Competition between magnetism and superconductivity in the 2D Hubbard model from weak to strong coupling

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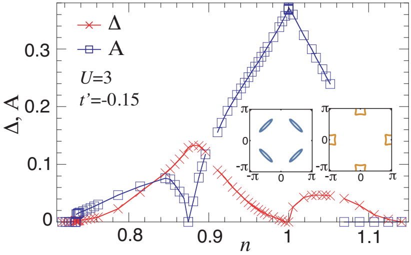
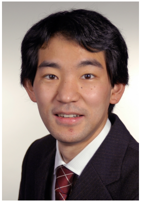


Coworkers



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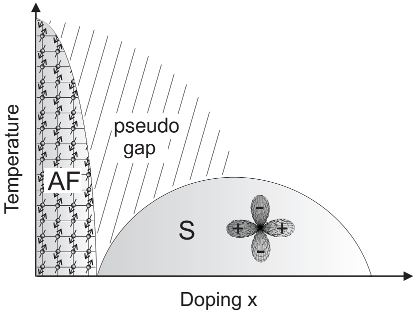
Outline

- Cuprate superconductors and Hubbard model
- Functional RG for fermions
- Computation of order parameters
- Superconductivity versus magnetism
- Functional RG for strongly interacting Fermi systems

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

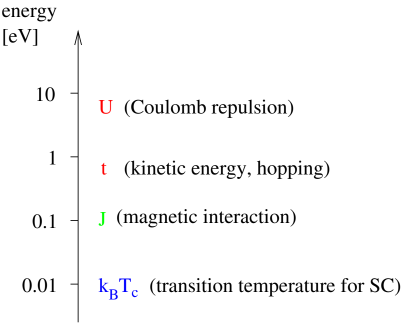
CuO_2 high temperature superconductors



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

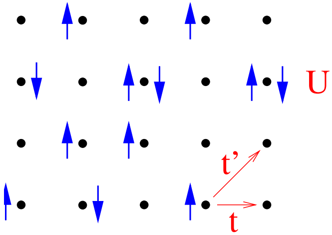
Vast hierarchy of energy scales:

Magnetic interaction and superconductivity generated from kinetic energy and Coulomb interaction



Two-dimensional Hubbard model

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



Hamiltonian $H = H_{kin} + H_I$

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

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

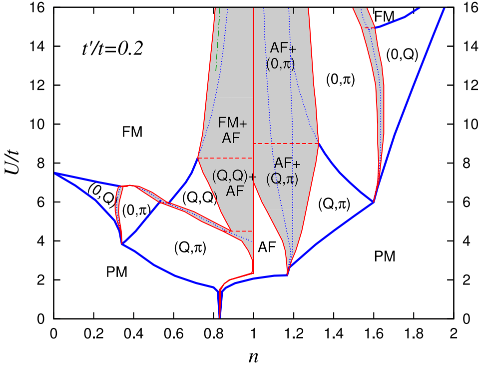
Antiferromagnetism at/near half-filling for sufficiently large U

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



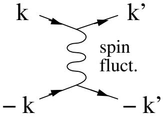
- Néel antiferromagnet at half-filling
- spin density wave with incommensurate wave vectors $\mathbf{Q} = (Q, \pi)$ away from half-filling for weak – moderate interactions

Superconductivity from spin fluctuations

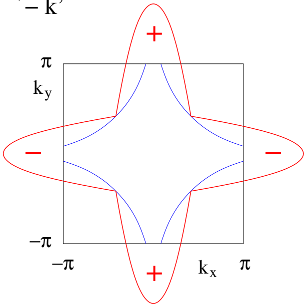
Miyake, Schmitt-Rink, Varma 1986; Scalapino, Loh, Hirsch 1986

Effective BCS interaction from exchange of spin fluctuations

$V_{kk'}$ =



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

Exact flow of effective action

Deform bare propagator G_0 to scale dependent G_0^Λ
(Λ momentum or energy cutoff, or any other parameter)

