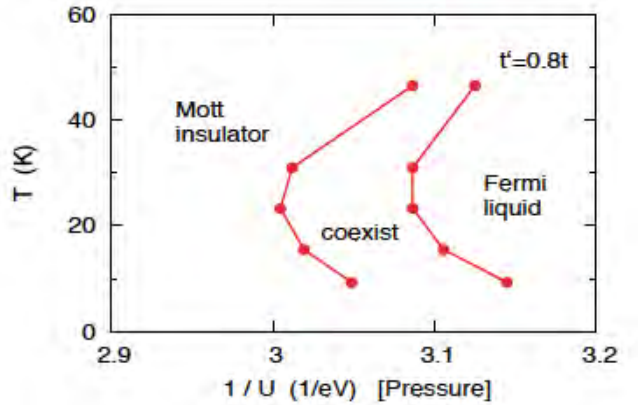
2d triangular lattice

Liebsch et al arXiv:0903.2063



t=0.04eV=>U_c~9t
single site: ~15t

=>apparently, substantial corrections to single-site behavior here also

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Recent results on 2D square lattice

Emanuel Gull, Olivier Parcollet, Philipp Werner, and Andrew J. Millis, Phys. Rev. B80, 245102 (2009).

Emanuel Gull, Michel Ferrero, Olivier Parcollet, Antoine Georges, Andrew J. Millis, Phys. Rev. B82 155101 (2010)

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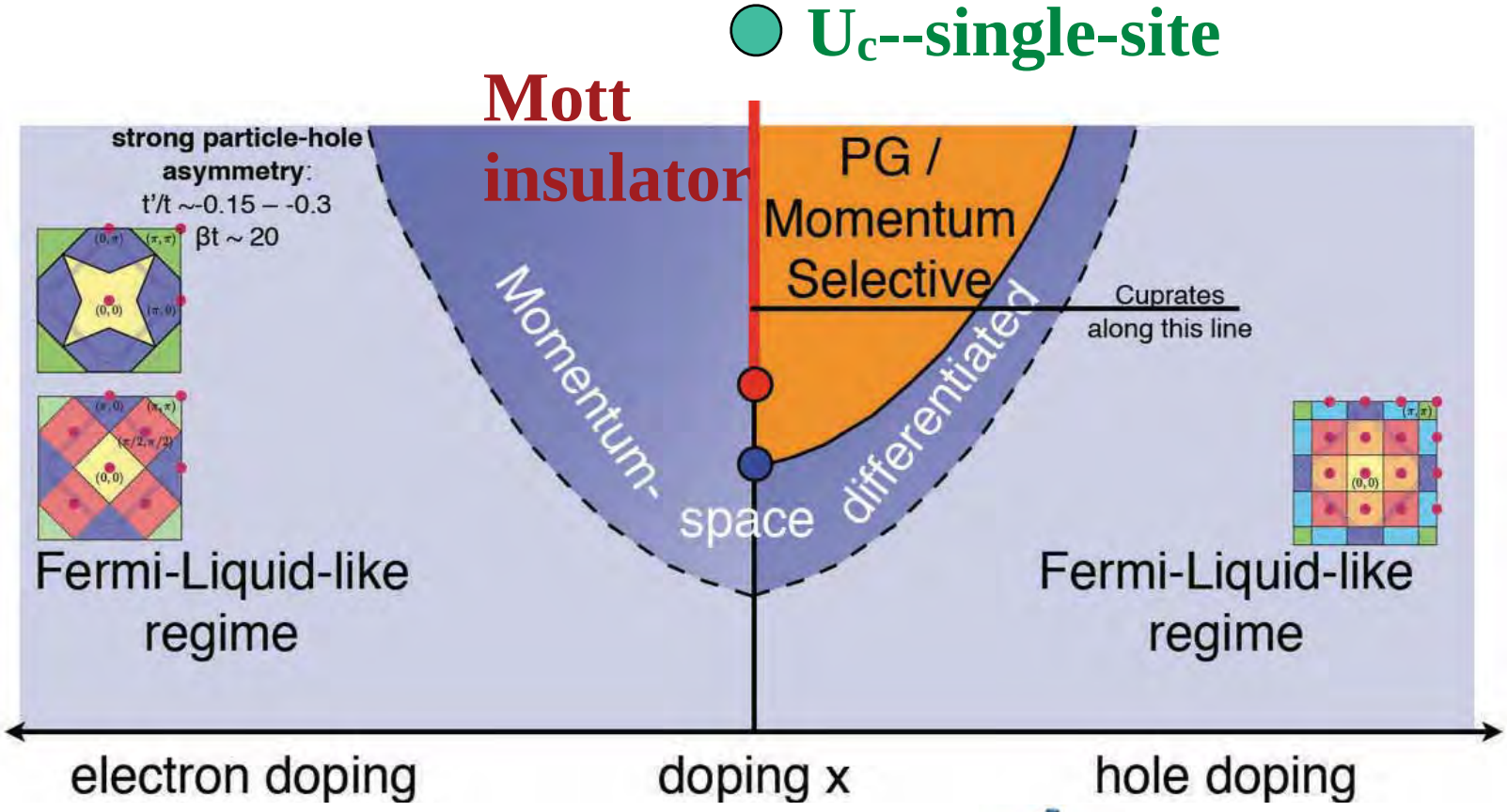
New finding: 2d square lattice correlation-driven metal-paramagnetic insulator transition is generically multi-stage



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How do we see that this is true

$$\varepsilon_k = -2t\,(\cos k_x + \cos k_y) - 4t'\cos k_x \cos k_y$$

look first at

$$\beta G(\tau = \frac{\beta}{2}) = \beta \int \frac{dx}{4\pi} \frac{A_{sector}(x)}{cosh\frac{x}{2T}} = \int \frac{dy}{4\pi} \frac{A_{sector}(2Ty)}{coshy}$$

Integral is peaked at y~1 =>T->0
picks out fermi level density of states
Directly measured.
No analytic continuation. No interpolation

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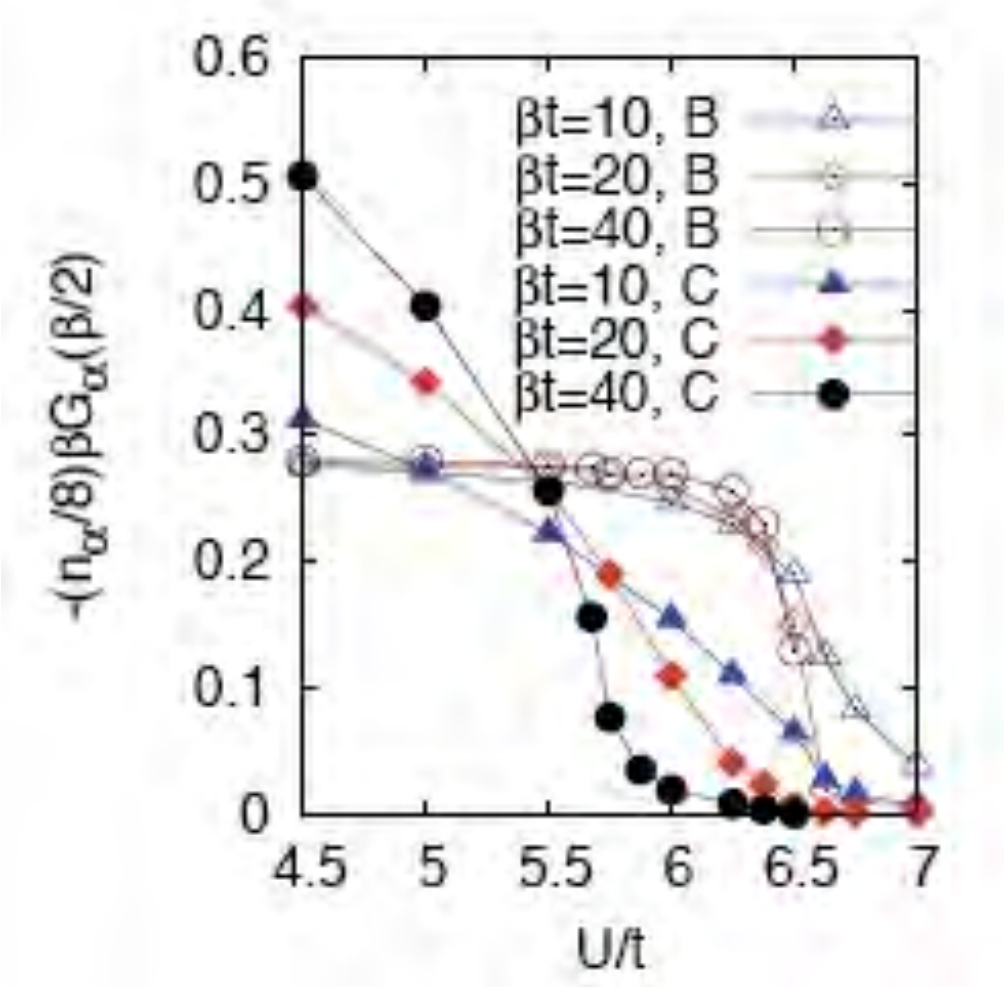
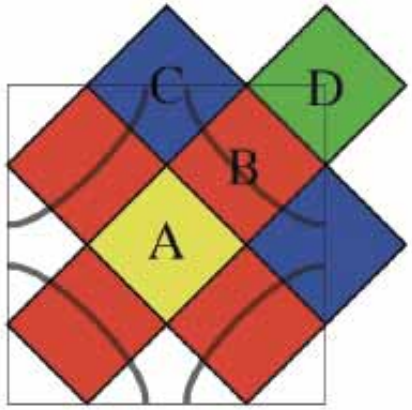
n=1, vary U
sector-selective transition

t'=0; 8 sites





van Hove singularity in sector C=>T-dependence

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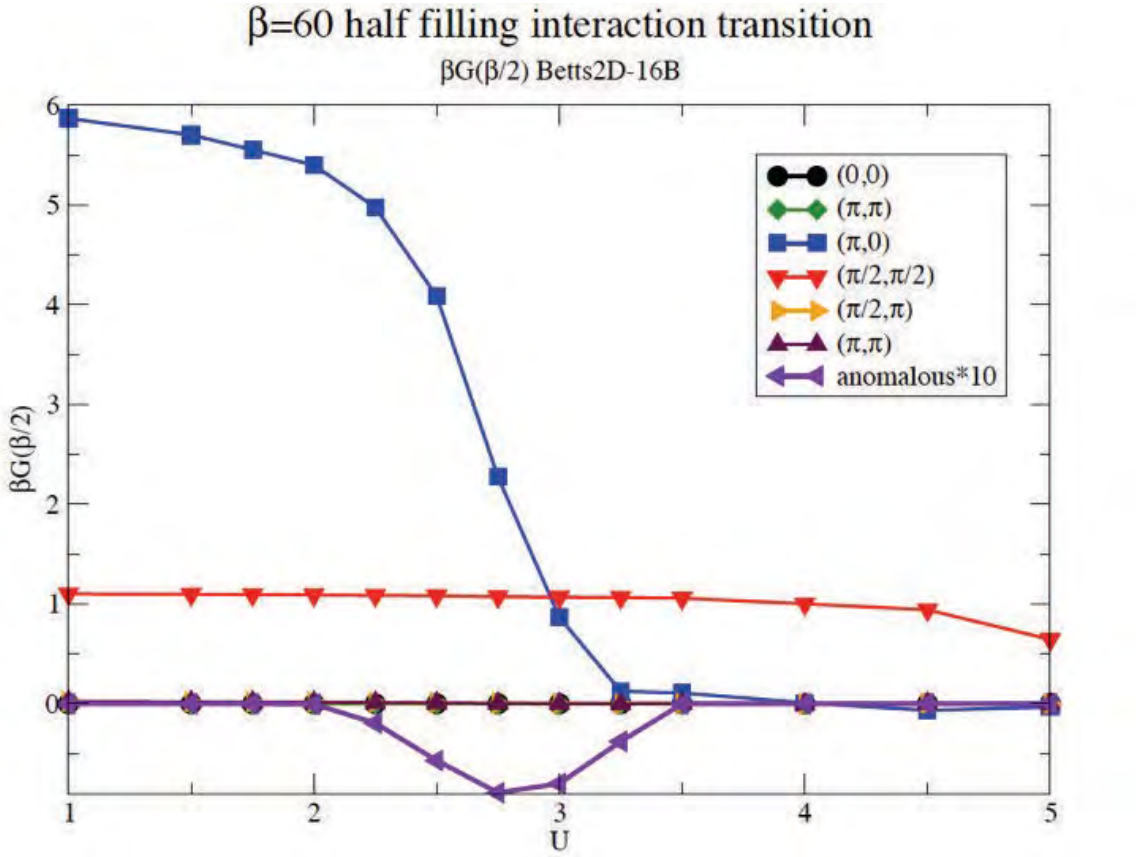
16 sites t'=0



