Large cluster dynamical mean field calculations and the momentum-selective Mott transition

Emanuel Gull

April 22, 2011

Funding: NSF-DMR-1006282

A.J. Millis
A. Georges, M. Ferrero, N. Lin, O. Parcollet, P. Werner
S. Fuchs, P. Staar, P. Nukala, M. Summers, T. Pruschke, T. Schulthess, T. Maier
L. Pollet, E. Kozik, E. Burovski, M. Troyer

Overview

• Introduction: the pseudogap in High Tc

• Methods and tools I: Cluster DMFT

• Methods and tools II: Impurity solvers

• Controlling DCA: Benchmarking the 3D Hubbard model

• Results for the 2D Hubbard model: Momentum selectivity, pseudogaps, Optical conductivities, Raman, ...
Experiments: Pseudogap

in high-Tc materials: Electronic spectral function is suppressed along the BZ face, but not along zone diagonal.

Key physics dependence on momentum around Fermi surface, Difference of spectral function around Fermi surface.

Doping dependence of region with quasiparticles


Bi2212 sample with Tc=30K, measured at 140K.
Experiments: Pseudogap

FIG. 1. Phase diagram of $n$- and $p$-type superconductors, showing superconductivity (SC), antiferromagnetic (AF), pseudogap, and normal-metal regions.

Pseudogap* appears only on the hole doped side.

Dopings smaller than optimal doping.

Temperatures up to ~ 300K.

Signatures also in NMR, Tunneling, c-axis conductivities, Raman...
Angle dependent magneto-resistance:

Data analysis:

\[ \rho(T) = A + BT + CT^2 \]

Angle dependent analysis:

\[ \gamma_{iso} \sim A + CT^2 \]
\[ \gamma_{aniso} \sim BT (+CT^2) \]

Anisotropic component of scattering rate: maximal near antinodal point, minimal near nodal point.

Momentum space differentiation!
Questions to theory

‘Explain’ momentum space differentiation

‘Explain’ pseudogap

‘Explain’ experimental probes:
ARPES, ADMR, optical conductivities, Raman, NMR,…

.............we will try to give an answer in this talk...........
Simulations of phase diagrams

Large enough systems to show which features are robust

Variation of cluster size, cluster geometry, etc to control approximation

Computation of experimental probes

Hubbard model, with t’-anisotropy, treated in a cluster DMFT approximation.

No long range order (AFM, stripes, …), no multi-orbital physics

Open theoretical question (addressed in this talk): how much of the physics already contained in this model?
Cluster DMFT

Approximation to self energy:

\[\Sigma(k, \omega) = \sum_n \Sigma_n(\omega) \phi_n(k) \approx \sum_n \Sigma_n(\omega) \phi_n(k)\]

Systematic truncation with cluster sites \(N_c\)

Basis functions

Example: Tiling of the BZ:

\[\epsilon_p = -2t(\cos(p_x) + \cos(p_y)) - 4t' \cos(p_x) \cos(p_y)\]

‘Machinery’ for obtaining approximated self energy: Cluster scheme. We use the DCA: \(\phi\) constant on patches in the BZ

Cluster DMFT is a **controlled approximation**, exact for \(N_c \rightarrow \infty\)

Restriction to paramagnetic bath (no long-ranged AFM here)

Georges, Kotliar, Phys. Rev. B 45, 6479 (1992),
Jarrell, Phys. Rev. Lett. 69, 168 (1992),
Georges et al., Rev. Mod. Phys. 68, 13 (1996),

Cluster DMFT – impurity solvers

\[ \Sigma(k, \omega) = \sum_n \Sigma_n(\omega) \phi_n(k) \approx \sum_n \Sigma_n(\omega) \phi_n(k) \]

Algorithm that produces \( \sum_n(\omega) \): Mapping onto a quantum impurity problem & self-consistent hybridization with a “bath”.

\[ H_{QI} = H_{\text{loc}} + H_{\text{hyb}} + H_{\text{bath}} \]

\[ H_{\text{loc}} = \sum_i \epsilon_i (n_{i\uparrow} + n_{i\downarrow}) + U n_{i\uparrow} n_{i\downarrow} \]

\[ H_{\text{bath}} = \sum_{k\alpha} \epsilon_{k\alpha} c_{k\alpha}^\dagger c_{k\alpha} \]

\[ H_{\text{hyb}} = \sum_{k\alpha b} V_{k}^{\alpha b} c_{k\alpha}^\dagger d_{b} + H.c. \]

Computationally hard part: obtaining the impurity Green’s function / self energy from this Hamiltonian:

• Solve large cluster impurity problems, at and away from half filling, for small and large interactions (density-density), at finite temperature.

