June 24, 2014
(ISSP workshop)

Dual fermion approach to unconventional superconductivity and spin/charge density wave

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Outline

i. Introduction

ii. Extension of DMFT: Dual fermion approach

local correlation + long-range correlation

iii. Demonstrative results for 2D Hubbard model:

- AFM
- Unconventional superconductivity
- Charge instability (phase separation)
- Unconventional SDW/CDW

iv. Further development: dual boson

short-range correlation

Strongly correlated superconductors

Magnetism and Superconductivity...

- appear nearby in phase diagrams
- coexist

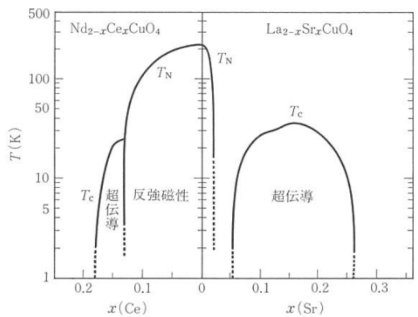


図 7.1 酸化物高温超伝導体 $La_{2-x}Sr_xCuO_4$ と $Nd_{2-x}Ce_xCuO_4$ の相図 [十倉好紀：固体物理 **25**, 618 (1990)]

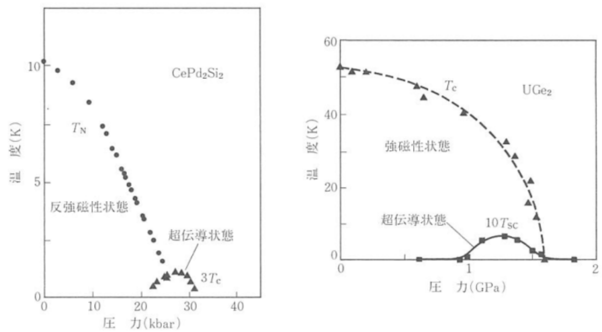


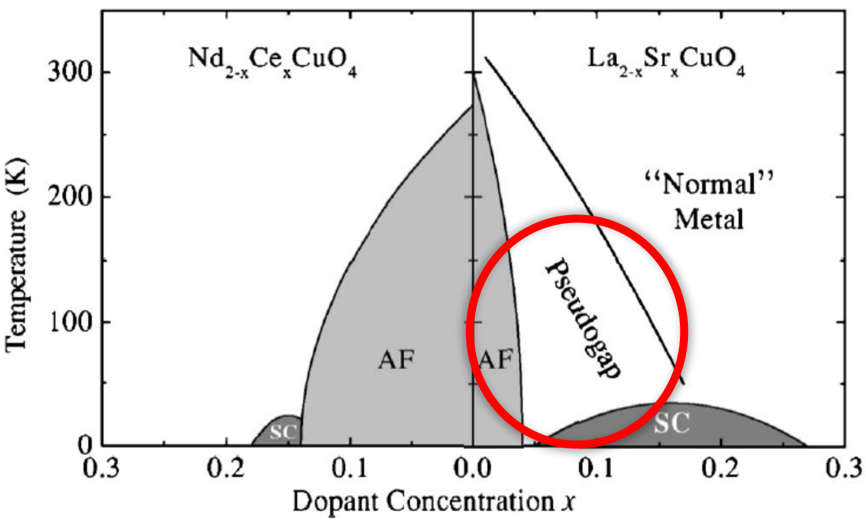
図 7.2 $CePd_2Si_2$[N. D. Mathur et al.: Nature **394**, 39 (1998)] と UGe_2[S. S. Saxena et al.: Nature **406**, 587 (2000)] の圧力–温度相図

From Shiba 2001

- Theory for superconductivity
  - Weak-coupling expansion (RPA, FLEX)
  - Numerically, two-dimensional system is most challenging.
- Theory for Mott-Insulator, heavy fermion (formation and treatment of local moments)
  - Dynamical mean-field theory (DMFT)
- Challenge
  - Unified treatment of magnetism and superconductivity
  - How itinerant and local natures can be dealt with at the same time
    Kuramoto, Miyake 1990, Ohkawa 1992, ...