$\Rightarrow$ Scale dependent effective action $\Gamma^\Lambda[\psi, \bar{\psi}]$

$\Gamma^\Lambda[\psi, \bar{\psi}]$ interpolates between solvable (usually bare) action for $\Lambda = \Lambda_0$ and final effective action $\Gamma[\psi, \bar{\psi}]$ for $\Lambda \to 0$

Exact flow equation (Wetterich 1993):

$$\frac{d}{d\Lambda}\Gamma^\Lambda[\psi, \bar{\psi}] = \pm\frac{1}{2}\mathrm{tr}\frac{\partial_\Lambda (G_0^\Lambda)^{-1}}{\partial^2_{(\psi,\bar{\psi})}\Gamma^\Lambda[\psi, \bar{\psi}] + (G_0^\Lambda)^{-1} - G_0^{-1}}$$

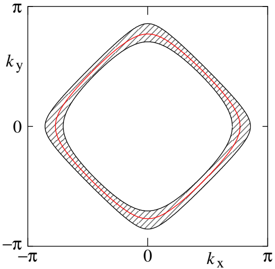
bosons
fermions

Flow parameter for interacting fermions

Fermi surface singularity at $\omega = 0$, $\xi_{\mathbf{k}} = \epsilon_{\mathbf{k}} - \mu = 0$

Infrared cutoff $\Lambda > 0$

- Momentum cutoff: $G_0^\Lambda(\mathbf{k}, i\omega) = \dfrac{\Theta(|\xi_{\mathbf{k}}| - \Lambda)}{i\omega - \xi_{\mathbf{k}}}$
- Frequency cutoff: $G_0^\Lambda(\mathbf{k}, i\omega) = \dfrac{\Theta(|\omega| - \Lambda)}{i\omega - \xi_{\mathbf{k}}}$



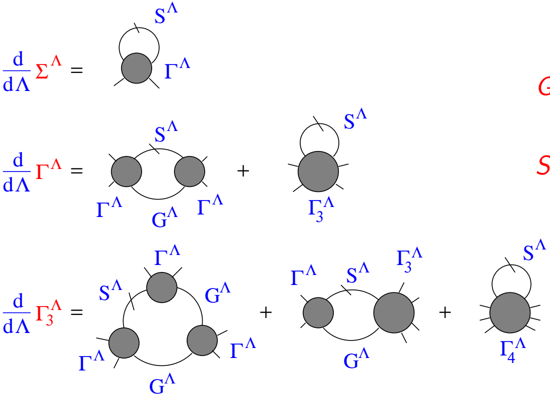
Many other choices: mixed momentum-frequency, smooth cutoff etc.

Initial condition: Λ_0 = band width (momentum) or ∞ (frequency)

Flow equations for vertex functions

Expansion of flow equation for effective action in powers of fields

$\Rightarrow$ Exact hierarchy of flow equations for vertex functions



$$G^\Lambda = \left[(G_0^\Lambda)^{-1} - \Sigma^\Lambda \right]^{-1}$$

$$S^\Lambda = \frac{d}{d\Lambda} G^\Lambda \Big|_{\Sigma^\Lambda \text{ fixed}}$$

Starting point for approximations

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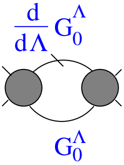
Stability analysis at weak coupling

Leading instabilities of 2D Hubbard model?

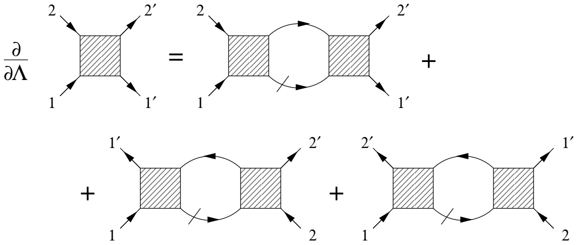
$$\frac{d}{d\Lambda}\Gamma^{\Lambda} \quad =$$



Truncated flow of two-particle vertex

Higher order corrections small for weak (effective) interactions.