• No further approximations (\( \Delta \tau \) - errors, bath discretization, ...).

Cluster DMFT – impurity solvers

\[ \Sigma(k, \omega) = \sum_n \Sigma_n(\omega) \phi_n(k) \approx \sum_n \Sigma_n(\omega) \phi_n(k) \]

Algorithm that produces \( \sum_n(\omega) \): Mapping onto a quantum impurity problem & self-consistent hybridization with a “bath”.

\[ H_{QI} = H_{loc} + H_{hyb} + H_{bath} \]

\[ H_{loc} = \sum_i \epsilon_i(n_{i\uparrow} + n_{i\downarrow}) + Un_{i\uparrow}n_{i\downarrow} \]

\[ H_{bath} = \sum_{k\alpha} \epsilon_{k\alpha} c_{k\alpha}^{\dagger} c_{k\alpha} \]

\[ H_{hyb} = \sum_{k\alpha b} V_{k}^{\alpha b} c_{k\alpha}^{\dagger} d_{b} + H.c. \]

Only Candidates: Continuous-Time quantum Monte Carlo algorithms. We use: Continuous-Time Auxiliary Field (CT-AUX) algorithm.

Continuous-Time quantum Monte Carlo impurity solvers

Diagrammatic expansion of the partition function of an impurity model in the interaction or the hybridization, sampling of the resulting series stochastically up to infinite order.

\[ H_{QI} = H_a + H_b \]

\[ Z = \text{Tr} \int_0^\beta d\tau e^{-\beta H_a} \exp \left[ - \int_0^\beta d\tau H_b(\tau) \right] = \sum_k (-1)^k \int_0^\beta d\tau_1 \cdots \int_{\tau_{k-1}}^\beta d\tau_k \text{Tr} \left[ e^{-\beta H_a} H_b(\tau_k) H_b(\tau_{k-1}) \cdots H_b(\tau_1) \right] \]

Hybridization Expansion

\[ H_a = H_{\text{loc}}; \]
\[ H_b = H_{\text{hyb}} + H_{\text{bath}} \]

Exponential scaling in size of local Hilbert space

Continuous-Time Auxiliary Field

\[ H_a = H_{\text{bath}} + H_{\text{hyb}} + H_{\text{loc}}^0; \]
\[ H_b = H_{\text{loc}}^I \]

Efficiency dependent on type of interaction in \( H_{\text{loc}}^I \)

Continuous-Time Auxiliary Field impurity solver

Auxiliary field decoupling of interaction term \( s = \pm 1 \)

\[
Z = \sum_{k=0}^{\infty} \sum_{s_1, \ldots, s_k = \pm 1} \int_0^\beta d\tau_1 \cdots \int_{\tau_{k-1}}^\beta d\tau_k \left( \frac{K}{2\beta} \right)^k Z_k(\{ s_k, \tau_k \}),
\]

\[
Z_k(\{ s_i, \tau_i \}) \equiv \text{Tr} \prod_{i=k}^1 \exp(-\Delta \tau_i H_0) \exp(s_i \gamma(n^\uparrow - n^\downarrow)).
\]

\[
1 - \frac{\beta U}{K} \left( n^\uparrow n^\downarrow - \frac{n^\uparrow + n^\downarrow}{2} \right) = \frac{1}{2} \sum_{s = \pm 1} \exp \left( \gamma s (n^\uparrow - n^\downarrow) \right),
\]

\[
\cosh(\gamma) = 1 + \frac{U\beta}{2K}.
\]

Stochastic sampling of diagrams of the partition function:

No truncation of expansion!
Continuous-Time Auxiliary Field impurity solver

Stochastic sampling of diagrams of the partition function:

Auxiliary field decoupling of interaction term \( s = \pm 1 \)

\[
Z = \sum_{k=0}^{\infty} \sum_{s_1, \ldots, s_k = \pm 1} \int_{0}^{\beta} d\tau_1 \cdots \int_{\tau_{k-1}}^{\beta} d\tau_k \left( \frac{K}{2\beta} \right)^k Z_k(\{s_k, \tau_k\}),
\]

\[
Z_k(\{s_i, \tau_i\}) \equiv \text{Tr} \prod_{i=k}^{1} \exp(-\Delta \tau_i H_0) \exp(s_i \gamma(n_\uparrow - n_\downarrow)).
\]