E. Gull

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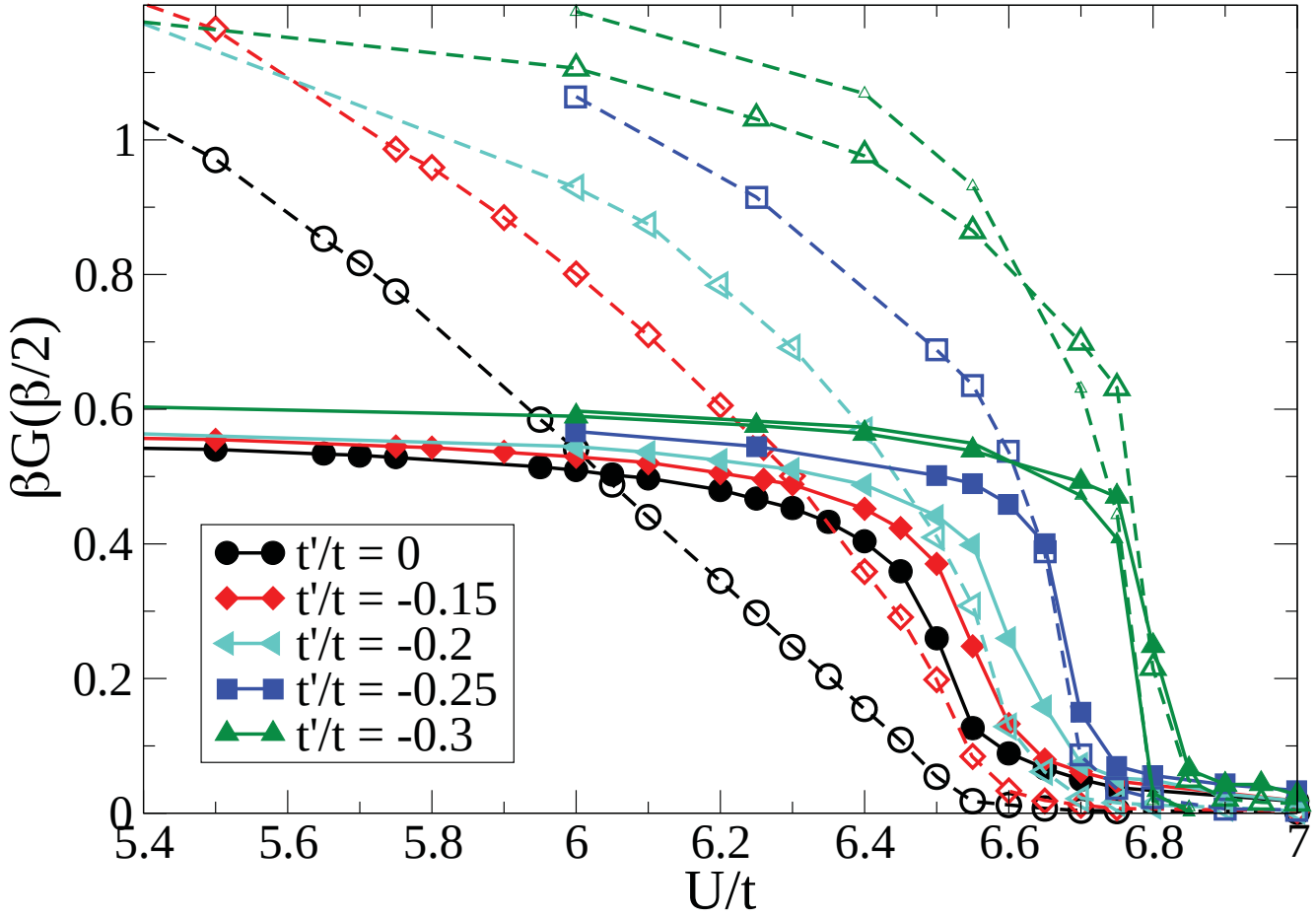
change t': transitions coalesce, seem to become 1st order



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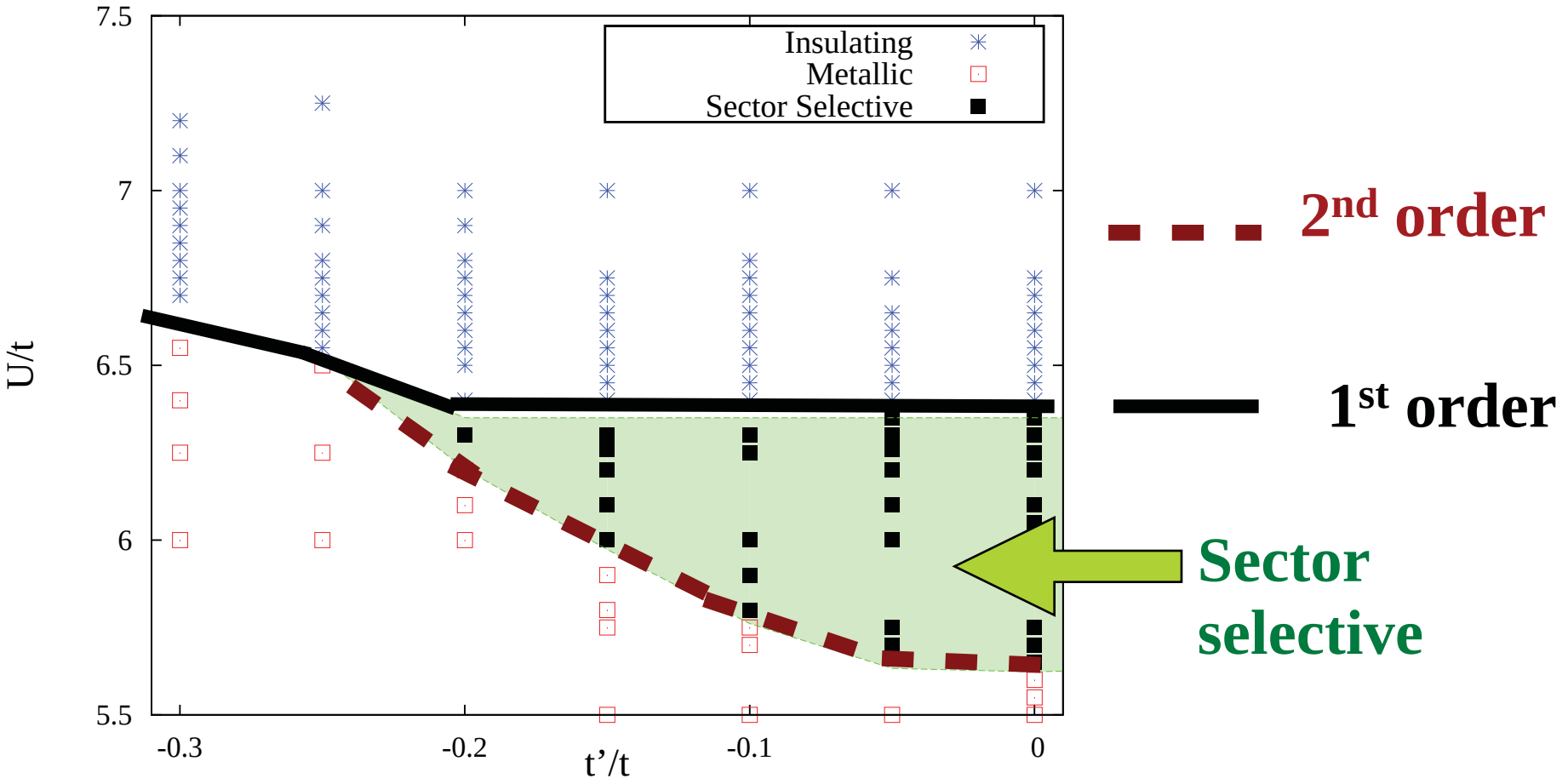
Phase diagram: n=1
(second order nature of transition confirmed down to T=t/60)



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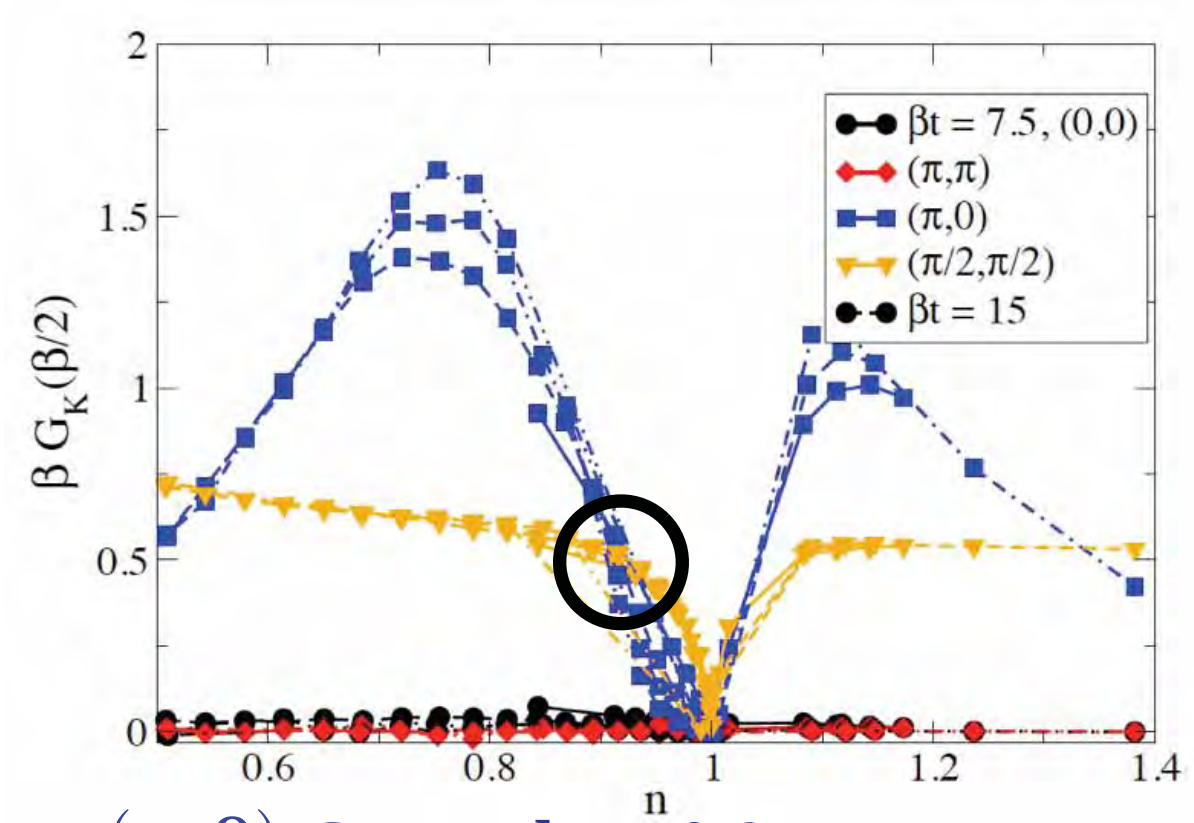
Doping driven transition: U=7t, t'=-0.15t