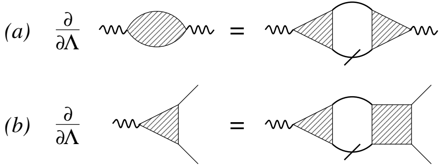
Stability analysis at weak coupling



3 "channels"

All channels (particle-particle, particle-hole) captured on equal footing.

Flow equations for susceptibilities



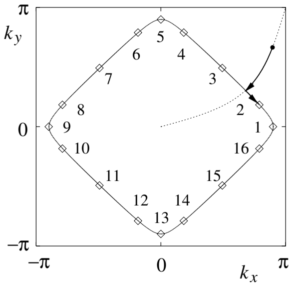
Parametrization of two-particle vertex

- Neglect frequency dependence ("irrelevant")
- Neglect momentum dependence normal to Fermi surface ("irrelevant")

$$\Rightarrow \quad \Gamma^\Lambda(\mathbf{k}'_1, \mathbf{k}'_2; \mathbf{k}_1, \mathbf{k}_2) \approx \Gamma^\Lambda(\mathbf{k}'_{F1}, \mathbf{k}_{F1} + \mathbf{k}_{F2} - \mathbf{k}'_{F1}; \mathbf{k}_{F1}, \mathbf{k}_{F2})$$

$\mathbf{k}_{F1}, \ldots$ = projection of $\mathbf{k}_1, \ldots$ on Fermi surface.

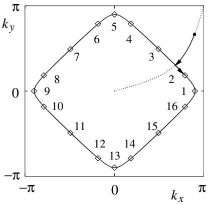
Tangential momentum dependence discretized (here 16 points).

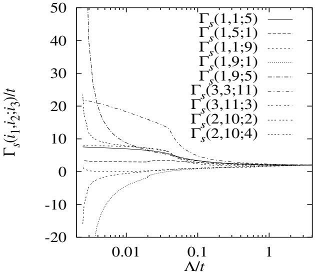


Equivalent to discretization via partition of Brillouin zone in "patches"

Effective interaction and susceptibilities in Hubbard model:

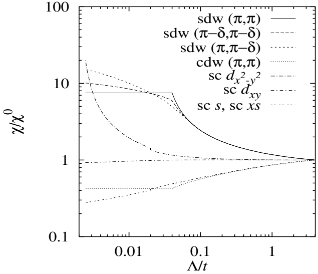
1-loop flow of
interactions





Singlet vertex
$\Gamma_s^\Lambda(k_1', k_2'; k_1, k_2)$
for various choices
of k_1, k_2, k_1'

1-loop flow of
susceptibilities



Divergence
at critical scale Λ_c
indicates instability

$n = 0.984$
$U = t$
$t' = 0$

Zanchi & Schulz '97-'00
Halboth & wm '00
Honerkamp et al. '01

Better parametrization: Channel decomposition

Each of the 3 channels contributing to Γ^Λ generates strong frequency and momentum dependences in one bosonic variable, such as $k_1 + k_2$

$\Rightarrow$ Channel decomposition

Karrasch et al. 2008
Husemann & Salmhofer 2009

$$\Gamma^\Lambda = U + (\text{charge} + \text{magnetic} + \text{pairing}) \text{ fluctuations}$$

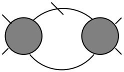
Accurate parametrization of *one* frequency and momentum variable in each channel

Frequency dependence important already at moderate interactions:

Pairing scale overestimated in static approximation!