1 - \( \beta U K \left( n_{i\uparrow} n_{i\downarrow} - \frac{n_{i\uparrow} + n_{i\downarrow}}{2} \right) \) = \( \frac{1}{2} \sum_{s=\pm 1} \exp(\gamma s (n_{i\uparrow} - n_{i\downarrow})) \),

\[
\cosh(\gamma) = 1 + \frac{U \beta}{2K}.
\]

Compute trace of product of exponentials of one-body operators as determinant of matrix.
Continuous-Time Auxiliary Field impurity solver

Auxiliary field decoupling of interaction term $s=\pm 1$

\[
Z = \sum_{k=0}^{\infty} \sum_{s_1, \ldots, s_k = \pm 1} \int_{0}^{\beta} d\tau_1 \cdots \int_{\tau_{k-1}}^{\beta} d\tau_k \left( \frac{K}{2\beta} \right)^k Z_k(\{s_k, \tau_k\}),
\]

\[
Z_k(\{s_i, \tau_i\}) \equiv \text{Tr} \prod_{i=k}^{1} \exp(-\Delta \tau_i H_0) \exp(s_i \gamma (n_\uparrow - n_\downarrow)).
\]

\[
1 - \frac{\beta U}{K} \left( n_{i\uparrow} n_{i\downarrow} - \frac{n_{i\uparrow} + n_{i\downarrow}}{2} \right) = \frac{1}{2} \sum_{s=\pm 1} \exp \left( \gamma s (n_{i\uparrow} - n_{i\downarrow}) \right),
\]

\[
cosh(\gamma) = 1 + \frac{U \beta}{2K}.
\]

Stochastic sampling of diagrams of the partition function:

No truncation of expansion!
Continuous-Time Auxiliary Field impurity solver

Auxiliary field decoupling of interaction term $s=\pm 1$

$$Z = \sum_{k=0}^{\infty} \sum_{s_1, \ldots, s_k=\pm 1} \int_0^\beta d\tau_1 \cdots \int_{\tau_{k-1}}^\beta d\tau_k \left( \frac{K}{2\beta} \right)^k Z_k(\{s_k, \tau_k\}),$$

$$Z_k(\{s_i, \tau_i\}) \equiv \text{Tr} \prod_{i=k}^1 \exp(-\Delta \tau_i H_0) \exp(s_i \gamma(n_\uparrow - n_\downarrow)).$$

Compute trace of product of exponentials of one-body operators as determinant of matrix.

Stochastic sampling of diagrams of the partition function:

No truncation of expansion!
Continuous-Time Auxiliary Field impurity solver

Auxiliary field decoupling of interaction term $s=\pm 1$

\[
Z = \sum_{k=0}^{\infty} \sum_{s_1, \ldots, s_k = \pm 1} \int_0^\beta d\tau_1 \cdots \int_{\tau_{k-1}}^\beta d\tau_k \left( \frac{K}{2\beta} \right)^k \mathbb{Z}_k(\{s_k, \tau_k\}),
\]

\[
\mathbb{Z}_k(\{s_i, \tau_i\}) \equiv \text{Tr} \prod_{i=k}^1 \exp(-\Delta \tau_i H_0) \exp(s_i \gamma (n_\uparrow - n_\downarrow)).
\]

\[
1 - \frac{\beta U}{K} \left( n_\uparrow n_\downarrow - \frac{n_\uparrow + n_\downarrow}{2} \right) = \frac{1}{2} \sum_{s=\pm 1} \exp(\gamma s(n_\uparrow - n_\downarrow)),
\]

\[
\cosh(\gamma) = 1 + \frac{U\beta}{2K}.
\]

Stochastic sampling of diagrams of the partition function:

No truncation of expansion!
Continuous-Time Auxiliary Field impurity solver

Auxiliary field decoupling of interaction term $s=\pm 1$

$$Z = \sum_{k=0}^{\infty} \sum_{s_1, \ldots, s_k = \pm 1} \int_0^\beta d\tau_1 \cdots \int_0^\beta d\tau_k \left( \frac{K}{2\beta} \right)^k Z_k(\{s_k, \tau_k\}),$$

$$Z_k(\{s_i, \tau_i\}) \equiv \text{Tr} \prod_{i=k}^1 \exp(-\Delta \tau_i H_0) \exp(s_i \gamma (n_\uparrow - n_\downarrow)).$$

