Energetics of superconductivity in the two dimensional Hubbard model

Emanuel Gull

A.J. Millis, O. Parcollet

ES2013, College of William and Mary

Emanuel Gull, Andrew J. Millis, Oliver Parcollet, Phys. Rev. Lett. 110, 216405 (2013)

Emanuel Gull and Andrew J. Millis, arXiv:1304.6406 (2013)

Emanuel Gull and Andrew J. Millis, Phys. Rev. B 86, 241106(R) (2012)

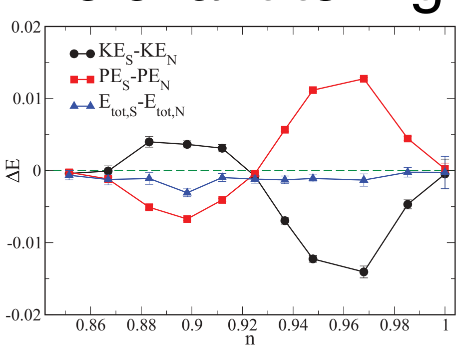
Energetics of superconductivity in the two dimensional Hubbard model

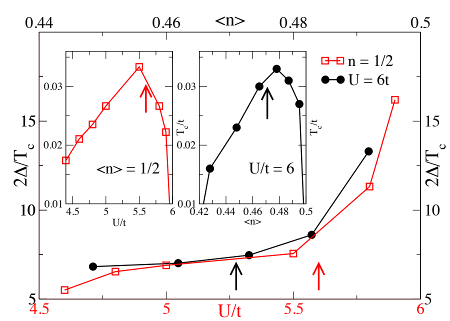
Main result: semi-quantitative solution of the **Hubbard model** in the **normal** and **superconducting** state, down to T~100K: **energetics**, **spectral functions**, optics.

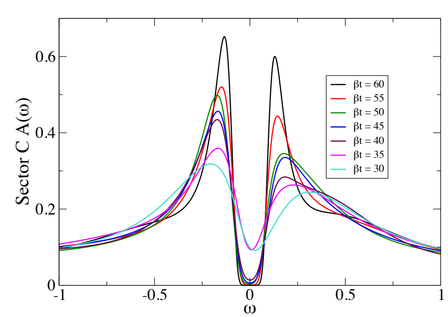
Results from cluster dynamical mean field theory.

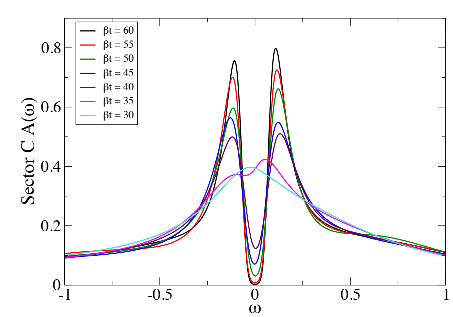
Cluster sizes large enough to see finite size effects.

Parameter ranges (interaction strength, filling, temperature) relevant to high Tc superconductivity.



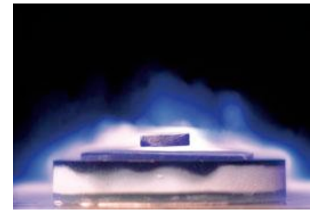


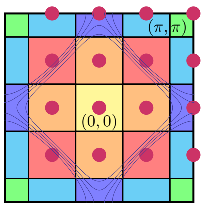




Outline

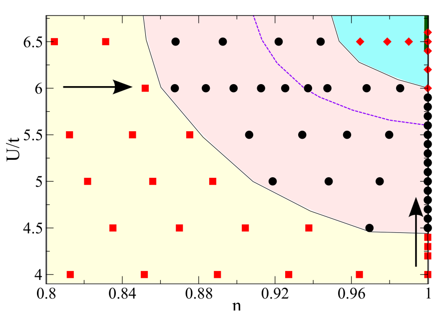
Motivation: Cuprate Experiments

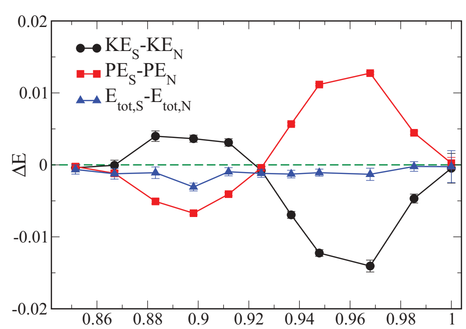


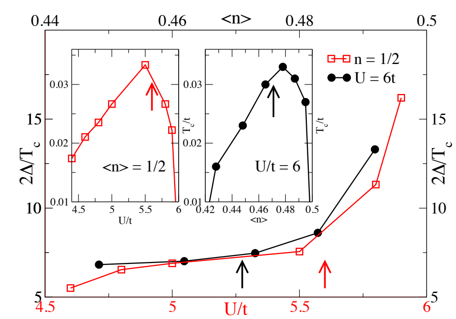


Theoretical and Numerical Methods

Phase Diagram and Results in the normal and superconducting state, energetics







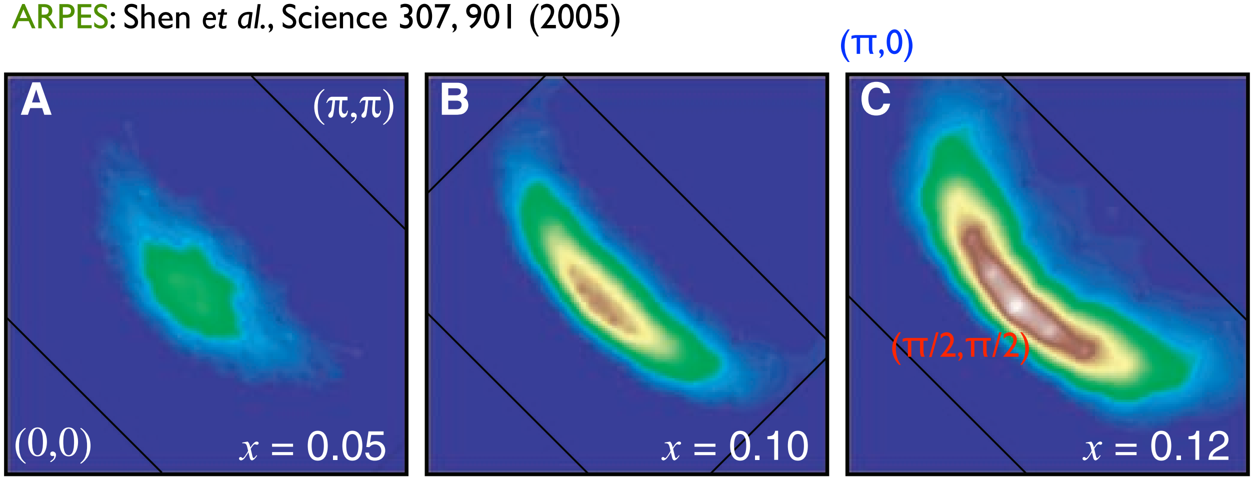
Experiments: Pseudogap

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

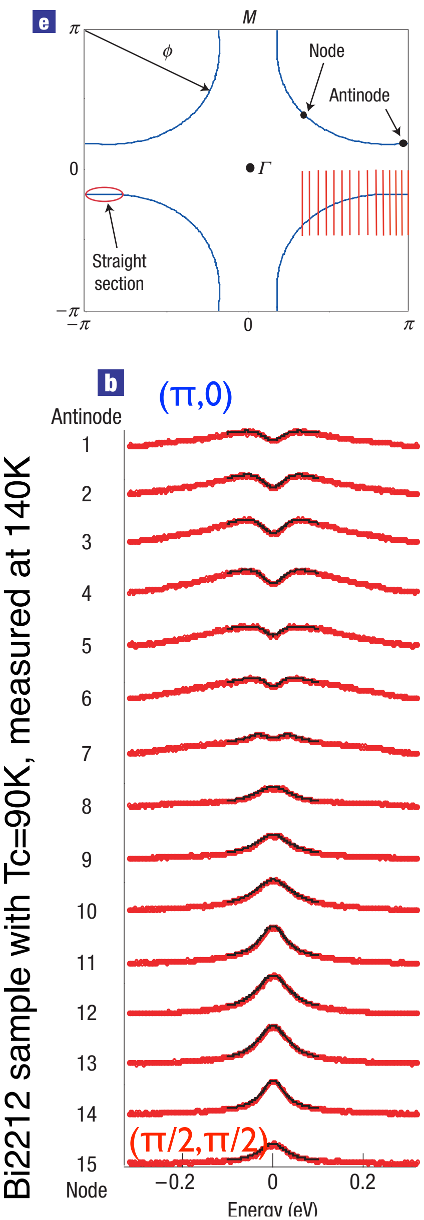
Key physics dependence on momentum around Fermi surface, Difference of spectral function around Fermi surface.

Doping dependence of region with quasiparticles

ARPES: Shen *et al.*, Science 307, 901 (2005)



ARPES: Kanigel *et al.*, Nature Physics 2, 447 - 451 (2006).
Bi2212 sample with Tc=90K, measured at 140K



Experiments: Pseudogap

Damascelli *et al.*, Rev. Mod. Phys 75, 2 (2003)

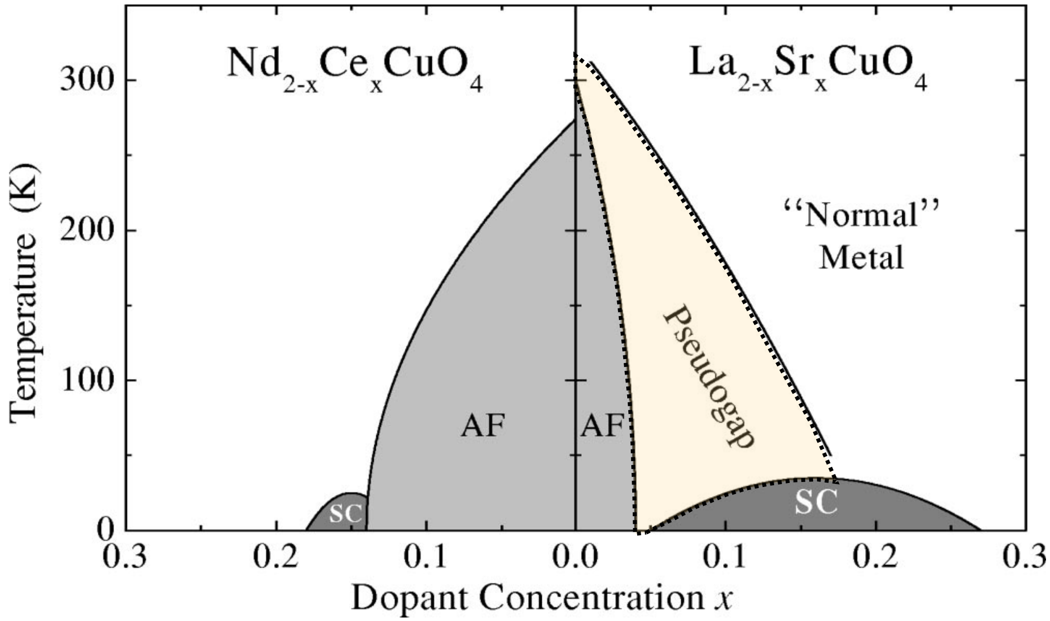
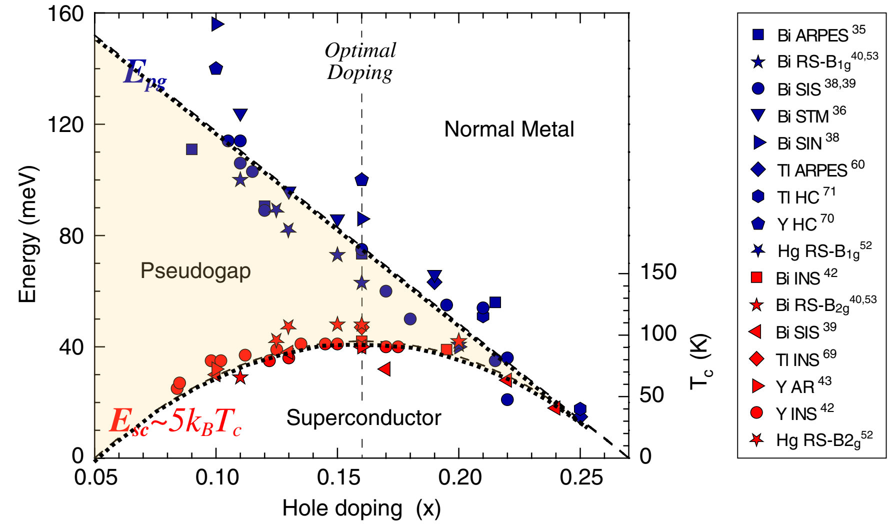


FIG. 1. Phase diagram of n- and p-type superconductors, showing superconductivity (SC), antiferromagnetic (AF), pseudogap, and normal-metal regions.

