Dynamical Mean Field Theory for Correlated Electron Physics

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Outline

1. The dynamical electronic structure question
2. From DFT (Density Functional band Theory) to DMFT (Dynamical Mean Field Theory)
3. Application: density fluctuation induced by muon
4. Application: pseudogaps in high Tc
5. Response functions (in process)
6. Where next?

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The dynamical electronic structure problem: Why is it hard?

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We know the Hamiltonian

$$\mathbf{H} = \sum_i \frac{-\nabla_i^2}{2m_e} + \sum_i V_{ext}(r_i) + \frac{1}{2}\sum_{i \neq j} \frac{e^2}{|r_i - r_j|}$$

We know the equation

$$\mathbf{H}\Psi_n = -i\partial_t \Psi_n$$

So stop complaining and solve it (?!)

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Not so fast!

Typical lattice constant: 4 Angstrom

Interesting length ~100 Angstrom

=> ~1000 electrons with 3 (x,y,z) coordinates.
Interaction 'entangles' coordinates=>

Schroedinger equation $\Psi(\vec{r}_1, \ldots.\vec{r}_{1000}\ldots)$ **Intractable**

Even worse: Ψ is fully antisymmetric function of spins and coordinates

``Fermion sign problem"

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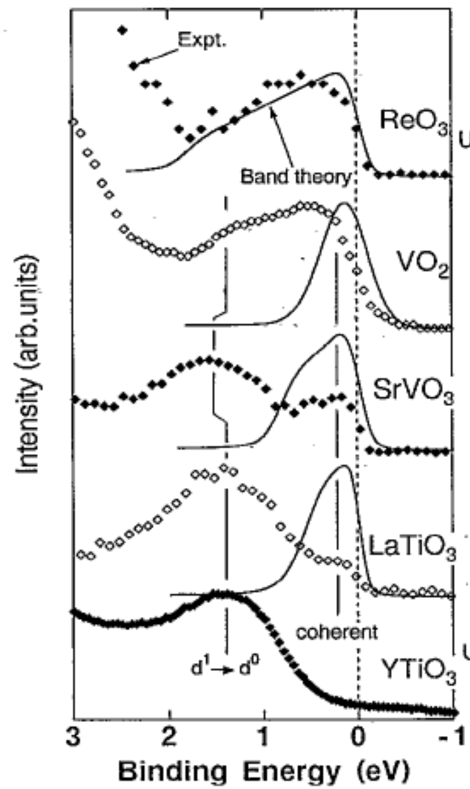
Perturbation theory (e.g. LDA+GW) inadequate in many cases

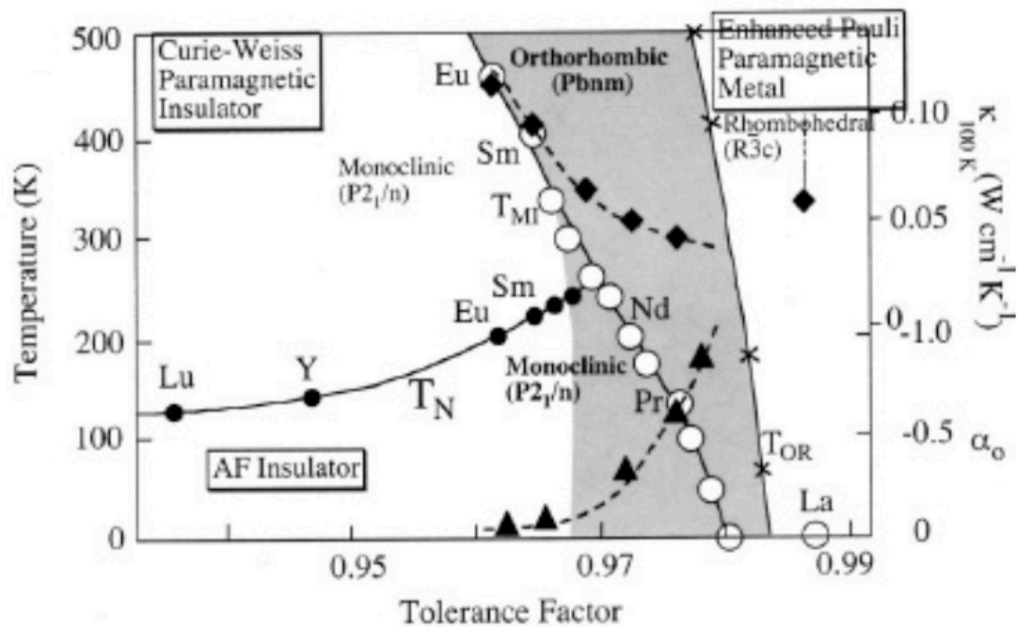
Excitation spectra



Fujiimori et al PRL 69

Phase Diagrams

ReNiO$_3$



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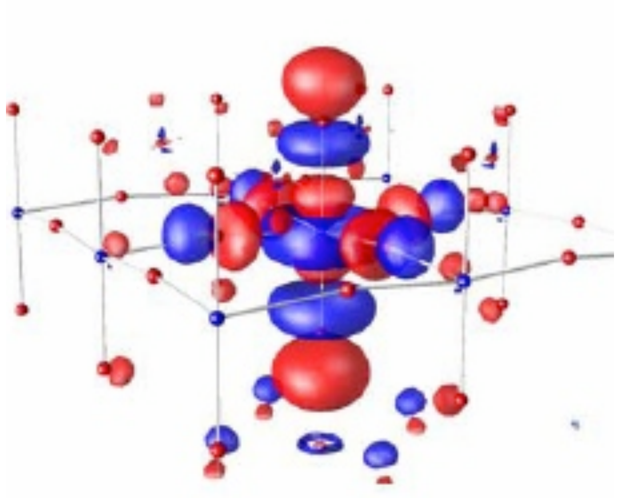
Model system:
'active subspace': correlated orbitals to be treated by refined technique
'passive' subspace: mean field theory

Representation of Wannier function for $LaNiO_3$



OK Andersen http://online.kitp.ucsb.edu/online/materials10/andersen/

=>Model system: matrix elements of Hamiltonian in restricted basis

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

Here: 1 band model

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BUT this is still not enough

N sites, P orbitals per site =>

Dimension of Hilbert space: 4^{NP}

Direct diagonalization: in general becomes impossible before reach large enough system

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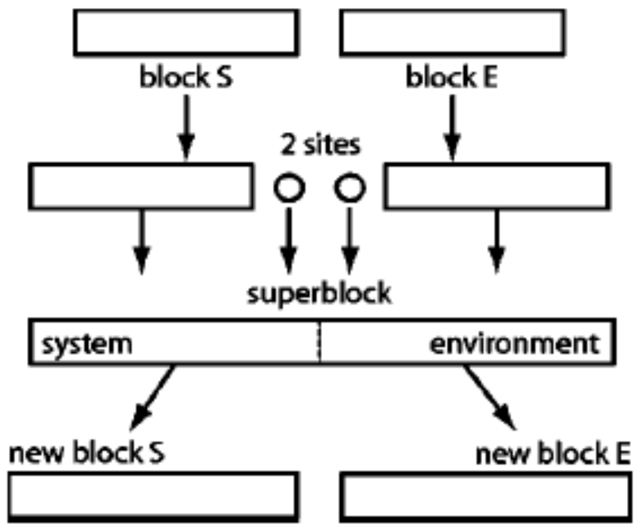
‘Indirect diagonalization’: density matrix renormalization group



U. Schollwoeck, RMP77 259

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

Method of choice for 1d model system problems

Becoming important tool in quantum chemistry

Interesting connections to quantum information theory

But: still cant do d>1

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Alternative: Stochastic (Monte-Carlo) exploration of configuration space

To estimate expectation value of some quantity A

$$\langle A \rangle_p = \frac{1}{Z} \int_C d\mathbf{x} \mathcal{A}(\mathbf{x}) p(\mathbf{x})$$

Here
Z=partition function
x=some configuration
p(x): contribution of x to partition function

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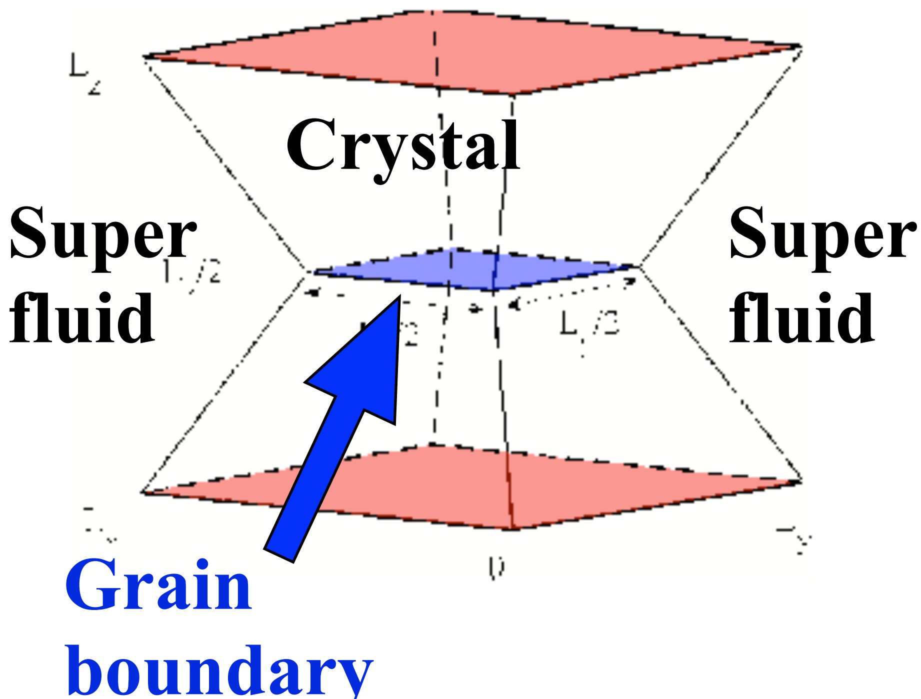
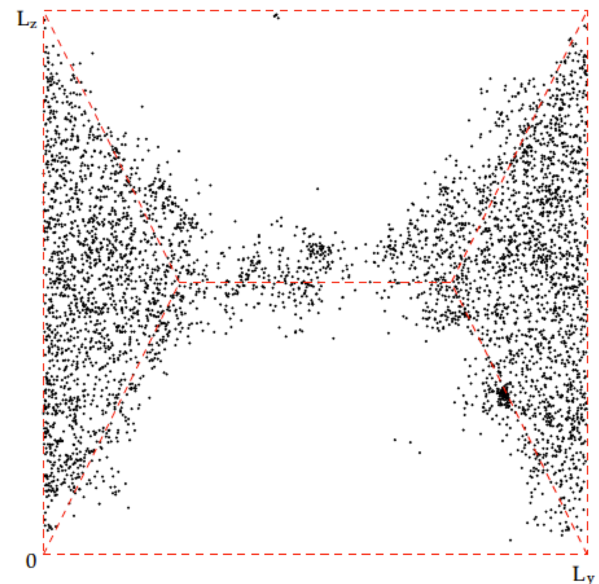
Method of choice for (unfrustrated) boson problems

Superfluidity of grain boundaries in solid He4



Density of points ~ condensate fraction



Pollett, Troyer et al 2007

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BUT for fermions

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

Sample $$\langle A \rangle_p = \frac{1}{Z}\int_C d\mathbf{x}\mathcal{A}(\mathbf{x})p(\mathbf{x})$$

using $\rho(x) = |p(x)|$

$$\langle \mathbf{A} \rangle_\mathbf{p} = \frac{\langle \mathbf{A}\ \mathbf{sign}[\mathbf{p}] \rangle_\rho}{\langle \mathbf{sign}[\mathbf{p}] \rangle_\rho} = \frac{\frac{1}{\mathbf{Z}}\int_\mathbf{C} \mathbf{dx}\mathbf{A}(\mathbf{x})\ \mathbf{sign}[\mathbf{p}(\mathbf{x})]|\mathbf{p}(\mathbf{x})|}{\frac{1}{\mathbf{Z}}\int_\mathbf{C} \mathbf{dx}\ \mathbf{sign}[\mathbf{p}(\mathbf{x})]|\mathbf{p}(\mathbf{x})|}$$

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

$$\langle sign \rangle = Z = e^{-\frac{F_{fermion}}{T}}$$

Partition function of fermion system

|p(x)|: weight of configuration of ``boson" system

$$|p(x)| \sim Exp[-\frac{F_{\text{``}boson''}}{T}]$$ **with** $\mathbf{F}_{\text{``}\mathbf{boson}''} < \mathbf{F}_{\mathbf{fermion}}$

$$\langle \mathbf{sign} \rangle = \frac{\mathbf{Z}}{\mathbf{Z}_{\rho}} = \mathbf{Exp}\left[-\left(\frac{\mathbf{F}_{\mathbf{fermion}} - \mathbf{F}_{\mathbf{boson}}}{\mathbf{T}}\right)\right]$$

Vanishes exponentially as T->0 or system size-> infinity

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

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Because direct approach inadequate,

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

Best known example: density functional theory

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Recall density functional theory

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

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

Kohn and Sham:

Minimize by solving auxiliary (band theory) problem with self-consistently determined potential V_{XC}

V_{XC} found from uncontrolled but apparently reasonable approximation (LDA, GGA, B3LYP....)

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Recent success: parallel development of many body theory

Density functional <=> ‘Luttinger Ward functional

Kohn-Sham equations <=> quantum impurity model

Particle density <=> electron Green function

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Many-body formalism: Luttinger-Ward functional

$$\mathbf{F}[\{\boldsymbol{\Sigma}(\mathbf{p},\omega)\}] = \boldsymbol{\Phi}_{\mathbf{univ}}[\{\boldsymbol{\Sigma}\}] + \mathbf{Tr}\mathbf{ln}\left[\mathbf{G}_{\mathbf{0}}^{-1} - \boldsymbol{\Sigma}\right]$$

G_0: Green function of noninteracting reference problem (contains lattice potential)

Φ_{univ}: sum of all vacuum to vacuum diagrams. 'Universal': Depends only on band structure and interactions

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

Stationarity: Dyson equation

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For almost 40 years, situation analogous to density functional theory after Hohenberg-Kohn paper

F_{univ} not known except perturbatively

No way known to carry out minimization

Kotliar and Georges found analogue of Kohn-Sham result: ‘uncontrolled’ approximation for F and way to carry out minimization via auxiliary problem

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Approximate the space dependence of self energy in terms of frequency-independent basis functions

$$\Sigma_p(\omega) \rightarrow \Sigma_p^{approx}(\omega) = \sum_a \phi_a(p)\Sigma_a(\omega)$$

Here p is some position coordinate (will be momentum in much of what follows)

Different choices of basis function $\phi_a(p)$=> different "flavors" of DMFT (1-site, DCA, CDMFT....).