Cuprates

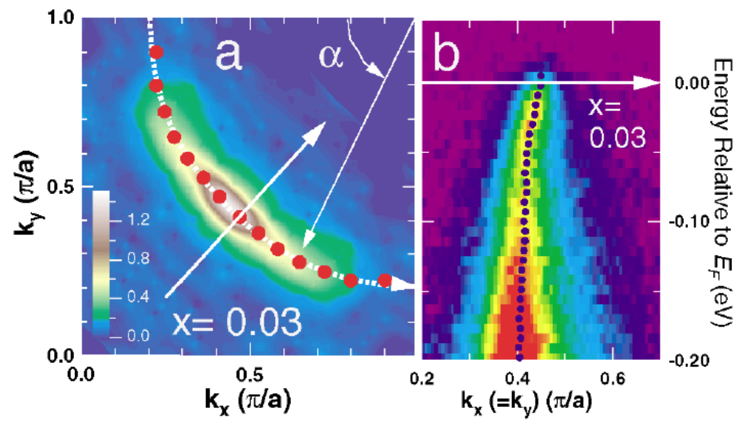
Phase diagram



From Damascelli et al. 2003

pseudo-gap "phase" or crossover?

ARPES spectra (Fermi arcs)



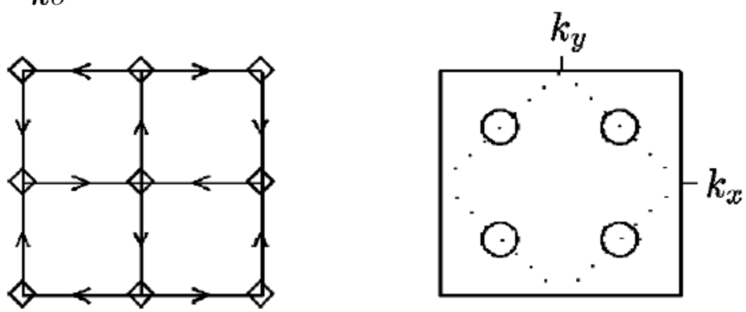
From Yoshida et al. 2003

Pseudo-gap state
For a review, Timusk, Statt 1999

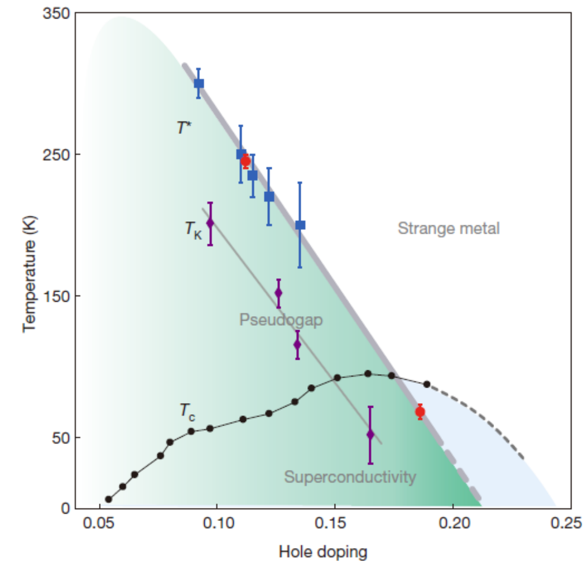
Staggered flux state / d-density wave

"hidden order" as the origin of pseudo gap

$$y = i \sum_{\boldsymbol{k}\sigma} f(\boldsymbol{k}) \langle c^{\dagger}_{\boldsymbol{k}+\boldsymbol{Q},\sigma} c_{\boldsymbol{k}\sigma} \rangle, \;\; f(\boldsymbol{k}) = \cos k_x - \cos k_y$$



Chakravarty et al, 2001, Nayak 2000



Strong-coupling limit (t-J model)
Kotliar, Liu, 1988
Affleck et al. 1988
Ubbens, Lee, 1992
Wen, Lee, 1995

slave-boson MF

broken time-reversal symmetry
Fauque et al, 2006
Shekhter et al. 2013

Numerical calculations in Hubbard model:
Honerkamp et al. 2002 (fRG)
Stanescu, Phillips, 2001 (Hubbard op)
Macridin et al. 2004 (DCA)
Lu et al, 2012 (variational cluster)
Yokoyama et al. arXiv (VMC)

No evidence of the transition

Unconventional SDW/CDW discussed in URu_2Si_2
Ikeda, Ohashi, 1998, Varma, Zhu, 2006, Fujimoto, 2011