Hüfner *et al.*, Rep. Prog. Phys. 71, 062501(2008)



Takigawa *et al.*, Phys. Rev. B 43, 247

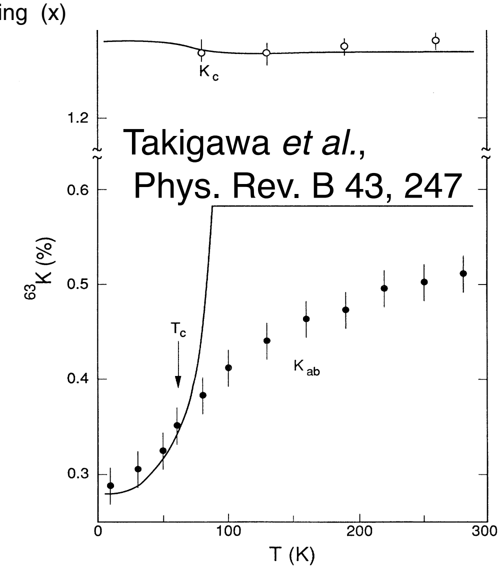


FIG. 3. Temperature dependence of the Cu(2) Knight shift (^{63}K) for $H \parallel c$ (K_c) and $H \perp c$ (K_{ab}) together with the results in the $y \simeq 0$ material reported by Barrett *et al.* (Ref. 25) (solid line). The arrow indicates the value of T_c at 10 Oe.

Pseudogap* appears only on the hole doped side.

Dopings smaller than optimal doping.

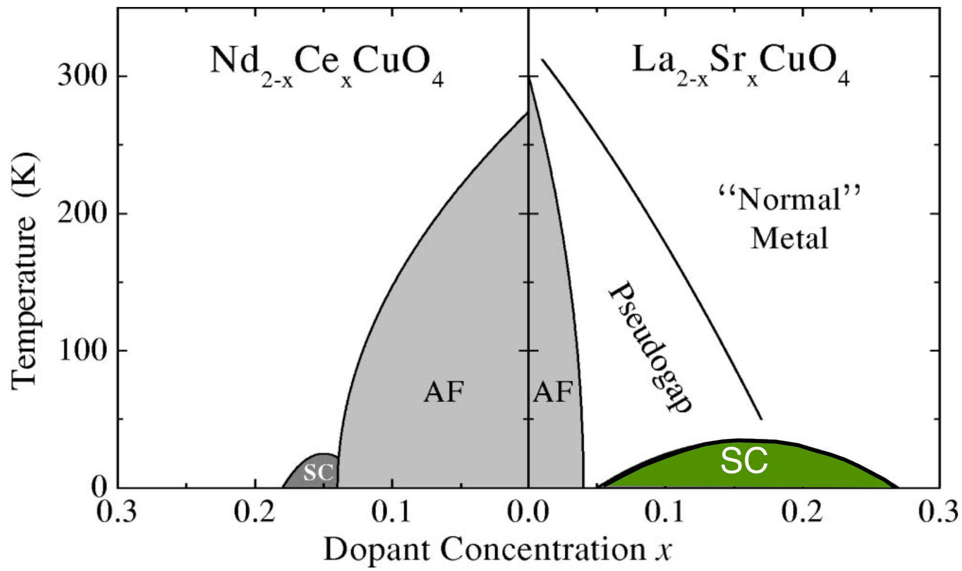
Temperatures up to ~ 300K.

Signatures also in NMR, Tunneling, c-axis conductivities, Raman…

*...of this type...

Experiments: d-wave superconductivity

Damascelli *et al.*, Rev. Mod. Phys 75, 2 (2003)



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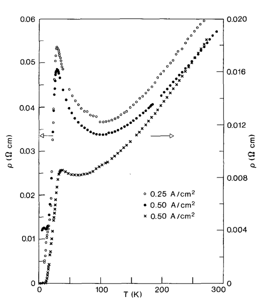
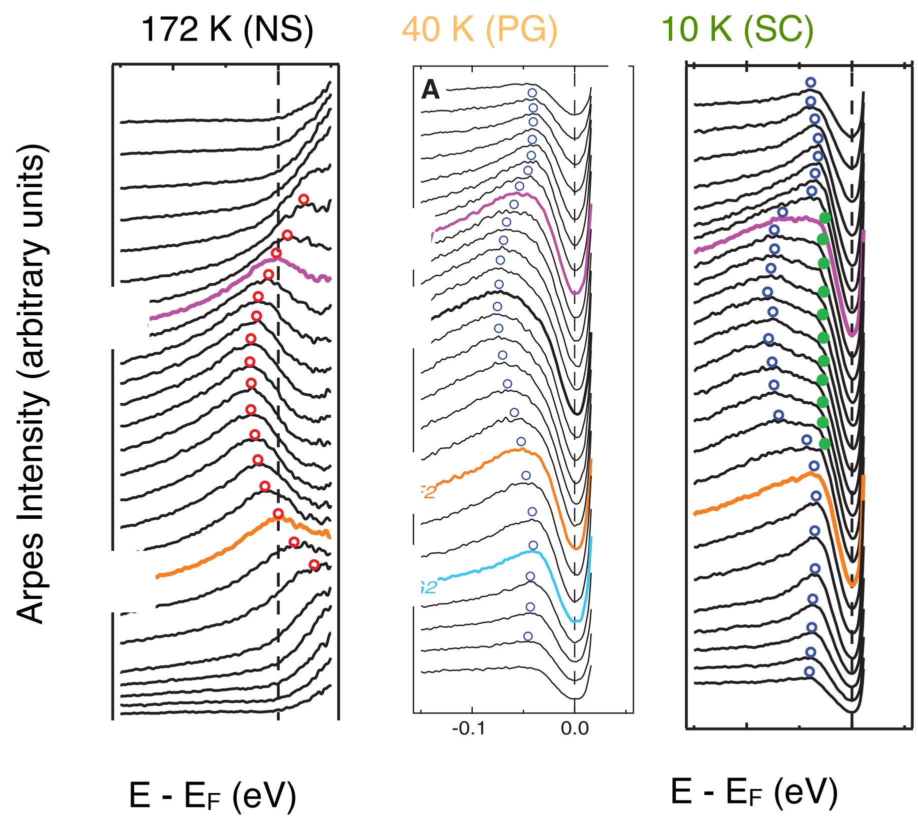
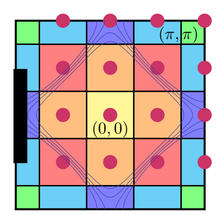


Fig. 1. Temperature dependence of resistivity in $Ba_xLa_{5-x}Cu_5O_{5(3-y)}$ for samples with x(Ba) = 1 (upper curves, left scale) and x(Ba) = 0.75 (lower curve, right scale). The first two cases also show the influence of current density

Bednorz and Müller, Z. Phys. B 64, 189 (1986)

He *et al.*, Science 331, 1579 (2011)





Arpes EDC for cuts along Brillouin-zone boundary (near $(\pi,0)$), almost optimally doped Pb-Bi2201 with T_c of 38K, T* of 132K

Questions to theory

Superconductivity at intermediate interaction strengths

Pseudogap at intermediate interaction strengths

Coexistence, precursor, competition, ?

Experiments: ARPES, ADMR, optical conductivities, Raman,…

Contained within a well-defined model + systematic and controllable approximation?

………..we will present a potential answer in this talk………

Theory: Hubbard model

Restrict to simple minimal model with kinetic and potential energy terms: Hubbard model:

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

Open theoretical question: **how much of the physics on the last pages is contained in this model?**

Even for the most simple model, when kinetic energy ~ potential energy we have no working theoretical tools: **quantum many-body theory needs numerical methods**!

Here: **Cluster DMFT**: diagrammatic approximation based on mapping of the system onto a self-consistently adjusted multi-orbital quantum impurity model, solved by numerically exact **'continuous-time' QMC**.

Simulations of **wide parameter regimes, for a range of cluster sizes/geometries.** Determine which features are robust, which may be artifacts of the model

E. Gull, O. Parcollet, A.J. Millis, Phys. Rev. Lett. 110, 216405 (2013)

Cluster DMFT

Approximation to self energy:

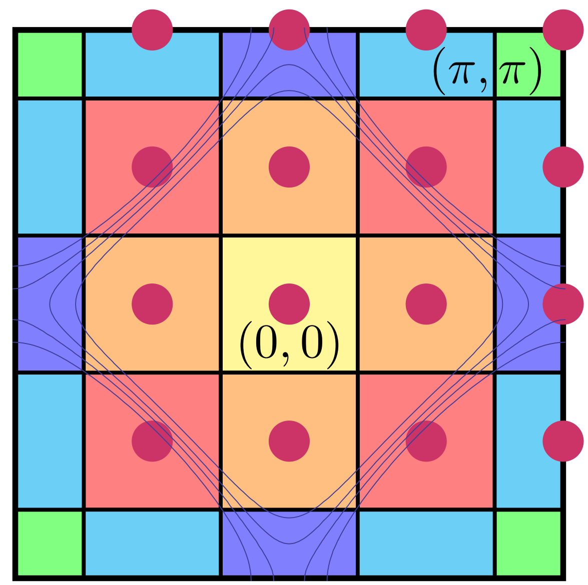
$$\Sigma(k,\omega) = \sum_{n} \Sigma_n(\omega)\phi_n(k) \approx \sum_{n}^{N_c} \Sigma_n(\omega)\phi_n(k)$$

Systematic truncation with cluster size N_c

Basis functions

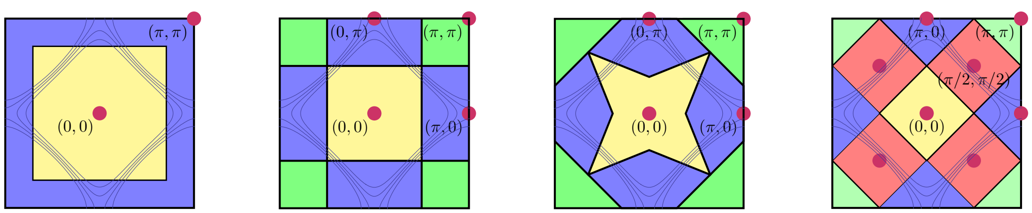
Cluster DMFT: **controlled** approximation, **exact for $N_c \to \infty$**; 'single site' DMFT for $N_c = 1$. Small parameter $1/N_c$

Example tiling of the BZ: 2d, $N_c = 16$



Cluster scheme: 'Dynamical Cluster Approximation' (DCA), basis functions ϕ constant on patches in BZ

Example tiling of the BZ: 2d, N_c = 2, 4, 4, 8



Resulting lattice system mapped onto impurity model & self-consistency

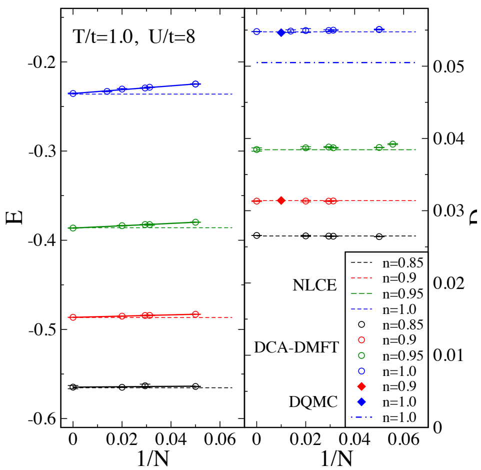
DMFT: Metzner, Vollhardt, Phys. Rev. Lett. 62, 324 (1989),
Georges, Kotliar, Phys. Rev. B 45, 6479 (1992),
Jarrell, Phys. Rev. Lett. 69, 168 (1992),
Georges et al., Rev. Mod. Phys. 68, 13 (1996)

DCA: Hettler et al., Phys. Rev. B 58, R 7475 (1998),
Lichtenstein, Katsnelson, Phys. Rev. B 62, R9283 (2000),
CDMFT: Kotliar et al., Phys. Rev. Lett. 87, 186401 (2001),
Review: T. Maier, et al., Rev. Mod. Phys. 77, 1027 (2005).

High-T: extrapolations & exact results

Results from a series of clusters with typical sizes cluster sizes: 50-100

Quantitative, numerically exact, stringent comparisons to other methods (linked cluster [very high T], lattice QMC [1/2 filling])



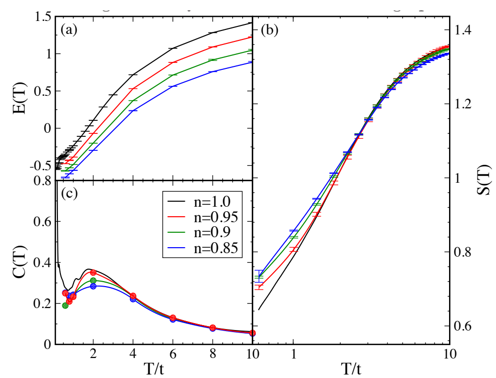
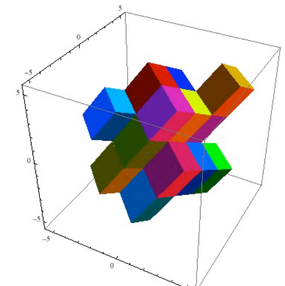
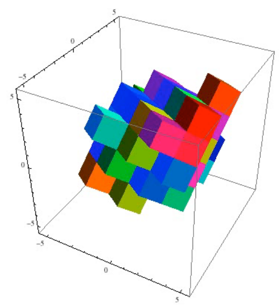


FIG. 6. (Color online) Energy, $E(T)$, entropy, $S(T)$, and specific heat capacity, $C(T)$, as functions of T/t extrapolated to the TL for $U/t = 8$ for filling values of $n = 0.85$, 0.9, 0.95, and 1.0 (half-filled).