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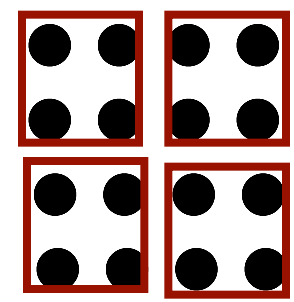
CDMFT: real space approach

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

Tile lattice with equal size cells, write Hamiltonian, G as matrix within supercell. Neglect terms in Σ which go outside cell



$$\textbf{Full self energy } \Sigma(i,j,\omega)$$
$$\rightarrow \mathbf{\Sigma}(I,I) \text{ (matrix inside supercell)}$$

$$\mathbf{G}(I,J,\omega) = \left[\omega\mathbf{1} - \mathbf{T}_{I,J} - \mathbf{\Sigma}_{I,I}(\omega)\right]^{-1}$$

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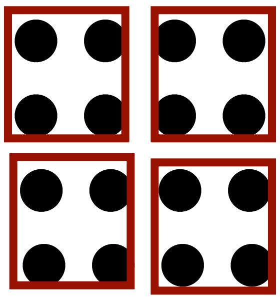
CDMFT breaks translation invariance (unless 'cluster' contains only 1 cell)



Components of Σ within cluster are kept but not components between clusters

treatment of intersite interactions also inconsistent

Discussion in literature of *periodization* (reconstructing periodic function from result of calculation)

see e.g. Tudor D. Stanescu and Gabriel Kotliar Phys. Rev. B **74**, 125110 (2006)

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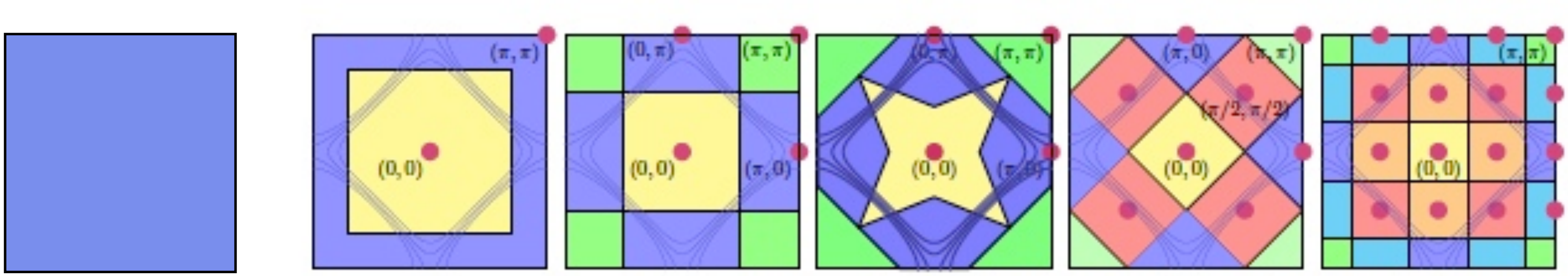
‘DCA’

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

Momentum space approach: tile Brillouin zone
Choose N momenta K_a, draw an equal area patch around each one



1 2 4 4* 8 16

$$\Sigma_p(\omega) \rightarrow \Sigma_p^{approx}(\omega) = \sum_a \phi_a(p)\Sigma_a(\omega)$$

$\phi_a(p) = 1$ **if** p **is in the patch containing** K_a **and is 0 othewise**

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Use approximate form of self energy in Luttinger-Ward function

$$\mathbf{F}[\{\boldsymbol{\Sigma}\}] \rightarrow \mathbf{F}[\{\boldsymbol{\Sigma}^{\mathbf{approx}}\}] \equiv \mathbf{F}^{\mathbf{approx}}[\{\boldsymbol{\Sigma}_{\mathbf{a}}(\omega)\}]$$

is a functional of a finite number of functions $\boldsymbol{\Sigma}_{\mathbf{a}}(\omega)$

$$\mathbf{F}^{\mathbf{approx}}[\{\boldsymbol{\Sigma}_{\mathbf{a}}\}] = \boldsymbol{\Phi}^{\mathbf{approx}}_{\mathbf{univ}}[\{\boldsymbol{\Sigma}_{\mathbf{a}}\}] - \mathbf{Trln}[\mathbf{G}_{\mathbf{0}}^{-1} - \sum_{\mathbf{a}} \phi_{\mathbf{a}}(\mathbf{p})\boldsymbol{\Sigma}_{\mathbf{a}}]$$

Φ^{approx}_{univ} **is a functional of a finite number of functionals of frequency; thus is the universal functional of some 0 space+1 time dimensional quantum field theory and its derivative is a Green function of this model**

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Stationarity

$$-\frac{\delta\Phi_{univ}^{approx}[\{\Sigma_a\}]}{\delta\Sigma_a} = G_a^{QI} = Tr_p\left[\phi_a(p)G_{lattice}(\Sigma^{approx})\right]$$

Thus, a la Kohn-Sham: determine approximation to self energy of full lattice problem from solution of auxiliary problem and self consistency condition. Dont evaluate directly: define model from self consistency condition and solve.

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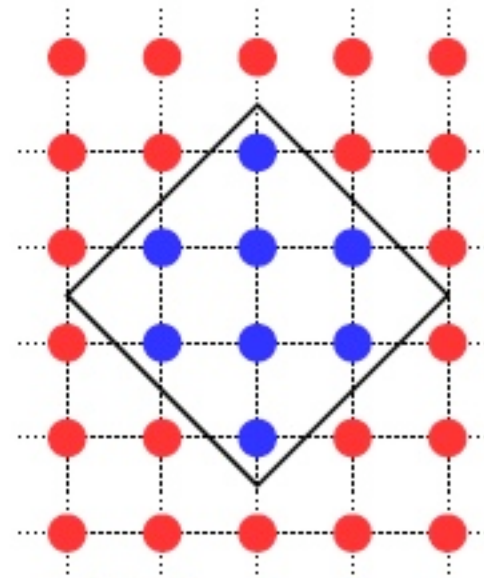
Useful to view auxiliary problem as 'quantum impurity model' (cluster of sites coupled to noninteracting bath)



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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Technical challenge: “impurity solver”

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

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

Until recently, could only be done, inefficently for simplest models (‘Hirsh-Fye’ QMC)

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 p. 349 (2011)**

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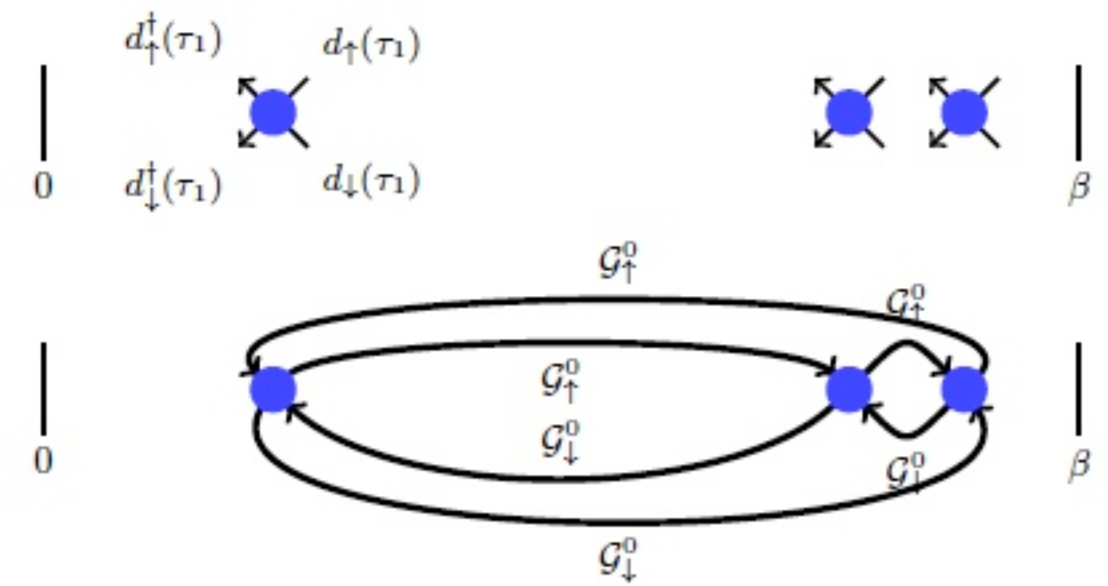
CT-INT: sample interaction perturbation diagram series stochastically



Vertex <=> particle
Propagator <=> interparticle interaction

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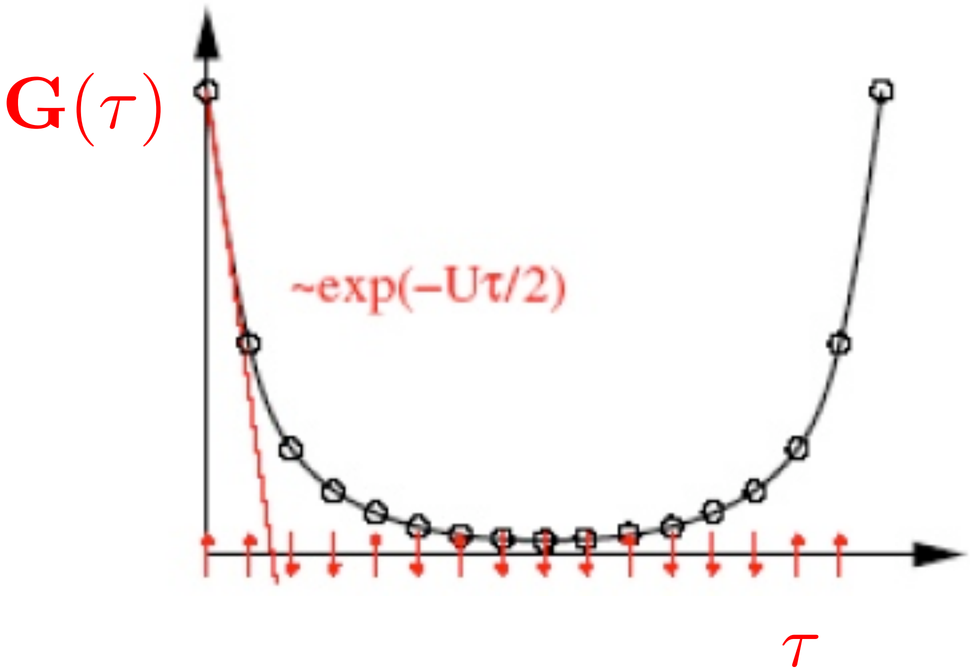
Method works in continuous time

Previously used methods needed time discretization =>difficulty representing behavior of Green function at small times. CT-QMC: many-body adaptive grid



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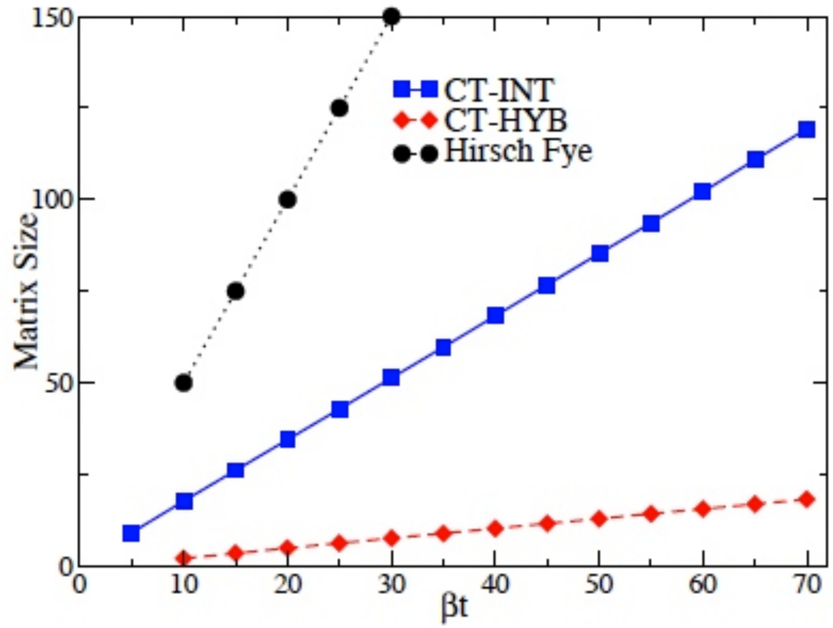
Consequence

All methods involve manipulating matrices.

Cost ~ cube of typical matrix size.

In new approaches: much smaller matrix is needed



Improved efficiency=> surveys (of doping, temp) and study of larger clusters possible

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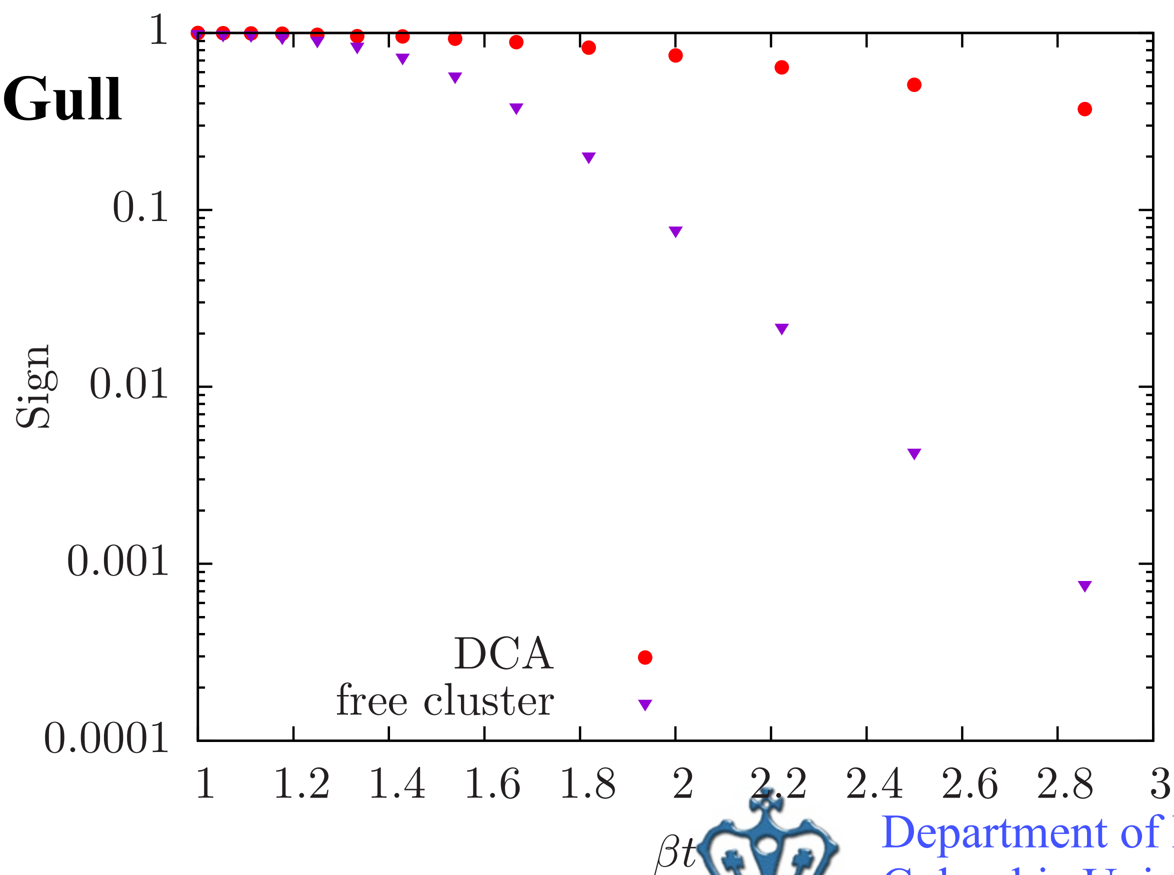
Second advantage:
SIGN PROBLEM MUCH BETTER

3d Hubbard model

$\mathrm{N}_c = 64 \qquad U = 8t$

$\mu = -7t \qquad n = 0.2$

S. Fuchs and E. Gull



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Nontrivial questions

- Does F^{approx} exist?
- How to construct the theory which gives G^{QI}
- What basis functions are acceptable
- Do the solutions make any sense at all, given the brutality of the approximation involved
- Can we generalize this to functionals of (approximations to) two particle correlators

