Competition between magnetism and superconductivity in the Hubbard model and in the cuprates

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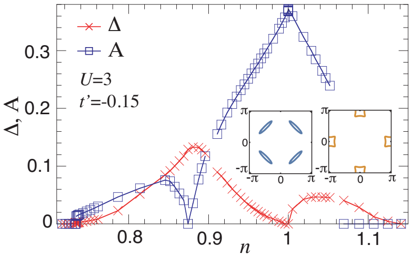
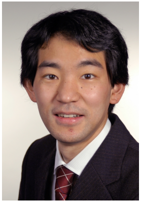


Coworkers



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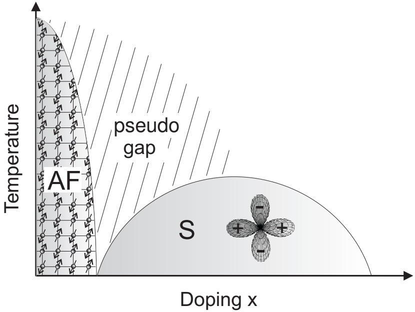
Outline

- Introduction
- Computation of order parameters
- Superconductivity versus magnetism

PRL **116** 096402 (2016)
PRL **117**, 187001 (2016)
PRB **98**, 195126 (2019)

CuO_2 high temperature superconductors

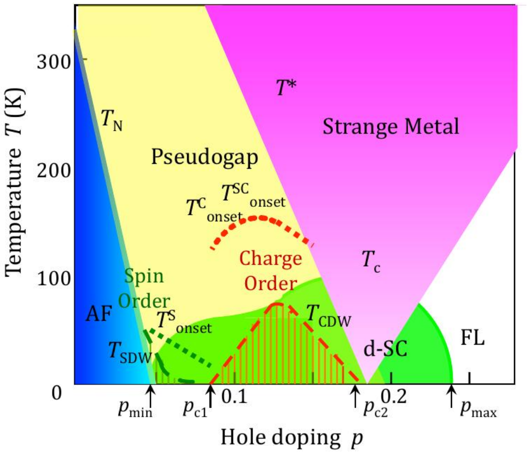
Theorist's phase diagram (the essentials):



- antiferromagnetism in undoped compounds
- d-wave superconductivity at sufficient doping
- Pseudo gap, non-Fermi liquid in "normal" phase at finite T

CuO_2 high temperature superconductors

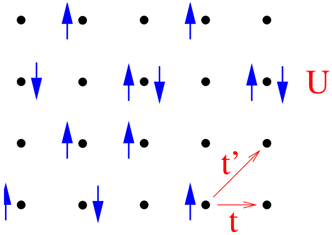
Complete (experimental) phase diagram:



Keimer et al. 2015

Two-dimensional Hubbard model

Effective single-band model for CuO_2-planes in HTSC:
(Anderson 1987, Zhang & Rice 1988)



Hamiltonian $H = H_{kin} + H_I$

$$H_{kin} = \sum_{\mathbf{i},\mathbf{j}} \sum_{\sigma} t_{\mathbf{ij}}\, c^{\dagger}_{\mathbf{i}\sigma} c_{\mathbf{j}\sigma} = \sum_{\mathbf{k},\sigma} \epsilon_{\mathbf{k}}\, n_{\mathbf{k}\sigma}$$

$$H_I = U \sum_{\mathbf{j}} n_{\mathbf{j}\uparrow} n_{\mathbf{j}\downarrow}$$

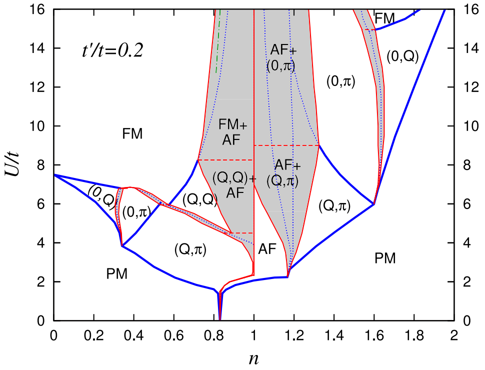
Antiferromagnetism at/near half-filling for sufficiently large U