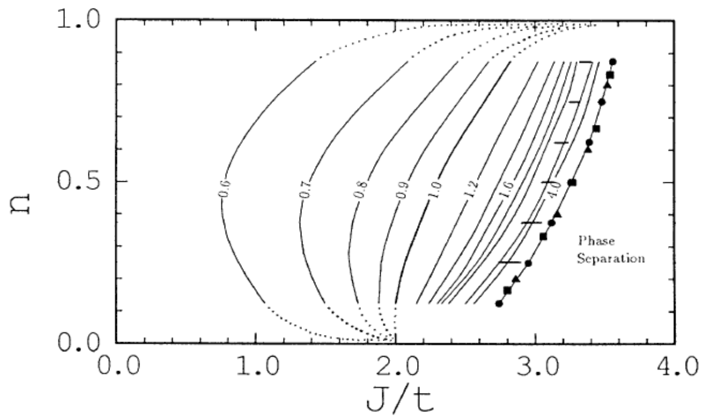
Charge instability (phase separation)

Phase separation (q=0 charge instability)

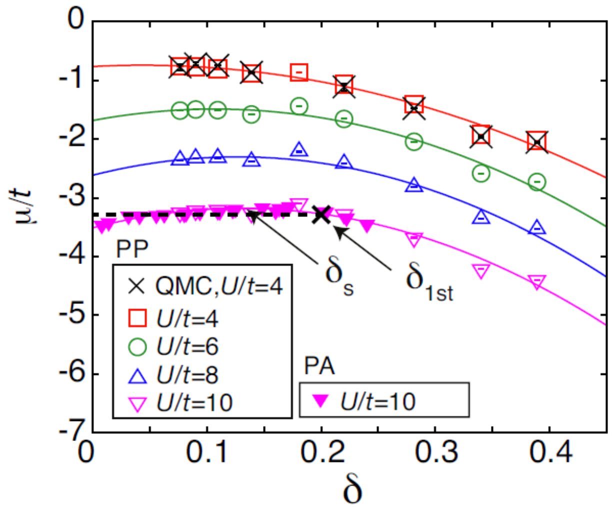
c.f. q≠0: Stripe order

t-J model
Emery, Kivelson, 1990

1D t-J model
Ogata et al, 1991



Hubbard model
Misawa, Imada, arXiv (VMC)



Random-coupling t-J model
JO, Vollhardt, 2013

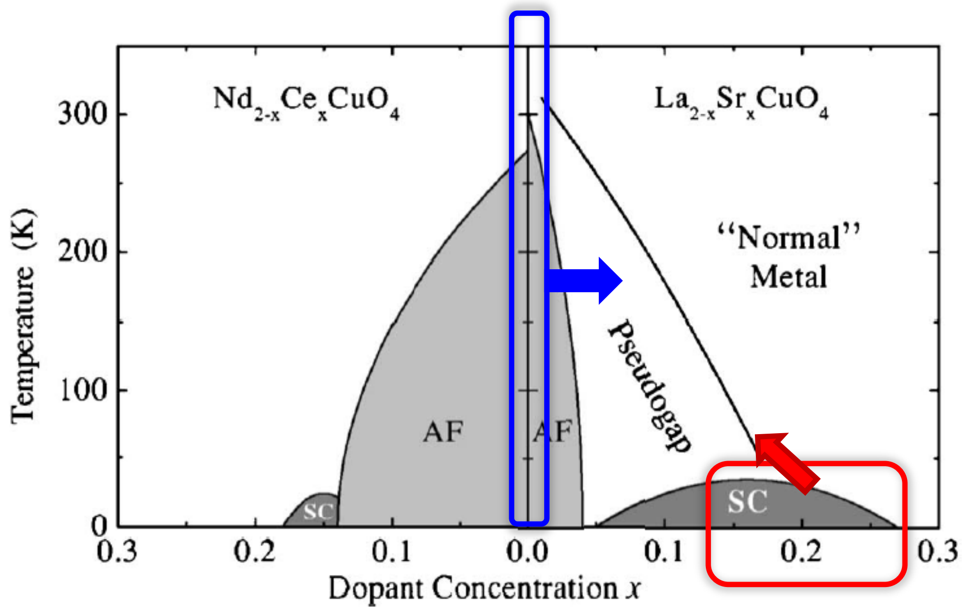
Hubbard model as a prototypical model

Doped Mott insulator:
- peculiar spectra
- d-DW / staggered flux state
- Charge instability (phase separation)

Hubbard model on a square lattice

$$H = \sum_{\boldsymbol{k}\sigma} \epsilon_{\boldsymbol{k}} c^{\dagger}_{\boldsymbol{k}\sigma} c_{\boldsymbol{k}\sigma} + U \sum_{\boldsymbol{r}} n_{\boldsymbol{r}\uparrow} n_{\boldsymbol{r}\downarrow}$$