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But note advantages

*'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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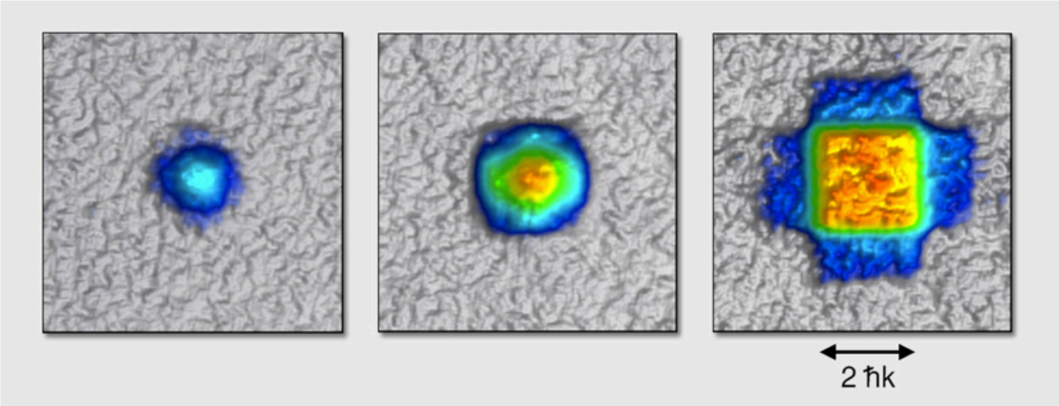
Application

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



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

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

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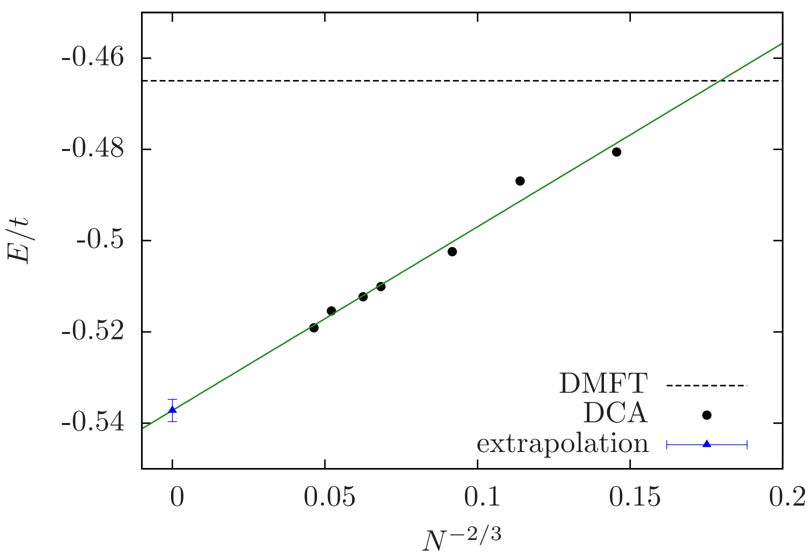
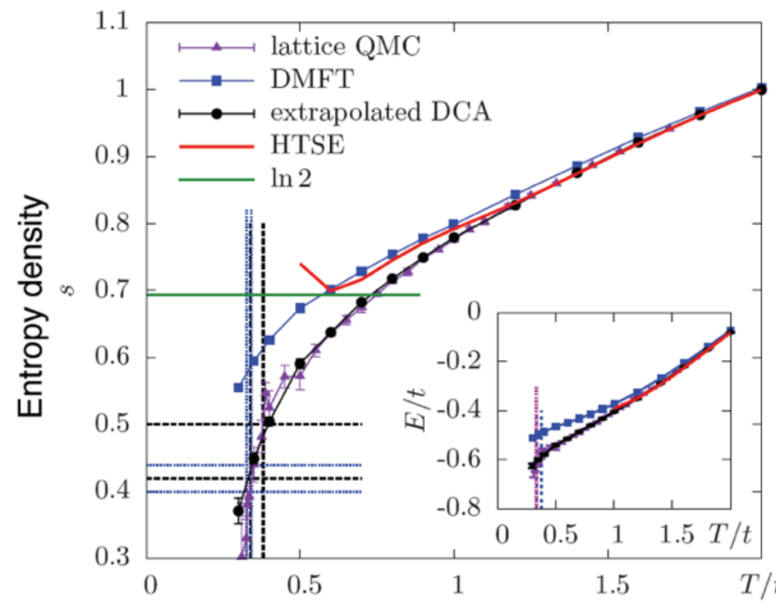
3 dimensional Hubbard model

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

cluster sizes up to 100 sites



U=8t, Temp=0.4t



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

DMFT: Optical emulator emulator

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Remark:

very large clusters--'heroic' calculations, for Hubbard model only.
More typical: study range of modest size clusters--can work out cluster artifacts and obtain qualitative behavior--not quantitative with error bars

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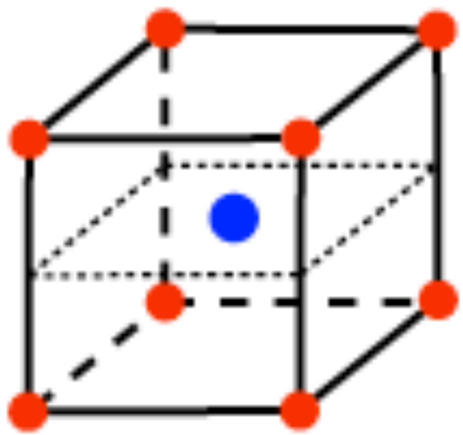
Response of a correlated system to a local charge



- Charged impurity
- lattice sites for electrons

Question: how do strong correlations (Mott gap) affect electron density response

H. T. Dang, E. Gull and AJM PRB 81 235124 (2010)

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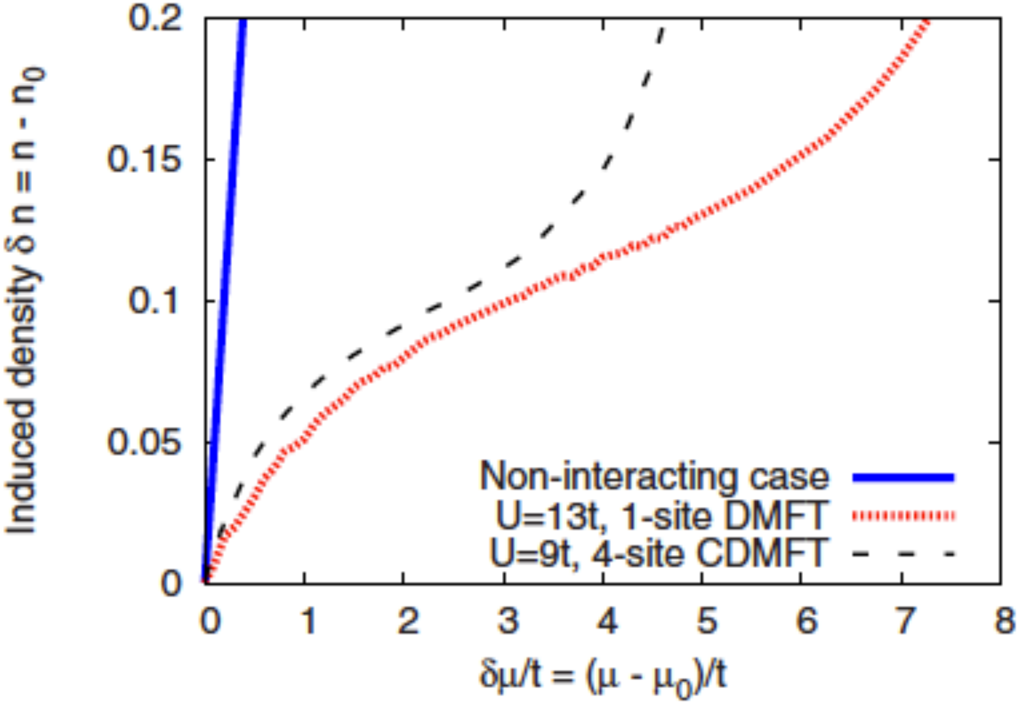
Hubbard model:
Local charge response



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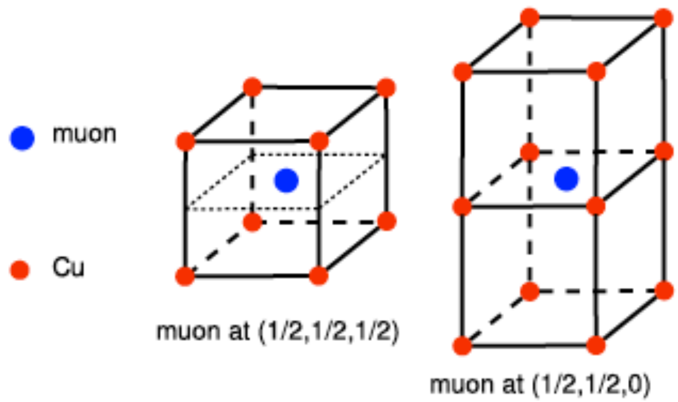
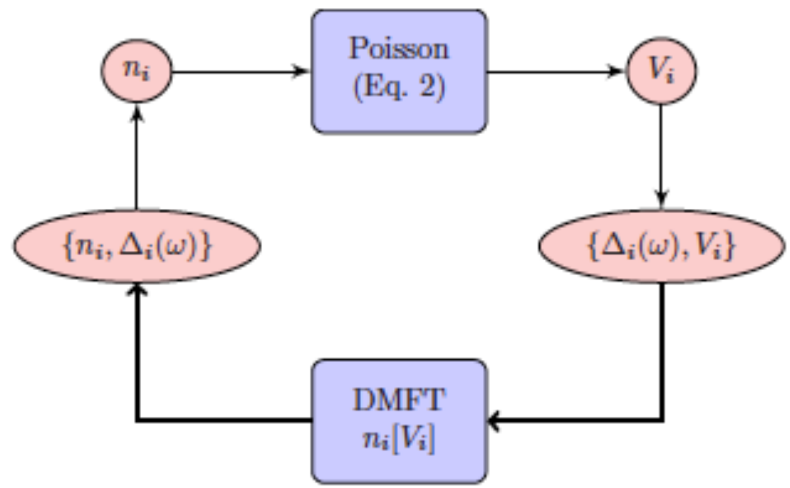
Charged impurity:
CDMFT + Self consistent Hartree



Hubbard model +long ranged Coulomb

$$V_i = -\frac{e^2}{\epsilon|\vec{R}_i - \vec{R}_\mu|} + \frac{e^2}{\epsilon}\sum_{j\neq i}\frac{\delta n_j}{|\vec{R}_i - \vec{R}_j|}$$



Open question: value of ϵ

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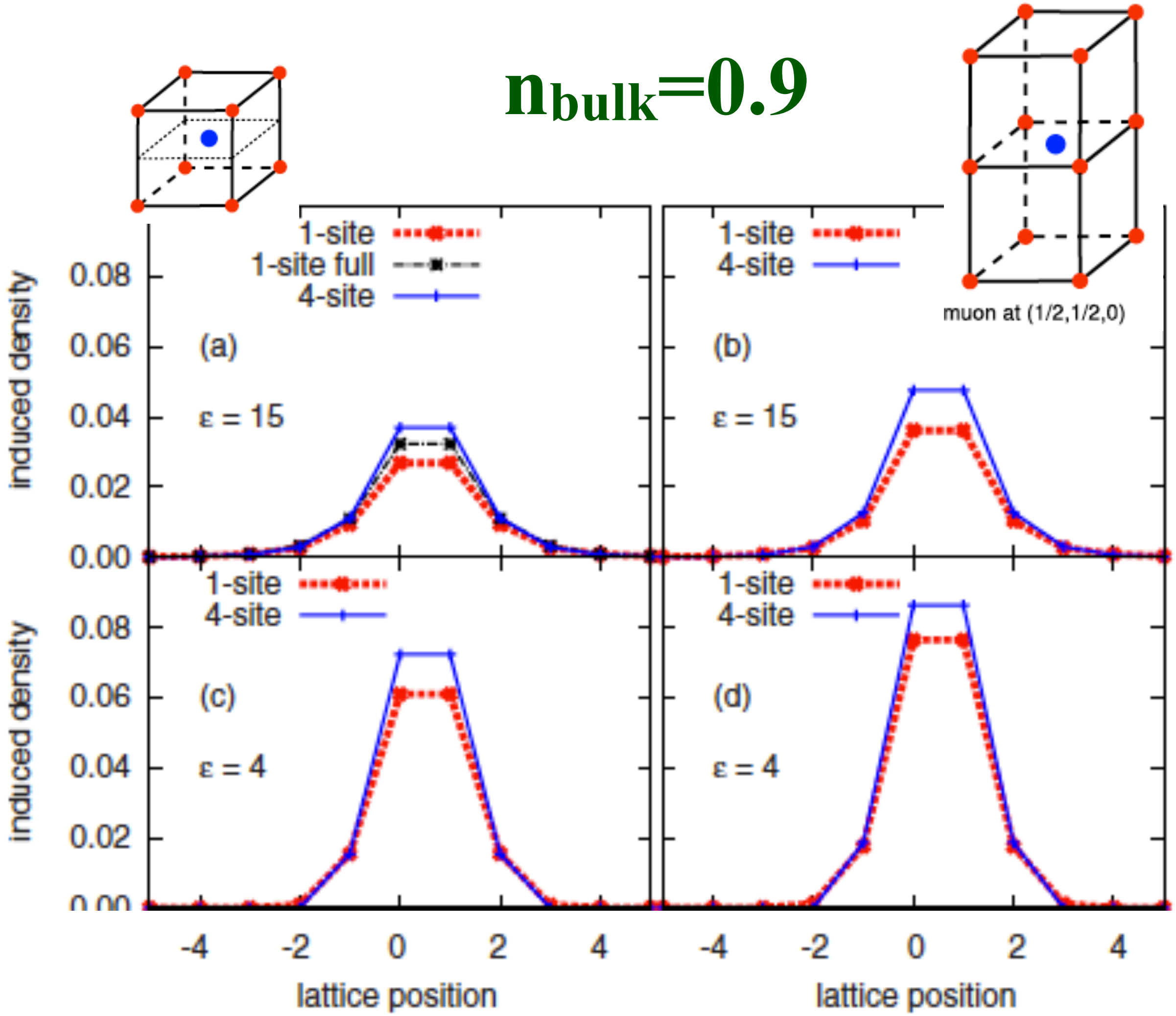
2d Hubbard + Coulomb

n_{bulk}=0.9



$$\delta \mathbf{n} \sim \frac{\mathbf{n} - \mathbf{n}_{Mott}}{2}$$

Density along line (1,0)

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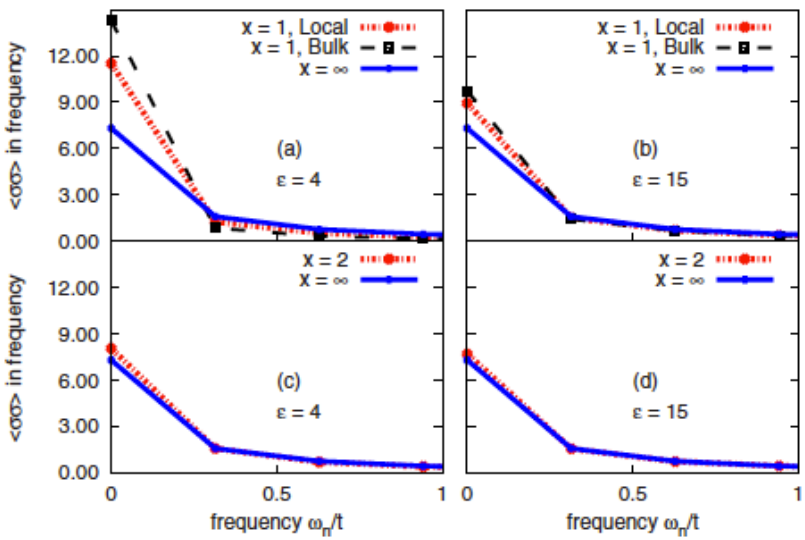
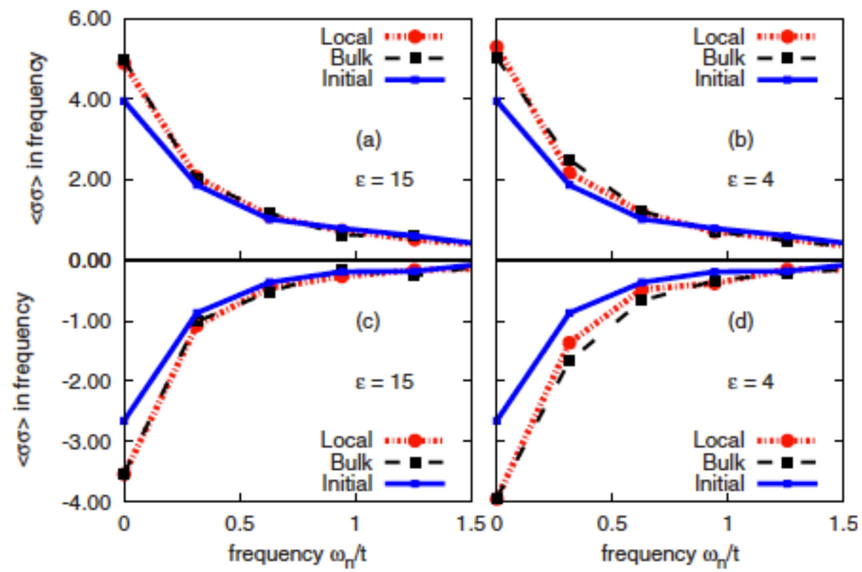
physical consequence of density change