Antiferromagnetism generates d-wave pairing and competes with it
(perturbation theory, RG, cluster DMFT, variational MC, some QMC)

Spin density waves in the Hubbard model

Ground state phase diagram of 2D Hubbard model in *mean-field theory*

Igoshev et al. 2010

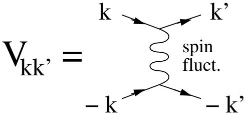


- Néel antiferromagnet at half-filling
- spin density wave with incommensurate wave vectors $\mathbf{Q} = (Q, \pi)$ away from half-filling for weak – moderate interactions

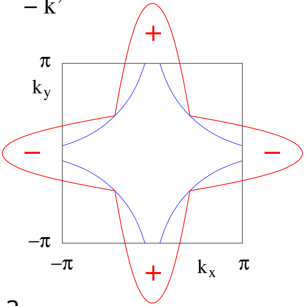
Superconductivity from spin fluctuations

Miyake, Schmitt-Rink, Varma 1986; Scalapino, Loh, Hirsch 1986

Effective BCS interaction
from exchange of
spin fluctuations



peaked for
$\mathbf{k}' - \mathbf{k} = (\pi, \pi)$



$\Rightarrow$ Gap equation

$$\Delta_{\mathbf{k}} = -\sum_{\mathbf{k}'} V_{\mathbf{k}\mathbf{k}'} \frac{\Delta_{\mathbf{k}'}}{2E_{\mathbf{k}'}}$$

has solution with d-wave symmetry

What about other (than AF spin) fluctuations?
Treat all particle-particle and particle-hole channels on equal footing
$\Rightarrow$ Summation of parquet diagrams (hard) or renormalization group

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Functional RG for quantum many-body systems

A natural way of dealing with diverse energy scales and a powerful source of new approximations

- Applicable to microscopic models (not only effective field theory)
- Works for finite and infinite systems (thermodynamic limit)
- RG treatment of infrared singularities built in
- Access to universal and non-universal quantities
- Possibility to glue distinct approximations on different energy scales without adjustable parameters

Review on functional RG for interacting fermion systems:
wm, Salmhofer, Honerkamp, Meden, Schönhammer, Rev. Mod. Phys. 2012

Flow equations

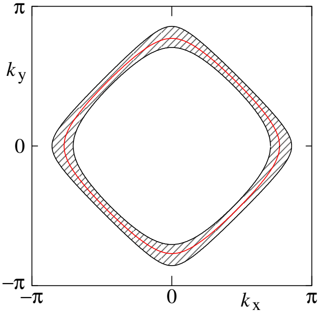
Scale-by-scale functional integration with flowing cutoff Λ

- Momentum cutoff:

$$G_0^\Lambda(\mathbf{k}, i\omega) = \frac{\Theta(|\xi_\mathbf{k}| - \Lambda)}{i\omega - \xi_\mathbf{k}} \quad , \quad \xi_\mathbf{k} = \epsilon_\mathbf{k} - \mu$$

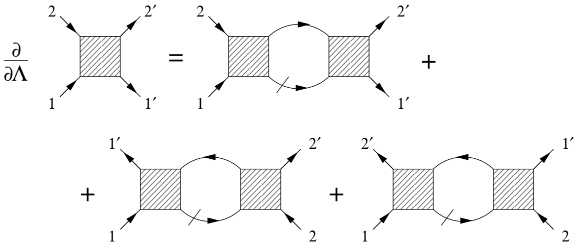
- Frequency cutoff:

$$G_0^\Lambda(\mathbf{k}, i\omega) = \frac{\Theta(|\omega| - \Lambda)}{i\omega - \xi_\mathbf{k}}$$



Flow equations for effective interactions obtained from derivative with respect to Λ (Wetterich 1993)

Effective two-particle interaction at one-loop level



dash: $\frac{\partial}{\partial \Lambda}$

2-particle vertex only

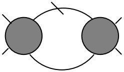
3 "channels"

Initial condition: Γ^{Λ_0} = bare interaction

All channels (charge, spin, pairing) captured on equal footing.