Extrapolation to the TD limit using known finite size relations in 2d and 3d


18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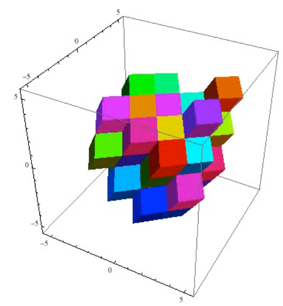
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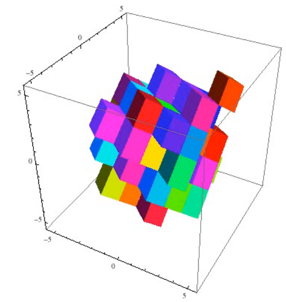

56

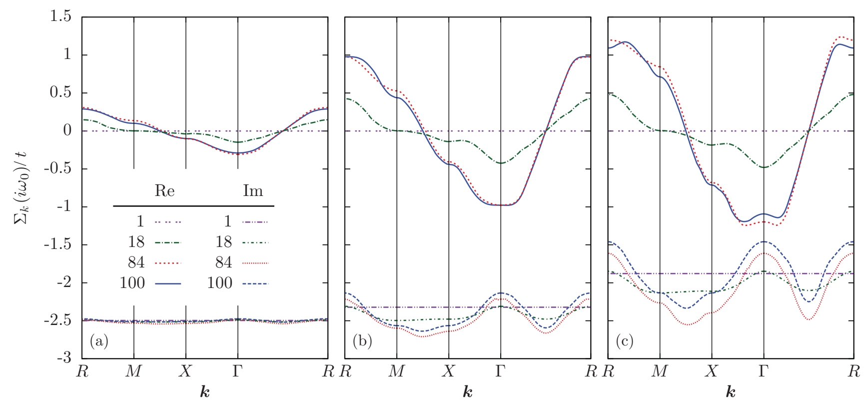
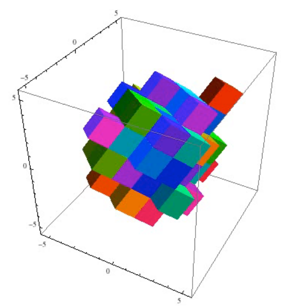


FIG. 6. (Color online) Real and imaginary parts of the lowest Matsubara frequency of the interpolated DCA cluster self-energy $\Sigma(k, i\omega_0)$ of a 3D Hubbard model above the Néel temperature,[44] for $U/t = 8$, $T/t = 1$ (left panel), $T/t = 0.5$ (middle panel), and $T/t = 0.35$ (right panel), at half filling. The lines denote DMFT results (horizontal straight lines) and results for clusters of size 18, 84, and 100. The interpolation follows a path along the high-symmetry points $\Gamma = (0,0,0)$, $X = (\pi,0,0)$, $M = (\pi,\pi,0)$, and $R = (\pi,\pi,\pi)$.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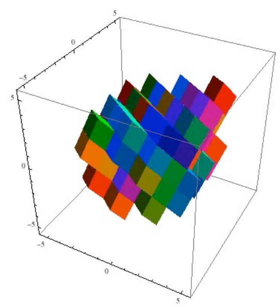
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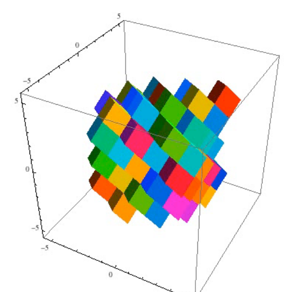
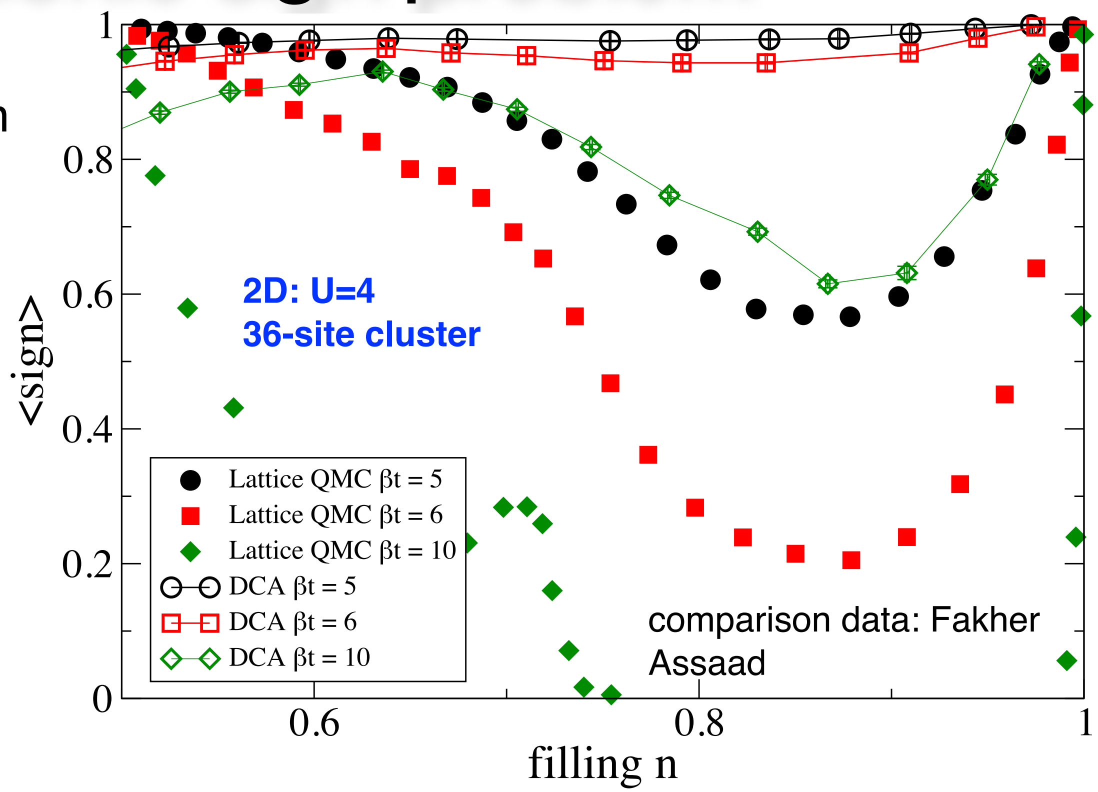

100

E. Gull, P. Staar, S. Fuchs, et al., Phys. Rev. B 83, 075122 (2011)

Low-T: fermionic sign problem



For 2D at physically interesting interaction strengths and temperatures: **No quantitative extrapolation** to TD limit.

Variation of cluster sizes and geometries, establish robustness of results and trends. What is **artifact**, what is **general**?

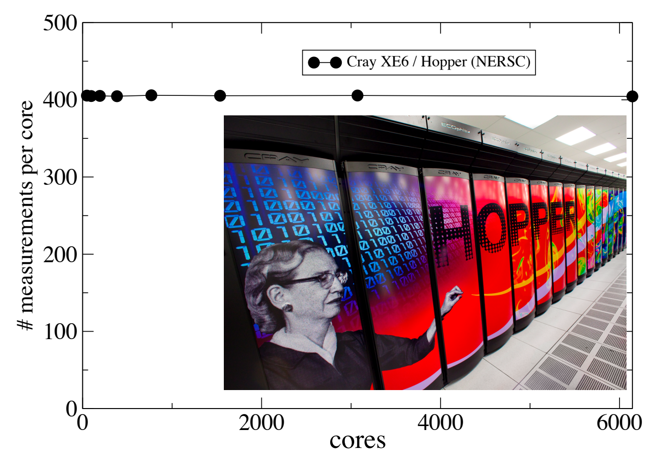
For superconductivity: cluster geometries of size 4–16.

In practice: **only** hard limitation given by **fermionic sign problem** of QMC solver

Dynamical mean field bath helps to increase <sign>, convergence to TD limit becomes more regular, absence of shell effects.

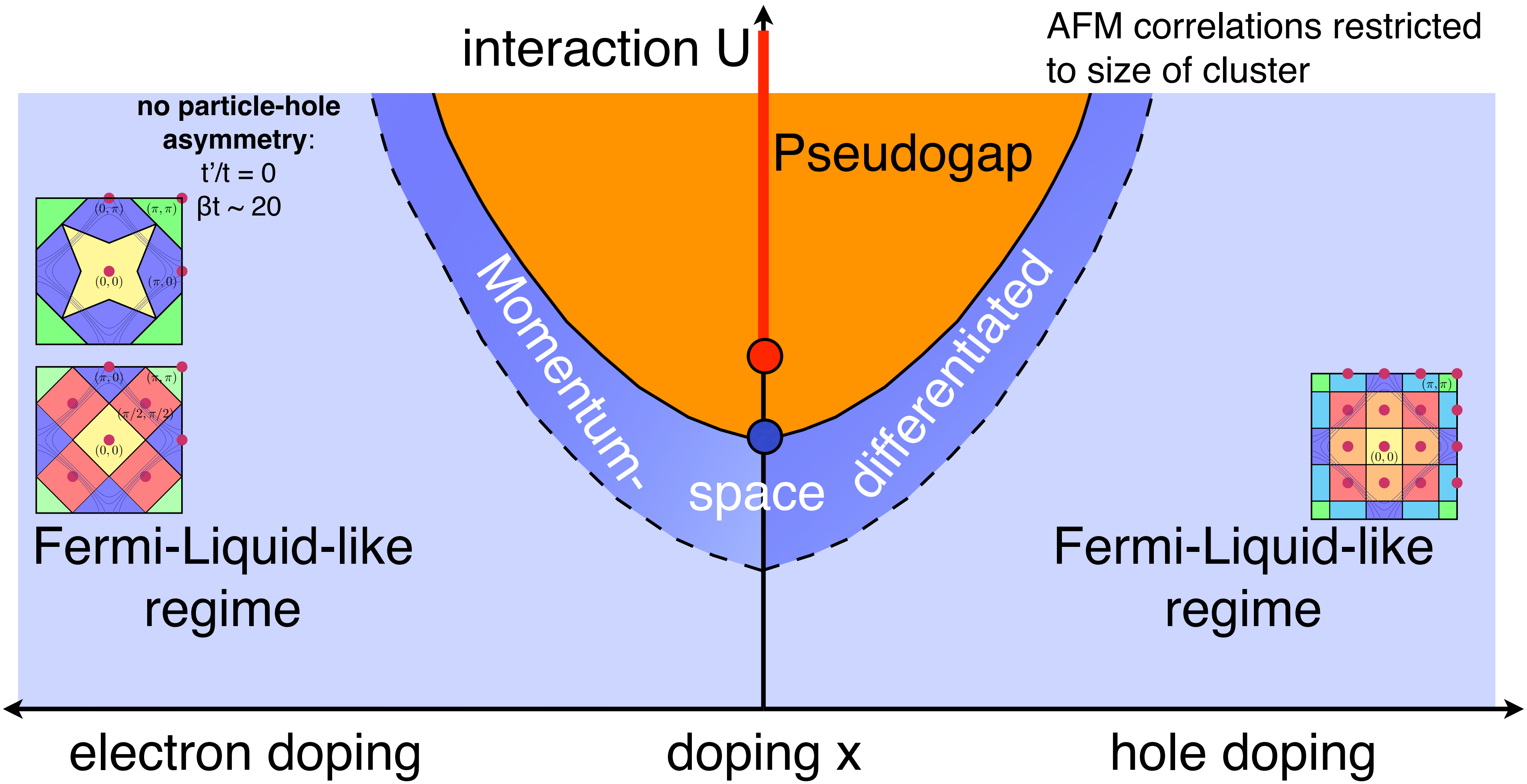
Approximation to Sigma, not G.

MC possible to scale to 10'000s of compute cores (ALPS libraries)



E. Gull, O. Parcollet, A.J. Millis, Phys. Rev. Lett. 110, 216405 (2013)

Generic U/doping Phase Diagram (high T, no t', disordered phase, ~ 200K)



P. Werner, E. Gull, O. Parcollet, A. J. Millis, Phys. Rev. B 80, 045120 (2009) (interaction)
E. Gull, O. Parcollet, P. Werner, A. J. Millis, Phys. Rev. B 80, 245102 (2009) (doping, t')
E. Gull, M. Ferrero, O. Parcollet, A. Georges, A.J. Millis, Phys. Rev. B 82, 155101 (2010) (cluster size)