Local spin correlators



single site DMFT



4 site CDMFT

Spin correlators ~ those of bulk system with local density

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Muon may not be a 'soft probe'

To firm up conclusion: band theory (more realistic treatment of dielectric screening) + DMFT

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Global properties of Hubbard model and high Tc pseudogap

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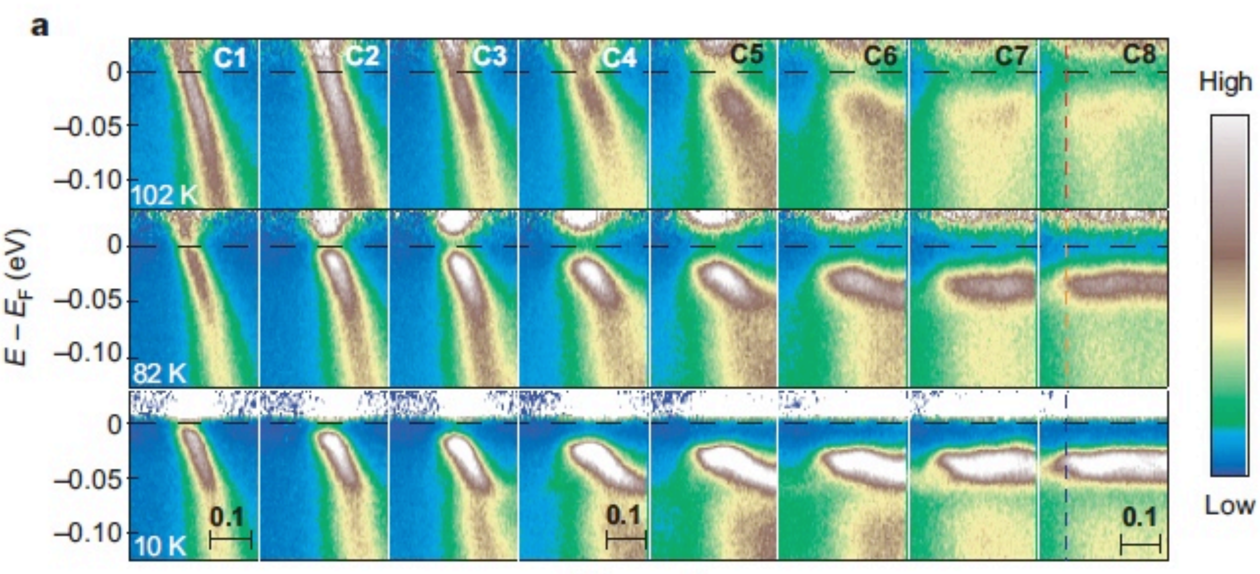
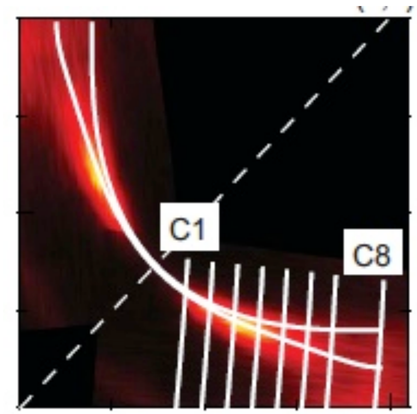
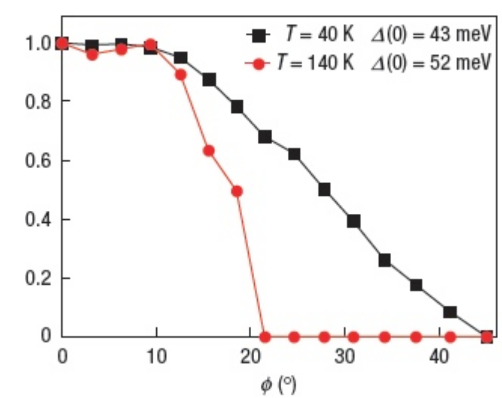
`Pseudogap'

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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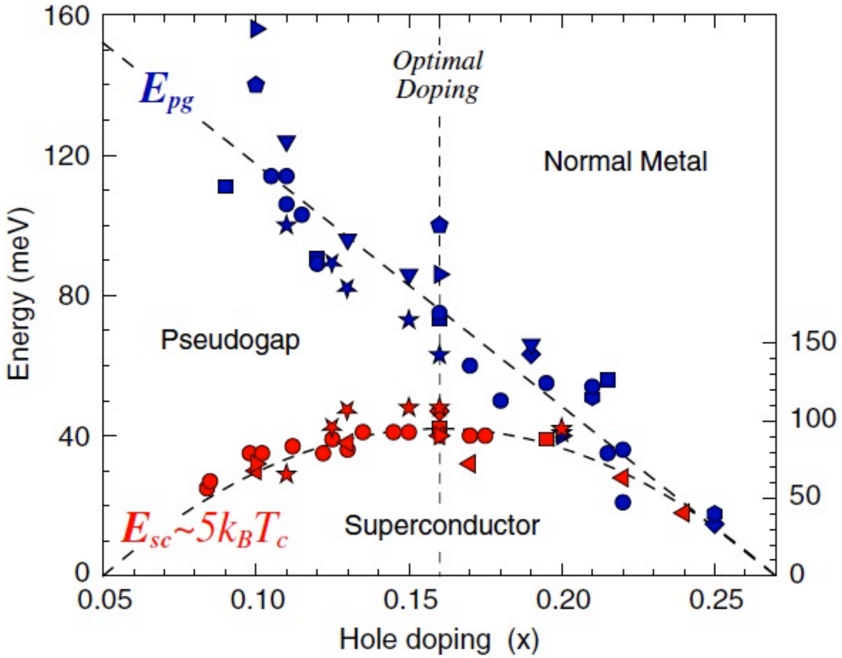
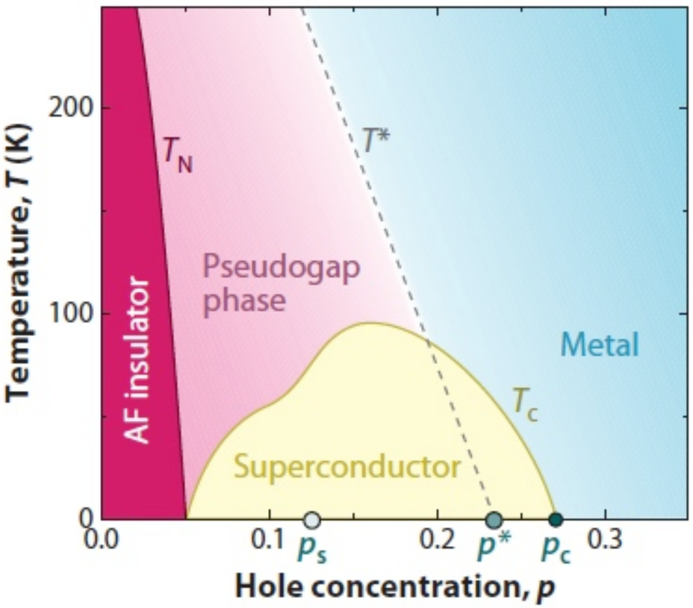
`Pseudogap'

Magnitude increases as doping decreases

Onset temp. increases as doping decreases



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



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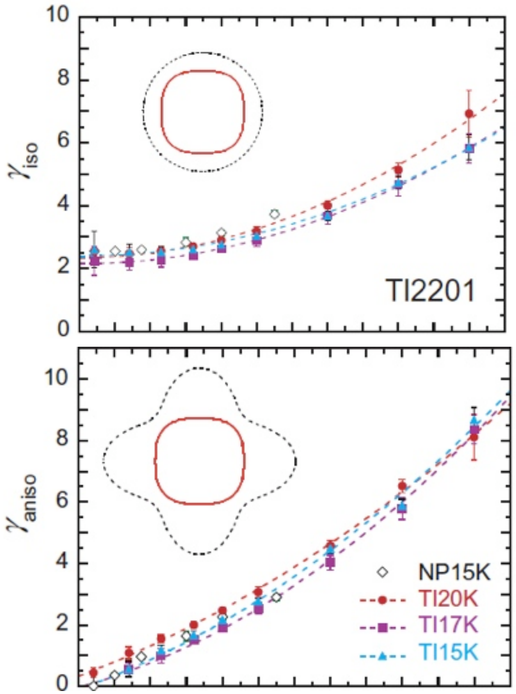
Precursor of pseudogap in momentum-space dependent scattering rate

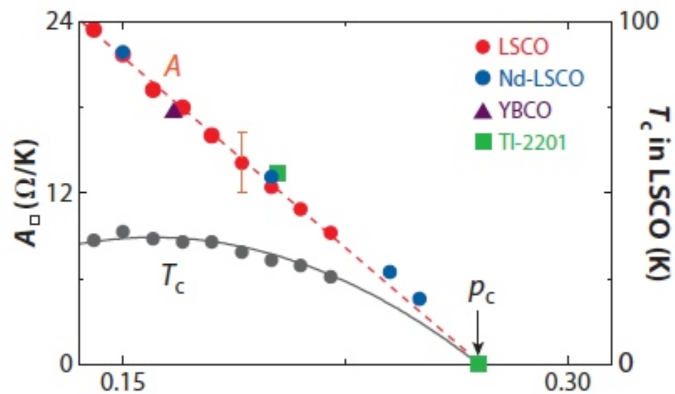


Temperature

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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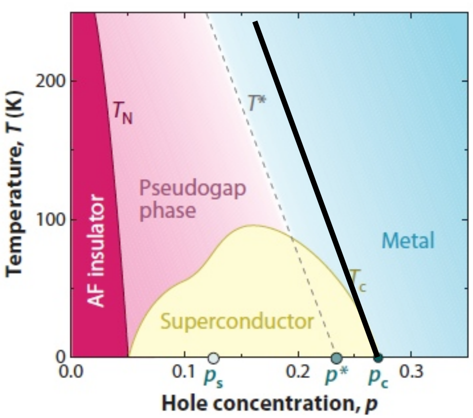
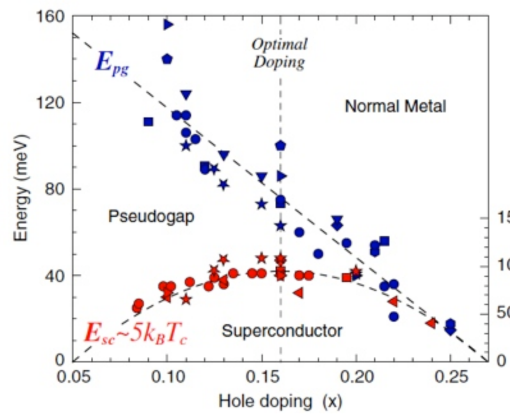
Question

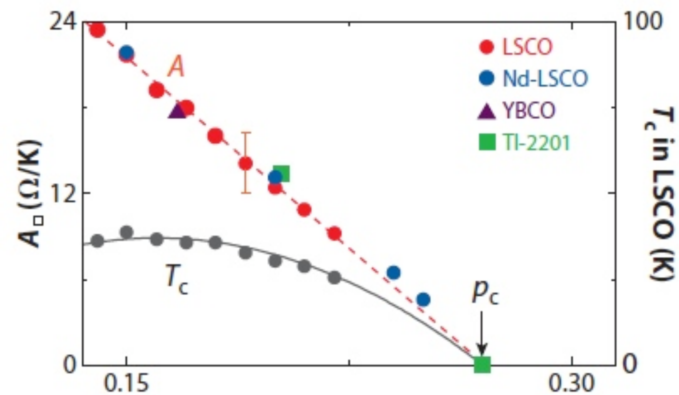
Phase diagram



Pseudogap



Scattering rate



Are these phenomena properties of a theoretical model?

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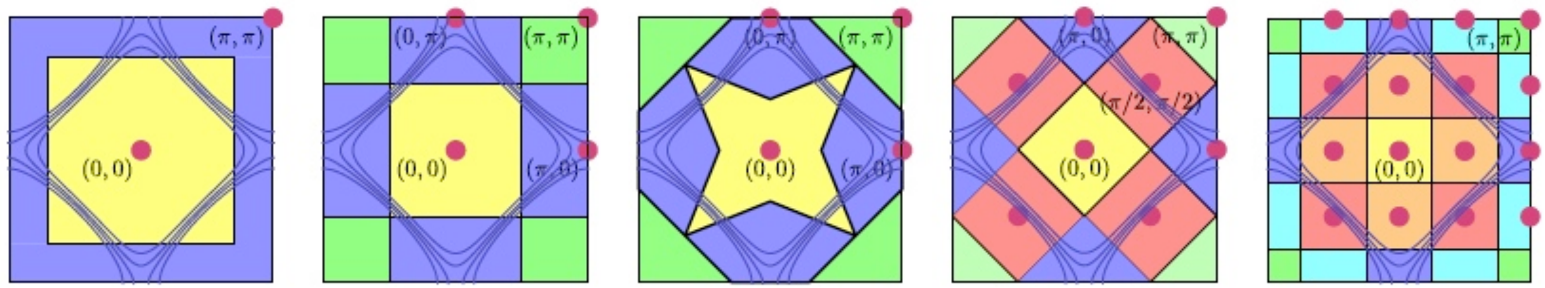
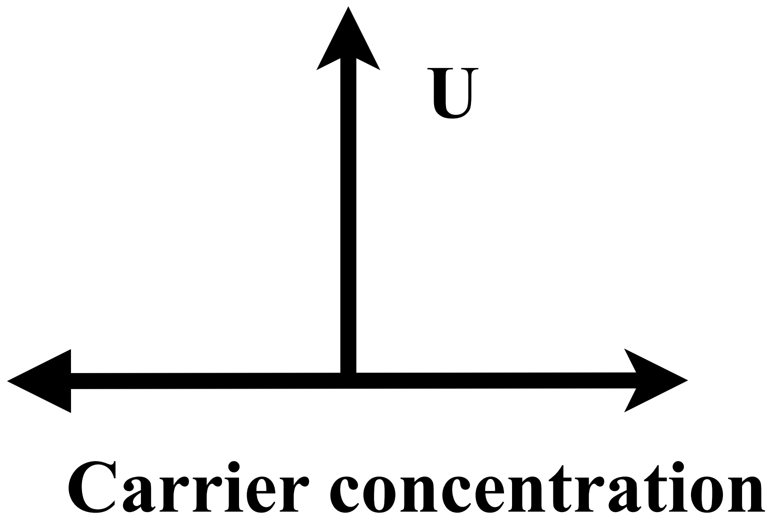
2,4,8,16 site cluster DMFT