Higher order corrections small for weak interactions.

Lessons learned from one-loop flow

$$\frac{d}{d\Lambda}\Gamma^\Lambda \quad = $$  one-loop truncation

- Strong antiferromagnetic correlations near half-filling
- Antiferromagnetic correlations drive d-wave pairing instability
- Other pairing correlations suppressed
- Conventional charge density waves suppressed
- d-wave charge correlations generated (but no instability)

Zanchi & Schulz 2000, Halboth & wm 2000, Honerkamp et al. 2001

Caveats

Truncation of flow equation hierarchy justified only for weak interactions

Mott insulator physics in strongly interacting Hubbard model
not captured by weak coupling expansion!

Commonly used static approximation for two-particle vertex overestimates pairing already for moderate interactions
Husemann, Giering, Salmhofer 2012; Vilardi, Taranto, wm 2017

Leap to strong coupling:

Start flow from DMFT ($d = \infty$)

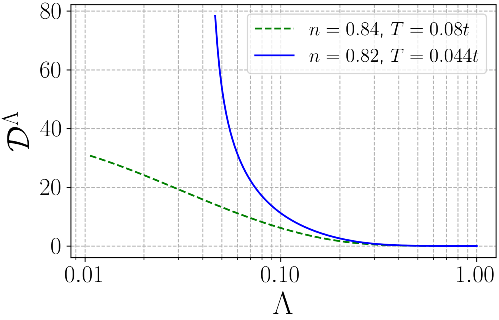
Local correlations captured non-perturbatively

Taranto et al. 2014
Vilardi, Taranto, wm 2019

Extremely demanding flow equations due to strong and non-separable frequency dependence of two-particle vertex at strong coupling

Pairing instability at strong coupling

Vilardi, Taranto, wm 2019



Flow of d-wave pairing interaction at 16 and 18 percent hole doping

$U/t = 8$, $t'/t = 0.2$

Almost diverging interaction indicates critical temperature for superconductivity T_c near 100 K.

Spontaneous symmetry breaking

Divergence of effective interaction at scale Λ_c signals instability

$\Rightarrow$ order parameter generated

Flow below critical scale Λ_c complicated due to anomalous effective interactions, especially in case of two order parameters

$\Rightarrow$ "Poor man's" approach:
Approximate flow below Λ_c by mean-field theory

Symmetry breaking via RG + MFT

"Poor man's approach": Functional RG + mean-field theory
(Reiss, Rohe, wm 2007; Wang, Eberlein, wm 2014)

1) fRG flow down to scale $\Lambda_{\mathrm{MF}} > \Lambda_c$: effective interaction $\Gamma^{\Lambda_{\mathrm{MF}}}$

2) Treat scales $\Lambda < \Lambda_{\mathrm{MF}}$ in mean-field theory with $\Gamma^{\Lambda_{\mathrm{MF}}}$ as input

- Equivalent to single-channel one-loop flow with self-energy
- Fluctuation driven order such as d-wave superconductivity captured
- In ground state, fluctuations below Λ_c usually less important (exception QCP)

Application to 2D Hubbard model:
Magnetic order and d-wave SC (coexistence allowed)

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Order parameters

Key players at scale Λ_c: magnetic and d-wave pairing fluctuations

Magnetic fluctuations peaked at wave vectors $\mathbf{Q} = (\pi - 2\pi\eta, \pi)$ with small incommensurability η