Partition function expansion

$$1 - \frac{\beta U}{K} \left( n_{i\uparrow} n_{i\downarrow} - \frac{n_{i\uparrow} + n_{i\downarrow}}{2} \right) = \frac{1}{2} \sum_{s=\pm 1} \exp(\gamma s (n_{i\uparrow} - n_{i\downarrow})), $$

$$\cosh(\gamma) = 1 + \frac{U \beta}{2K}.$$ 

Computes trace of product of exponentials of one-body operators as determinant of matrix.

Stochastic sampling of diagrams of the partition function:

No truncation of expansion!
Continuous-Time Auxiliary Field impurity solver

Auxiliary field decoupling of interaction term $s = \pm 1$

$$Z = \sum_{k=0}^{\infty} \sum_{s_1, \ldots, s_k = \pm 1} \int_0^\beta d\tau_1 \cdots \int_{\tau_{k-1}}^\beta d\tau_k \left( \frac{K}{2\beta} \right)^k Z_k(\{s_k, \tau_k\}),$$

$$Z_k(\{s_i, \tau_i\}) \equiv \text{Tr} \prod_{i=k}^{1} \exp(-\Delta \tau_i H_0) \exp(s_i \gamma (n_i^\uparrow - n_i^\downarrow)).$$

Stochastic sampling of diagrams of the partition function:

No truncation of expansion!

$$1 - \frac{\beta U}{K} \left( n_{i^\uparrow} n_{i^\downarrow} - \frac{n_{i^\uparrow} + n_{i^\downarrow}}{2} \right) = \frac{1}{2} \sum_{s=\pm 1} \exp(\gamma s (n_{i^\uparrow} - n_{i^\downarrow})), \quad \cosh(\gamma) = 1 + \frac{U\beta}{2K}.$$
Continuous-Time Auxiliary Field impurity solver

Auxiliary field decoupling of interaction term $s=\pm 1$

$$Z = \sum_{k=0}^{\infty} \sum_{s_1, \ldots, s_k=\pm 1} \int_0^\beta d\tau_1 \cdots \int_0^\beta d\tau_k \left( \frac{K}{2\beta} \right)^k Z_k(\{s_k, \tau_k\}),$$

$$Z_k(\{s_i, \tau_i\}) \equiv \text{Tr} \prod_{i=k}^1 \exp(-\Delta \tau_i H_0) \exp(s_i \gamma (n_i^\uparrow - n_i^\downarrow)).$$

Partition function expansion

Compute trace of product of exponentials of one-body operators as determinant of matrix.

Stochastic sampling of diagrams of the partition function:

No truncation of expansion!
Continuous-Time Auxiliary Field impurity solver

Expansion order

Average expansion order as a function of interaction

Average expansion order as a function of inverse temperature

32-site cluster
- U/t=8, βt=2
  half filling

2d Hubbard DCA

Interaction expansion
Hybridization expansion

Bethe lattice βt=30

Interaction expansion
Hybridization exp.
Discrete time

Bethe lattice U/t=4
Sub-Matrix updates

Standard updates in auxiliary field impurity solvers: rank one operations (ger), $O(N^2)$ operations for $O(N^2)$ data: dominated by data access.

Sub-Matrix updates: based on matrix (gemm) operations: $O(N^3)$ operations on $O(N^2)$ data: runs at speed of (fast) CPU/Cache.

Linear algebra reformulated, overhead grows with size of $\Gamma$ but operations 10x faster.
Sub-Matrix updates

Scaling as a function of problem size

Scaling as a function of # of CPUs (single particle measurements)
‘Optical Lattice Emulator’: Goal is to experimentally simulate simple model Hamiltonians using cold atomic (fermionic) gases

Test model: 3D Hubbard

\[ H = - \sum_{\langle ij \rangle, \sigma} t_{ij}(c_{i\sigma}^\dagger c_{j\sigma} + c_{j\sigma}^\dagger c_{i\sigma}) + U \sum_i n_{i\uparrow} n_{i\downarrow}. \]

Temperatures in experiment are high (for now).
Questions to theory

When will we reach $T_N$?