Focus on quantities for which all clusters give (qualitatively) the same answers



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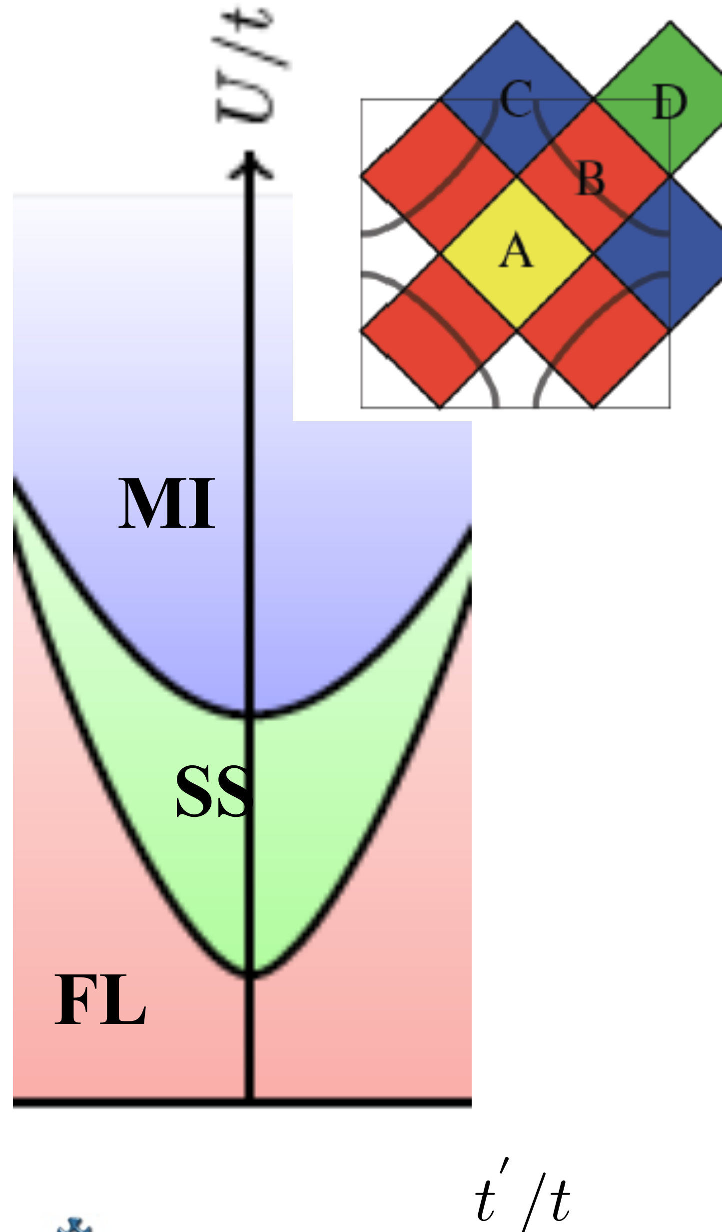
Phase diagram: Interaction-driven transition, half filled 2D Hubbard model

New result: 'Sector Selective' (partially gapped) phase separates Mott Insulator and Fermi liquid phases



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Doping phase diagram
U=7t

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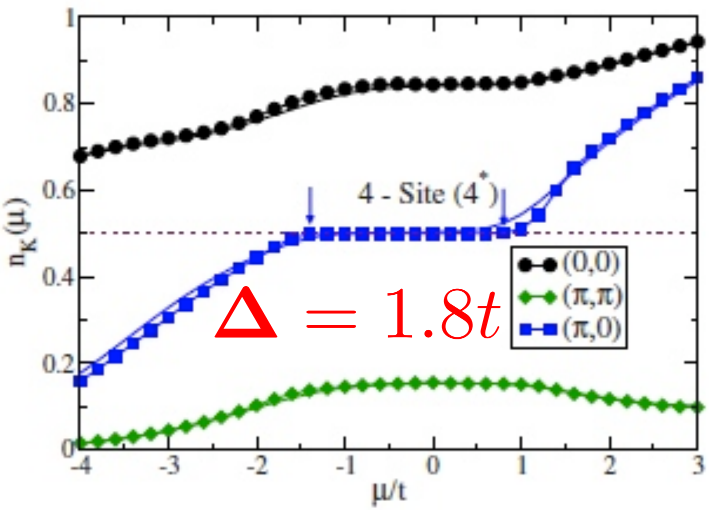
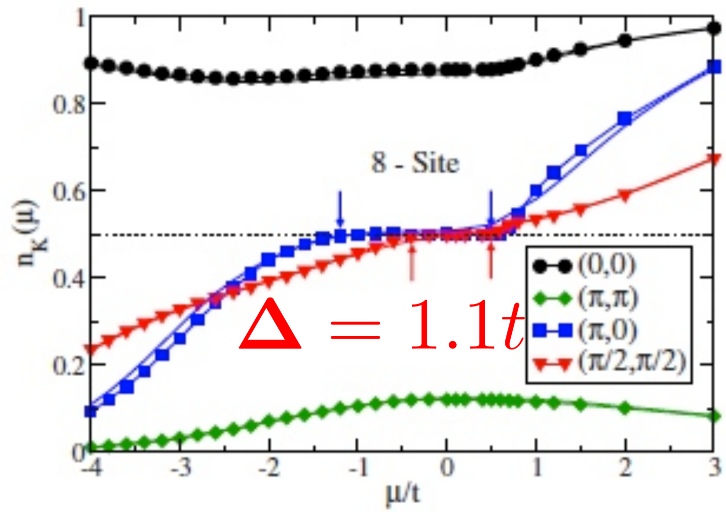
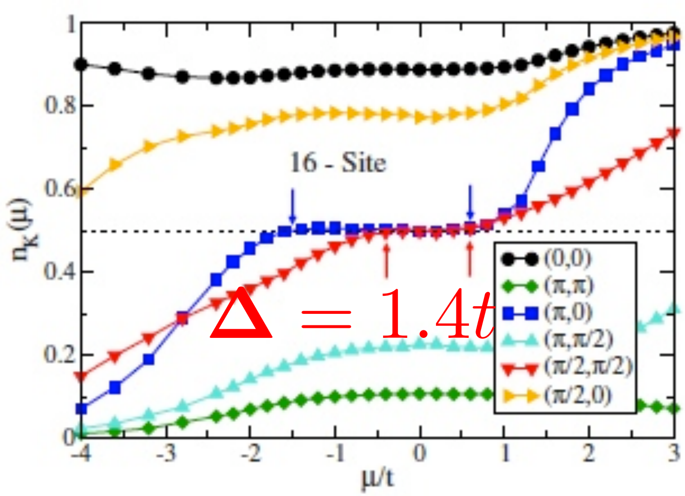
Momentum sector occupancy vs chemical potential







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

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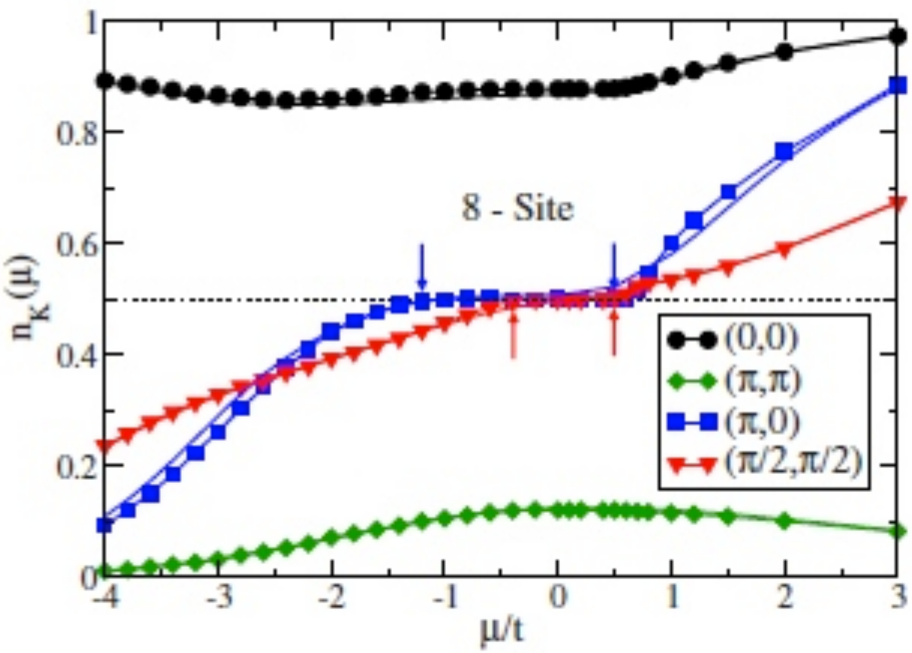
‘Sector selective’ transition: region near (0,Pi) remains gapped on doping



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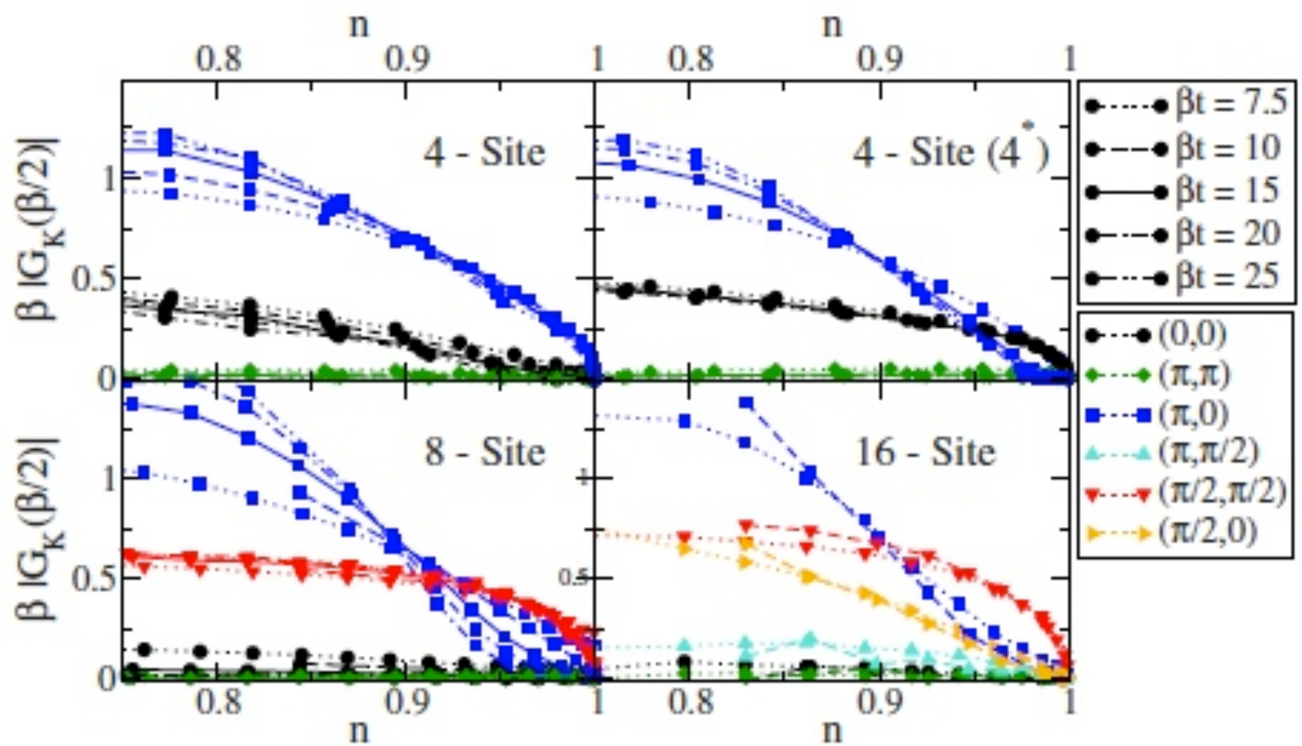
Additional evidence for 'sector selectivity'



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

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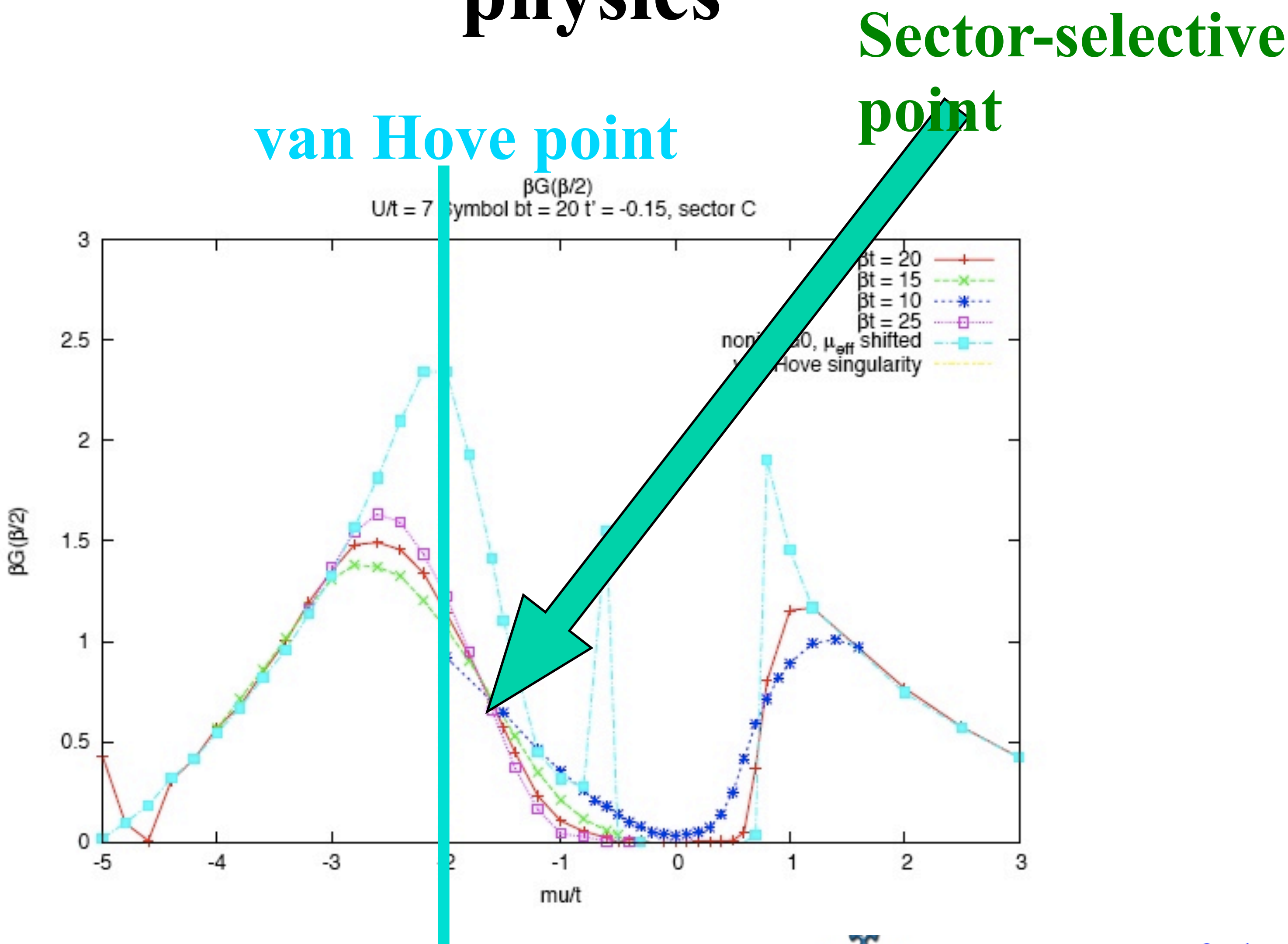
Transition not controlled by van Hove physics