Mott insulator by DMFT



SC by weak-coupling theory
(RPA, FLEX)

Challenge:
- New theoretical framework
  * treating magnetism and superconductivity
  * Mott insulator by DMFT + momentum dependence
- Possible symmetry breaking and excitations from microscopic models

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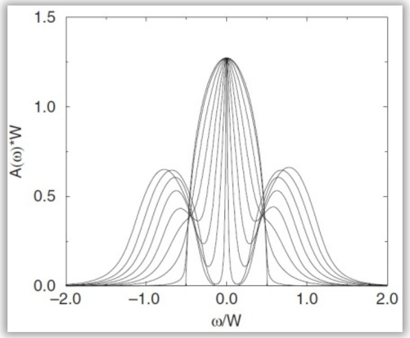
DMFT —Exact solution of non-trivial d=∞ limit of SCES

Many applications...

$$\Sigma(i\omega, \boldsymbol{k}) \rightarrow \Sigma(i\omega)$$

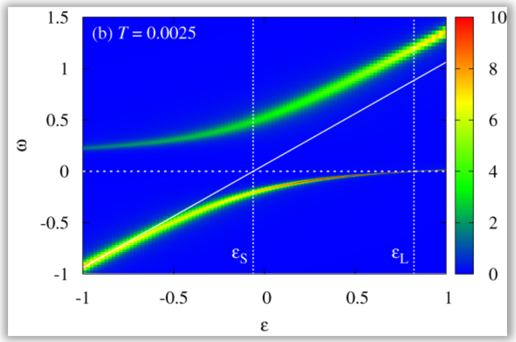
Metzner, Vollhardt 1989
Georges, Kotliar 1992
Georges et al. 1996

Mott insulator



From Vollhardt et al. 2005

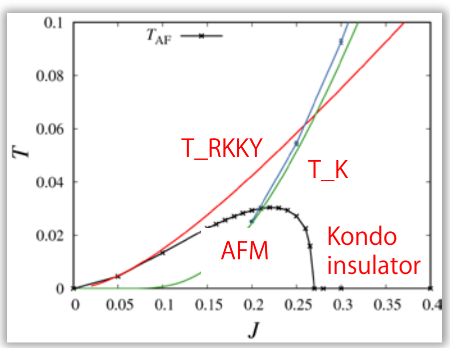
Heavy fermion



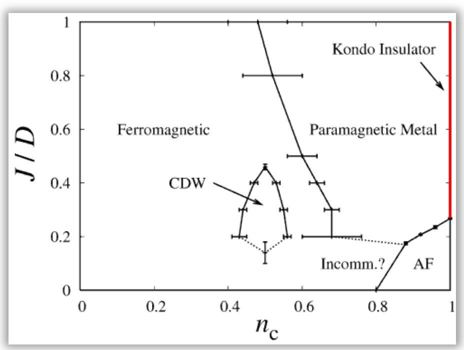
From JO et al. 2009

- Band-structure calculation (LDA + DMFT)
- Local degrees of freedom (multi-orbital, f^2 configuration, Holstein-phonon...)
- Non-equilibrium

Kondo lattice model



Kondo effect vs. RKKY interaction



magnetic and CDW phases

From JO et al. 2009

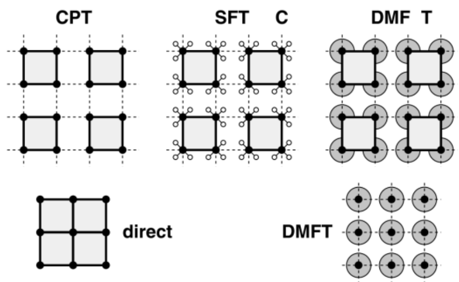
What cannot be addressed
- unconventional superconductivity
- quantum critical phenomena
...

An extension needed

Extension of DMFT —to incorporate non-local correlation

- Cluster extensions Maier et al. 2005
  - Cellular DMFT Kotliar et al. 2001
  - Dynamical cluster approximation Hettler et al. 1998
  - Self-energy functional theory Potthoff 2003

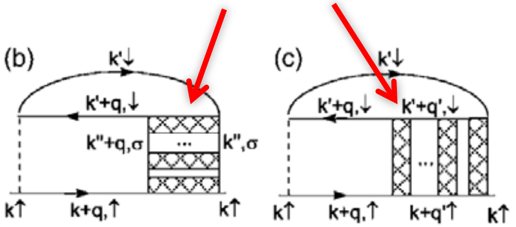
  finite-size effect, sign problem in QMC, ...