$(\pi, 0)$ **Gapped, n>0.9**

$(\frac{\pi}{2}, \frac{\pi}{2})$ **Ungapped until (perhaps) lowest doping**

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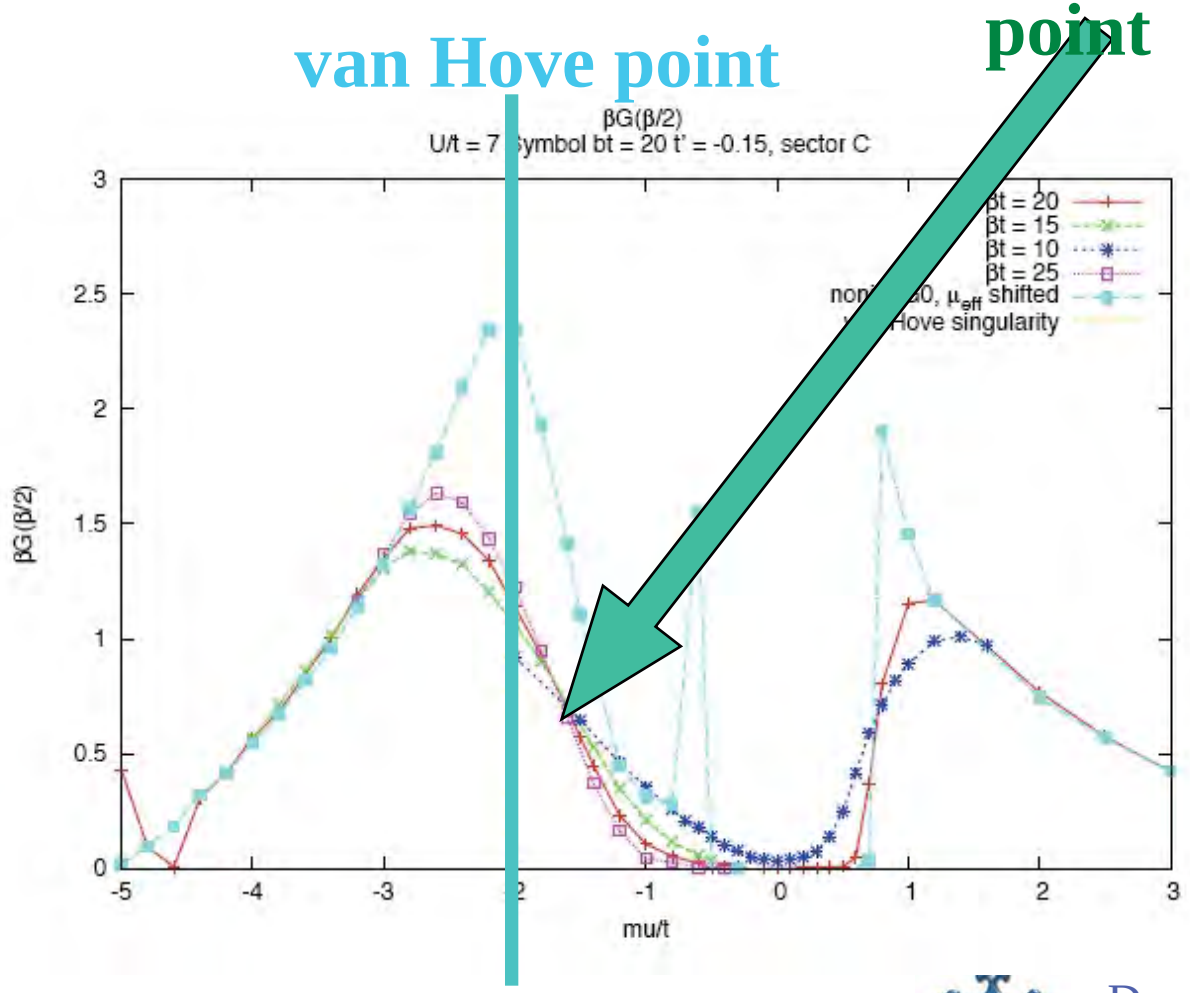
Transition not controlled by van Hove physics



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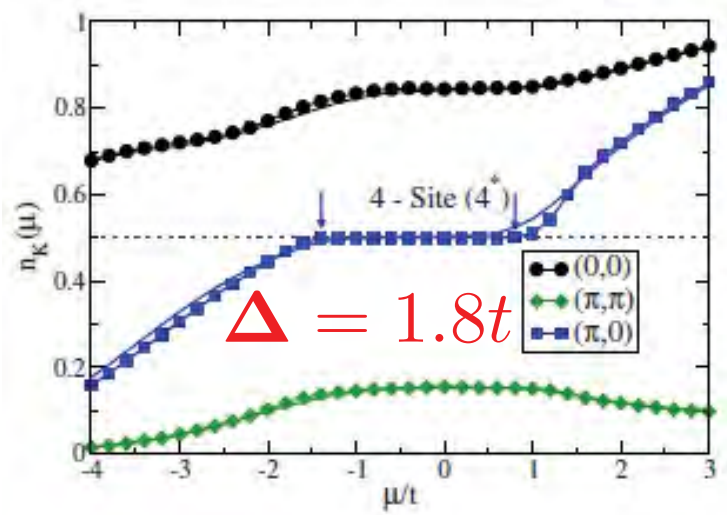
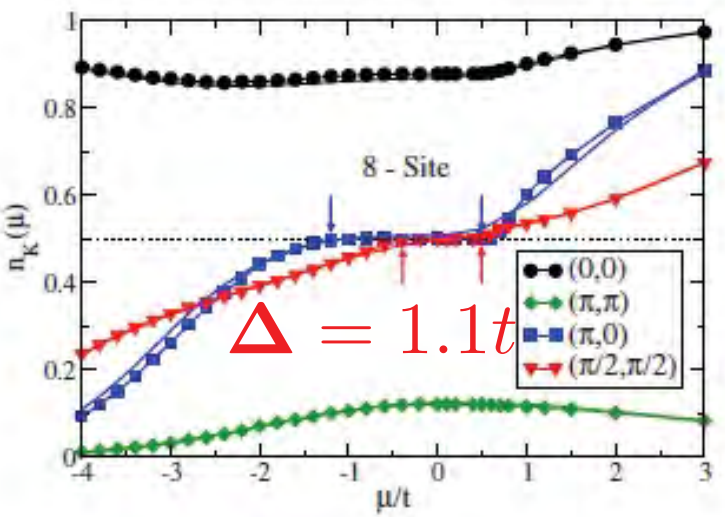
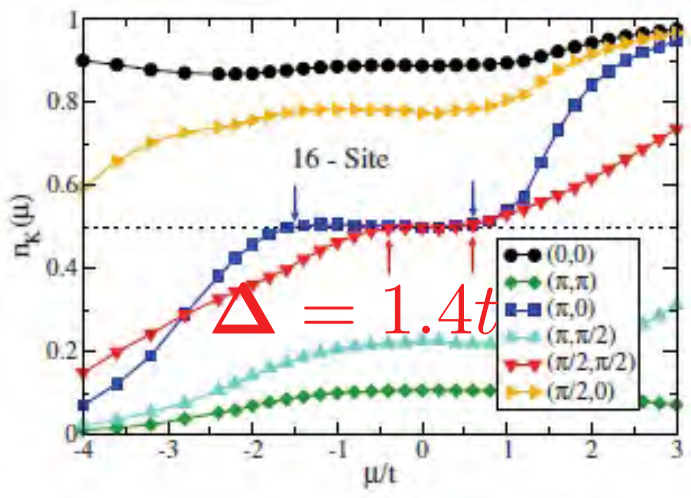
Momentum sector occupancy vs chemical potential







All sizes: n=1=>gap (different in different momenta) =>paramagnetic (Mott) insulator, reasonable estimate of gap~1.4t

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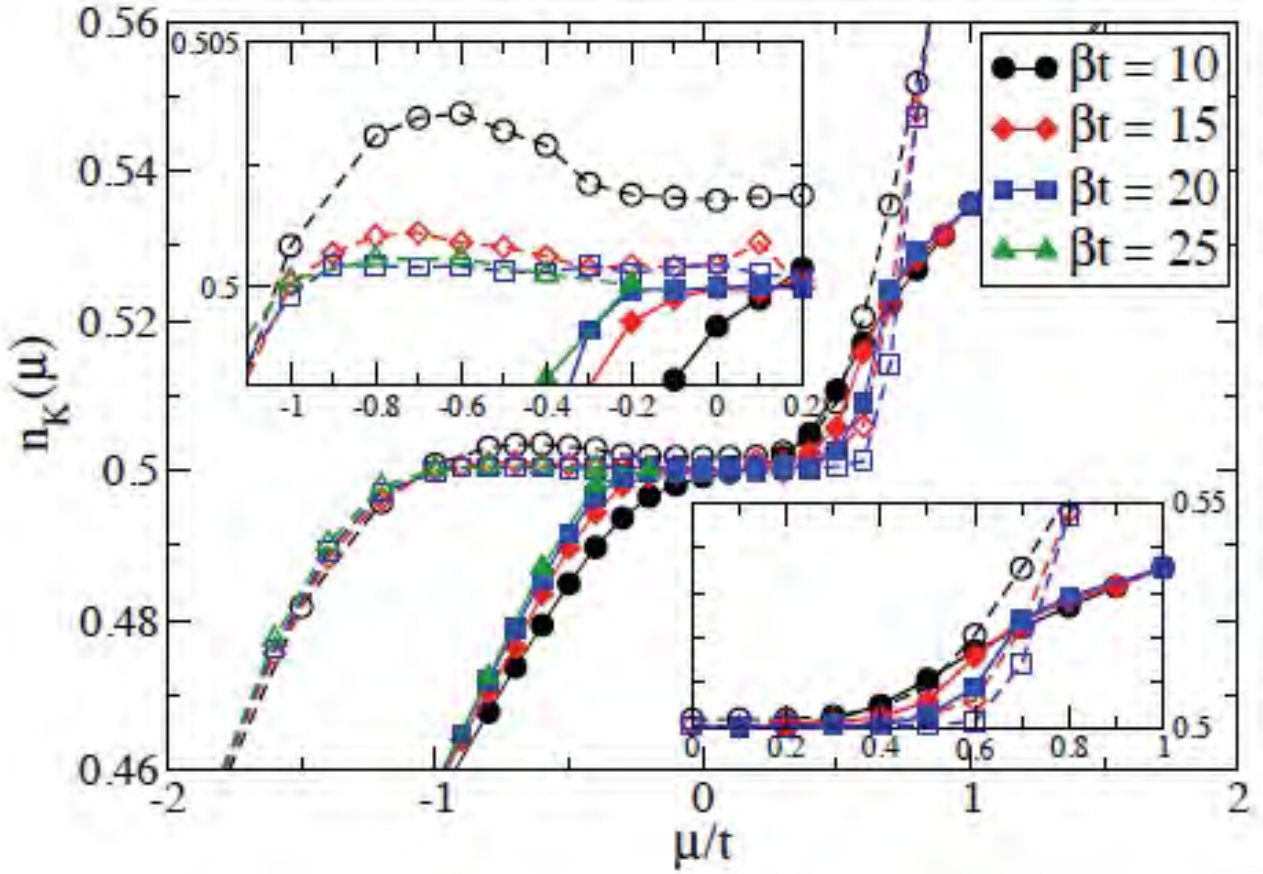
Density per sector vs chemical potential
U=7t, t'=-0.15t



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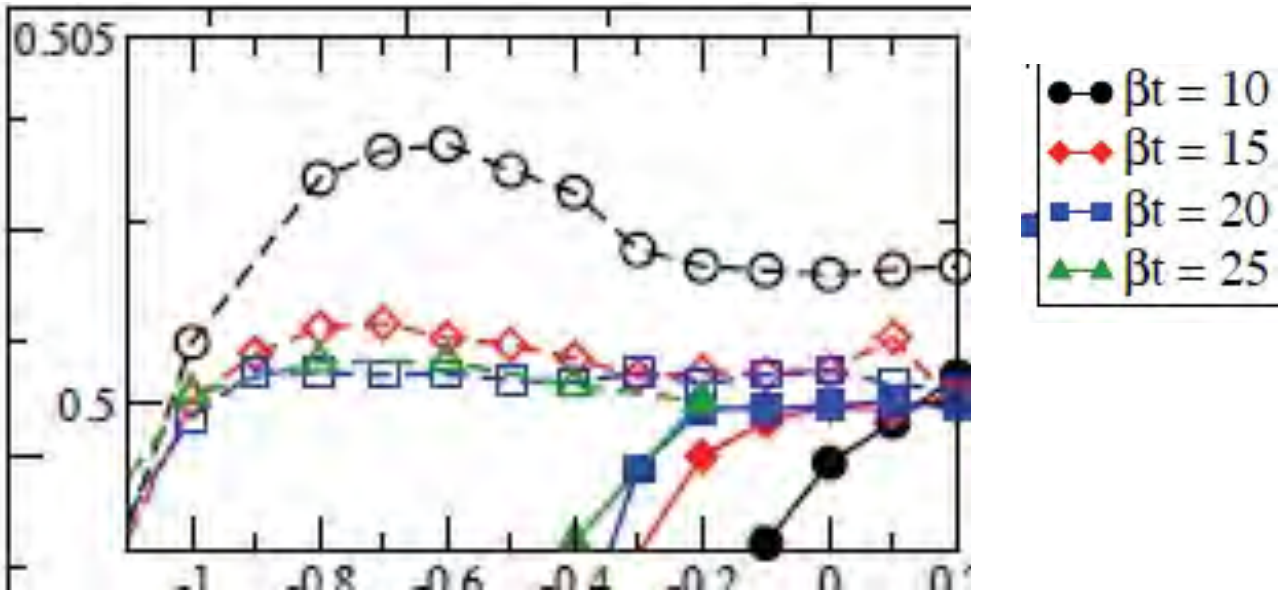
Blow-up