E. Gull, O. Parcollet, A.J. Millis, Phys. Rev. Lett. 110, 216405 (2013)

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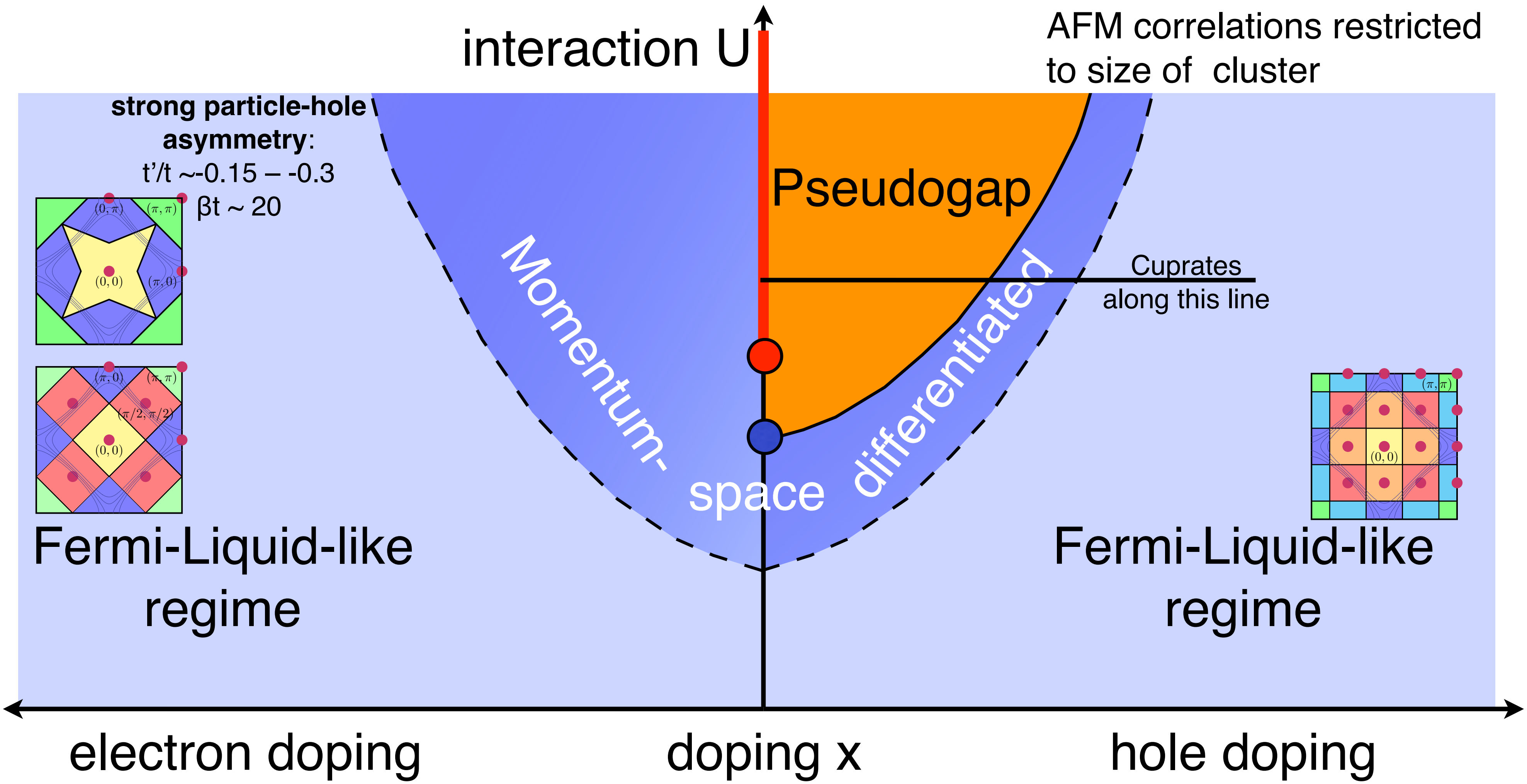

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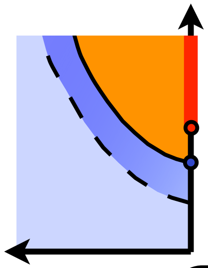
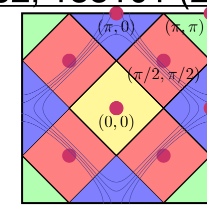
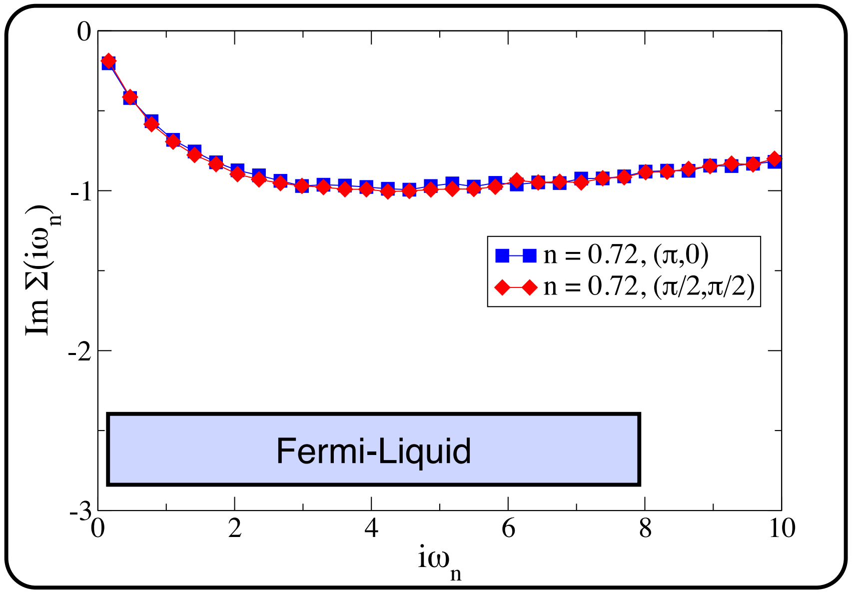
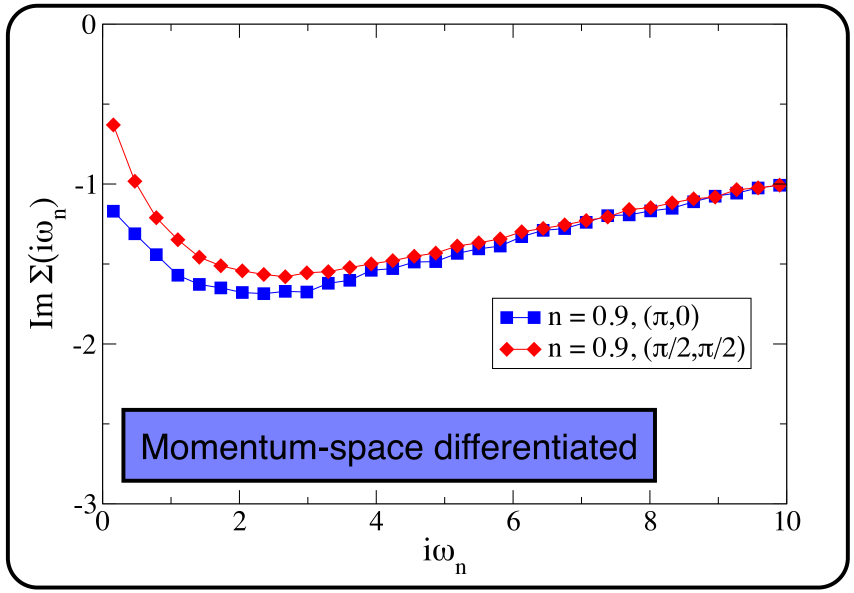


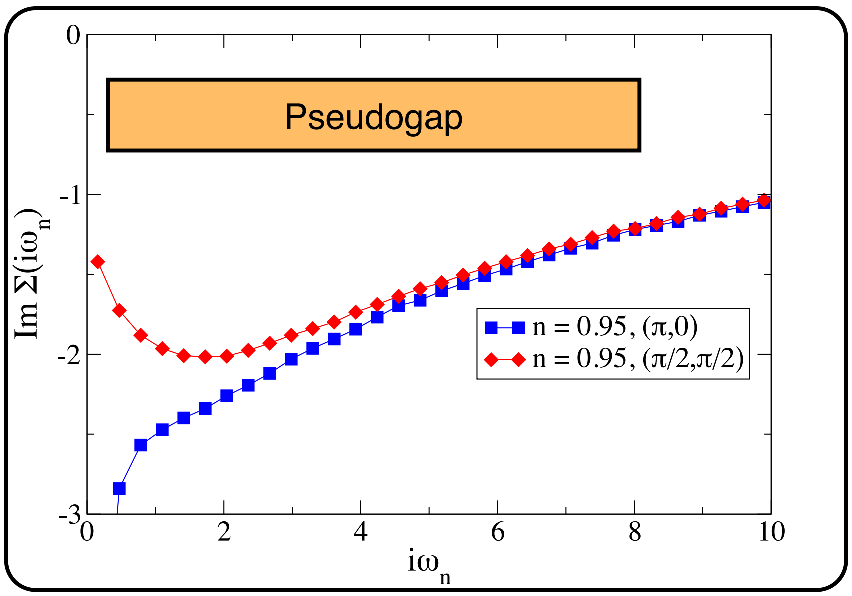
Four main phases

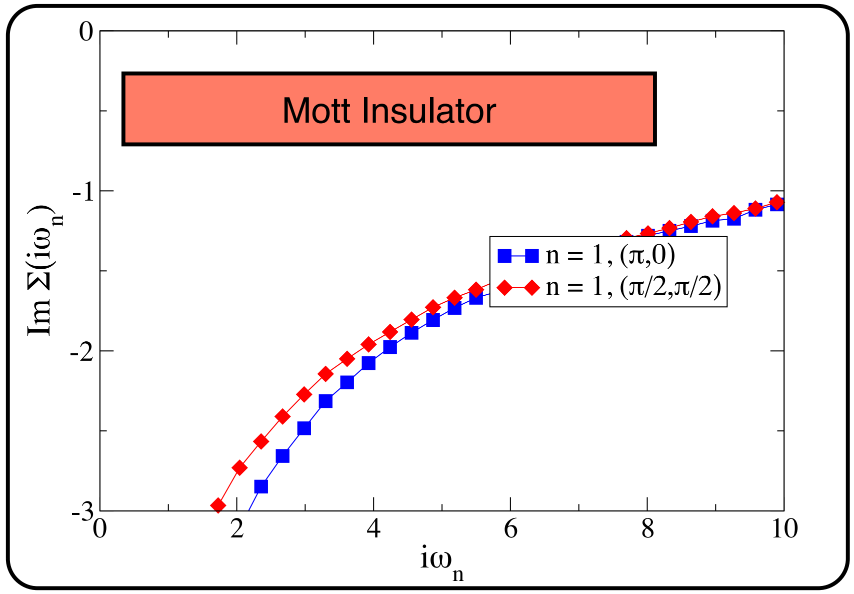


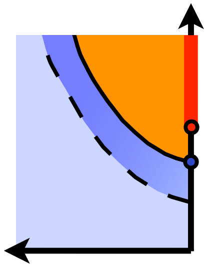
8-site Matsubara self-energy: blue: antinode. red: node









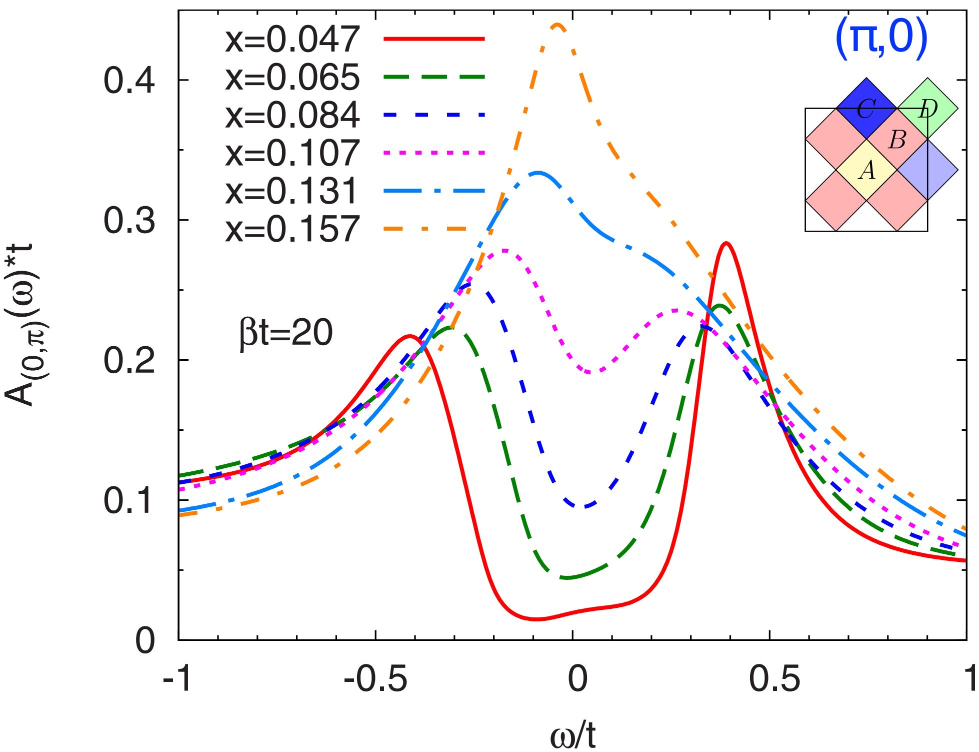


N. Lin, E. Gull, and A.J. Millis, Phys. Rev. B 82, 045104 (2010)

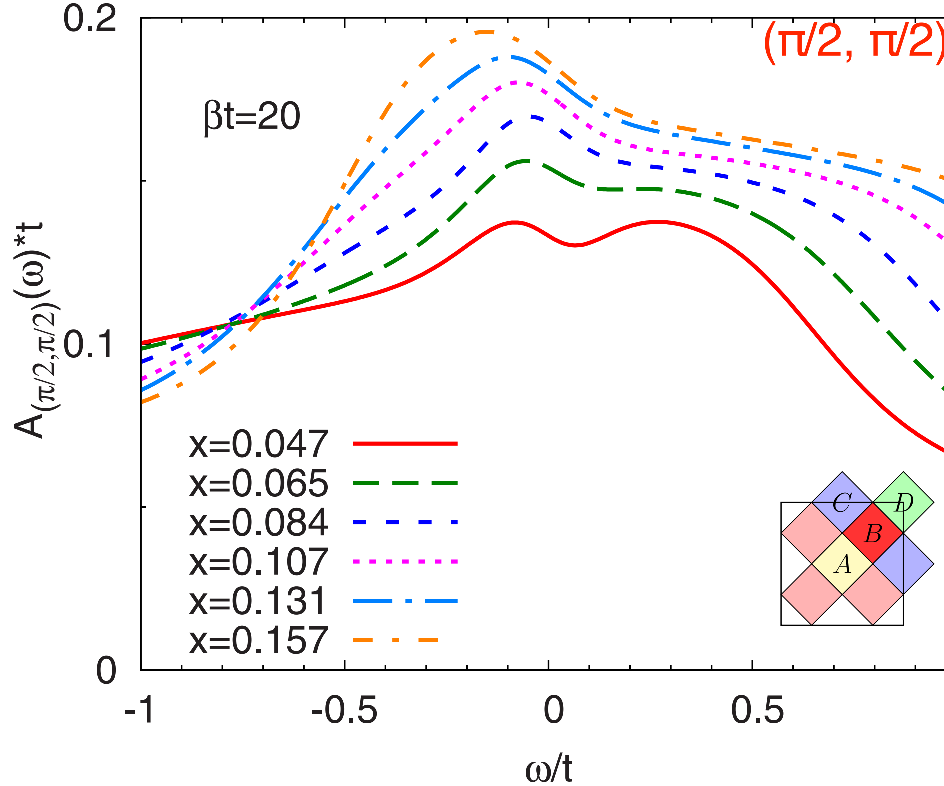
Pseudogap Regime: Spectra

Analytically continued* spectral function A(ω): U = 7t, t'/t=0.15, βt=20
(for various dopings, as a function of frequency)

for the antinodal region



for the nodal region.