(Husemann, Giering, Salmhofer 2012; Vilardi et al. 2017)

Lessons learned from one-loop flow

$$\frac{d}{d\Lambda}\Gamma^{\Lambda} =$$ 

- 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)

Two-loop extension: Eberlein 2014

Multi-loop extension = parquet approximation: Kugler & Delft 2018

Routes to symmetry breaking

Divergence of effective interaction at scale Λ_c signals instability

$\Rightarrow$ order parameter generated

Routes to spontaneous symmetry breaking in functional RG for fermions:

- Hubbard Stratonovich bosonization (Baier, Bick, Wetterich 2004)
- Fermionic flow with order parameter (Salmhofer et al. 2004)
- fRG + mean-field theory (Reiss et al. 2007)

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 $\Lambda_{\rm MF} > \Lambda_c$: effective interaction $\Gamma^{\Lambda_{\rm MF}}$

2) Treat scales $\Lambda < \Lambda_{\rm MF}$ in mean-field theory with $\Gamma^{\Lambda_{\rm MF}}$ 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 $\mathbf{Q}$

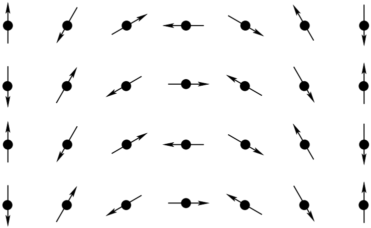
$$\Delta_{\mathbf{k}} = \int_{\mathbf{k}'} V_{\mathbf{k}\mathbf{k}'} \langle a_{-\mathbf{k}'\downarrow} a_{\mathbf{k}'\uparrow} \rangle$$

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

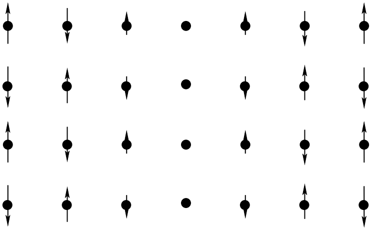
For $\mathbf{Q} = (\pi, \pi)$: spiral state = Néel state

Spiral versus collinear SDW

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



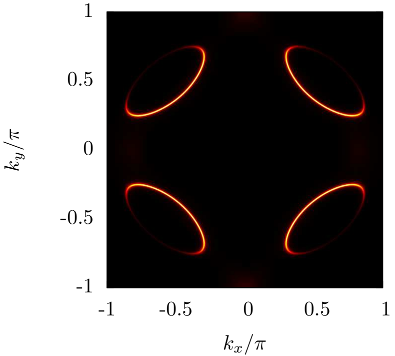
In collinear SDW smaller energy gain from regions with reduced magnetization amplitudes



Electron spectral function in spiral state

Underdoped regime

Eberlein, wm, Sachdev, Yamase 2016

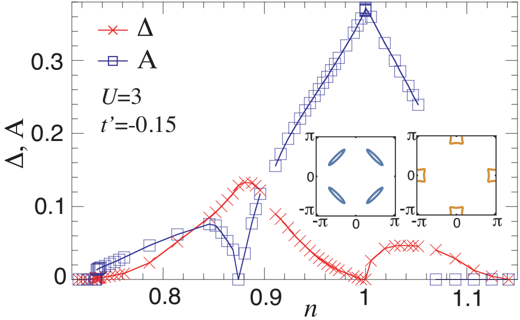


Strongly momentum dependent spectral weight makes pockets look like Fermi arcs

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

Antiferromagnetism & superconductivity vs. density

Yamase, Eberlein, wm 2016



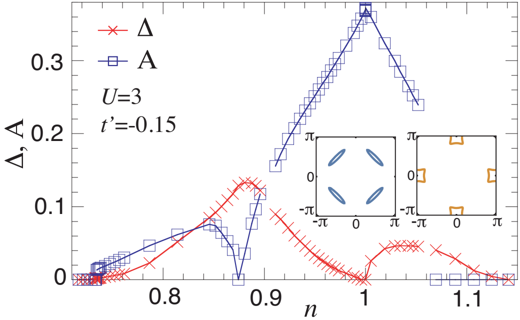
Ground state
order parameters
vs. density