$\Rightarrow$ Magnetic and superconducting order parameters:

$$A_{\mathbf{k}} = \int_{\mathbf{k}'} U_{\mathbf{k}\mathbf{k}'}(\mathbf{Q}) \langle a^{\dagger}_{\mathbf{k}'\uparrow} a_{\mathbf{k}'+\mathbf{Q}\downarrow} \rangle$$

Spiral spin density wave, $U_{\mathbf{k}\mathbf{k}'}(\mathbf{Q})$ magnetic interaction with momentum transfer $\mathbf{Q}$

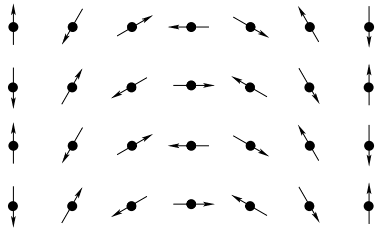
$$\Delta_{\mathbf{k}} = \int_{\mathbf{k}'} V_{\mathbf{k}\mathbf{k}'} \langle a_{-\mathbf{k}'\downarrow} a_{\mathbf{k}'\uparrow} \rangle$$

Spin-singlet pairing, $V_{\mathbf{k}\mathbf{k}'}$ pairing interaction

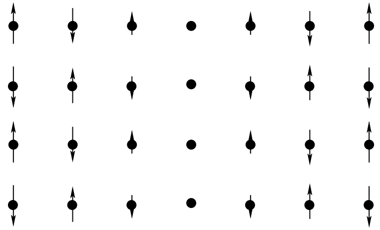
For $\mathbf{Q} = (\pi, \pi)$: spiral state = Néel state

Spiral versus collinear SDW

For small η, spiral state gains almost the same magnetic energy as Néel state



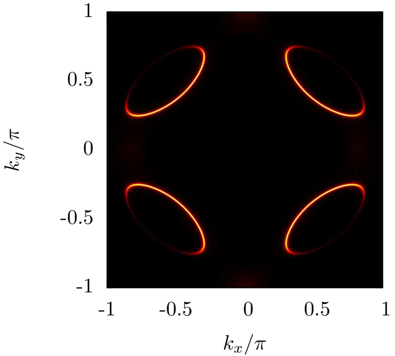
In collinear SDW smaller energy gain from regions with reduced magnetization amplitudes



Electron spectral function in spiral state

Underdoped regime

Eberlein, wm, Sachdev, Yamase 2016

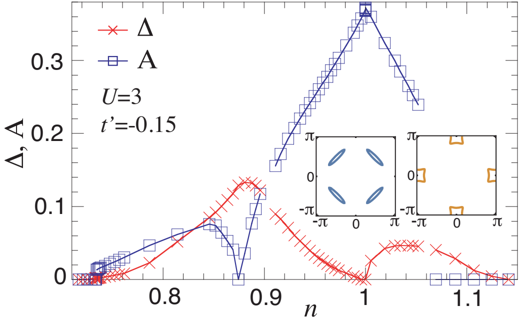


Strongly momentum dependent spectral weight makes pockets look like Fermi arcs

Electron spectral function $\mathcal{A}(\mathbf{k}, 0)$

Antiferromagnetism & superconductivity vs. density

Yamase, Eberlein, wm 2016



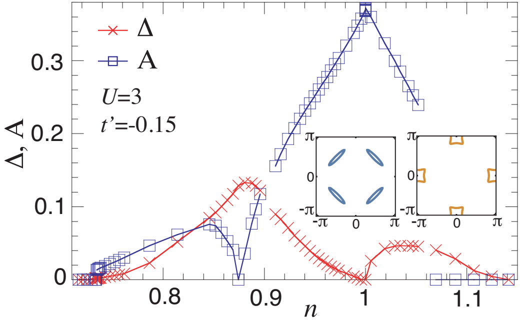
Ground state order parameters vs. density

Inset:
Electron and hole pockets in Néel state near half-filling

- Coexistence of magnetism and superconductivity away from half-filling due to Cooper instability in electron or hole pockets
- Néel state near half-filling, incommensurate antiferromagnet for $n < 0.9$
- Magnetism suppressed by superconductivity at van Hove filling