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

*Maximum entropy of self-energy data

Emanuel Gull, Andrew J. Millis, Oliver Parcollet, Phys. Rev. Lett. 110, 216405 (2013)
Emanuel Gull and Andrew J. Millis, Phys. Rev. B 86, 241106(R) (2012)

d-wave Superconductivity

Low enough temperature to access the superconducting phase

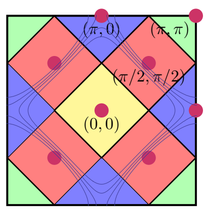
- **Large clusters that have a clear pseudogap state, different geometries**!

- **Interactions strong enough** that half-filled system is Mott insulating

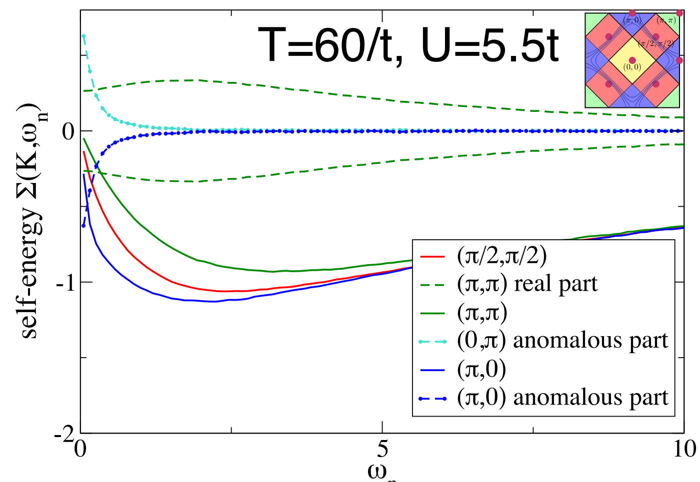
- **Numerically exact algorithms** (no bath fitting, no imaginary time discretization)

- Increase of CPU power makes **surveys of phase space** possible

- Precision good enough to perform reliable analytic continuation



d-wave superconductivity:
anomalous antinodal self-energy
(- - - -) at (pi,0) and (- - - -) at (0,pi)

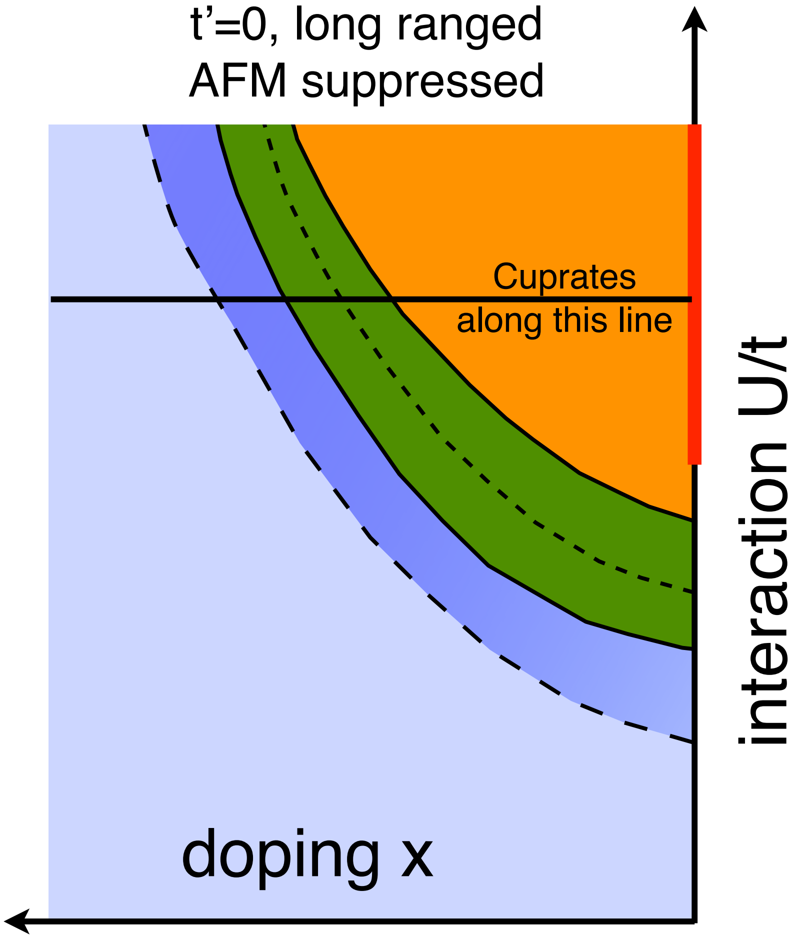


Previous work: Large clusters, phase boundary from normal state susceptibilities, U/t=4: **Maier, Jarrell**, et al., Phys. Rev. Lett. 95, 237001 (2005)

4-site clusters (Hirsch Fye), formalism: **Lichtenstein, Katsnelson**: Phys. Rev. B 62, R9283 (2000), NCA: **Maier, Jarrell, Pruschke, Keller**, Phys. Rev. Lett. . 85, 1524–1527 (2000), ED: **Kancharla** et al, PRB ’08, **Civelli** et al, PRL 08,09, PRB 08, CT-HYB: Sordi et al., arxiv 1201.1283

E. Gull, O. Parcollet, A.J. Millis, Phys. Rev. Lett. 110, 216405 (2013)

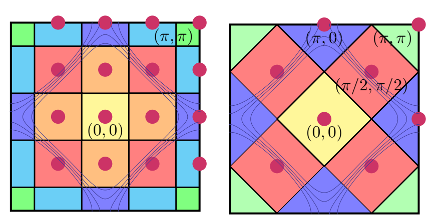
Generic U/doping Phase Diagram (low T, superconducting phase, ~ 100K)



Additional low-T phase:

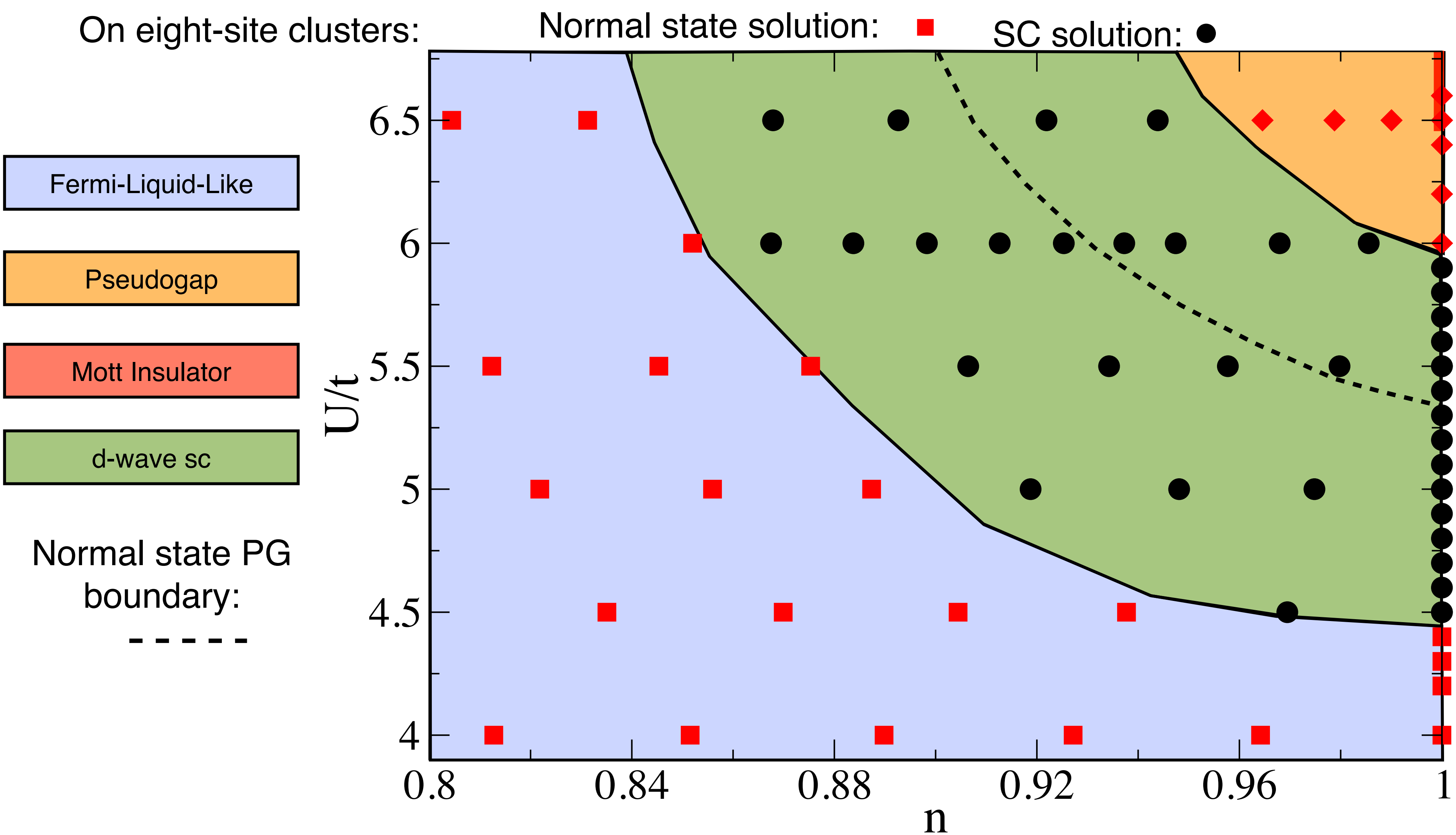
- d-wave superconductivity
- Mott Insulator
- Non-superconducting pseudogap regime
- Momentum-space differentiated regime [no sc]
- Non-superconducting Fermi-Liquid-like regime

On clusters large enough to allow for nodal/antinodal differentiation:



E. Gull, O. Parcollet, A.J. Millis, Phys. Rev. Lett. 110, 216405 (2013)

Phase Diagram
(T/t = 1/60)



E. Gull, O. Parcollet, A.J. Millis, Phys. Rev. Lett. 110, 216405 (2013)

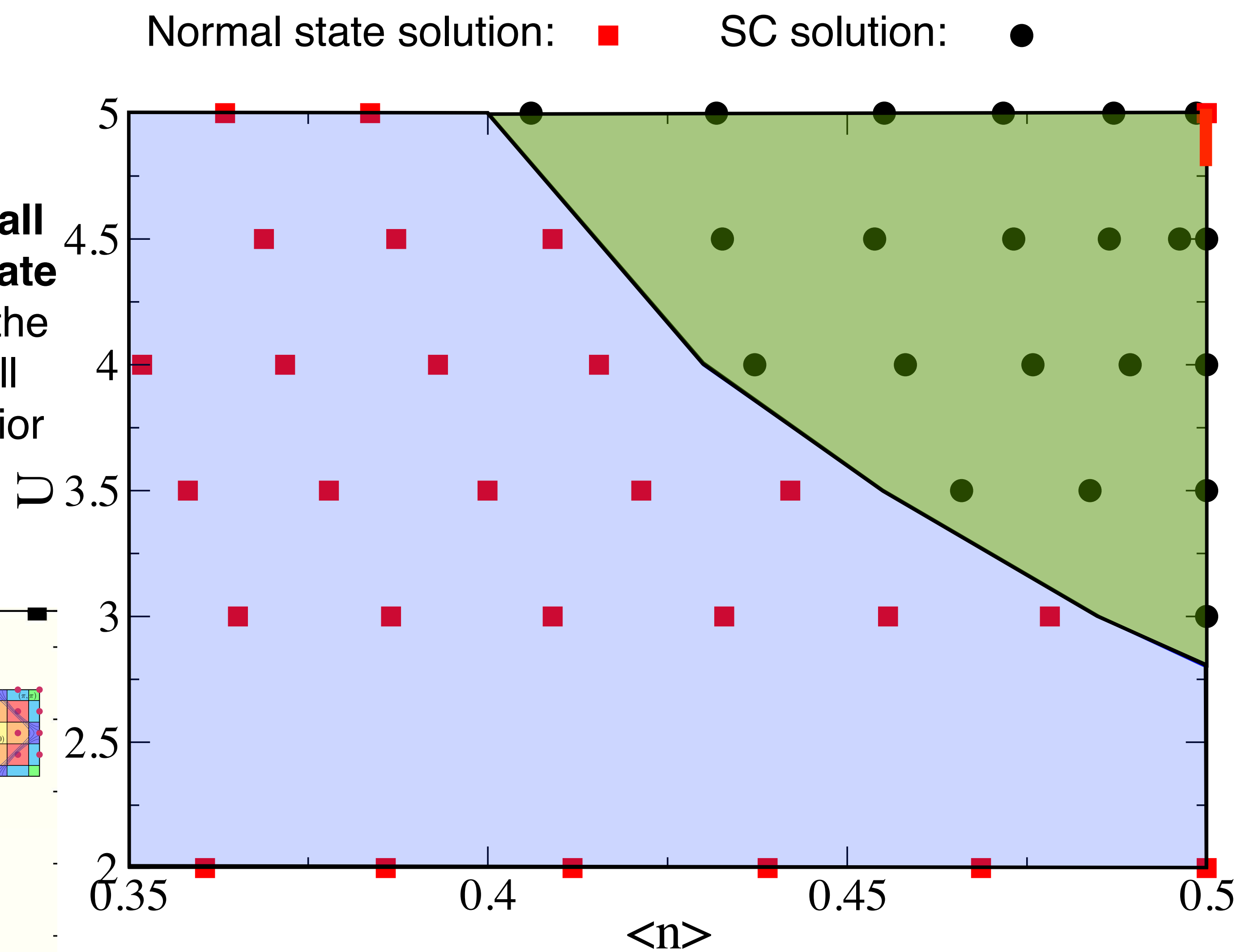
Geometry dependence of superconducting region