Sector-selective transition<=>pinning of sector density to half filling
=>Mott-like transition

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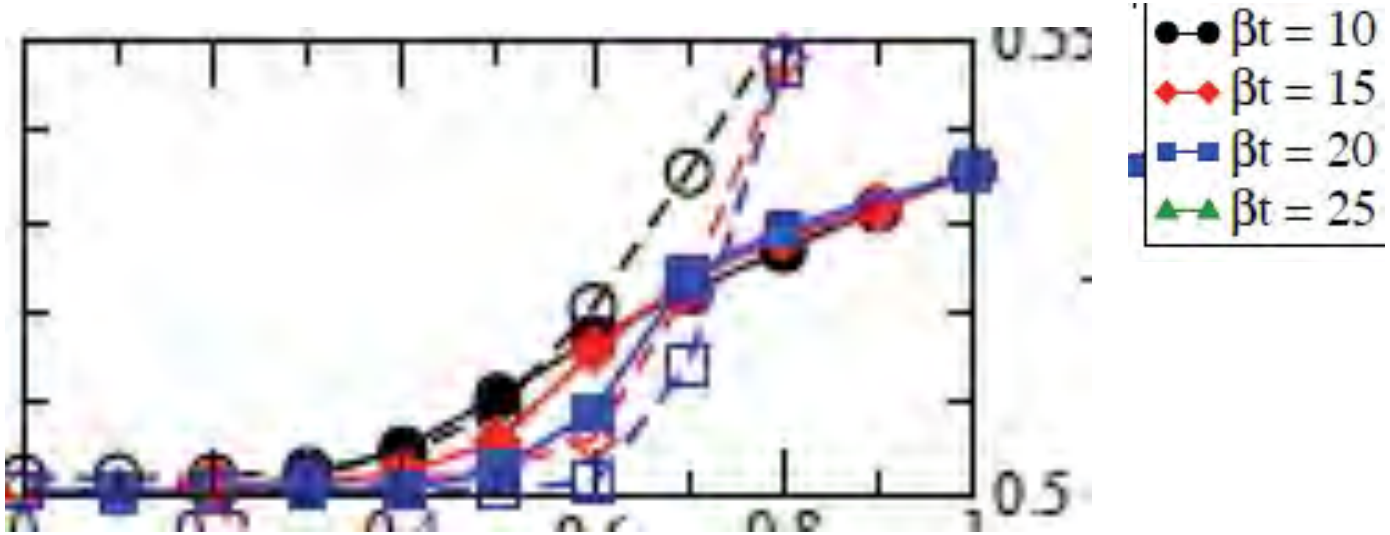
Blow-up: electron-doped side



Doping transition (weakly) first order

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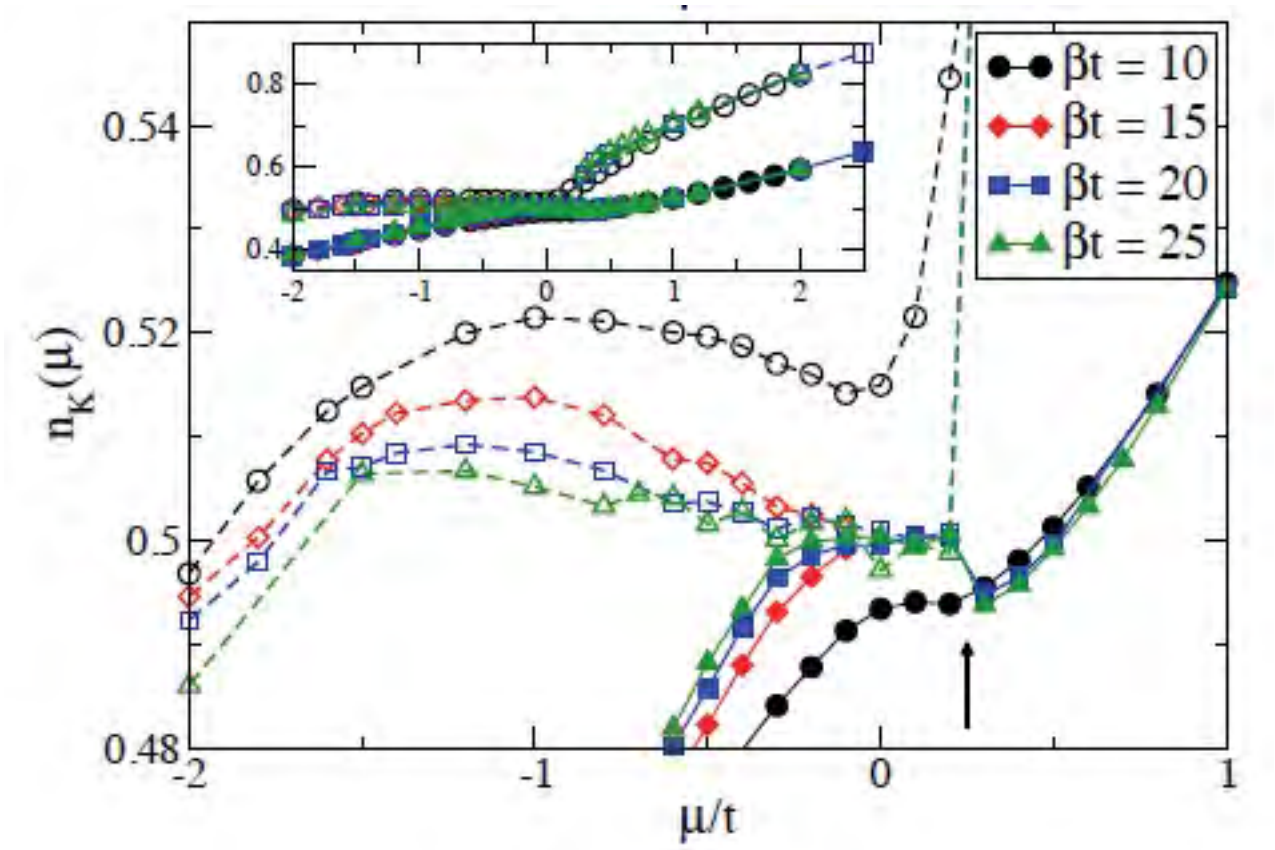
t'=-0.3t



e-doping: transition strongly first order

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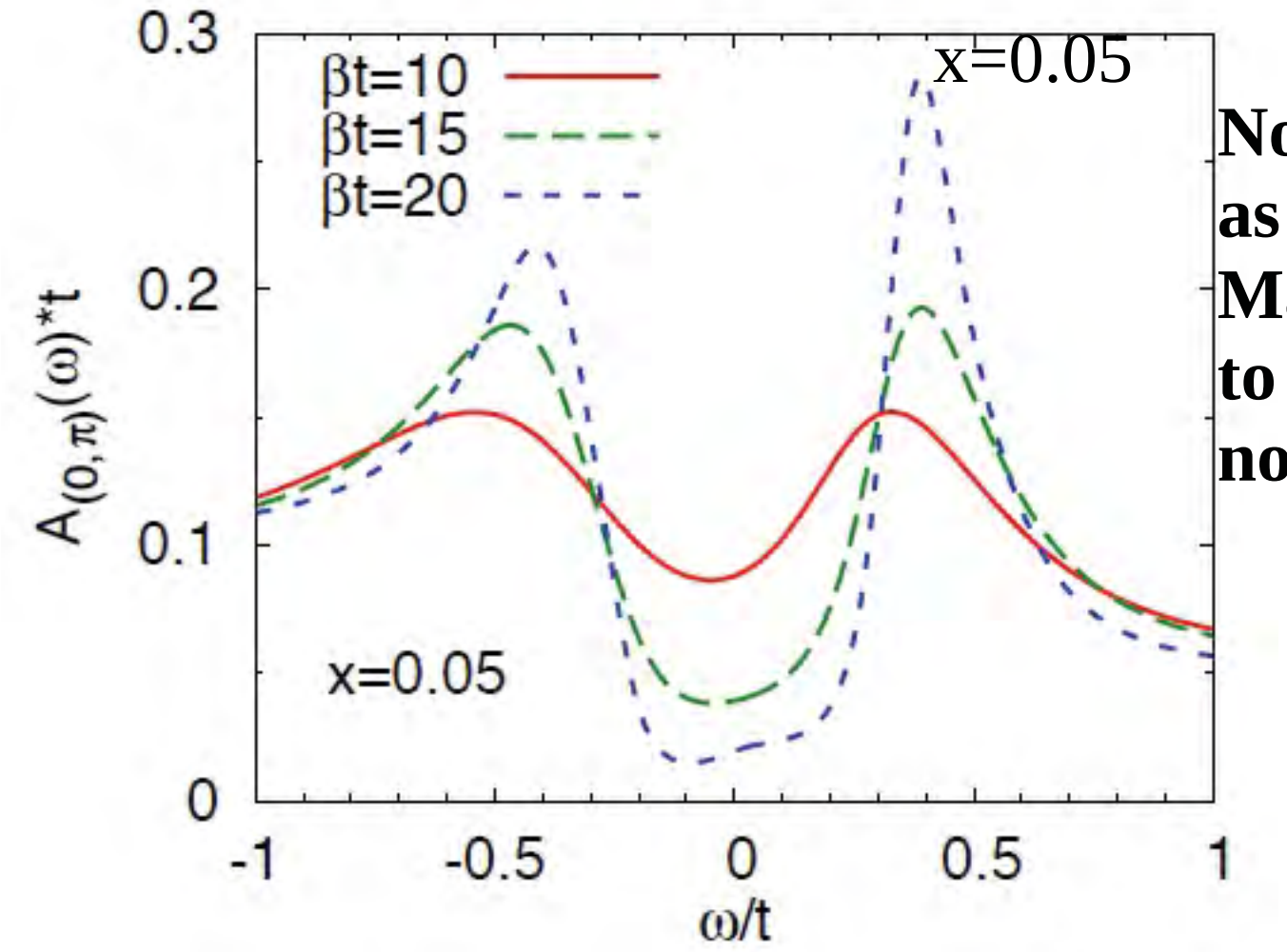
Closer look at the pseudo--or is it real--gap: maximum entropy analytical continuation



Note: gap 'fills in' as T increases. Magnitude (peak to peak distance) not changed much

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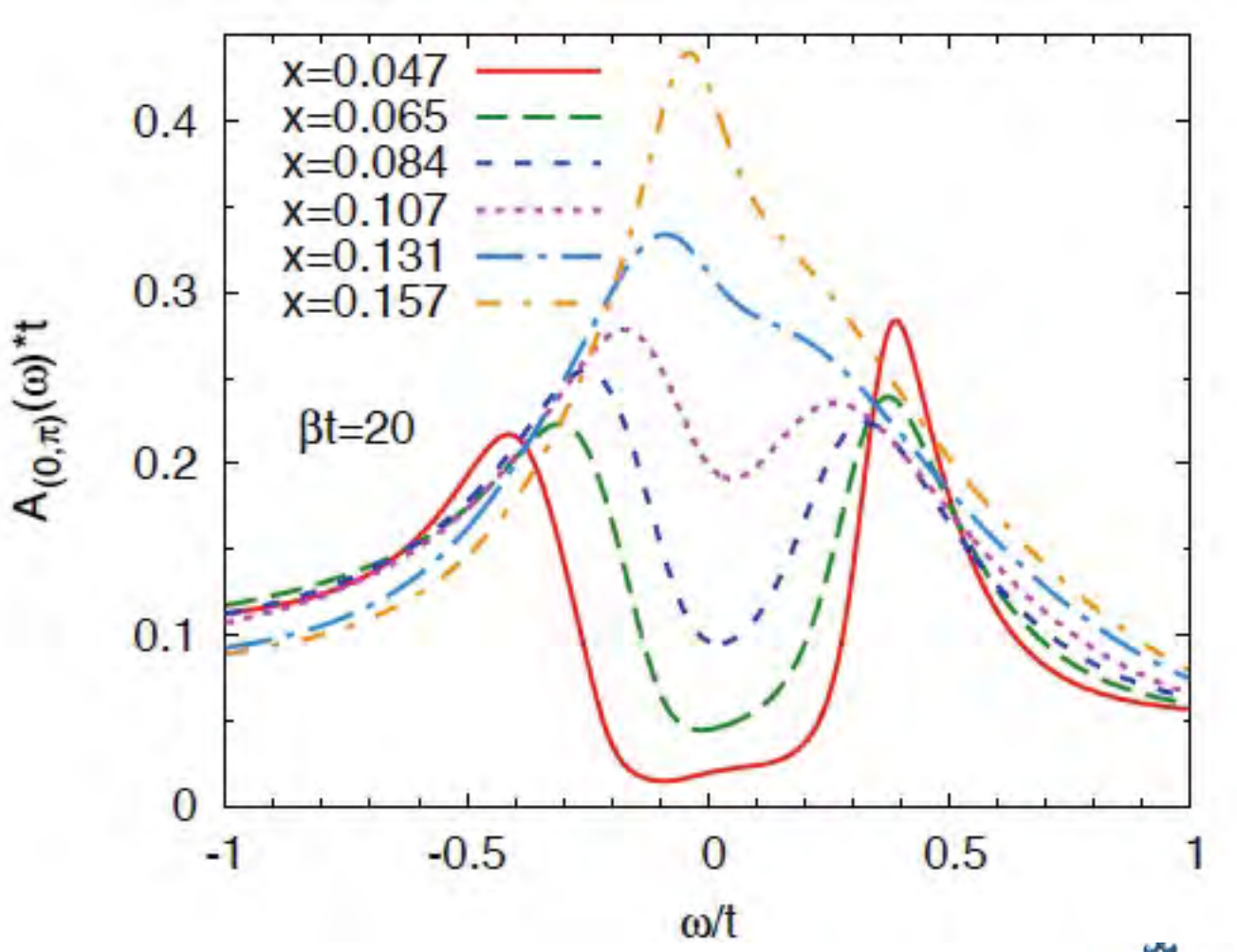
Doping dependence