Antiferromagnetism & superconductivity vs. density

Yamase, Eberlein, wm 2016



Ground state
order parameters
vs. density

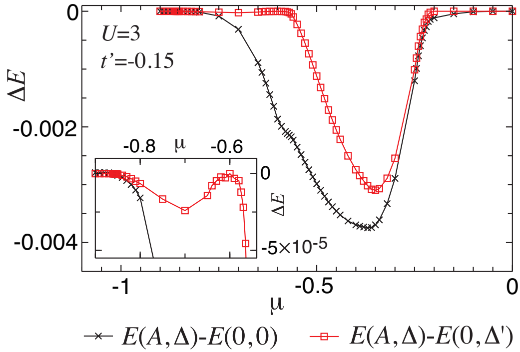
Inset:
Electron and hole
pockets in Néel state
near half-filling

Coexistence of Néel order and superconductivity near half-filling also found in cluster calculations at stronger interactions:

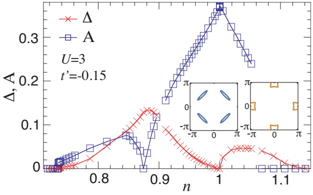
Lichtenstein & Katsnelson 2000; Capone & Kotliar 2006; Aichhorn et al. 2006; Kancharla, Kyung, ..., Tremblay 2008; B.-X. Zheng & G. K.-L. Chan 2016

"Gossamer magnetism"

"Gossamer" synonymous for fragile: "Gossamer superconductivity" (Laughlin)



Total condensation energy
$E(A,\Delta) - E(0,0)$
magnetic condensation energy
$E(A,\Delta) - E(0,\Delta')$



Tiny magnetic energy gain in incommensurate regime ($\mu < 0.57$, $n < 0.9$) compared to a superconducting state without magnetic order

$\Rightarrow$ Magnetic order extremely fragile in presence of superconductivity!

“Gossamer magnetism”

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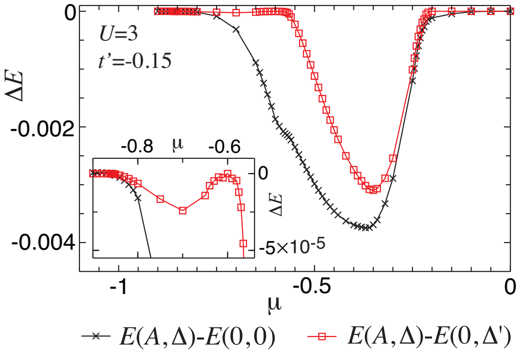

Total condensation energy
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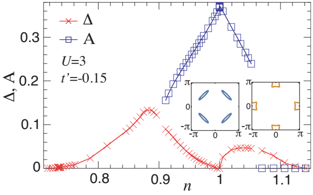

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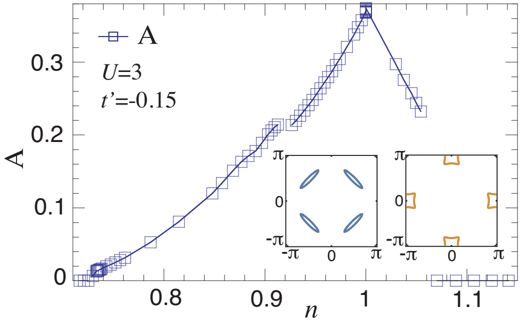
Suppressing superconductivity

Magnetic order could be stabilized by suppressing superconductivity, e.g. by a high external magnetic field