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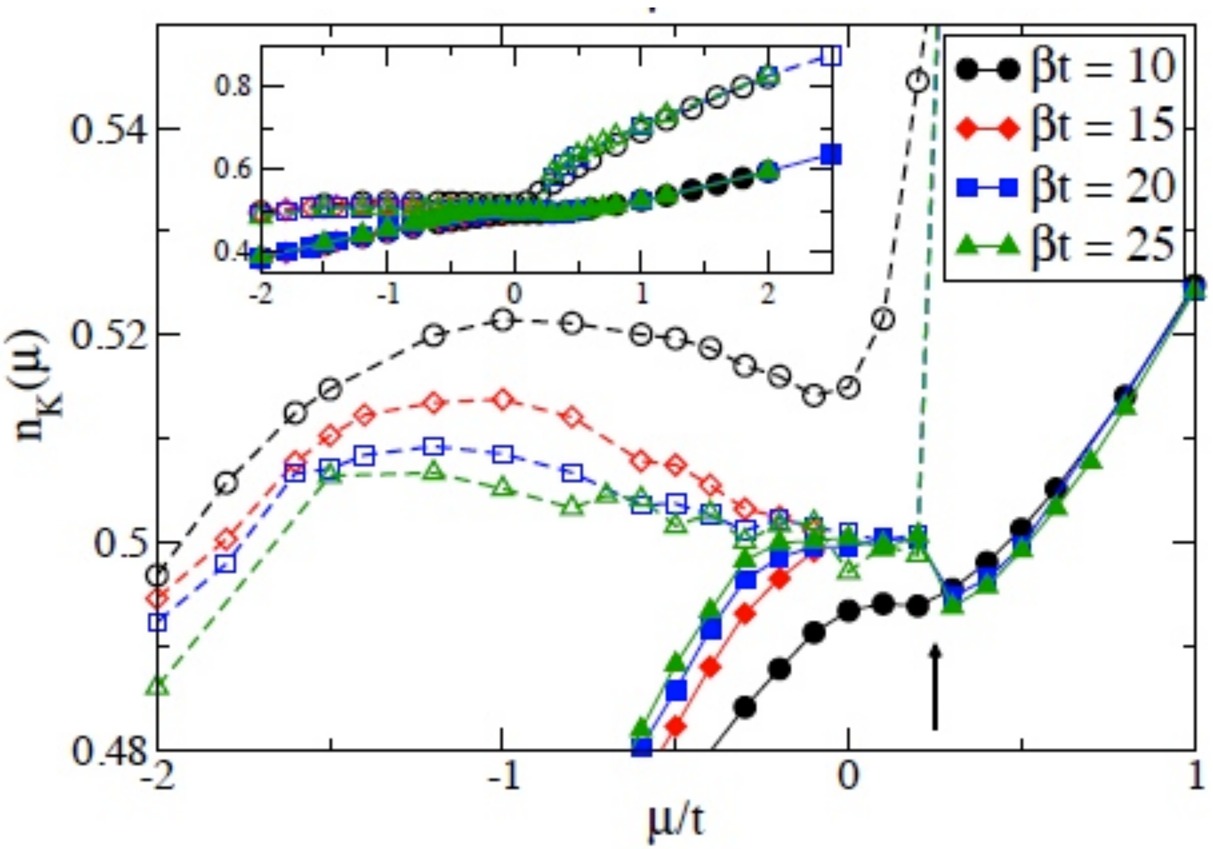
t'=-0.3t



e-doping: transition strongly first order

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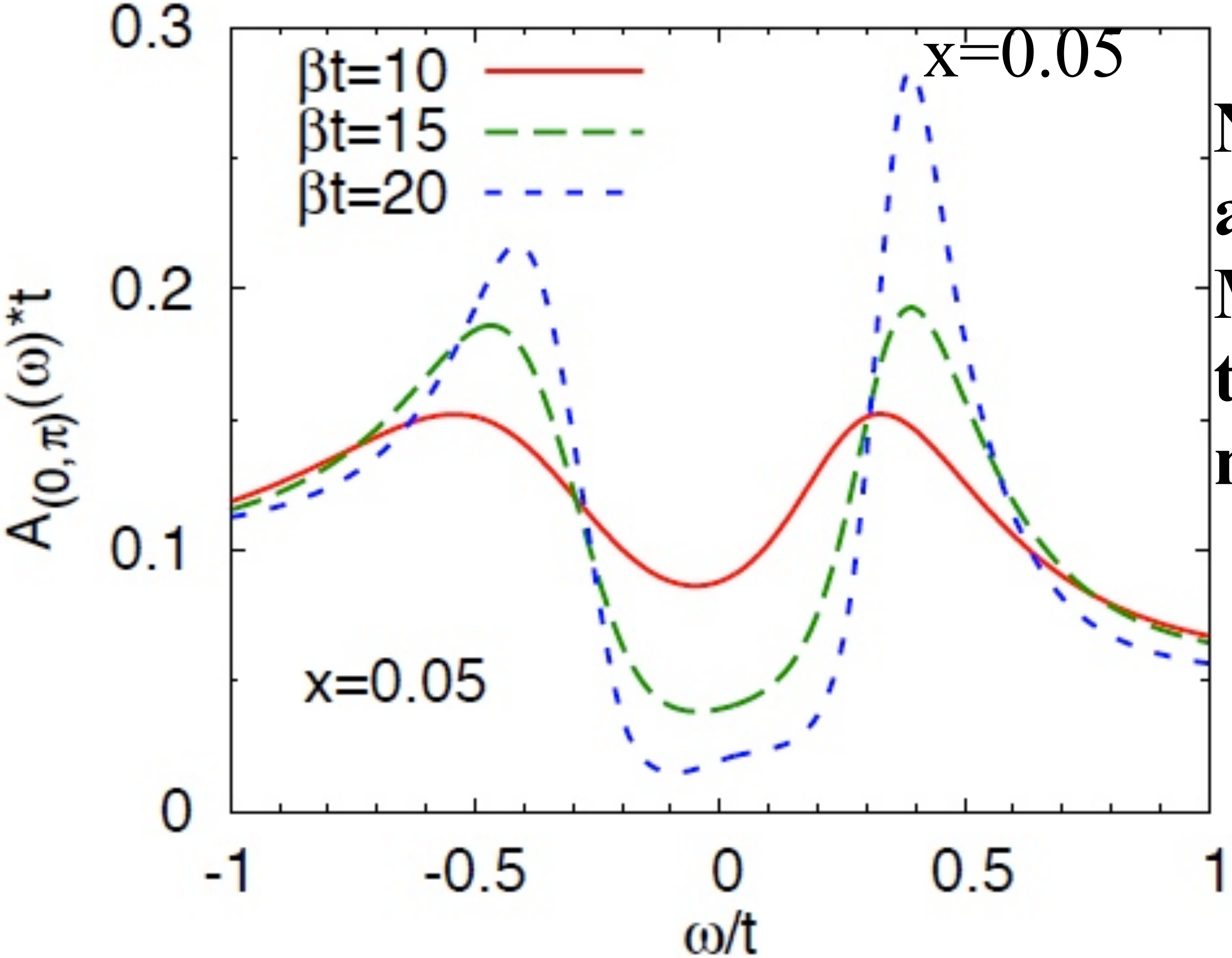
Closer look at the pseudo--or is it real--gap: maximum entropy analytical continuation



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

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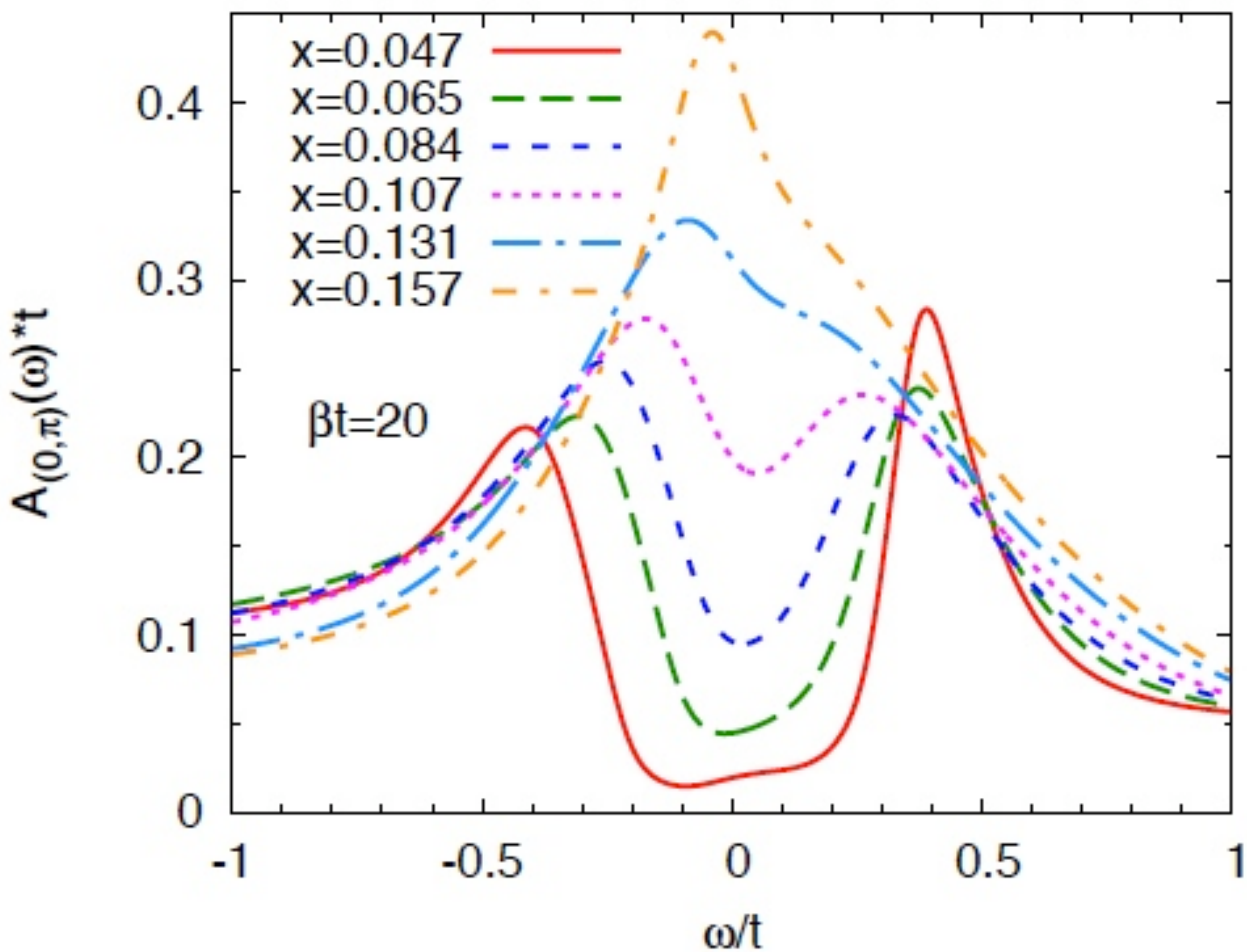
Doping dependence



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

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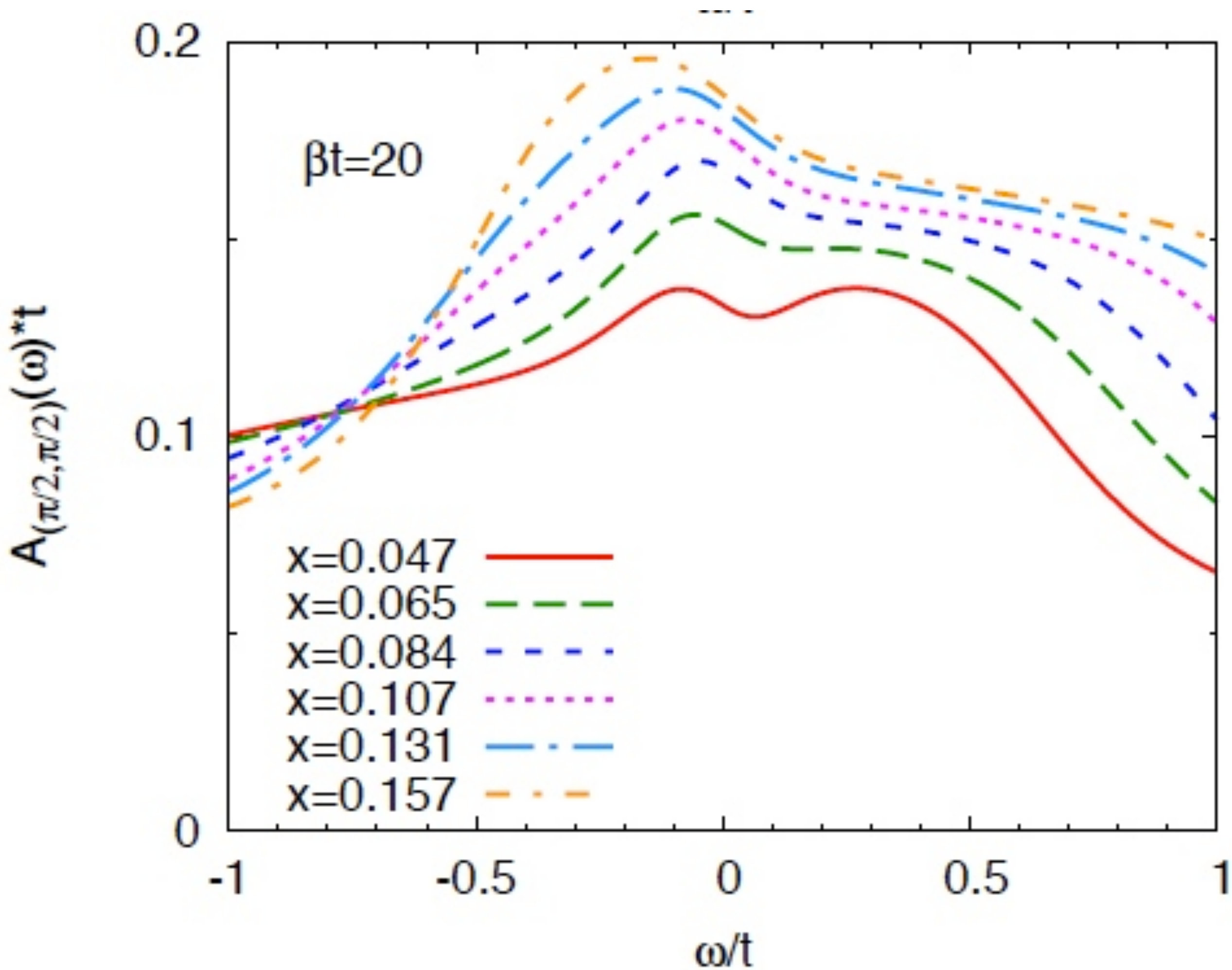
Zone diagonal sector