From Potthoff 2005

- Other extensions within single-site approximation
  - Kusunose 2006
  - Dynamical vertex approximation Toschi et al. 2007
  - Dual fermion approach
    Rubtsov et al. 2008, Hafermann et al. 2009
  - GW + DMFT
    Biermann et al. 2003, Sun, Kotliar 2004, Ayral et al. 2013
  - Slezak et al. 2009
  - DMFT + fRG Taranto et al. 2013

spin & charge fluctuations
constructed with local vertex



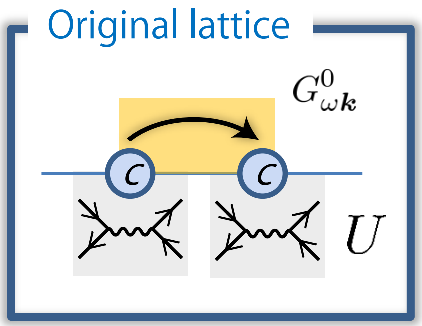
From Toschi et al. 2007

combine...
- local correlation by DMFT
- long-range correlation (collective modes) by RPA, FLEX

how to formulate? → **dual fermion approach**

Dual fermion approach I: Overview

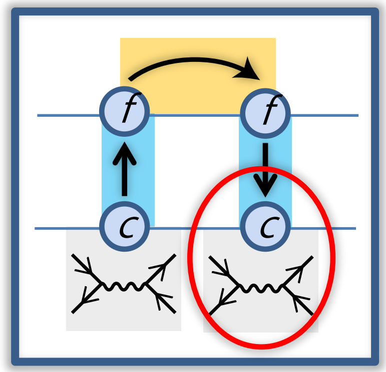
Rubtsov et al. 2008



Hubbard model

$$\mathcal{S}[c^*, c] = \sum_i \left\{ \sum_{\omega\sigma} c^*_{\omega i\sigma} \left(-i\omega - \mu\right) c_{\omega i\sigma} + U \int d\tau n_{i\uparrow}(\tau) n_{i\downarrow}(\tau) \right\} + \sum_{\omega \boldsymbol{k} \sigma} \epsilon_{\boldsymbol{k}} c^*_{\omega \boldsymbol{k}\sigma} c_{\omega \boldsymbol{k}\sigma}$$

Auxiliary fermion f (dual fermion)
Hopping-term "decoupled"

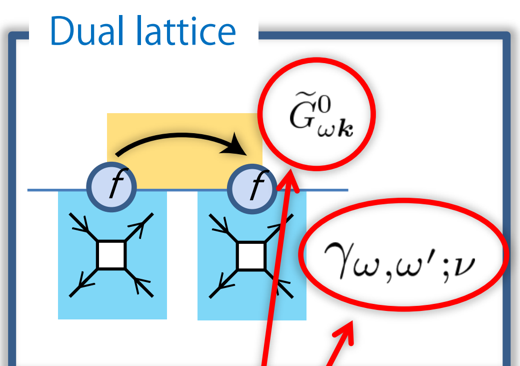


local w.r.t. c variables

bath $\Delta_\omega c^*_{\omega i\sigma} c_{\omega i\sigma}$

Solving the lattice problem in two steps

① integrate out c at each site (solve impurity problem)



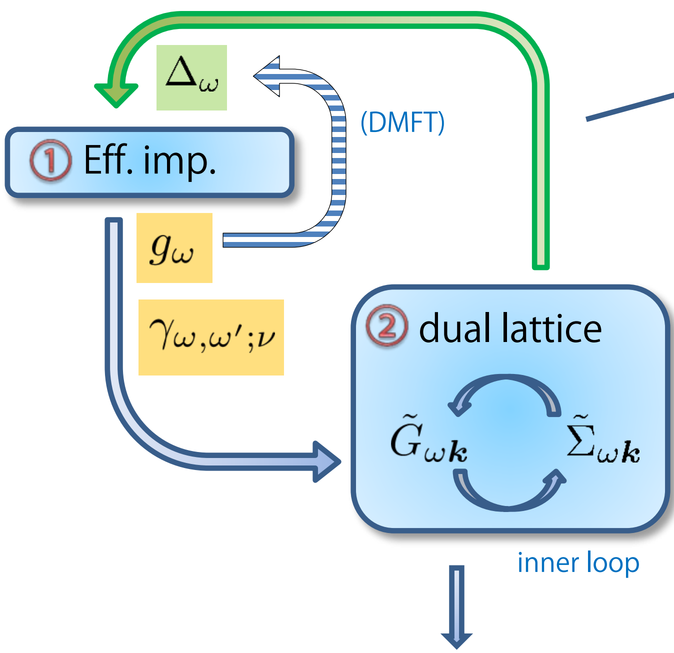
$$\tilde{\mathcal{S}}[f^*, f] = -\sum_{\omega \boldsymbol{k} \sigma} (\tilde{G}^0_{\omega \boldsymbol{k}})^{-1} f^*_{\omega \boldsymbol{k}\sigma} f_{\omega \boldsymbol{k}\sigma} + \frac{1}{4} \sum \gamma^{\sigma_1\sigma_2\sigma_3\sigma_4}_{\omega,\omega';\nu} f^*_{k\sigma_1} f^*_{k'+q,\sigma_2} f_{k'\sigma_3} f_{k+q,\sigma_4} + \cdots$$