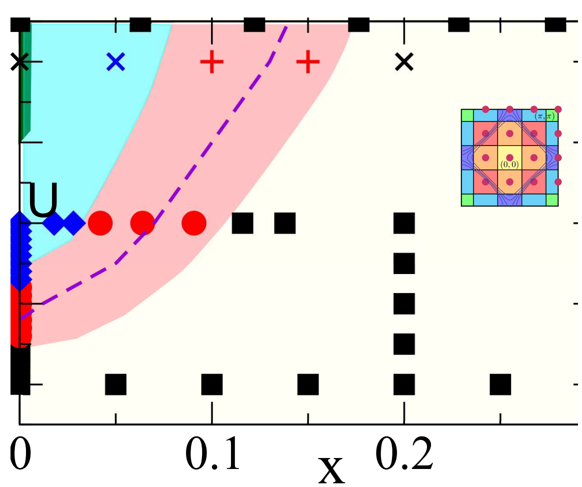
Fermi-Liquid/MSD

Mott Insulator

d-wave sc

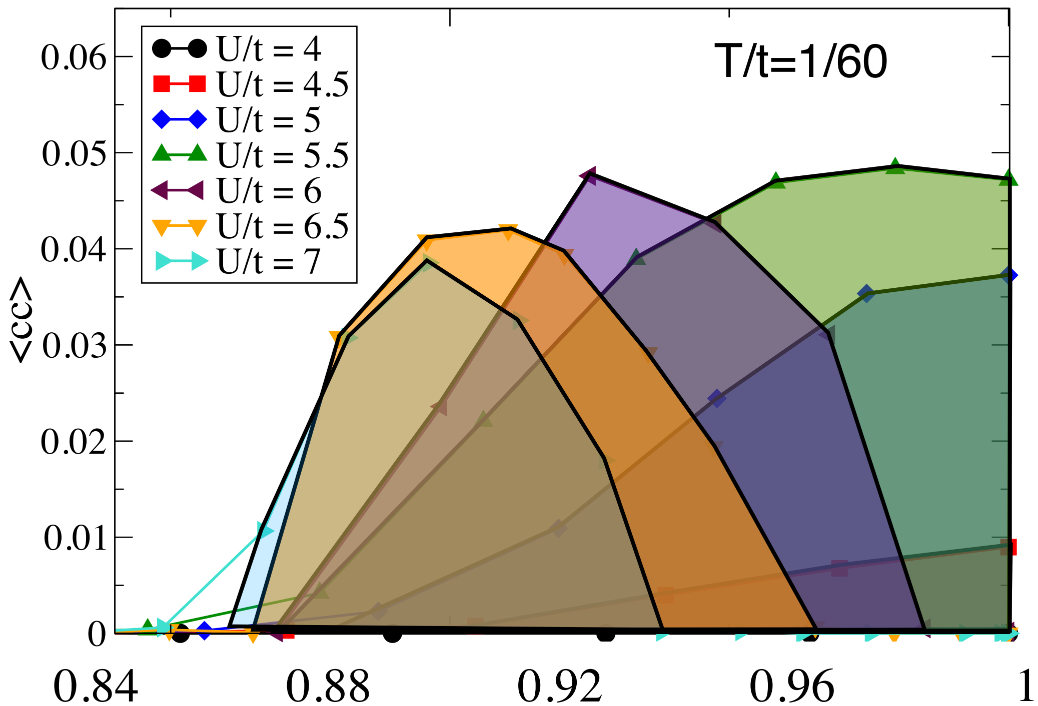
4-site Cluster **too small to support intermediate PG phase**; nature of the PG different on small clusters; nodal behavior not separated from antinodal behavior!

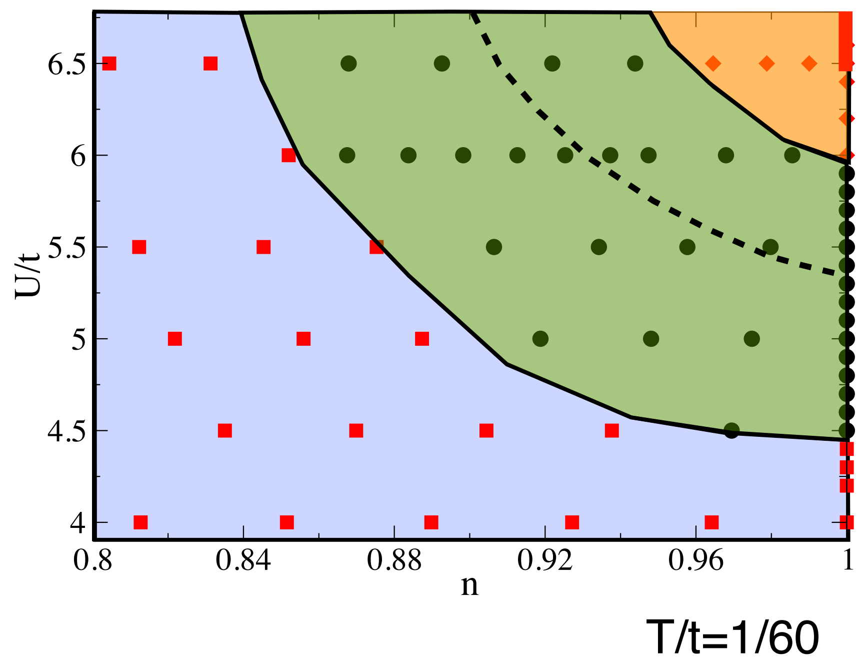




E. Gull, O. Parcollet, A.J. Millis, Phys. Rev. Lett. 110, 216405 (2013)

Superconducting order parameter doping transition





For weak interactions: superconductivity at and near half filling (no long-ranged AFM in this calculation).

For large interactions: superconductivity around 10% doping.

- Superconducting dome does not extend to half filling (on clusters with N_c>4)

- Strength of superconductivity decreases as interaction is increased

E. Gull, A.J. Millis, Phys. Rev. B 86, 241106(R) (2012)

Energy differences (doping)

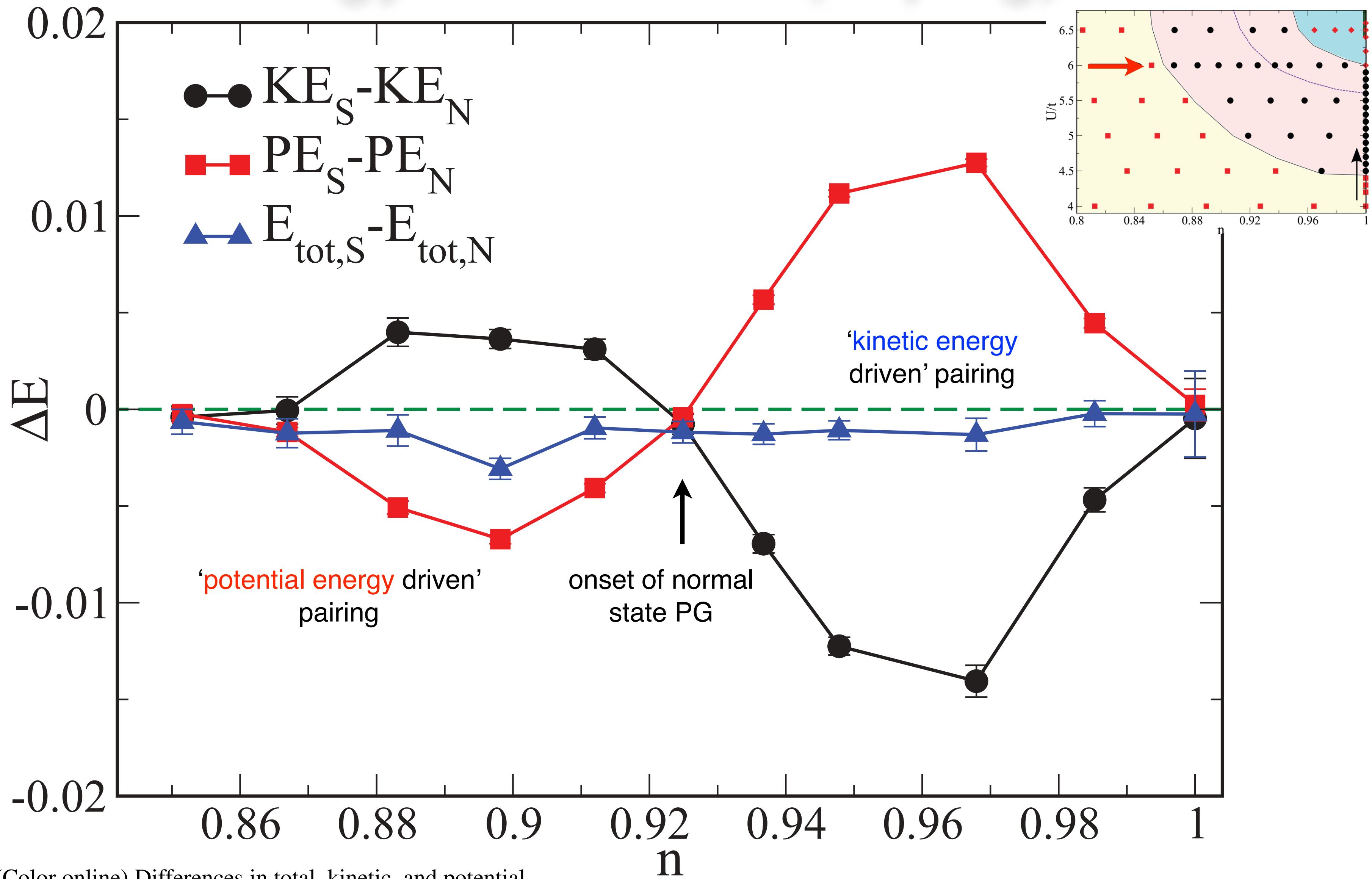
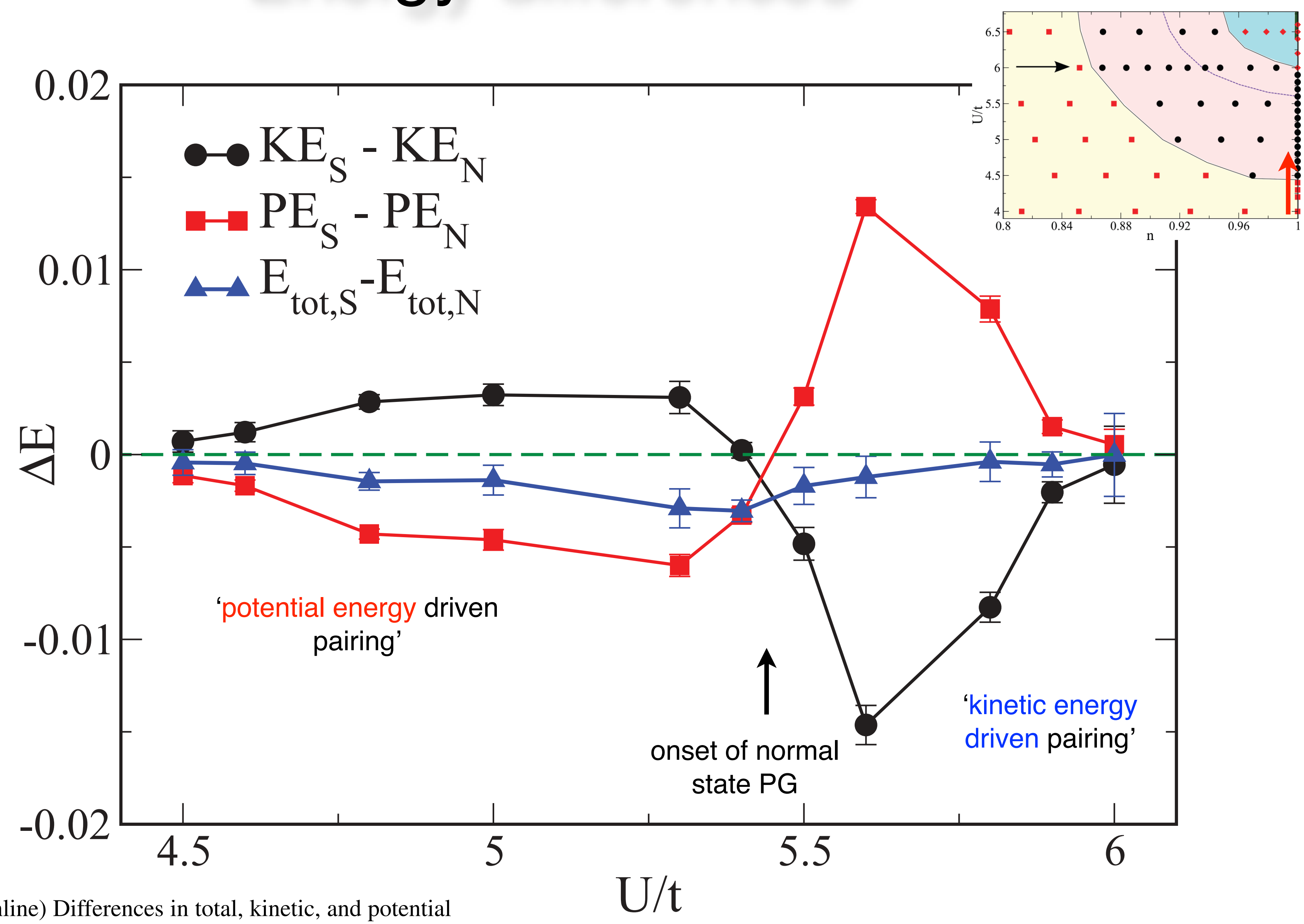


FIG. 2. (Color online) Differences in total, kinetic, and potential energies (per site, in units of hopping t) between normal and superconducting states, obtained as described in the text at density $n = 1$ varying interaction strength (upper panel) and as function of density at fixed interaction strength $U = 6t$ (lower panel).