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

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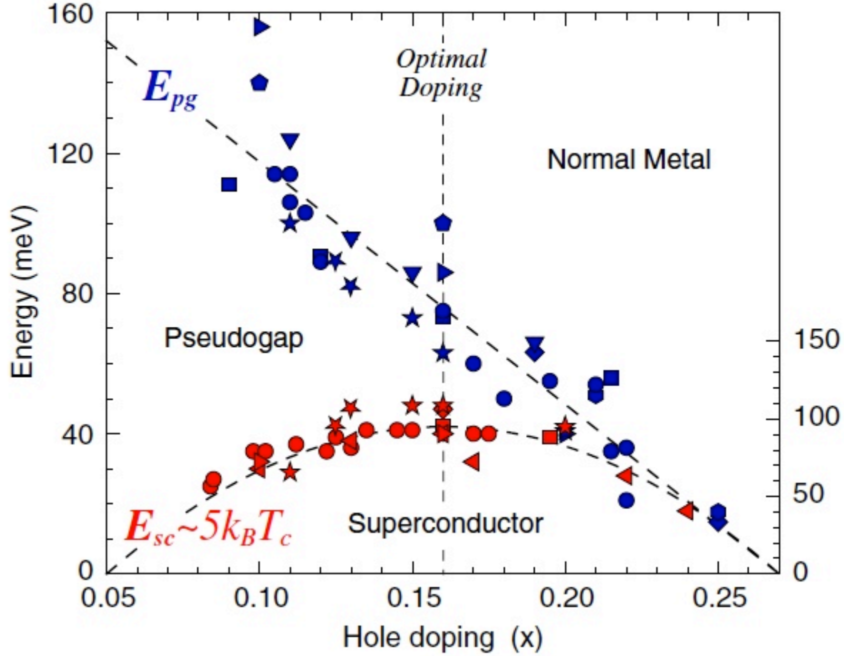
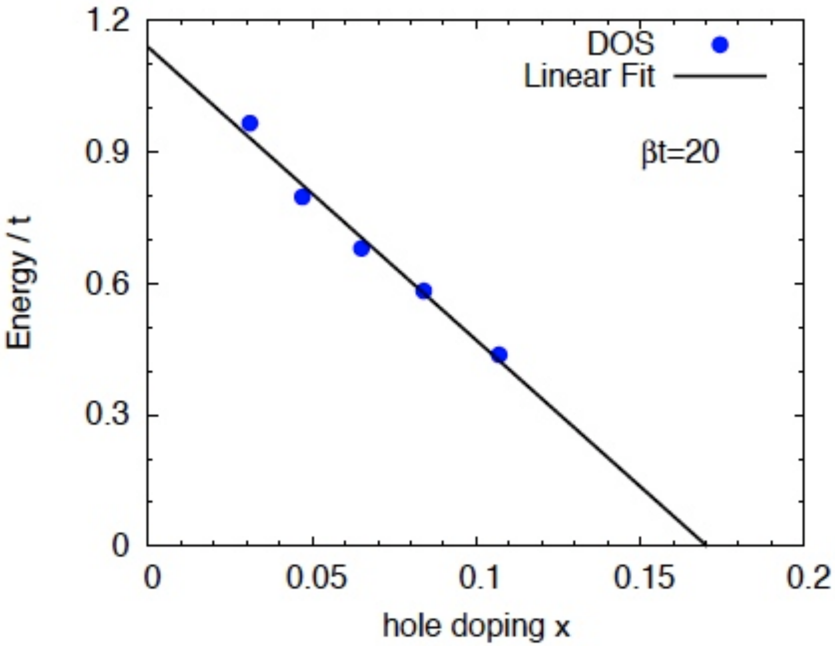
Summary of gap size

Compilation of data



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

Calculation (t=300meV)



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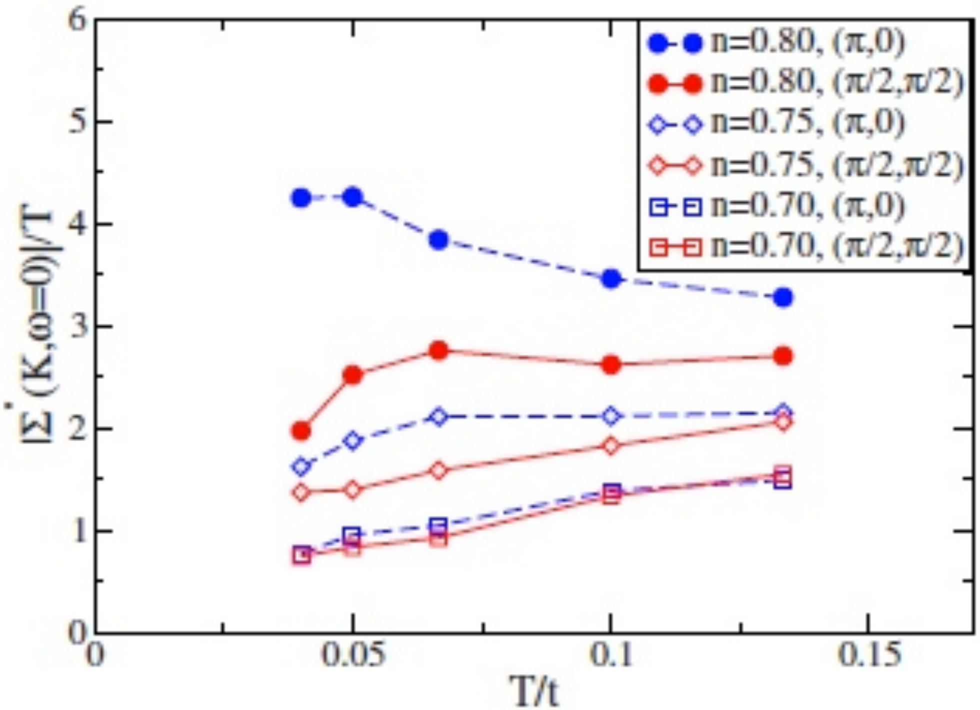
Higher doping: electron scattering rate divided by T



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

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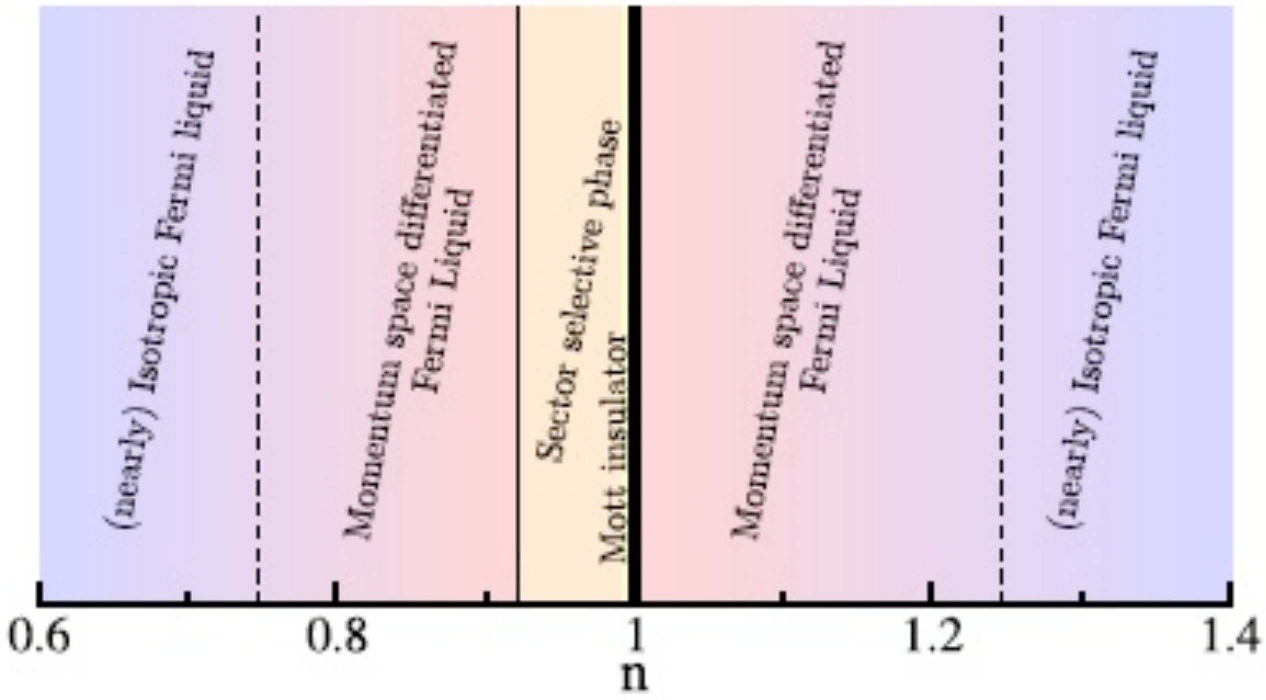
Doping phase diagram
U=7t



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Summary

New methods beginning to yield quantitative results for dynamical quantities, at least for model systems. Example: pseudogap physics of high-T_c

- **insulating behavior from short ranged correlations at n=1**
- **Particle-hole assymmetry**
- **new mechanism for metal-insulator transition**
- **Nodal/antinodal differentiation and pseudogap**
- **Behavior of optical conductivity**

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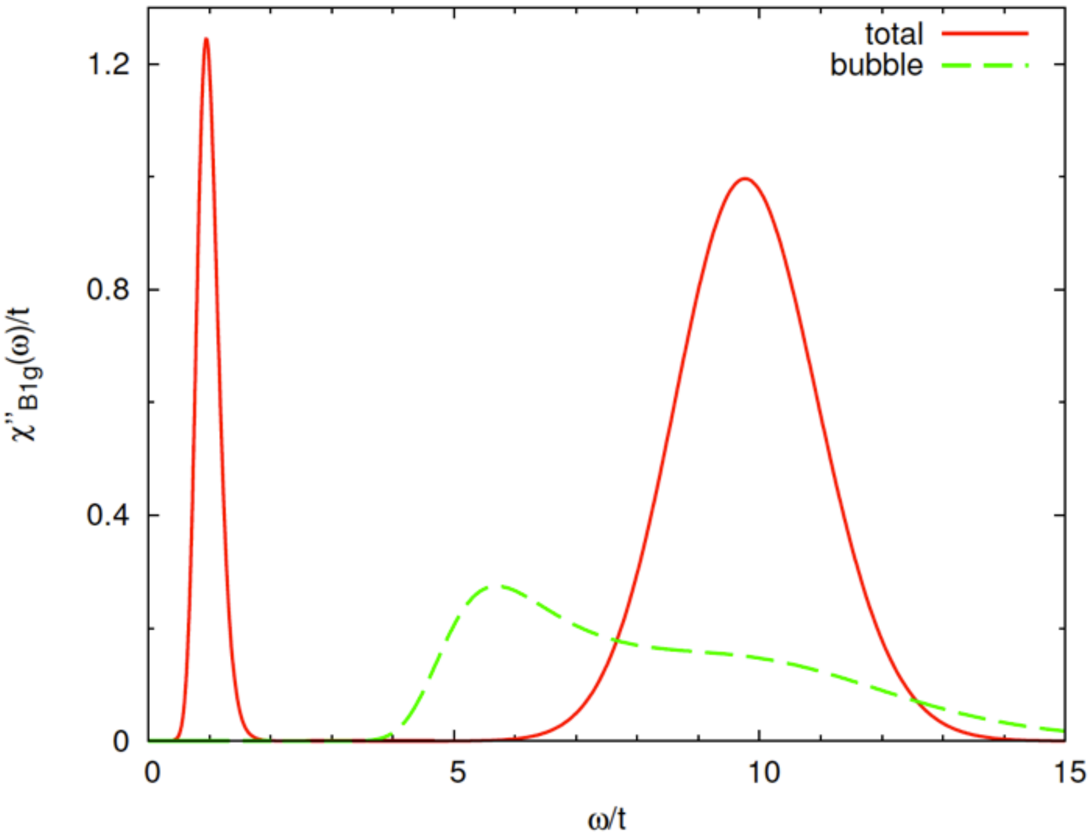
2 particle response functions (N. Lin, E. Gull, AJM in preparation)



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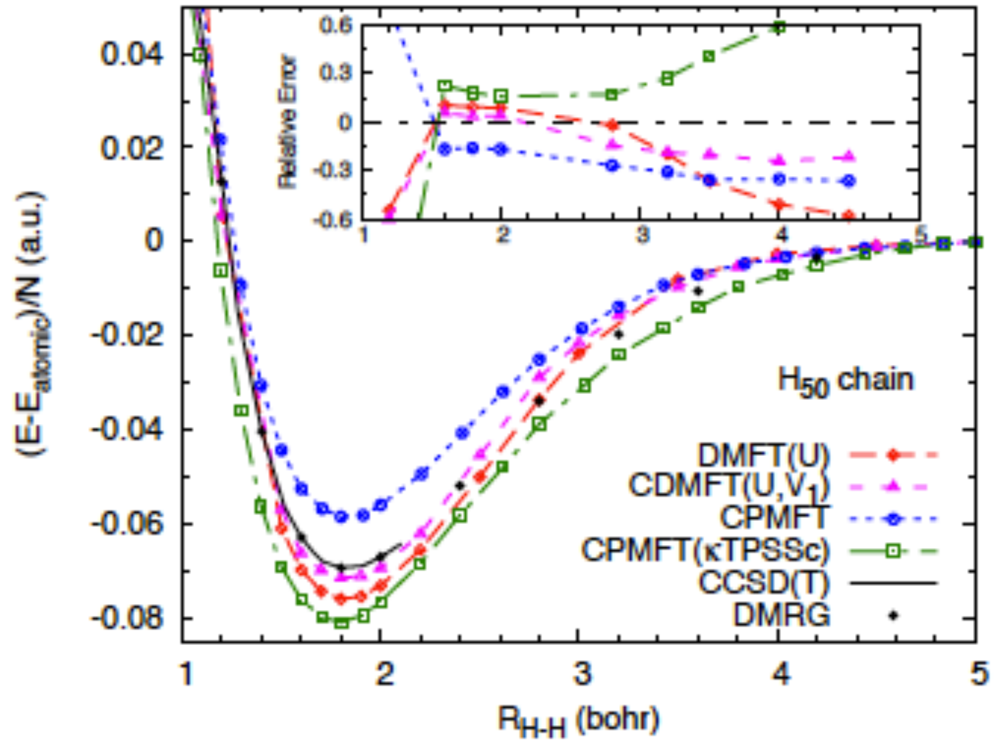
Methods may be useful for quantum chemistry

Quantum chemical test-bed: H_n molecule



Nan Lin, C. Marianetti, A. J. Millis, and D. Reichman, Phys. Rev. Lett. **106**, 096402 (2011).

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Prospects

- Quantitative extrapolation to thermodynamic limit now coming on line (for simple models with density interaction)
- Vertex corrections: two particle responses
- Wide range of other questions

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Gottfried Wilhelm von

Leibniz' dream...

"If controversies were to arise, there would be no more need of disputation between two philosophers than between two accountants. For it would suffice to take their pencils in their hands, and say to each other, 'Let us calculate.'"

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Open Issues

- **Non-hubbard models:**
  - **Multiplet interactions: possible (so far) only with single site DMFT**
  - **non-local interactions ('V')**

- **Mapping real materials onto many-body models:**
  - **'the double counting correction'**
  - **screening**

- **Real time: response functions and neq dynamics**

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Now this is not the end. It is not even the beginning of the end. But it is, perhaps, the end of the beginning.

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Open Issues

‘materials theory’ of correlated compounds

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Open Issues

'materials theory' of correlated compounds

meaning of models

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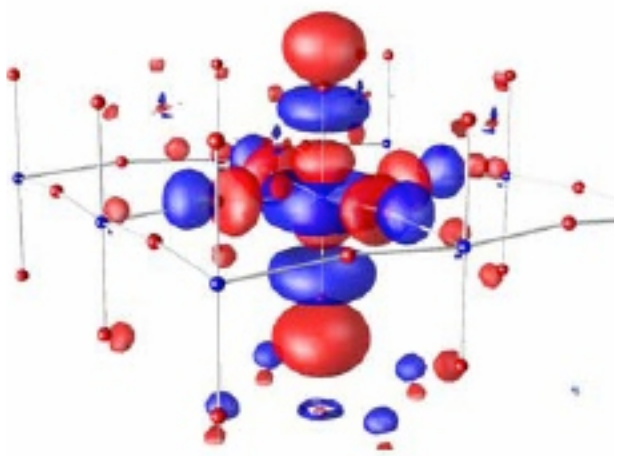
Define correlated orbitals: wave functions and so interactions depend on energy window

If project onto near fermi level states, wannier function spatially extended: longer ranged hopping and more complicated interactions

Representation of Wannier function for $LaNiO_3$



???