full account of
local correlations

② perturbation expansion w.r.t γ

Dual fermion approach II: Self-consistency loop

Rubtsov et al. 2008



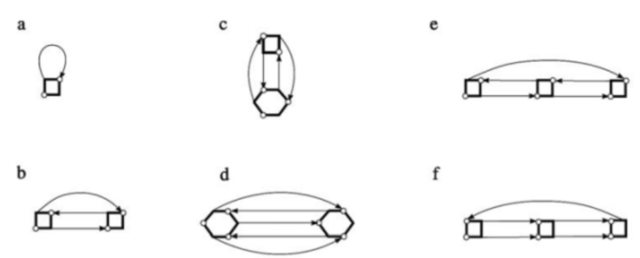
$$G^{-1}_{\omega\boldsymbol{k}} = (g_\omega + g_\omega \widetilde{\Sigma}_{\omega\boldsymbol{k}} g_\omega)^{-1} + \Delta_\omega - \epsilon_{\boldsymbol{k}}$$

Self-consistency condition

$$\left\langle \widetilde{G}_{\omega\boldsymbol{k}} \right\rangle_{\boldsymbol{k}} \equiv 0$$

reduced to DMFT in the lowest-order approximation

Self-energy diagrams



① $$S_{\mathrm{imp}}[c_i^*, c_i] = \sum_{\omega\sigma} c^*_{\omega i\sigma} \left(-i\omega - \mu + \Delta_\omega\right) c_{\omega i\sigma} + U \int d\tau n_{i\uparrow}(\tau) n_{i\downarrow}(\tau$$

② $$\tilde{S}[f^*, f] = -\sum_{\omega\boldsymbol{k}\sigma} (\widetilde{G}^0_{\omega\boldsymbol{k}})^{-1} f^*_{\omega\boldsymbol{k}\sigma} f_{\omega\boldsymbol{k}\sigma} + \frac{1}{4} \sum \gamma^{\sigma_1\sigma_2\sigma_3\sigma_4}_{\omega,\omega';\nu} f^*_{k\sigma_1} f^*_{k'+q,\sigma_2} f_{k'\sigma_3} f_{k+q,\sigma_4} + \cdots$$

$$\widetilde{G}^0_{\omega\boldsymbol{k}} = (g_\omega^{-1} + \Delta_\omega - \epsilon_{\boldsymbol{k}})^{-1} - g_\omega$$

Approximations

1. Retain only 2-body interactions
2. Sum up a certain set of diagrams

Dual fermion approach III: First few diagrams

Rubtsov et al. 2008

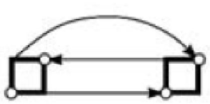
1st-order diagram

$$\tilde{\Sigma}^{(1)}_{\omega} =$$  $$\equiv 0$$

DMFT

from self-consistency condition $\left\langle \tilde{G}_{\omega \boldsymbol{k}} \right\rangle_{\boldsymbol{k}} \equiv 0$

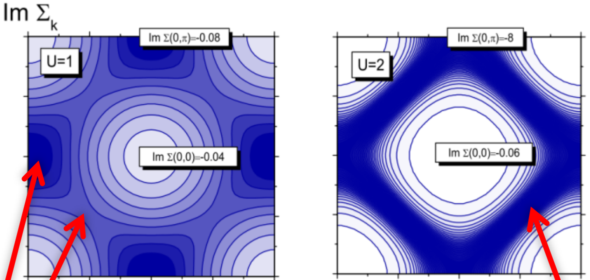
2nd-order diagram

$$\tilde{\Sigma}^{(2)}_{\omega \boldsymbol{k}} =$$ 

k-dependence

$\mathrm{Im}\Sigma(0, \boldsymbol{k})$

n=1, T/t=0.2



U/t=4 (metal)