What is the equation of state of this model? (for all fillings, as a function of $U/t$ and $T/t$?)

Exact answer needed.
Controlling DCA

Solve quantum impurity model self-consistently for a range of cluster sizes:

Compute thermodynamics: energy, density, entropy, free energy, double occupancy, spin correlation functions, ...: Observable estimates and errors for a finite size system.

Extrapolate observable estimate to the infinite system size limit using known finite size scaling.

$E/t$ vs $N^{-2/3}$

$U=8, n=1$

Controlling DCA

Validation against lattice QMC (1/2 filling) and HTSE (high T)

Comparison HTSE / DCA? (6th, 8th, 10th order)

HTSE order by order convergence: at U=8 correct down to $T \sim 1.6t$ (at half filling). Worse away from half filling.

Agreement of 10th order HTSE with DCA down to $T \sim 1.4t$.

Agreement with lattice QMC within error bars with for all T

How well does single site DMFT work? (Single Site, PM self consistency)

First deviations at half filling are visible at $T \sim 1.6t$ [ AFM $T_N$ at $\sim 0.5t$ ]

Away from half filling, for $n \leq 0.7$: same behavior as in 2D; DMFT is essentially exact, no momentum dependence of the self energy:

$$\Sigma(k, \omega) = \sum_n \Sigma_n(\omega) \phi_n(k) = \Sigma_{DMFT}(\omega)$$

$n < 0.7$
Solve quantum impurity model self-consistently for a range of cluster sizes:

- 18
- 36
- 48
- 56
- 64
- 84
- 100

Compute thermodynamics: energy, density, entropy, free energy, double occupancy, spin correlation functions, …: Observable estimates and errors for a finite size system.

Extrapolate observable estimate to the infinite system size limit using known finite size scaling.

Controlling DCA

Solve quantum impurity model self-consistently for a range of cluster sizes:

- 18
- 36
- 48
- 56
- 64
- 84
- 100

Compute thermodynamics: energy, density, entropy, free energy, double occupancy, spin correlation functions, …: Observable estimates and errors for a finite size system.

Extrapolate observable estimate to the infinite system size limit using known finite size scaling

Results for finite clusters without extrapolations are not accurate!

Controlling DCA

Solve quantum impurity model self-consistently for a range of cluster sizes:

18 36 48 56 64 84 100

Compute thermodynamics: energy, density, entropy, free energy, double occupancy, spin correlation functions, ...: Observable estimates and errors for a finite size system.

Extrapolate observable estimate to the infinite system size limit using known finite size scaling

Controlling DCA

k-dependence of the self energy systematically reintroduced, convergence for self energy observed: Approximation controlled

High temperature $T/t = 1$: Exact convergence of the self energy as a function of cluster size.
k-dependence of the self energy systematically reintroduced, convergence for self energy observed: Approximation controlled

High temperature $T/t = 1$: Exact convergence of the self energy as a function of cluster size.

Intermediate temperature $T/t = 0.5$: Convergence visible, extrapolation needed.
Controlling DCA

k-dependence of the self energy systematically reintroduced, convergence for self energy observed: Approximation controlled

High temperature $T/t = 1$: Exact convergence of the self energy as a function of cluster size.

Intermediate temperature $T/t = 0.5$: Convergence visible, extrapolation needed.

Low temperature $T/t = 0.35$: Convergence not obvious, critical regime with diverging correlation length not well captured. ($\sim T_N$)
Finite Size Simulations vs DCA

- **Convergence** in DCA is **faster**: results from 64-84-100 sites comparable to $6^3$, $8^3$, $10^3$ sites in lattice simulation.

- **Sign problem** is **better** (‘bath helps with sign problem’) near half filling.
3D Hubbard Model (conclusions)

We have solved the 3D Hubbard model (at high temperature)! Full tables, entire phase diagram with energies, densities, entropies, double occupancies, spin correlation functions available online

http://prl.aps.org/supplemental/PRL/v106/i3/e030401

Finite size scaling feasible for non-trivial systems in practice: change the status of cluster DMFT from an uncontrolled approximation to a method for obtaining controlled results with accurate error bars, similar to BSS / finite Lattice simulations

Nontrivial regime accessible: about 5x lower in temperature than HTSE & DMFT.
Cluster DMFT

Variation of cluster sizes and geometries, crucial to establish robustness of features!