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

OK Andersen http://online.kitp.ucsb.edu/online/materials10/andersen/

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As make energy range narrower

Miyake et al J. Phys. Soc. Jpn. 77 (2008) Supplement C pp. 99-102
Aichhorn et al Phys. Rev. B 80, 085101

- **Wave function more delocalized**
- **Interaction smaller**
- **Deviation from free space relations larger**

FeAs materials

d-p basis

band

$$U^{\sigma\bar{\sigma}}_{mm'}|_{\mathrm{cRPA}} = \begin{pmatrix} 3.77 & 2.35 & 2.21 & 2.71 & 2.71 \\ 2.35 & 3.94 & 2.87 & 2.44 & 2.44 \\ 2.21 & 2.87 & 3.31 & 2.29 & 2.29 \\ 2.71 & 2.44 & 2.29 & 3.48 & 2.29 \\ 2.71 & 2.44 & 2.29 & 2.29 & 3.48 \end{pmatrix}$$

‘averaged’ U, J (free space symm enforced)

$$U^{\sigma\bar{\sigma}}_{mm'} = \begin{pmatrix} 3.59 & 2.19 & 2.19 & 2.73 & 2.73 \\ 2.19 & 3.59 & 2.91 & 2.37 & 2.37 \\ 2.19 & 2.91 & 3.59 & 2.37 & 2.37 \\ 2.73 & 2.37 & 2.37 & 3.59 & 2.37 \\ 2.73 & 2.37 & 2.37 & 2.37 & 3.59 \end{pmatrix}$$

d-only basis

band

$$U^{\sigma\bar{\sigma}}_{mm'}|_{\mathrm{cRPA}} = \begin{pmatrix} 3.17 & 2.02 & 1.72 & 2.22 & 2.22 \\ 2.02 & 3.36 & 2.16 & 2.04 & 2.04 \\ 1.72 & 2.16 & 2.17 & 1.73 & 1.73 \\ 2.22 & 2.04 & 1.73 & 2.73 & 1.84 \\ 2.22 & 2.04 & 1.73 & 1.84 & 2.73 \end{pmatrix}$$

averaged U, J

$$U^{\sigma\bar{\sigma}}_{mm'} = \begin{pmatrix} 2.82 & 1.77 & 1.77 & 2.18 & 2.18 \\ 1.77 & 2.82 & 2.31 & 1.91 & 1.91 \\ 1.77 & 2.31 & 2.82 & 1.91 & 1.91 \\ 2.18 & 1.91 & 1.91 & 2.82 & 1.91 \\ 2.18 & 1.91 & 1.91 & 1.91 & 2.82 \end{pmatrix}$$

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Open Issues

‘materials theory’ of correlated compounds

meaning of models

values of parameters (screening)

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Screening

Other degrees of freedom react to screen charge fluctuations on correlated orbitals

(Arasetiywan): replace

$$U^{\sigma_1\sigma_2\sigma_3\sigma_4}_{m_1m_2m_3m_4} = e^2\int d^3r d^3r' \frac{\psi^\dagger_{m_1\sigma_1}(r)\psi_{m_3\sigma_3}(r)\psi^\dagger_{m_2\sigma_2}(r')\psi_{m_4\sigma_4}(r')}{|\vec{r}-\vec{r}'|}$$

$$\mathbf{W^{\sigma_1\sigma_2\sigma_3\sigma_4}_{m_1m_2m_3m_4}(\omega) = \int d^3r d^3r' \psi^\dagger_{m_1\sigma_1}(r)\psi_{m_3\sigma_3}(r) W(r,r',\omega) \psi^\dagger_{m_2\sigma_2}(r')\psi_{m_4\sigma_4}(r')}$$

$$\mathbf{W(r,r';\omega) = \frac{e^2}{|r-r'|} * \left[1 - P_r(\omega) * \frac{e^2}{|r-r'|}\right]^{-1}}$$

W is coulomb int screened by other bands

Arasetiyawan, et al Phys. Rev. B 70, 195104
Arasetiyawan, et al Phys. Rev. B 74, 125106
Miayke and Arasetiyawan Phys. Rev. B. 77, 085122

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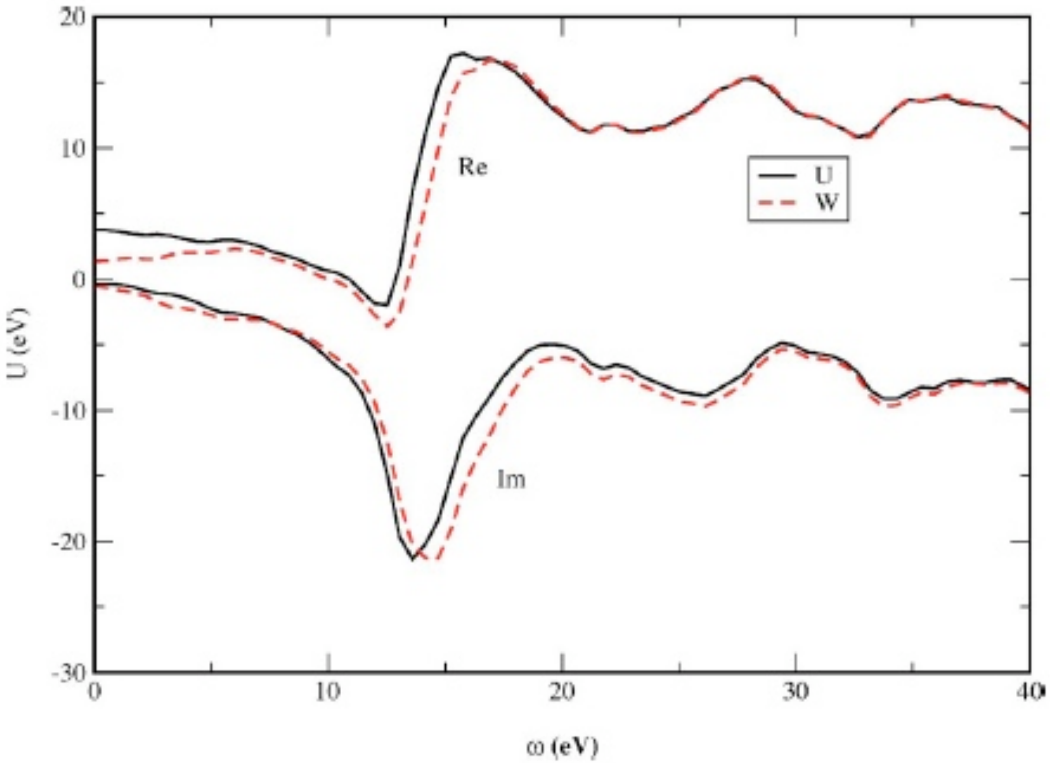
Typical result: $SrVO_3$



Strong screening on ~15eV scale (all electron plasma frequency)

Factor of 2 changes on ~5eV scale (screening by nearby orbitals)

Screening important (for 'U'). Open question: dynamical effects?

See P. Werner and AJM ArXiv1001.1377

Arasetiyawan, et al Phys. Rev. B 70, 195104

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Theory

Expectation value of current: $\vec{j}(t) = Tr\left[\mathbf{\vec{J}}(A)\mathbf{G}(t;\{\vec{A}\})\right]$

Current operator J and Green function G computed in presence of vector potential A

Hamiltonian: $\hat{H}[\{\mathbf{A}\}] = \hat{T}[\{\mathbf{A}\}] + \hat{U}$

Hopping: depends on A

Interaction: particle positions, not velocities

$$\vec{J} = \frac{\delta \hat{T}}{\delta \vec{A}} \qquad G = \left[i\partial_t - \hat{T}(\vec{A}) - \Sigma(\vec{A})\right]^{-1}$$

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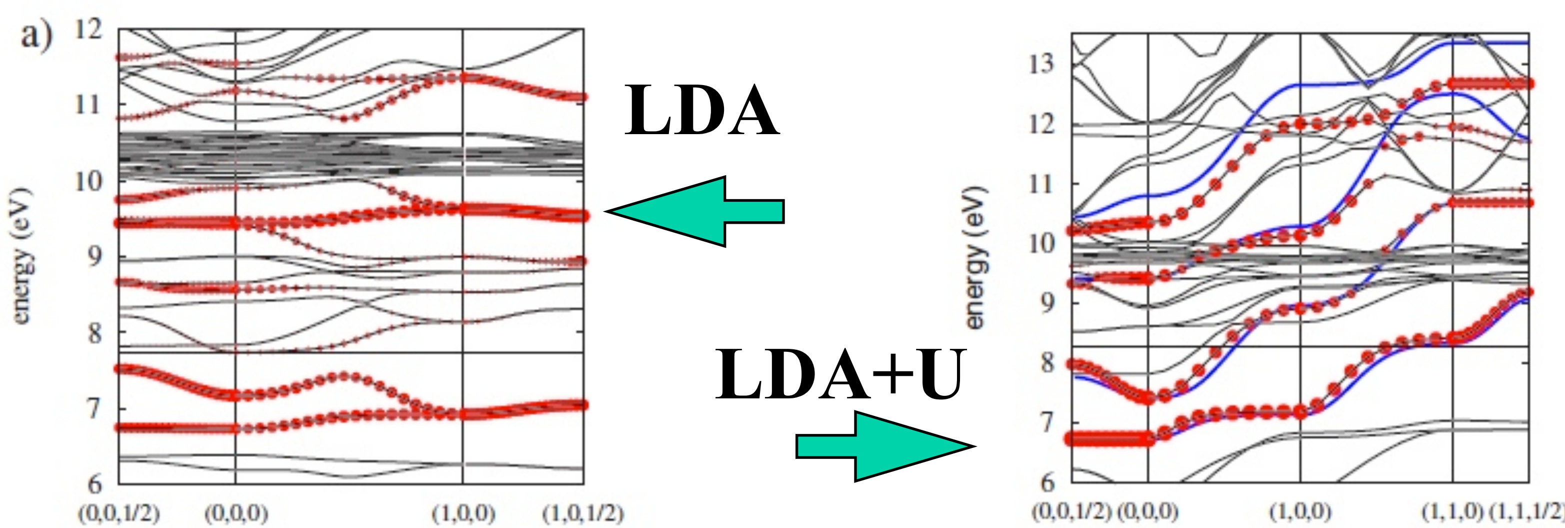
Double counting shifts d levels down by U/2 (roughly): consequences for mixing with other bands

ex: Ederer PRB76 155105 $LaMnO_3$:

Mn e_g symmetry d bands highlighted in red



Position, shape of e_g relative to other bands changes!

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Bottom line

- Techniques exist to extract correlated states
- For 'simple' structure of interactions, effective hamiltonian' should include other (e.g. oxygen degrees of freedom)
- Screening (at least of 'U') is important

Open questions:

--Is it enough to use the low freq. screened U

--d-p interactions??

--Are polarizibility effects correctly captured by RPA

--Double counting problem not well understood

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Open Issues

'materials theory' of correlated compounds

meaning of models
values of parameters (screening)
'double counting' problem--some interactions already in LDA

Solution of models

What we can do: single site, up to 5 (in some cases 7) orbitals, complicated interactions. cluster: only Hubbard models, mainly 1 and 2d.
meaning, reliability of cluster methods
Reliability of single-site DMFT in d=3?
Longer ranged interactions??

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The next few years

- Improve methods
  - Clusters
  - Mapping to materials (high energy physics)
  - Mapping to models (low energy effective field theories
- Apply to more systems and models.

Approach: do stuff. improve methods. see what works and what doesnt. A lot of things to do.

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Expanding

Vertex function: $$\Gamma = \frac{\delta \Sigma}{\delta \vec{A}}$$

=>usual 3 contributions to conductivity

$$\chi_{\rm dia}(t-t') = {\rm Tr}\left[\mathbf{K}\mathbf{G}(t=0)\right]\delta(t-t')$$

$$\chi_{\rm bubble}(t-t') = {\rm Tr}\left[\vec{\mathbf{J}}\mathbf{G}(t-t')\vec{\mathbf{J}}\mathbf{G}(t'-t)\right]$$

$$\chi_{\rm vertex}(t-t') = {\rm Tr}\left[\vec{\mathbf{J}}\mathbf{G}(t-t_1)\vec{\mathbf{\Gamma}}(t_1-t', t'-t_2)\mathbf{G}(t_2-t),\right]$$

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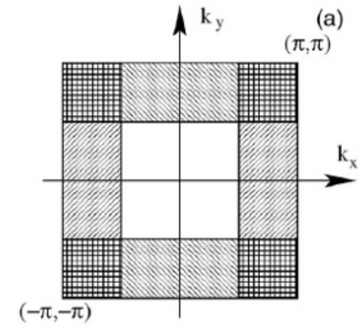
Vertex function: $$\Gamma = \frac{\delta\Sigma}{\delta\vec{A}}$$

In DCA:

$$\Sigma(k,\omega) = \sum_{a}^{N} \Sigma_a(\omega)\phi_a(k)$$

=>2 contributions to vertex:



From k dependence (delta functions where patches meet)

From dependence of cluster self energy on A

Vertex from k-dependence: line where patches "a" and "b" meet

$$\vec{\Gamma}^k(\omega+\Omega,\omega) = \vec{n}^{ab}\left(\Sigma_b(\omega+\Omega) - \Sigma_a(\omega)\right)\delta\left((\vec{k}-\vec{k}^{ab})\cdot\vec{n}^{ab}\right)$$

(Previous literature neglected this)

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Vertex from k-dependence: line where patches "a" and "b" meet

$$\vec{\Gamma}^k(\omega+\Omega,\omega) = \vec{n}^{ab}\left(\Sigma_b(\omega+\Omega) - \Sigma_a(\omega)\right)\delta\left((\vec{k}-\vec{k}^{ab})\cdot\vec{n}^{ab}\right)$$

(Previous literature neglected this)

Vertex from cluster self-energy: compute by linearizing self consistency equation in A

$$\delta\mathcal{G}_\alpha^{-1} - I_\Sigma[\{\delta\Sigma_\alpha\}] = -\vec{I}_v^\alpha\cdot\vec{A}$$

$$\vec{I}_v = -G_a^{-1}\left(\int_a (dk)G(k)\frac{\partial\varepsilon}{\partial\vec{k}}G(k)\right)G_a^{-1}$$

$$I_\Sigma = \delta\Sigma^a + G_a^{-1}\left(\int_\alpha (dk)G(k)\delta\Sigma^\alpha G(k)\right)G_a^{-1}$$

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Vertex from k-dependence: line where patches "a" and "b" meet

$$\vec{\Gamma}^k(\omega+\Omega,\omega) = \vec{n}^{ab}\left(\Sigma_b(\omega+\Omega)-\Sigma_a(\omega)\right)\delta\left((\vec{k}-\vec{k}^{ab})\cdot\vec{n}^{ab}\right)$$

(Previous literature neglected this)

Vertex from cluster self-energy: compute by linearizing self consistency equation in A

$$\delta\mathcal{G}_\alpha^{-1} - I_\Sigma[\{\delta\Sigma_\alpha\}] = -\vec{I}_v^\alpha\cdot\vec{A}$$

$$\vec{I}_v = -G_a^{-1}\left(\int_a (dk)G(k)\frac{\partial\varepsilon}{\partial\vec{k}}G(k)\right)G_a^{-1}$$

$$I_\Sigma = \delta\Sigma^a + G_a^{-1}\left(\int_\alpha (dk)G(k)\delta\Sigma^\alpha G(k)\right)G_a^{-1}$$

2 and 4 site clusters: I=0=> self energy A-indep.
8 site: vertex being implemented now

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