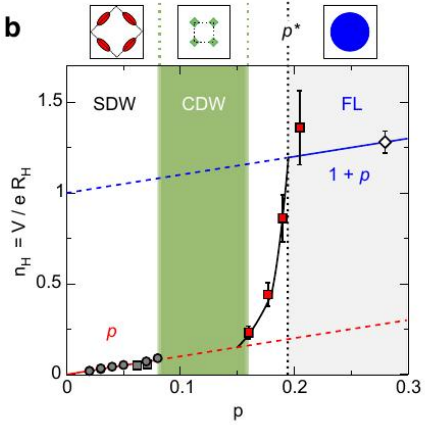


Magnetic order parameter with superconductivity suppressed

Hall effect in high magnetic fields

Hall number n_H in YBCO in very high magnetic fields drops from $1 + p$ to p for $0.16 < p < 0.19$ (Badoux et al. 2016)

Fermi surface reconstruction due to spin density wave stabilized by suppression of superconductivity?



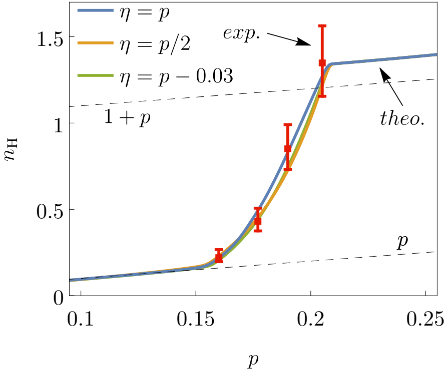
Observed Hall coefficient consistent with hole pockets in SDW state

Storey 2016; Eberlein, wm, Sachdev, Yamase 2016; Verret et al. 2017

Calculated Hall coefficient for spiral state

Standard formula (relaxation time app.) with quasi-particle bands $E_{\mathbf{k}}^{\pm}$ (Voruganti et al. 1992)

$$R_H = \frac{\sigma_H}{\sigma_{xx}\sigma_{yy}} \quad , \quad \sigma_H = -e^3\tau^2 \sum_{n=\pm} \int_{\mathbf{k}} f(E_{\mathbf{k}}^n) \left[\frac{\partial^2 E_{\mathbf{k}}^n}{\partial k_x^2} \frac{\partial^2 E_{\mathbf{k}}^n}{\partial k_y^2} - \left(\frac{\partial^2 E_{\mathbf{k}}^n}{\partial k_x \partial k_y} \right)^2 \right]$$

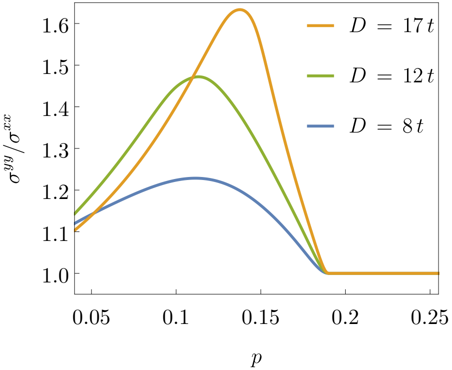


For sizeable $\Gamma = \tau^{-1}$ also interband contributions Mitscherling & wm 2018

Hall number $n_H = (eR_H)^{-1}$ for linear onset of spiral order $A(p) \propto p^* - p$

Longitudinal conductivity and nematicity in spiral state

- Longitudinal conductivities σ_{xx} and σ_{yy} also exhibit drop due to charge carrier reduction
- Pronounced doping-dependent nematicity:



Conductivity anisotropy versus doping for various choices of

$A(p) = D(p^* - p)$

Mitscherling & wm 2018

Qualitative agreement with experiments, e.g. by Ando et al. (2002)

Summary

- In ground state of 2D Hubbard model magnetic order coexists with superconductivity at *any* finite doping (in pure system)
- For sizable hole-doping incommensurate magnetic order with a tiny energy gain (*gossamer*) compared to a non-magnetic superconductor
- Robust magnetism expected upon suppression of superconductivity by strong magnetic field even at fairly large doping
  $\Leftrightarrow$ charge carrier drop in recent experiments
  $\Leftrightarrow$ very recent NMR evidence for frozen spins up to p^*! (Julien et al.)
- Functional RG at strong coupling with DMFT as a “booster rocket”