Gap decreases with increasing doping--but has filled in, not closed at x~0.11 boundary of sector selective phase

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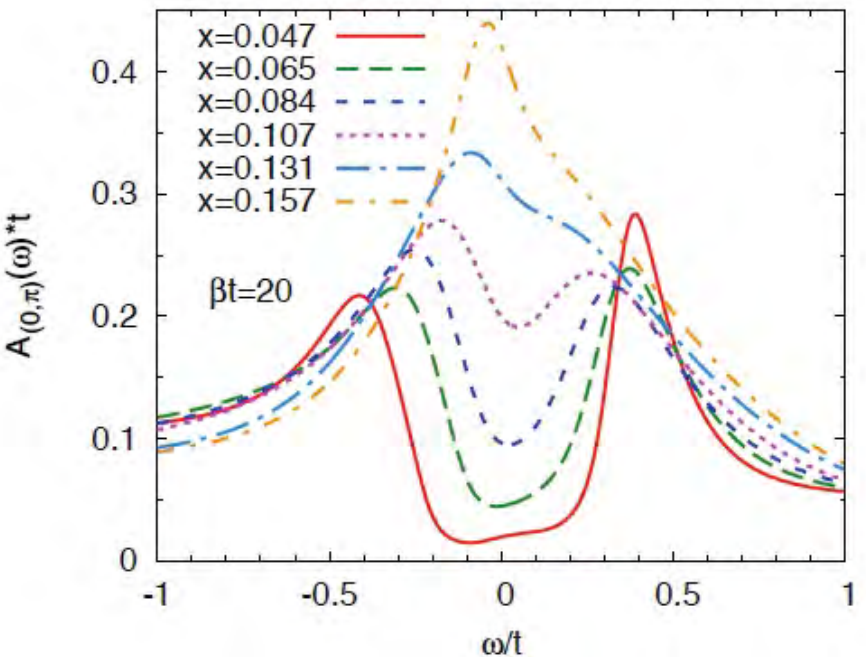
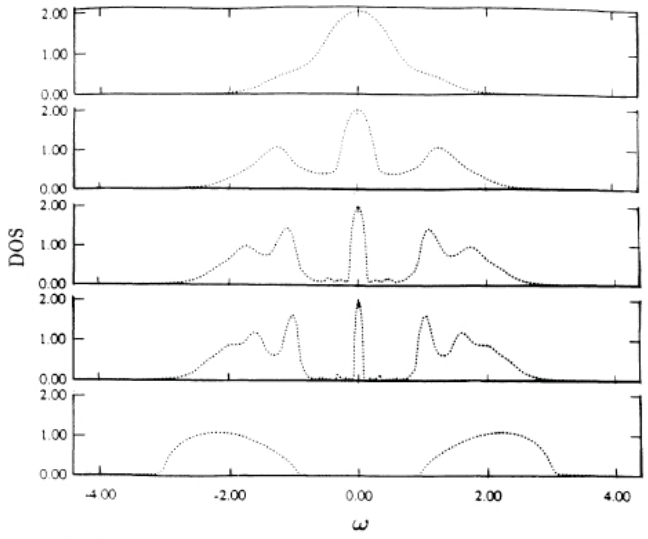
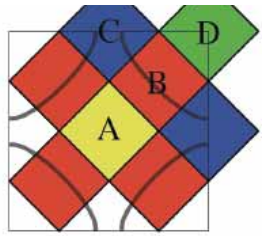
Doping driven transtion:

No sign of 2 pole structure







N. Lin, E. Gull, AJM arXiv:1004.2999

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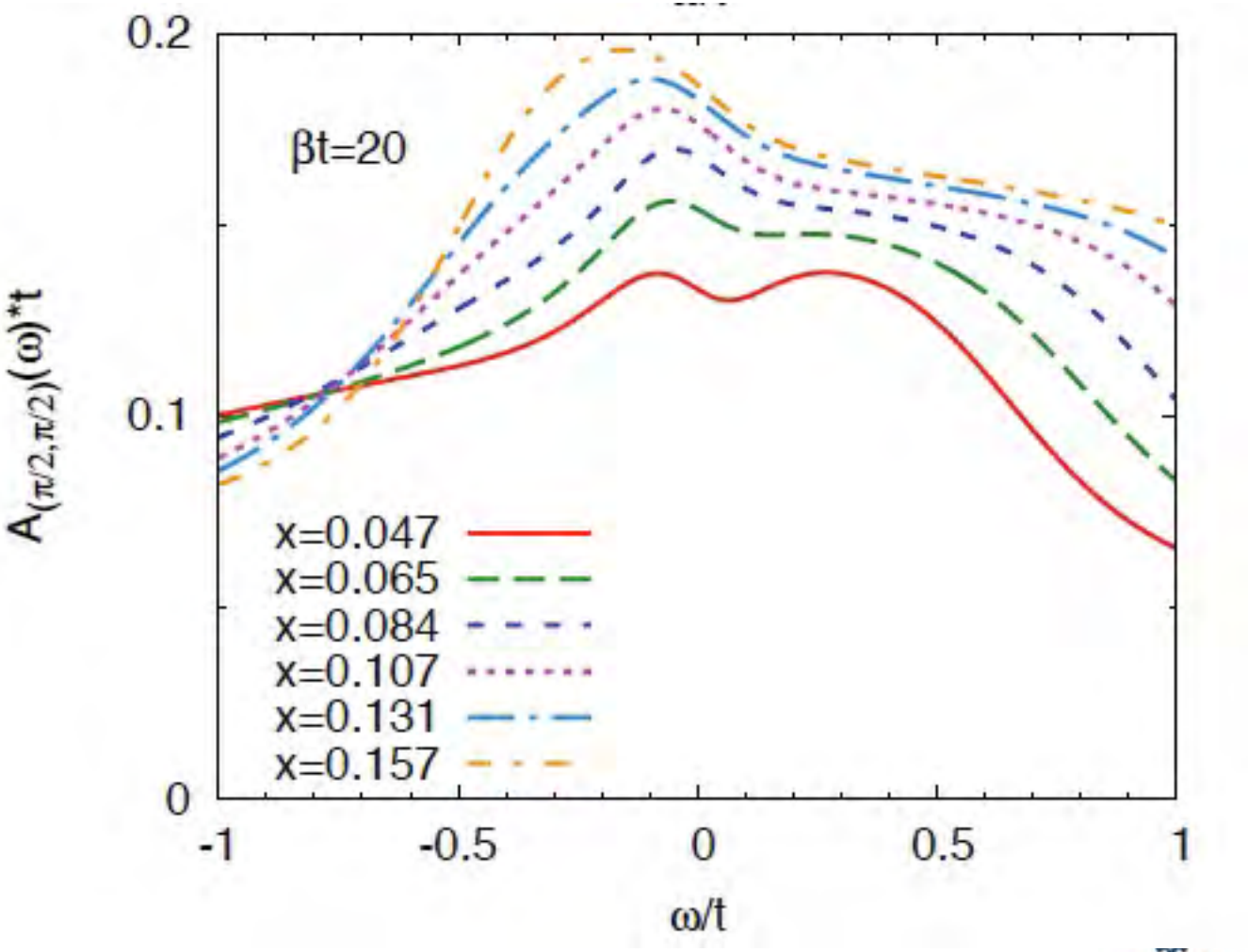
Zone diagonal sector



Possibly hint of gap at lowest dopings, but otherwise no gap

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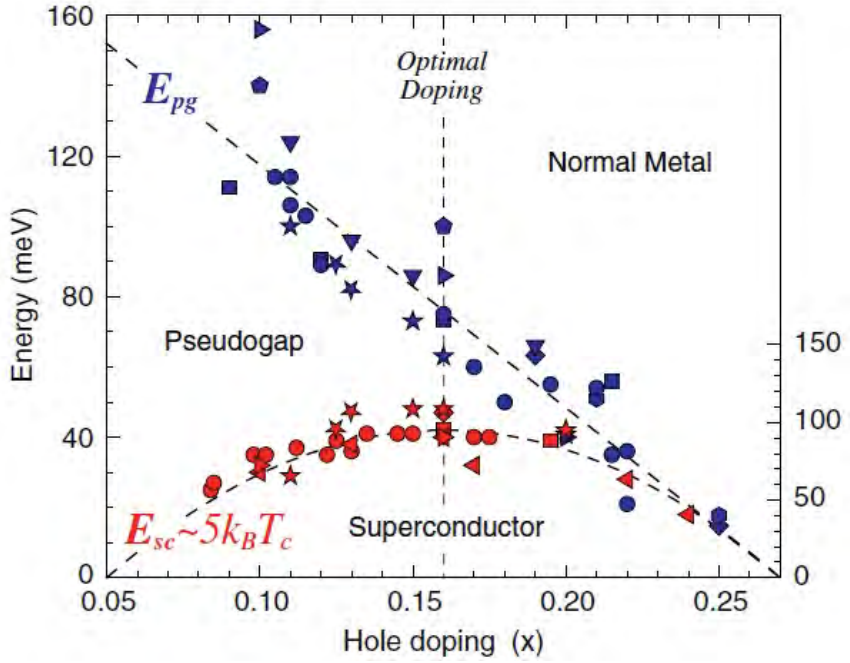
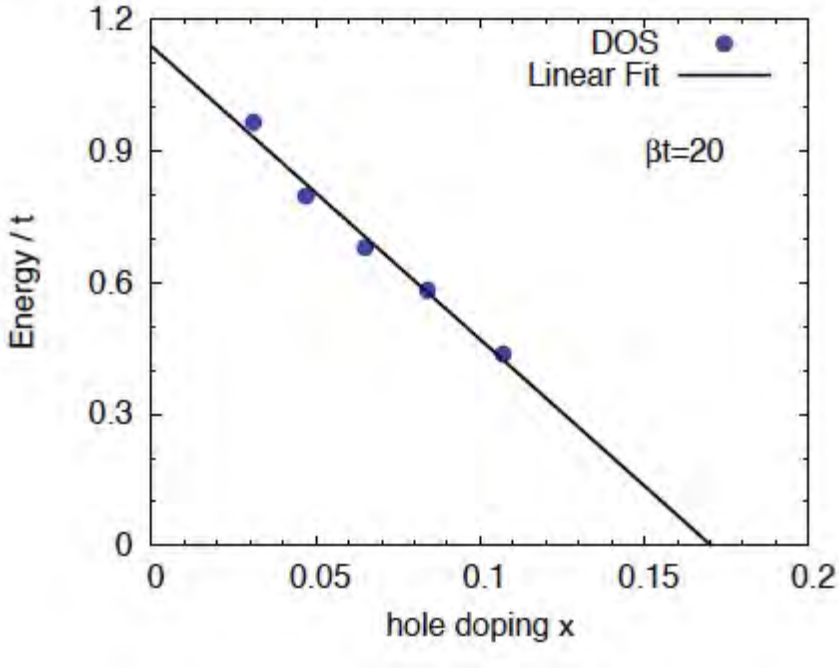
Summary of gap size