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

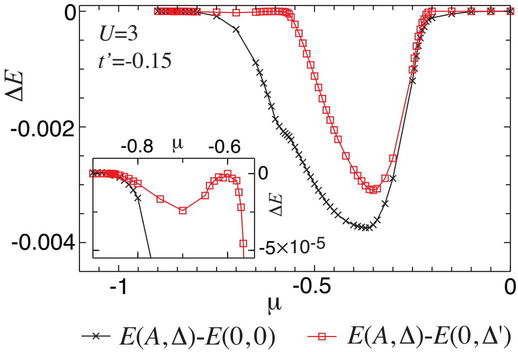
Inset:
Electron and hole pockets in Néel state near half-filling

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

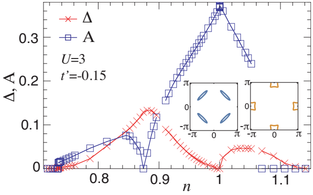
Lichtenstein & Katsnelson 2000; Capone & Kotliar 2006; Aichhorn et al. 2006; Kancharla, Kyung, ..., Tremblay 2008; B.-X. Zheng & G. K.-L. Chan 2016

“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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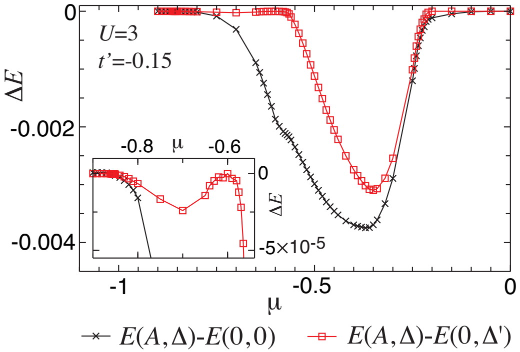

Total condensation energy
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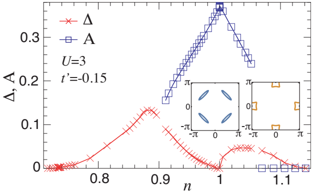

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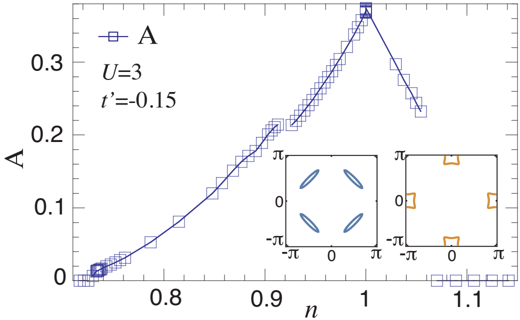
Suppressing superconductivity

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

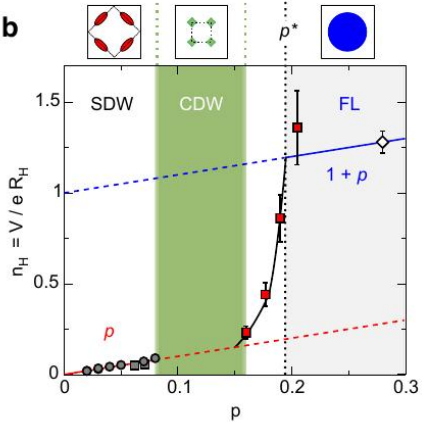


Magnetic order parameter with superconductivity suppressed

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?



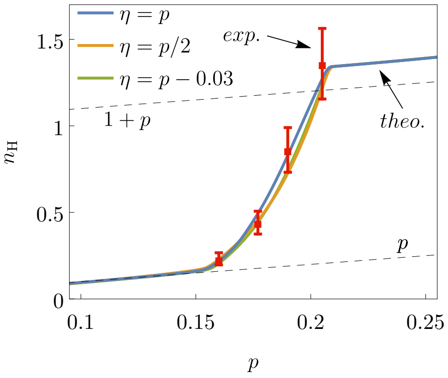
Observed Hall coefficient consistent with hole pockets in SDW state

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)

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



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

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

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DMFT as a booster rocket for functional RG

Truncation of flow equation hierarchy justified only for weak interactions

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

Leap to strong coupling:

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

Local correlations captured non-perturbatively

Taranto, Andergassen, Bauer, Held, Katanin, wm, Rohringer, Toschi 2014

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

Dynamical mean-field theory

wm & Vollhardt 1989

Georges & Kotliar 1992

DMFT = *local* approximation for self-energy and other vertex functions

Exact in infinite dimensions

Self-energy $\Sigma(\omega) \equiv \Sigma_{\mathbf{jj}}(\omega)$ functional of local propagator $G_{\mathrm{loc}}(\omega)$

Local self-energy same as that for local auxiliary action
$\leftrightarrow$ single-impurity Anderson model

$$\mathcal{S}_{\mathrm{loc}}[\psi, \bar{\psi}] = -\sum_{\omega,\sigma} \bar{\psi}_{\omega,\sigma} \mathcal{G}_0^{-1}(\omega) \psi_{\omega,\sigma} + U \int_0^\beta d\tau \, \bar{\psi}_\uparrow(\tau) \psi_\uparrow(\tau) \bar{\psi}_\downarrow(\tau) \psi_\downarrow(\tau)$$

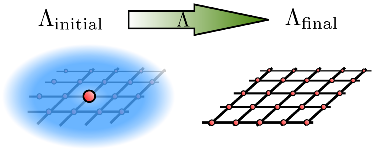
with Weiss field $\mathcal{G}_0^{-1}(\omega)$

Self-consistency condition: $G_{\mathrm{loc}}^{-1}(\omega) = \mathcal{G}_0^{-1}(\omega) - \Sigma(\omega)$

From infinite to finite dimensions

Taranto et al. 2014

Idea: Construct fRG flow that interpolates smoothly between DMFT action and exact action of *d*-dimensional system.



Wetterich's flow equation holds for *any* modification of quadratic part of action

Simple linear interpolation:

$$[G_0^\Lambda(k_0, \mathbf{k})]^{-1} = \Lambda\, \mathcal{G}_0^{-1}(k_0) + (1-\Lambda)\, G_0^{-1}(k_0, \mathbf{k})$$

Weiss field — bare lattice propagator

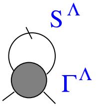
Initial condition: $\Sigma^{\Lambda_0} = \Sigma_{\mathrm{dmft}}$ $\quad \Gamma^{(2m)\Lambda_0} = \Gamma^{(2m)}_{\mathrm{dmft}}$ $\quad (\Lambda_0 = 1)$

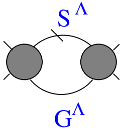
Truncation of flow for non-local correlations

Initially, no contribution from three-particle vertex,

if flow is set up such that $G^{\Lambda}_{\mathrm{loc}}|_{\Sigma^{\Lambda}=\Sigma_{\mathrm{dmft}}} = G_{\mathrm{loc,dmft}}$ for all Λ!

$\Rightarrow$ Keep only Σ^{Λ} and two-particle vertex Γ^{Λ} in flow equations:

$\frac{d}{d\Lambda}\Sigma^{\Lambda} =$ 

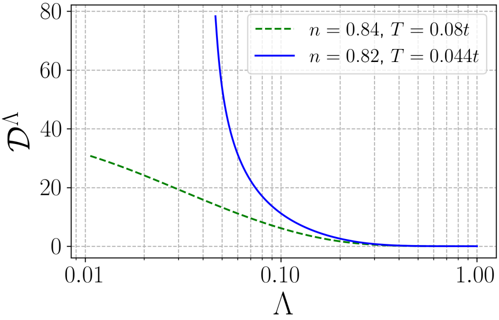
$\frac{d}{d\Lambda}\Gamma^{\Lambda} =$ 

Full frequency dependence of two-particle vertex (three variables!) required at strong coupling!

Hard, but managable by Italian Ferrari team (Taranto & Vilardi)

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.

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
- Functional RG at strong coupling with DMFT as a booster rocket: superconductivity at temperatures $T < 100K$