E. Gull, A.J. Millis, Phys. Rev. B 86, 241106(R) (2012)

Energy differences



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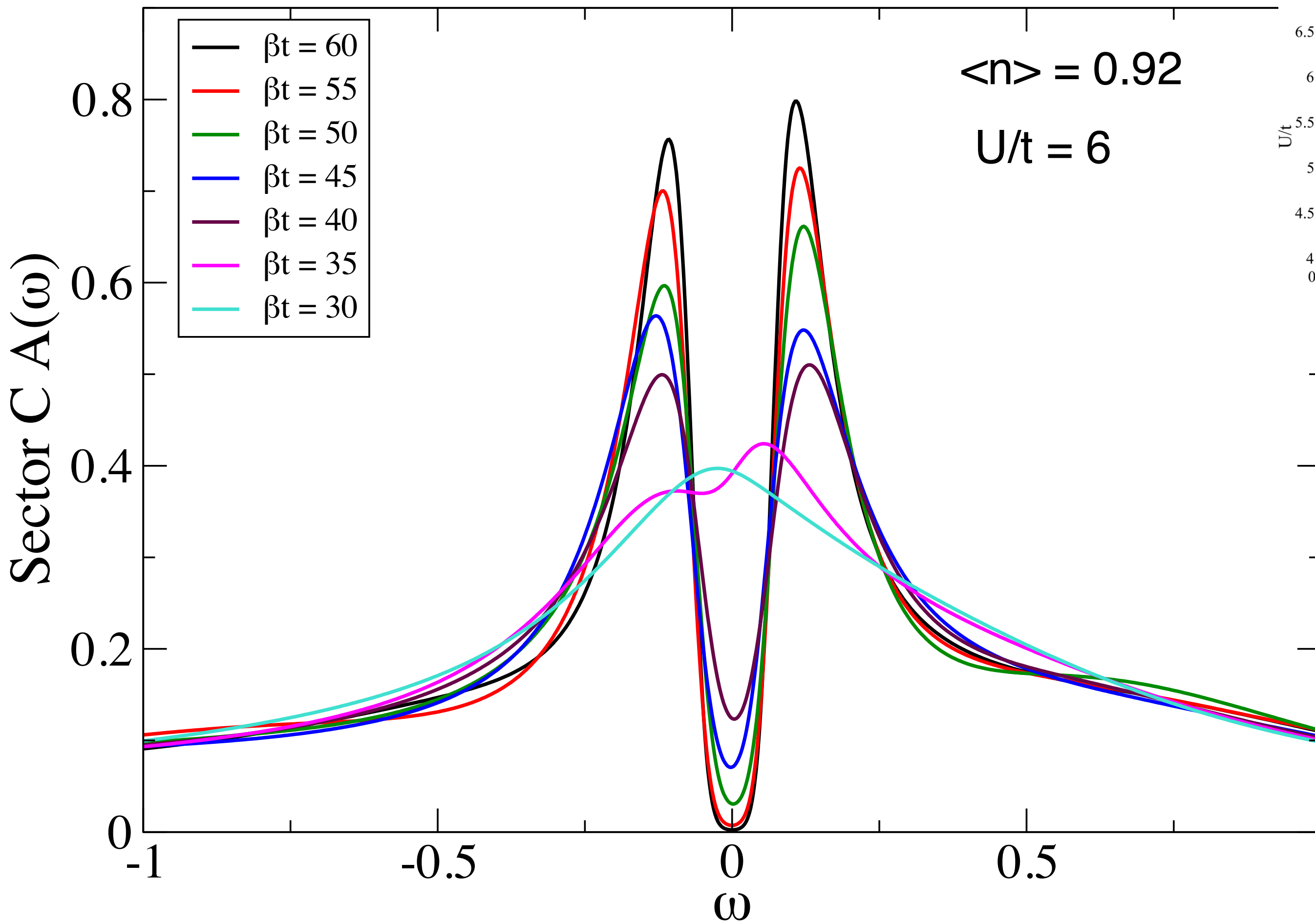
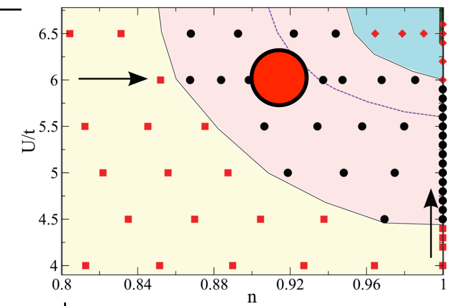
E. Gull, O. Parcollet, A.J. Millis, Phys. Rev. Lett. 110, 216405 (2013)

Superconducting spectral function overdoped / optimally doped region



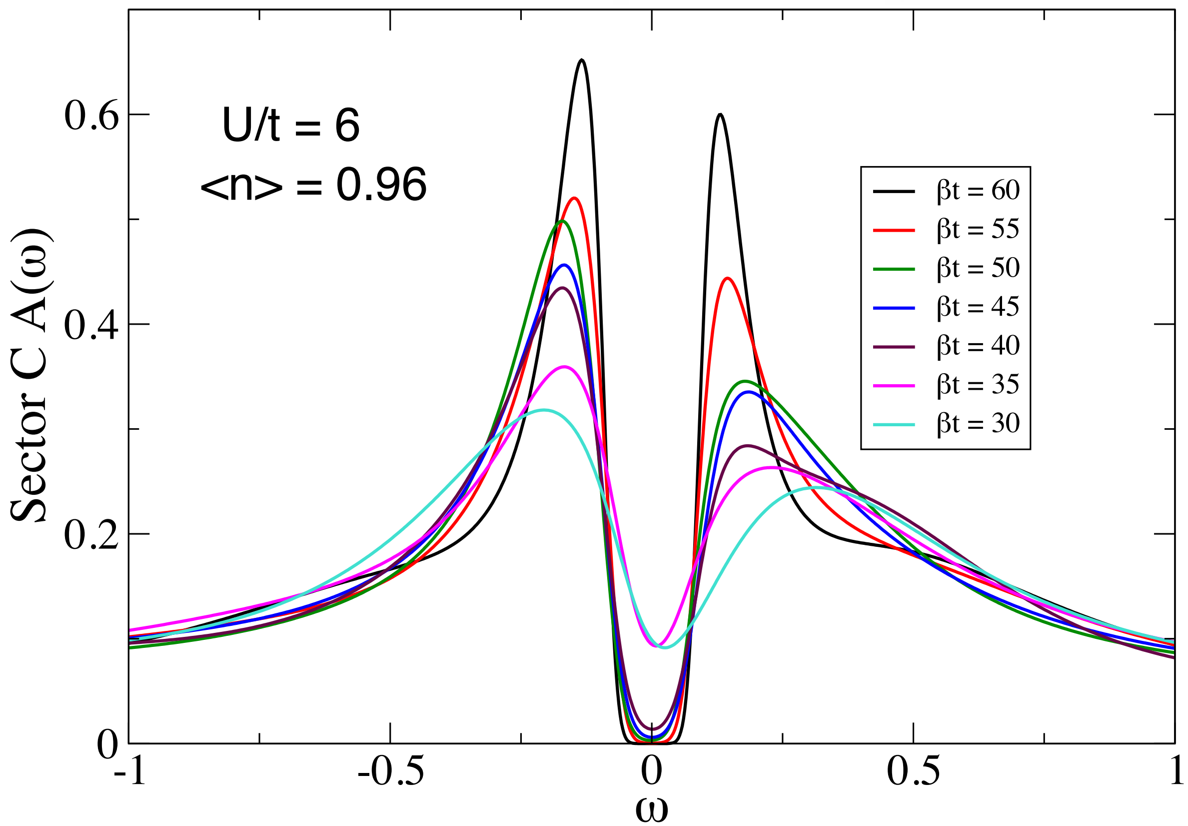


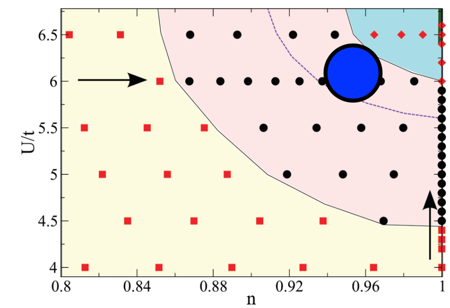
- symmetric spectral function, quasiparticle peaks on both sides. Weight in peaks from vicinity of Fermi energy

- superconducting gap at the antinode

E. Gull, O. Parcollet, A.J. Millis, Phys. Rev. Lett. 110, 216405 (2013)

Superconducting spectral function: underdoped region



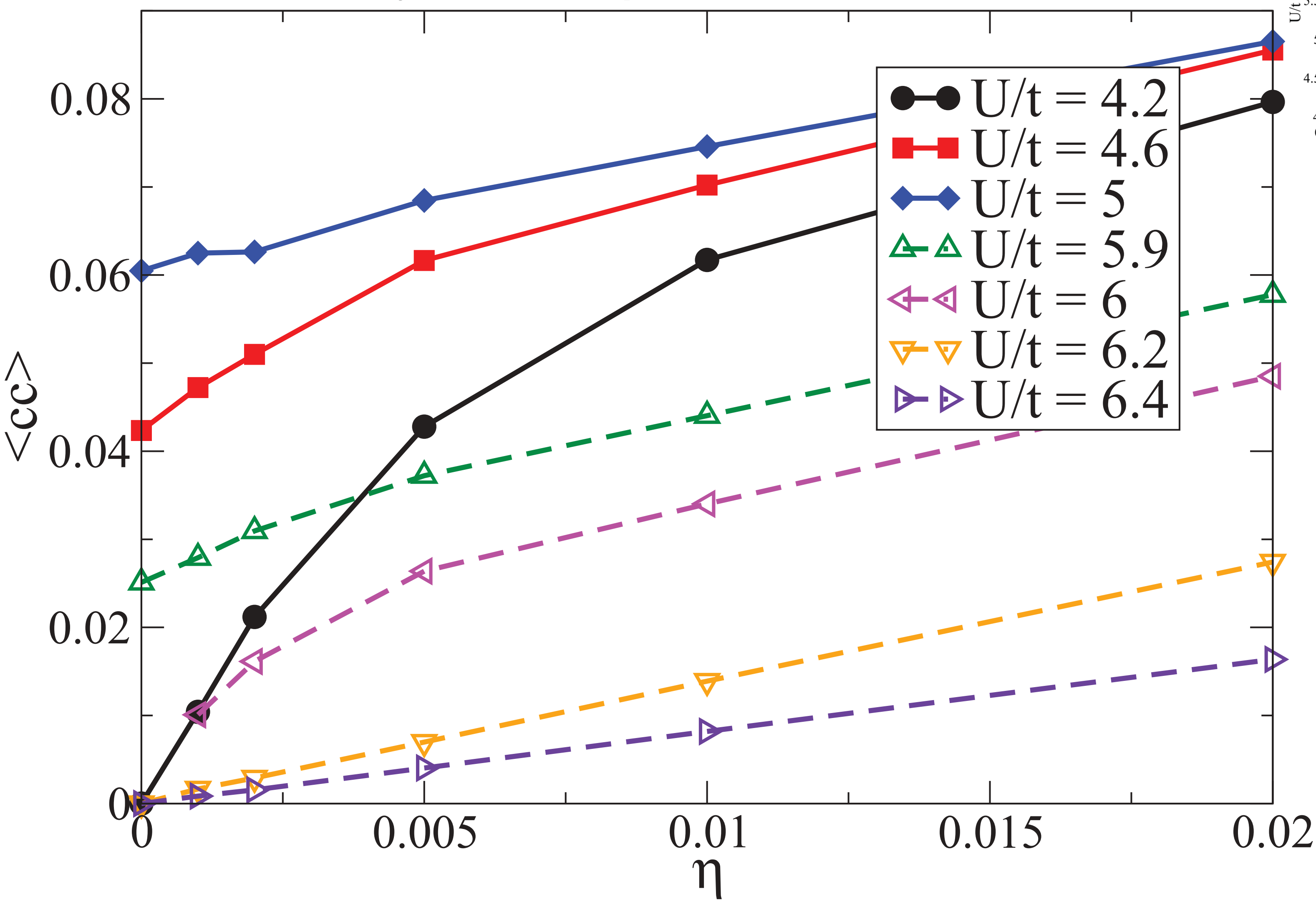


Pseudogap state at high T very different from SC state at low T: fundamental rearrangement of spectral weight on energy scales ≫ Δ. Superconducting gap significantly smaller than pseudogap. (conclusion independent of continuation)