Compilation of data



Calculation (t=300meV)



Huefner et al Rep. Prog. Phys. 71 062501 (2008)

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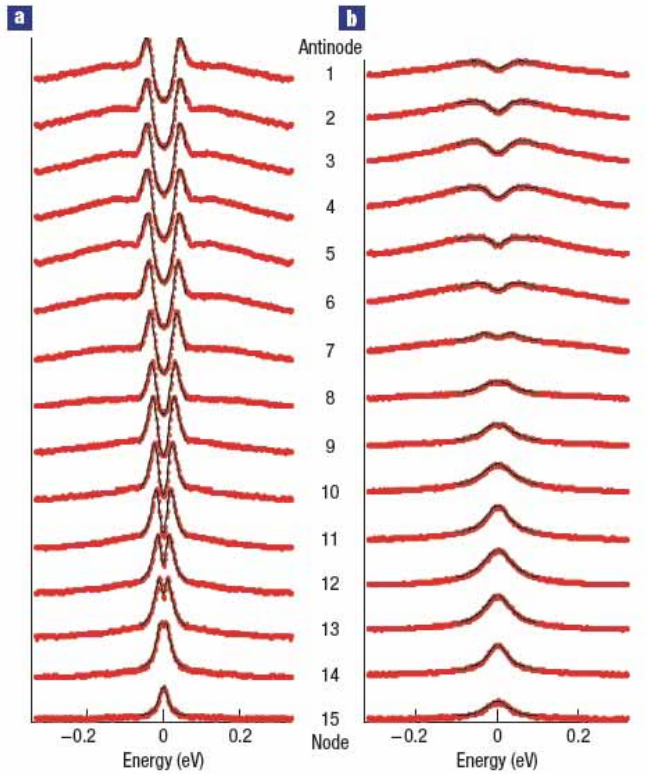
Pseudogap and zone diagonal velocity

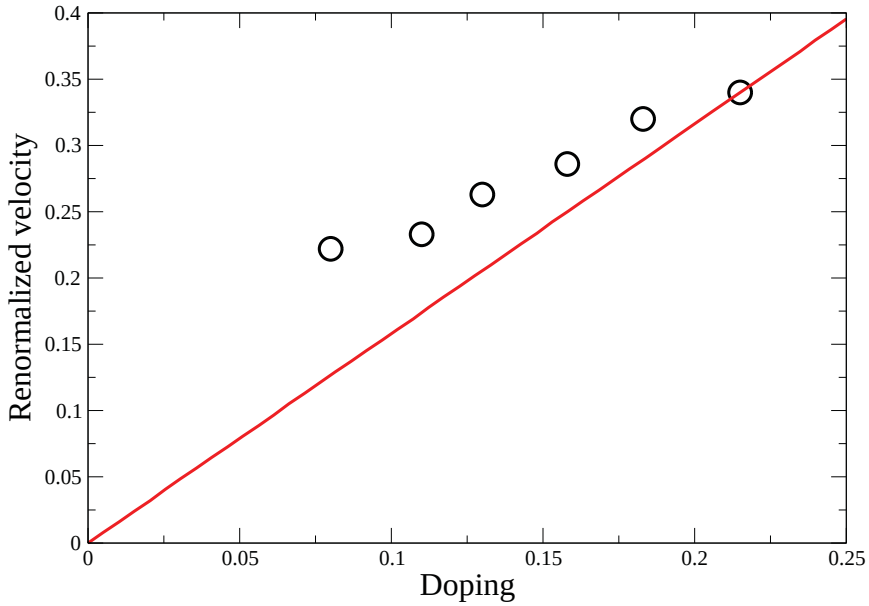
'Normal state gap' for states near 0,Pi

$T=40K<T_c$ $T=140K>T_c$



Kanigel et al, Nat. Phys 2 447 2006

Zone diagonal velocity NOT ~ doping



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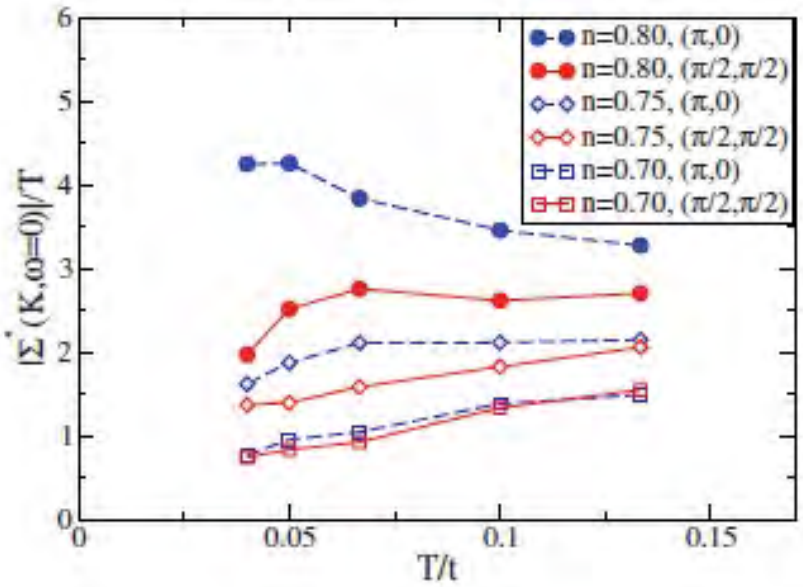
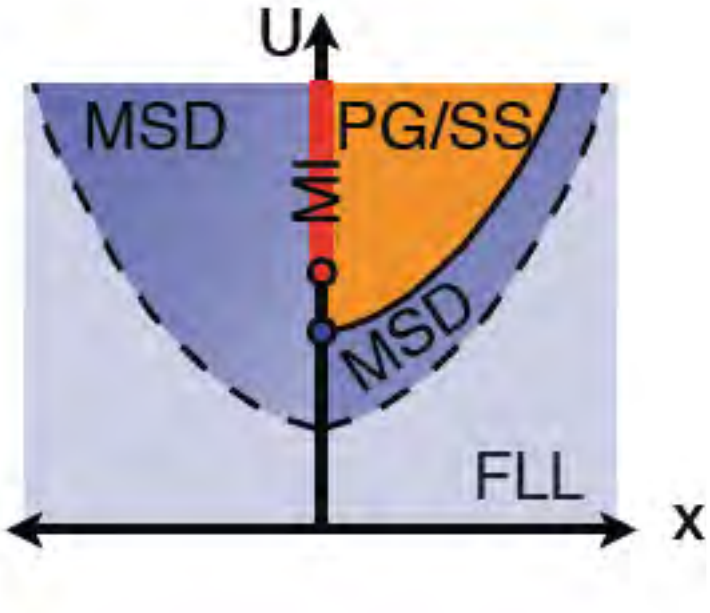
Higher doping: electron scattering rate divided by T





High doping: isotropic scattering
Intermediate doping: anisotropy in magnitude, T-dep

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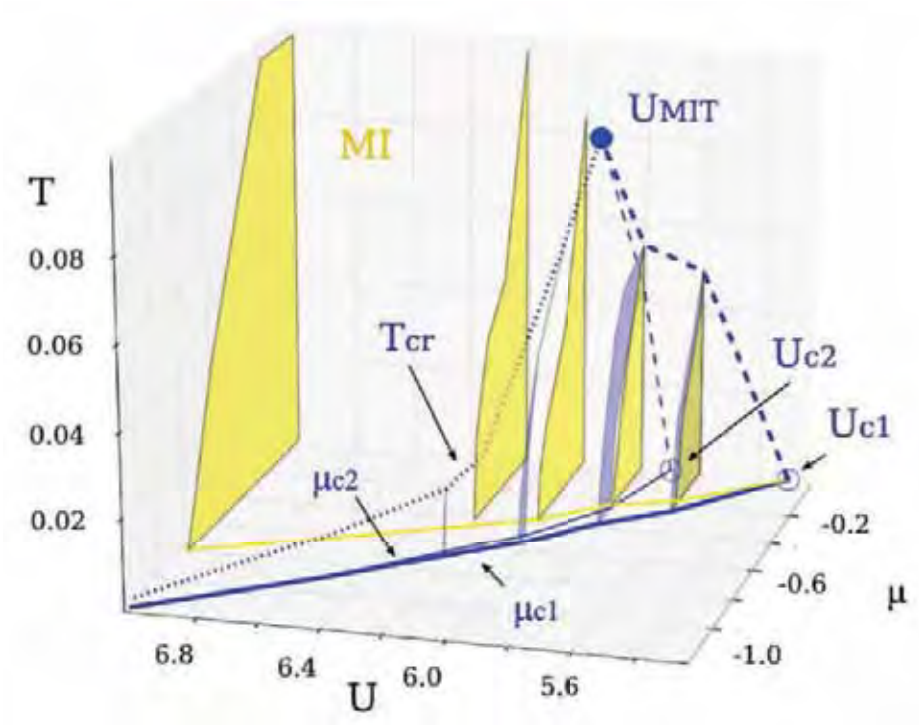
4 site cluster is different



Single first order metal-insulator transition at half filling.

First order line extends out in doping. Again only 1 transition (or crossover).

Sordi et al, PRL and PRB

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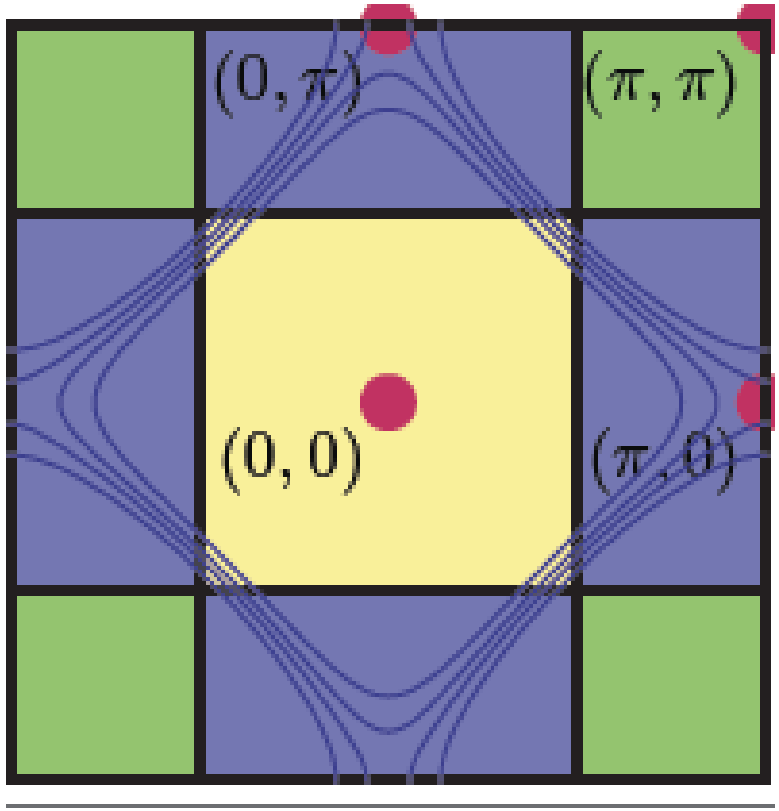
Standard 4-site cluster: fermi surface almost entirely contained in one sector