U/t=8 (Mott I)

k-dependent renormalization

Energy gap on the Fermi level

Fermi-surface structure + Strong local correlation

Dual fermion approach IV: Collective modes

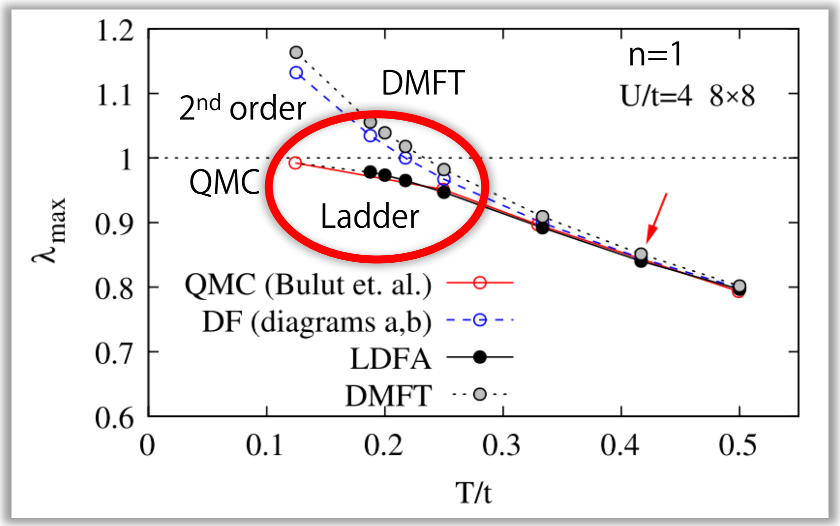
Spin and charge fluctuations (collective modes)

Hafermann et al. 2009

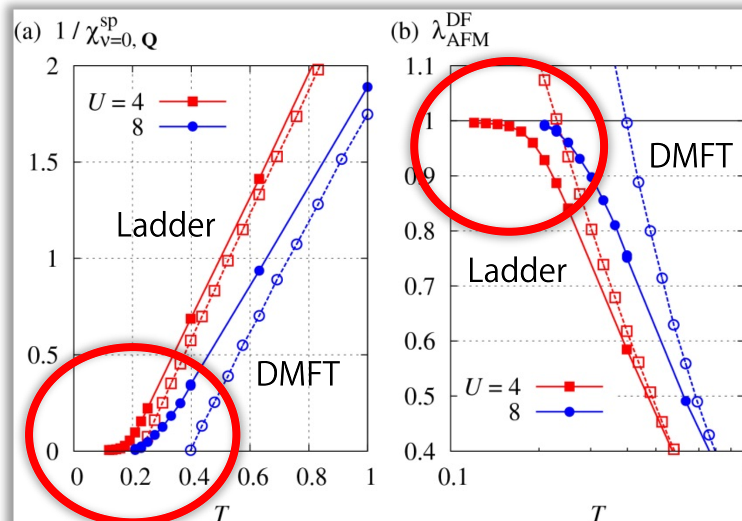
Ladder diagram (FLEX-type diagrams)

$$\tilde{\Sigma}^{(\text{ladder})}_{\omega \boldsymbol{k}} =$$

λ_{max}=1 corresponds to AFM transition



Recent improved calculation



Ladder diagrams suppress the AF transition.
(two-dimensionality is incorporated)
Mermin-Wagner theorem is fulfilled.

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Details of numerical calculations

Hubbard model on a square lattice

32 x 32 lattice sites

$$H = \sum_{\boldsymbol{k}\sigma} \epsilon_{\boldsymbol{k}} c^{\dagger}_{\boldsymbol{k}\sigma} c_{\boldsymbol{k}\sigma} + U \sum_{\boldsymbol{r}} n_{\boldsymbol{r}\uparrow} n_{\boldsymbol{r}\downarrow} \qquad \epsilon_{\boldsymbol{k}} = -2t(\cos k_x + \cos k_y), \quad t = 1, \; t' = 0$$

Impurity solver: Continuous-time QMC method (Rubtsov et al. 2005, Werner et al. 2006, Gull et al. 2011)