In DCA: No periodization / interpolation schemes.

In this talk: cluster geometries of size 2–16 (larger: hampered by sign problem)

Clear Nodal / Antinodal separation on clusters large enough.
Cluster DMFT

Variation of cluster sizes and geometries, crucial to establish robustness of features!

In DCA: No periodization / interpolation schemes.

In this talk: cluster geometries of size 2–16 (larger: hampered by sign problem)

Clear Nodal / Antinodal separation on clusters large enough.
2D Hubbard with $t'$: Generic Phase Diagram

See also:
M. Ferrero, P. S. Cornaglia, L. De Leo, O. Parcollet, G. Kotliar, and A. Georges, EPL 85, 57009 (2009)
…and several other studies…

New aspects:
Larger clusters, lower temperatures, scans of entire phase diagrams:
enabled by new computational methods.

Generic Phase Diagram

2D Hubbard: Phase diagram as a function of interaction and doping, on large clusters

Interaction U

Strong particle-hole asymmetry:
\[ t'/t \sim -0.15 \text{ to } -0.3 \]
\[ \beta t \sim 20 \]

Momentum space differentiated along this line

Cuprates along this line

PG / MomentumSelective

Fermi-Liquid-like regime

Momentum-differentiated

Fermi-Liquid-like regime

Electron doping

doping x

Hole doping


**Generic Phase Diagram**

2D Hubbard: Phase diagram as a function of interaction and doping, on large clusters

interaction $U$

strong particle-hole asymmetry:
$t'/t \sim -0.15 - -0.3$

$\beta t \sim 20$

**Fermi-Liquid-like regime**

**Momentum Selective**

**Cuprates** along this line

**Fermi-Liquid-like regime**


Generic Phase Diagram

2D Hubbard: Phase diagram as a function of interaction and doping, on large clusters

interaction U

strong particle-hole asymmetry:
\( t'/t \sim -0.15 \text{--} -0.3 \)
\( \beta t \sim 20 \)

PG /
Momentum Selective

Momentum differentiated

Cuprates along this line

Fermi-Liquid-like regime

Fermi-Liquid-like regime


Phase Diagram

8-site Matsubara self-energy: blue: antinode. red: node

Isotropic Fermi Liquid

Momentum Space Differentiation

Sector Selectivity / Pseudogap

Mott Insulator
Interaction transitions at half filling

For weak interaction: **Fermi-Liquid** (-like) phase (FLL)

Crossover: At slightly larger interaction **Momentum-Space Differentiation** (MSD), Each momentum sector consistent with Fermi Liquid, but variations between momentum sectors

**Transition 1**: (Continuous, at the $T$ accessible) to a **Sector Selective Phase**: Anti-nodal part of the Fermi surface gapped), nodal part metallic. Analogous to orbitally selective Mott transition

Momentum selectivity proposed in minimal 2-site model: M. Ferrero, P. S. Cornaglia, L. De Leo, O. Parcollet, G. Kotliar, and A. Georges, *EPL 85, 57009*

**Transition 2**: (First Order) to a **Mott insulating** Phase. All parts of the noninteracting Fermi surface gapped


see also: Liebsch, Tong, *Phys. Rev. B 80, 165126 (2009)* for CDMFT
On the hole doped side: same story as in interaction transition.

On the electron-doped side: direct transition to the **Mott Insulator**. Large $t'$: first order. Small $t'$: intermittent sector selective phase, continuous.

[1st order: see also Macridin et al., Phys. Rev. B 74, 085104 (2006)]


see also: M. Ferrero, P. S. Cornaglia, L. De Leo, O. Parcollet, G. Kotliar, and A. Georges, *EPL* 85, 57009
Doping transition at intermediate U

Direct Fermi level DOS estimator:

\[ \beta G \left( \frac{\beta}{2} \right) = \int \frac{d\omega}{2\pi T} \frac{A_K(\omega)}{\cosh \frac{\omega}{2t}} \xrightarrow{T \to 0} A_K(0) \]

Antinodal Fermi level DOS

Nodal Fermi level DOS


Doping transition at intermediate $U$

Doping transition at intermediate $U$

Direct Fermi level DOS estimator:

$$
\beta G \left( \frac{\beta}{2} \right) = \int \frac{d\omega}{2\pi T} \frac{A_K(\omega)}{\cosh \frac{\omega}{2t}} \quad T \to 0 \quad A_K(0)
$$