Sector selective transition is suppressed

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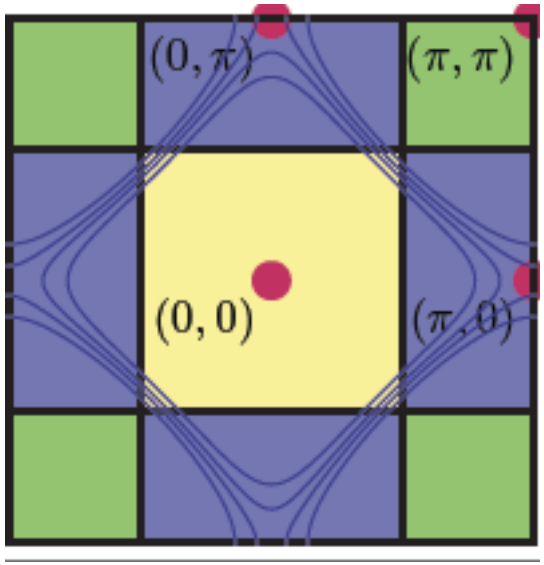
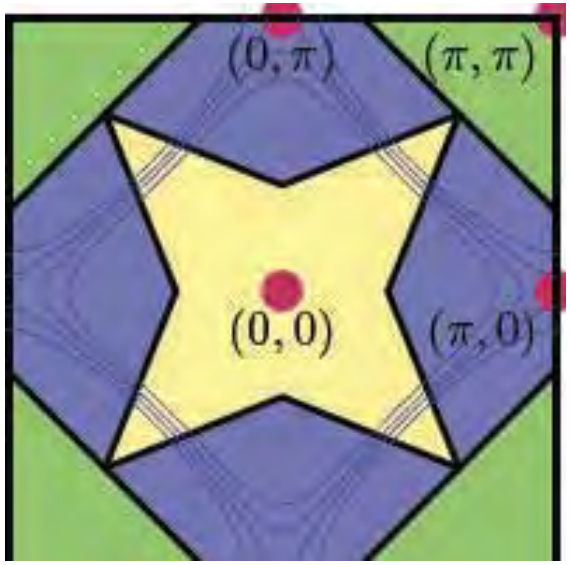
Georges/Ferrero alternative tiling

4



4*



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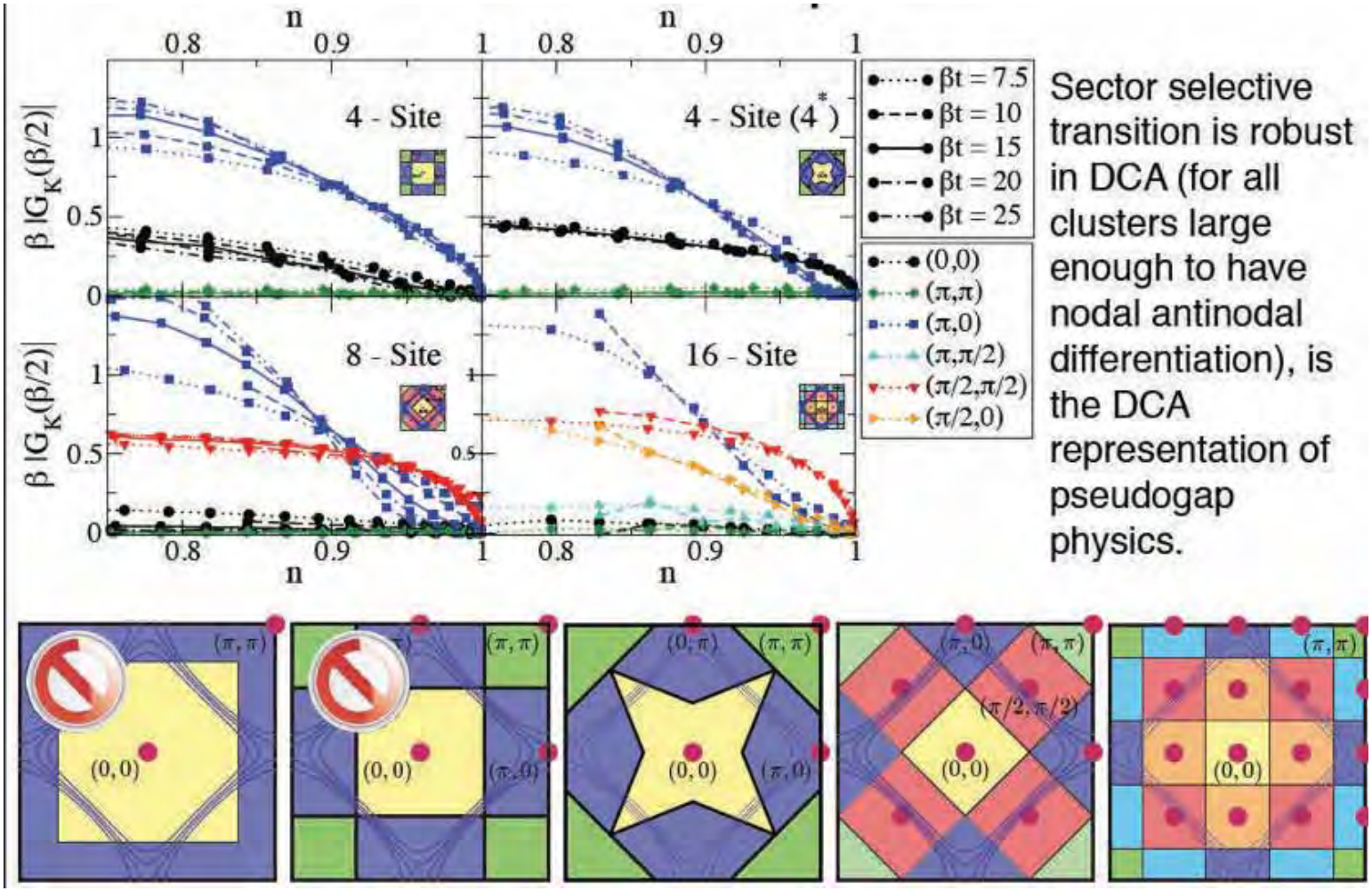
4* has the transition



Sector selective transition is robust in DCA (for all clusters large enough to have nodal antinodal differentiation), is the DCA representation of pseudogap physics.

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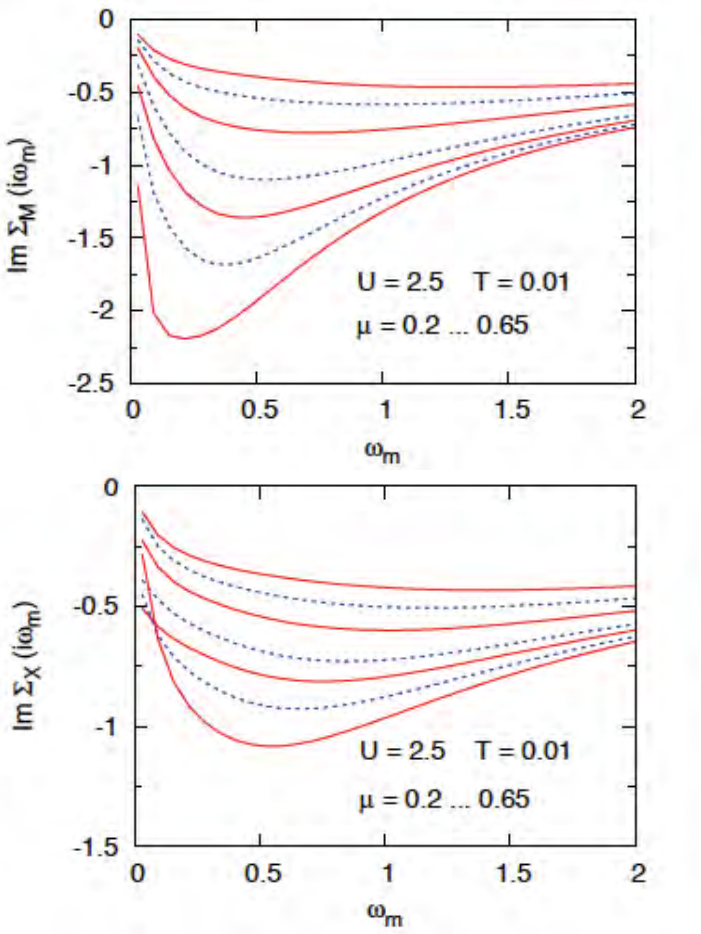
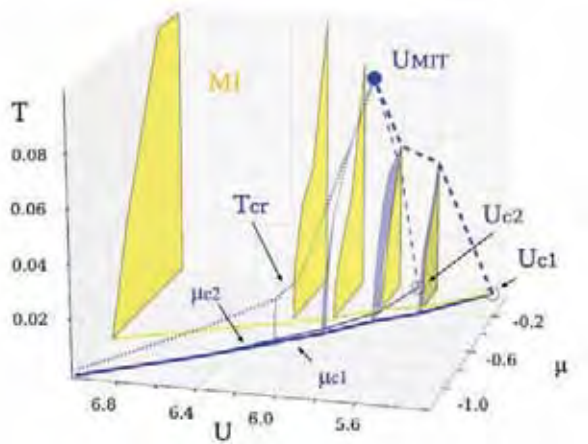
Standard 4-site cluster: captures much of physics despite lack of transition

Liebsch and Tong, 09

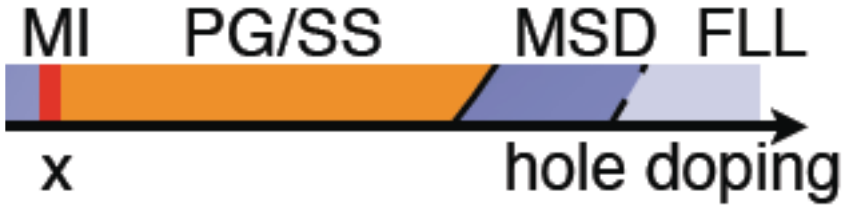


$\delta = 0.24,\ 0.18,\ 0.12,\ 0.08,\ 0.05,\ 0.03,\ 0.01$

Sordi 11



Onset of anisotropic scattering, suppression of DOS at x~0.15.



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Summary:

Present limits:
--Hubbard models (local, density-density interaction).

--Constrained by sign problem. Generic points in phase diagram, surveys of parameters: 8 sites, T>60. 16 sites: larger T.

--*Properly interpreted*, lots of information in small clusters

--Large cluster studies=> Hubbard model at moderate correlations--reasonable description of high Tc

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Extensions

Hubbard model:

--Multparticle response functions.

--superconductivity

--longer ranged interactions

--perturbative inclusion of other physics

Richer models??--probably need to go beyond CT-QMC

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2 particle response: Theory

Observable in presence of pertubation P:

$$\langle \mathrm{O} \rangle = \mathrm{Tr}\left[\hat{\mathrm{O}}(\mathrm{t})\mathrm{G}(\mathrm{t};\mathrm{P})\right]$$

Hamiltonian:

$$\mathrm{H}[\mathrm{P}] = \hat{\mathrm{T}} + \hat{\mathrm{I}} + \mathrm{P}\hat{\mathrm{O}}_{\mathrm{P}}$$

Unperturbed H

Perturbation

$$\text{Expand } \mathrm{G} = \left(\omega\hat{1} - \hat{\mathrm{T}} - \mathrm{P}\hat{\mathrm{O}}_{\mathrm{P}} - \hat{\Sigma}(\mathrm{P})\right)^{-1}$$

$$\text{to linear order in P}$$

$$\text{Vertex function } \Gamma = \frac{\delta\Sigma}{\delta\mathrm{P}}$$

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Formally

Expand $\mathbf{G} = \left(\omega\hat{\mathbf{1}} - \hat{\mathbf{T}} - \mathbf{P}\hat{\mathbf{O}}_{\mathbf{P}} - \hat{\mathbf{\Sigma}}(\mathbf{P})\right)^{-1}$
to linear order in P

response function $\chi = \chi_{\mathbf{bubble}} + \chi_{\mathbf{vertex}}$

$$\chi_{\mathbf{bubble}} = \mathbf{Tr}\left[\hat{\mathbf{O}}\mathbf{G}\hat{\mathbf{O}}_{\mathbf{P}}\mathbf{G}\right]$$

$$\chi_{\mathbf{vertex}} = \mathbf{Tr}\left[\hat{\mathbf{O}}\mathbf{G}\frac{\delta\mathbf{\Sigma}}{\delta\mathbf{P}}\mathbf{G}\right]$$

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Find (reducible) vertex from linearized DMFT equations

Presence of perturbation=>impurity model changes

$$\mathbf{S} = \mathbf{S_{int}} + \mathbf{T}\sum_{\omega}\left(\mathcal{G}_{\mathbf{0}}^{-\mathbf{1}}\right)_{\mathbf{eq}}(\omega)\mathbf{c}(\omega)\mathbf{c}^{\dagger}(\omega) + \mathbf{T^2}\sum_{\omega\omega'}\left(\mathcal{G}_{\mathbf{0}}^{-\mathbf{1}}\right)^{\mathbf{1}}(\omega',\omega)\mathbf{c}(\omega)\mathbf{c}^{\dagger}(\omega')$$