E. Gull, A.J. Millis, Phys. Rev. B 86, 241106(R) (2012)

Response to applied field

small response to sc field in pseudogap regime shows that PG and superconductivity are **in competition**



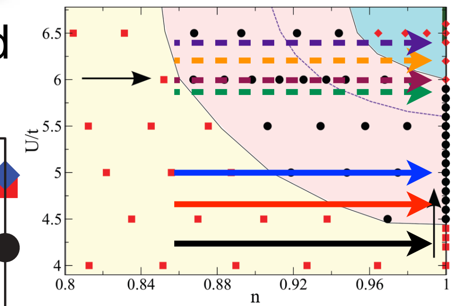
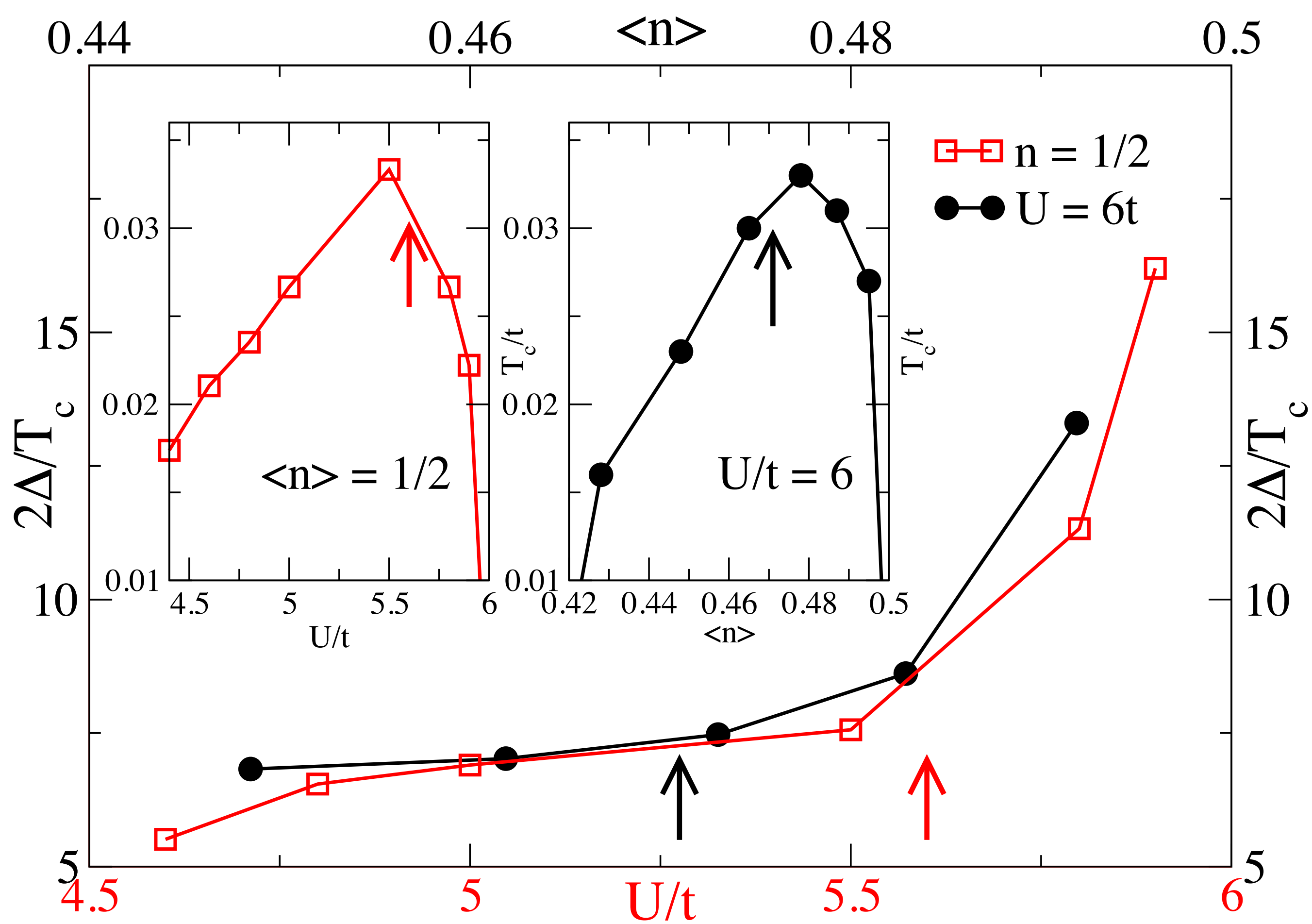


FIG. 3. (Color online) Anomalous expectation value in sector $K = (0,\pi)$ plotted against pairing field η at doping $x = 0$ for interaction strengths indicated.

E. Gull, O. Parcollet, A.J. Millis, Phys. Rev. Lett. 110, 216405 (2013)

Gap vs Tc (2 Δ/Tc)



Tc determined from simulations at different T. Gap size **Δ** measured by inter-peak distance (maxent) and verified by fitting a simple gap model (interaction transition)

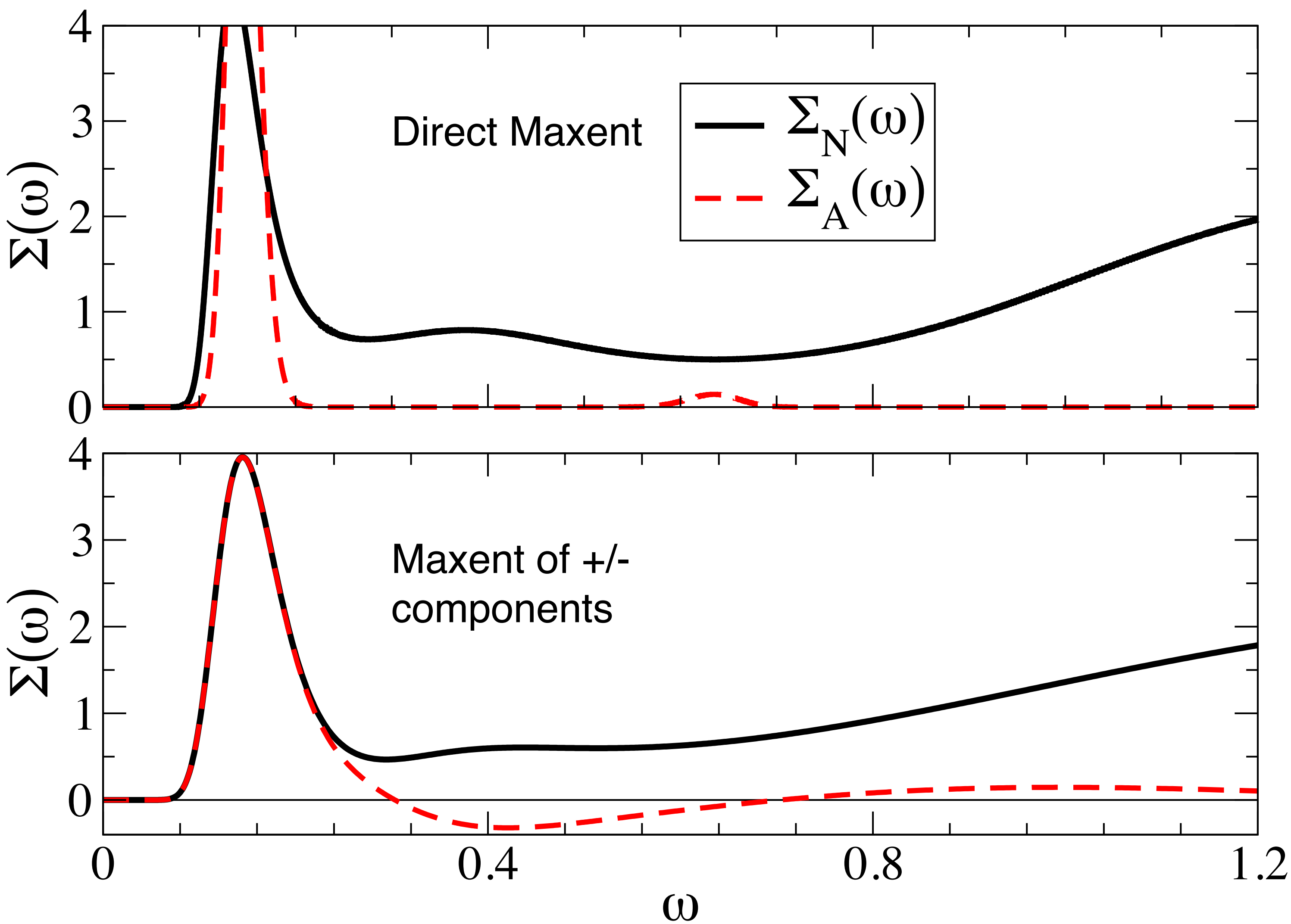
2 Δ/Tc about 2x larger than BCS (**7-8** instead of 3.5) for weak interaction / large doping.

rapid rise inside PG region.

Gap size Δ increasing slowly, linearly towards larger U/t, lower doping. Tc strongly suppressed in PG regime

E. Gull, O. Parcollet, A.J. Millis, Phys. Rev. Lett. 110, 216405 (2013)

Analytic continuation of self energies



Maxent procedures have very different uncertainties.
Both show single feature: peak at relatively low frequencies, followed by broad normal state features.

E. Gull, O. Parcollet, A.J. Millis, Phys. Rev. Lett. 110, 216405 (2013)

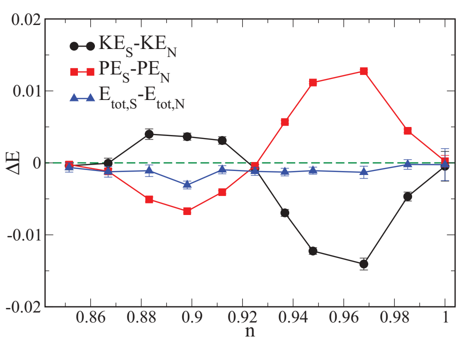
Brief overview – emerging picture

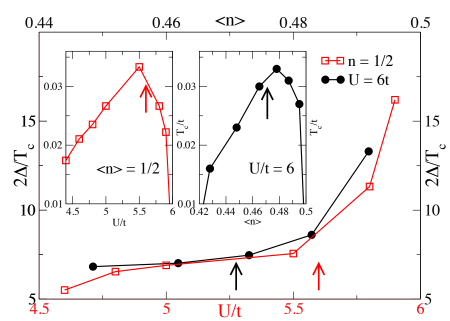
In part of the phase diagram **superconductivity** looks very **conventional**: more or less BCS-like, symmetric quasiparticle peak, interaction driven. Connected to weak coupling superconductivity.

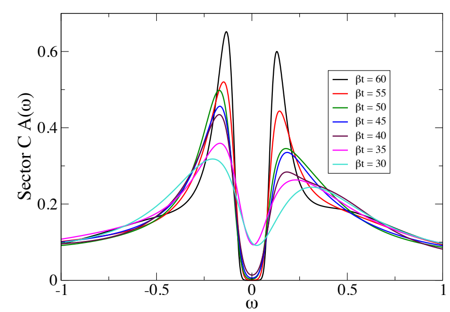
For larger U and lower doping, under the normal state **pseudogap** phase, superconductivity looks **very different** from the normal state: kinetic energy driven, non-BCS 2Δ/Tc.

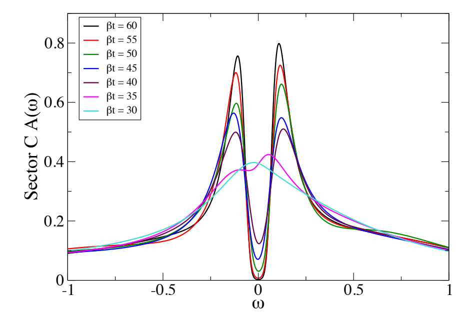
Eventually (even larger U and lower doping) the **PG state becomes energetically more favorable** than the SC state. This happens away from the Mott transition at half filling.

Doping transition and interaction transition (when long range AFM is suppressed) look remarkably similar – allows higher precision analysis at half filling in the absence of the sign problem.





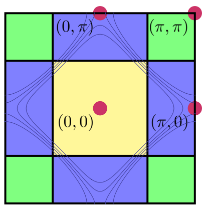


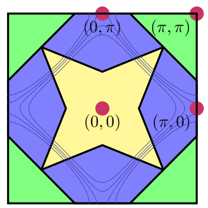


E. Gull, O. Parcollet, A.J. Millis, Phys. Rev. Lett. 110, 216405 (2013)

Acknowledgments

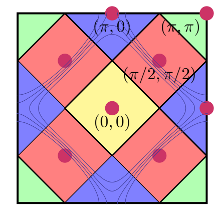
Many thanks to my collaborators:

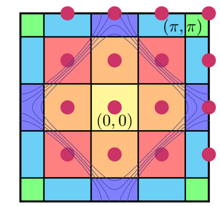




A. J. Millis
O. Parcollet

2d Hubbard:
J. Le Blanc





Emanuel Gull, Andrew J. Millis, Oliver Parcollet, Phys. Rev. Lett. 110, 216405 (2013)
Emanuel Gull and Andrew J. Millis, arXiv:1304.6406 (2013)
Emanuel Gull and Andrew J. Millis, Phys. Rev. B 86, 241106(R) (2012)

Columbia University in the City of New York → Max-Planck-Gesellschaft mpipks → Michigan

Computer time: the Center for Nanophase Materials Sciences at ORNL and Cray Hopper, NERSC

[redacted]