Antinodal Fermi level DOS

Nodal Fermi level DOS

$U = 7t, t' = -0.15t$


Doping transition at intermediate U

Direct Fermi level DOS estimator:

$$\beta G \left( \frac{\beta}{2} \right) = \int \frac{d\omega}{2\pi T} \frac{A_K(\omega)}{\cosh \frac{\omega}{2t}} \xrightarrow{T \to 0} A_K(0)$$

Antinodal Fermi level DOS

Nodal Fermi level DOS

Doping transition at intermediate U

Direct Fermi level DOS estimator:

\[ \beta G \left( \frac{\beta}{2} \right) = \int \frac{d\omega}{2\pi T} \frac{A_K(\omega)}{\cosh \frac{\omega}{2t}} \xrightarrow{T \to 0} A_K(0) \]

Antinodal Fermi level DOS

Nodal Fermi level DOS

\[ U = 7t, \ t' = -0.15t \]

Doping transition at intermediate $U$

Direct Fermi level DOS estimator:

$$\beta G \left( \frac{\beta}{2} \right) = \int \frac{d\omega}{2\pi T} \frac{A_K(\omega)}{\cosh \frac{\omega}{2t}} \quad T \to 0 \quad A_K(0)$$

**Antinodal** Fermi level DOS

**Nodal** Fermi level DOS


In momentum-selective phase pinned to Mott insulating value: antinode is incompressible, node is metallic.
for the antinodal sector.

for the nodal sector.

when reducing doping from $x=0.157$ to $x=0.047$: gap develops in the antinodal part of BZ, nodal part stays metallic.
Generic Phase Diagram

As a function of t'/t: Two transitions merging into one first order transition on the electron doped side


Sector selective transition is robust in DCA (for all clusters large enough to have nodal antinodal differentiation), is the DCA representation of pseudogap physics.
Sector selective transition is robust in DCA (for all clusters large enough to have nodal antinodal differentiation), is representative of the DCA (Fig. 2D), and our antinodal MDCs (Fig. 2C) are almost entirely dominated by nodal MDCs (Fig. 2B). To better quantify the Fermi surface splitting, and orthorhombic distortions and is summarized in Fig. 2E. The relatively weak node. To better quantify the Fermi surface splitting, and orthorhombic distortions and is contrast to the expected behavior of the van Hove singularity, where both the dispersion of the antinodal excitations is below 50 meV, in contrast to the dispersive effects of photoelectron matrix elements or differentiation), is approximately well nested and separated by approximately 100 meV. As will be discussed later, the doping dependence of the nodal and antinodal particle (QP) residue, state FS for conventional metallic or even pseudogap physics.
Sector Selective Regime: ARPES & Pseudogap

Sector selective transition is the cluster DMFT representation of pseudogap physics.

The pseudogap is a feature of the Hubbard model at intermediate correlation strength. No long range order is required. Remarkable agreement with other experimental probes: c-axis, in-plane optical conductivity, Raman.

FIG. 15. (Color online) Points: pseudogap size determined from electron spectral function as a function of hole doping $x$ for $U=7t$ and inverse temperature $\beta=20/t=200$ K. Line: linear fit to results.

Momentum space differentiation (n ~ 0.8): **Nodal** scattering rate vanishing more rapidly than **antinodal** scattering rate.

Isotropic Fermi Liquid regime (n ~ 0.7): **Nodal** and **Antinodal** scattering rate identical.

Similar to anisotropic component observed in Angle-Dependent Magneto-Resistance
Conclusions

We have established DCA as a reliable tool to obtain results for the thermodynamic limit (for the infinite (lattice) system).

**Algorithmic** and **numerical** improvements: much larger systems accessible, scans of phase space possible.

2D Hubbard model, phase diagram: contains many features observed in High-Tc experiments: Momentum space differentiation, pseudogap: Node metallic, antinode insulating. No long-ranged order required.

Sector selectivity is the Cluster DMFT signature of the pseudogap, Features are robust: observed for all clusters large enough, also in CDMFT, no interpolation / analytical continuation
Acknowledgments

Many thanks to my collaborators:

M. Ferrero, A. Georges, N. Lin, O. Parcollet, P. Werner


Funding: NSF-DMR-1006282

Computer time: Brutus cluster, ETH Zurich and the Center for Nanophase Materials Sciences at ORNL