=>first order change in G_{QI}

$$G_{\alpha\alpha}(\omega,\omega') = G^{eq}(\omega)\beta\delta_{\omega\omega'} + G^{eq}(\omega)\beta\delta_{\omega\omega'}T\sum_{\omega_1}G^{eq}(\omega_1)\left(\mathcal{G}_0^{-1}\right)^{1}(\omega_1\omega_1) - T^2\sum_{\omega_1\omega_2,\gamma}\Gamma_{\alpha,\alpha,\gamma,\gamma}(\omega,\omega',\omega_1,\omega_2)\left(\mathcal{G}_0^{-1}\right)^{1}_{\gamma,\gamma}(\omega_2,\omega_1)$$

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Must measure reducible 4 point functions of the impurity model

$$\mathbf{\Gamma}_{\alpha,\alpha,\gamma,\gamma}(\omega+\mathbf{\Omega},\omega,\omega_{\mathbf{1}}-\mathbf{\Omega},\omega_{\mathbf{1}}) = \left\langle \mathbf{c}_{\alpha}(\omega+\mathbf{\Omega})\mathbf{c}^{\dagger}_{\alpha}(\omega')\mathbf{c}_{\gamma}(\omega_{\mathbf{1}}-\mathbf{\Omega})\mathbf{c}^{\dagger}_{\gamma}(\omega_{\mathbf{1}})\right\rangle$$

(Need only reducible vertex; can do calc one external frequency at a time)

(Need ~100 Matsubara frequencies in each argument =>compute and store $N^2 10^6$ numbers)

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Combining Eq for $\mathbf{G}^1$ and self consistency Eq. gives linear equation for $\frac{\delta \mathbf{\Sigma}}{\delta \mathbf{P}}$ in terms of $\mathbf{\Gamma}_{\alpha,\alpha,\gamma,\gamma}(\omega + \mathbf{\Omega}, \omega, \omega_1 - \mathbf{\Omega}, \omega_1)$ and

$$\mathbf{P}(\omega, \omega') = \int' (\mathbf{dk}) \mathbf{G}^{\mathrm{eq}}_{\mathrm{lattice}}(\mathbf{k}, \omega) \hat{\mathbf{O}}_{\mathbf{P}} \mathbf{G}^{\mathrm{eq}}_{\mathrm{lattice}}(\mathbf{k}, \omega')$$

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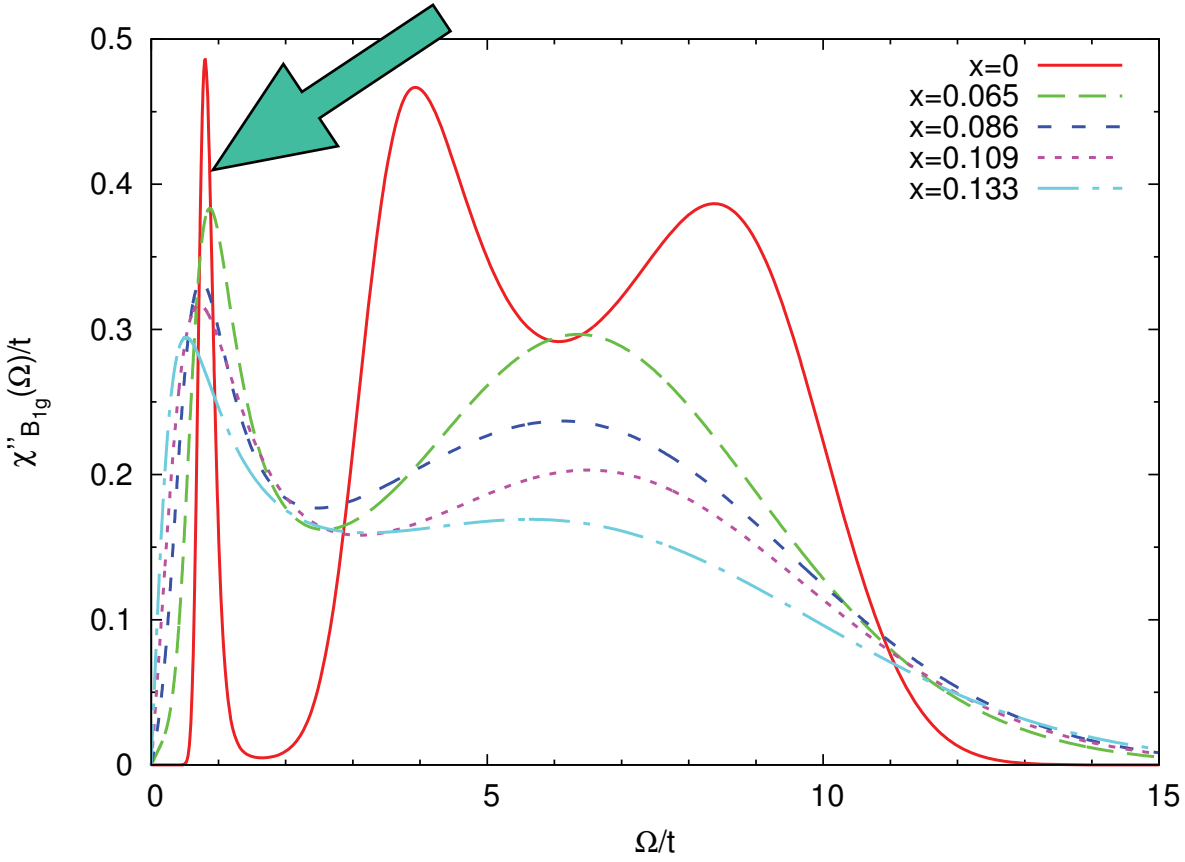
Raman spectra

two magnon peak inside insulating gap



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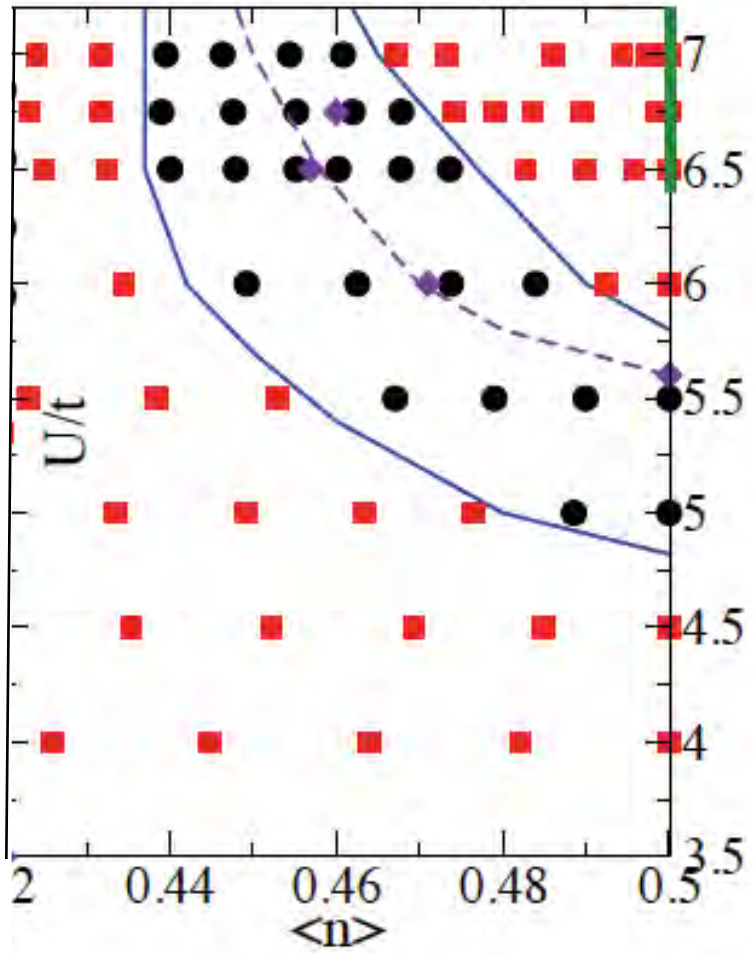
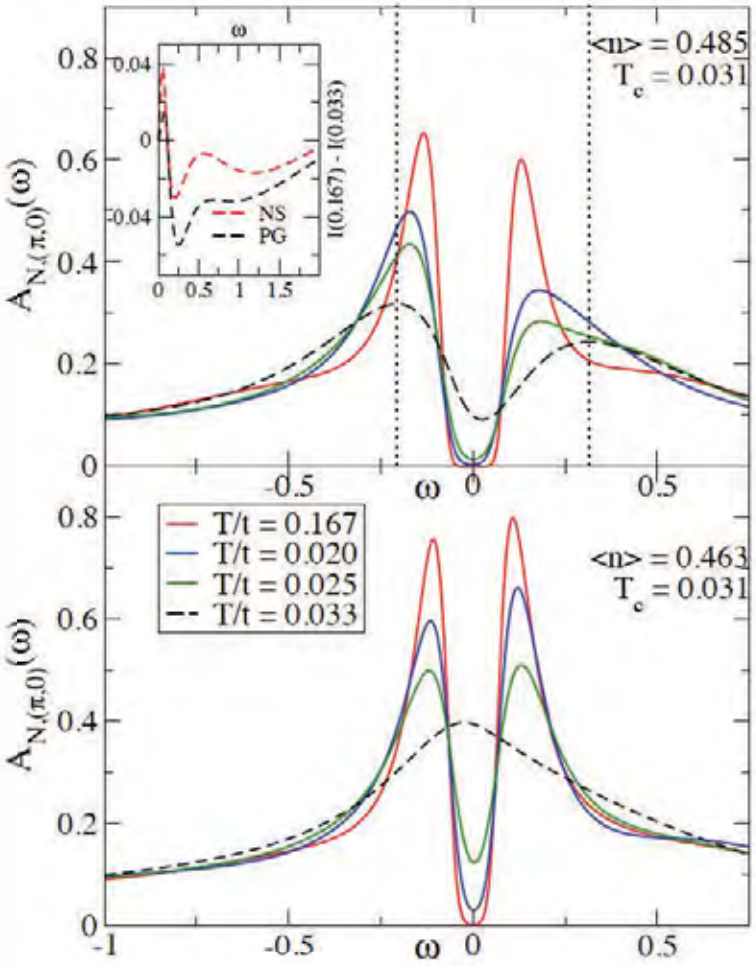
Superconductivity: preliminary results

8 sites; U=7t

Phase diagram



Spectral function



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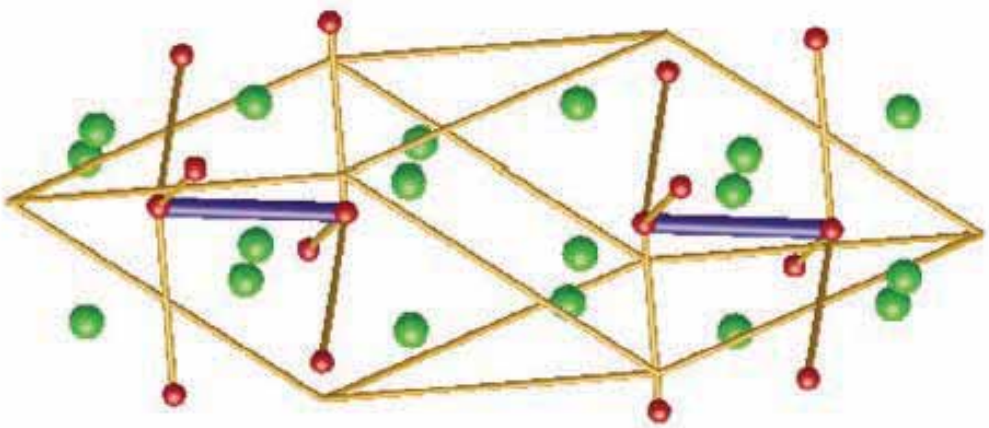
Non-local interactions

Naturally dimerized materials: CDMFT

NaV_2O_5 Mazurenko et al PRB 66 081104 (2002)

Ti_2O_3 Poteryaev et al PRL 93 086401 (2004)

Ti_2O_3



Intersite interaction essential to metal-insulator transition

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Not naturally dimerized: DCA

$$\mathbf{V(k_1, k_2, k_3, k_4) \rightarrow V(K_1, K_2, K_3, K_4)}$$

Hubbard: V indep of K

Longer ranged interactions=> more independent components of V.

Can include in QMC. Mikelsons (prvt comm) says: bad sign problem.

Alternative: treat non-local ints perturbatively

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Summary:

***`Cluster' DMFT: family of approximations--converge to exact result if cluster large enough**

***Requirement: solve N orbital impurity model.**

Text

***So far: can do this well only for Hubard model.**

--Convergence demonstrated

--2d model: pseudogap +sc 'similar to' high Tc

--vertex functions: coming under control

***?Extensions--an important open problem**

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