CT-HYB (Werner et al. 2006)

$$g_{\omega}, \quad \gamma_{\omega', \omega''; \nu}$$

Energy cutoff

For g : $N_1 = 2048, \cdots, 16384$

$|\omega| \le (2N_1 + 1)\pi T$

For γ : $N_2, N_3 = 10, \cdots, 60$

$|\omega'|, |\omega''| \le (2N_2 + 1)\pi T$

$|\nu| \le 2N_3 \pi T$

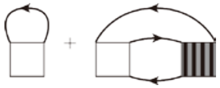
Δ_{ω}

Outer iteration (DMFT like)

dual-fermion self-energy

$$\tilde{G}^{-1}_{\omega \boldsymbol{k}} = (\tilde{G}^{0}_{\omega \boldsymbol{k}})^{-1} - \tilde{\Sigma}_{\omega \boldsymbol{k}}$$

$$\tilde{\Sigma}_{\omega \boldsymbol{k}} =$$



Inner iteration (FLEX like)
FFT applicable to k-sum

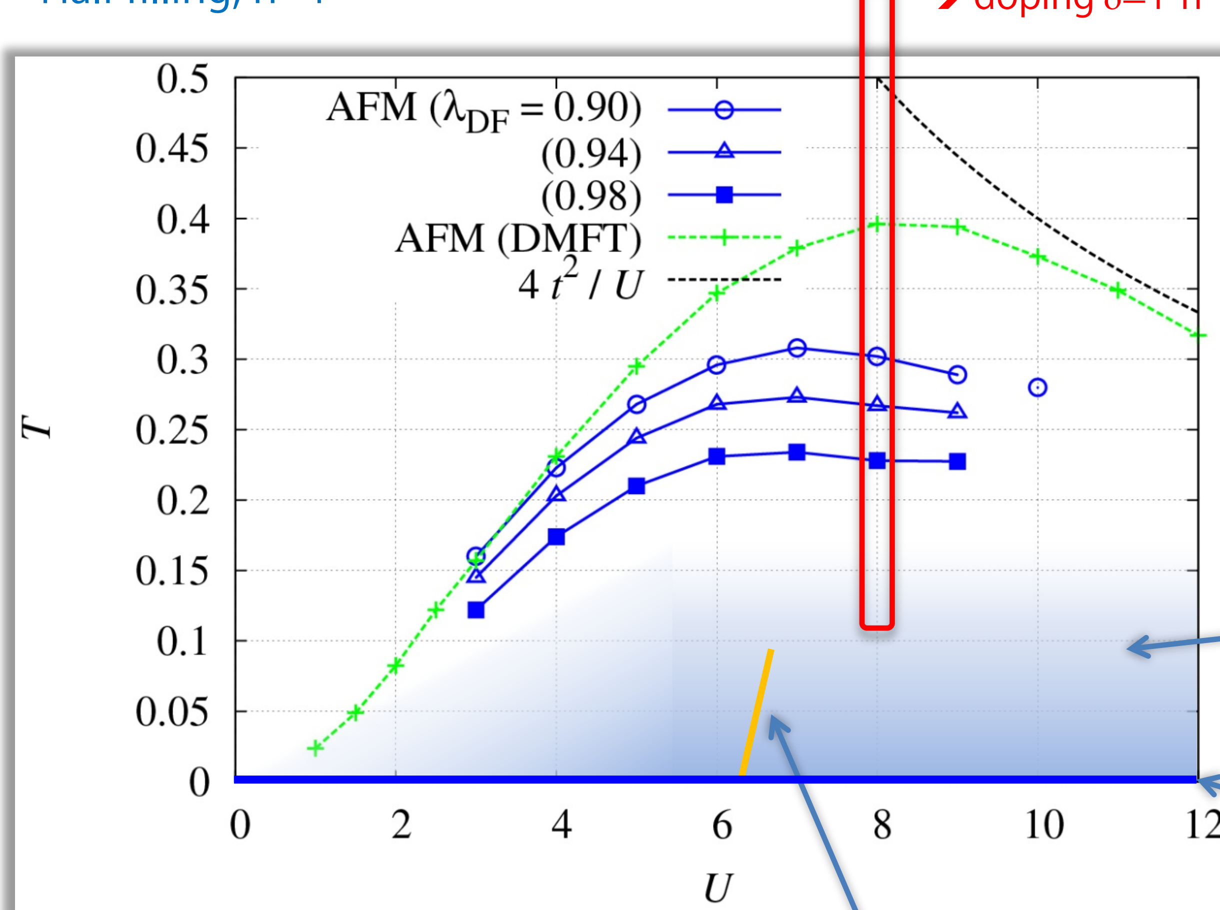
We investigate...

- AFM
- d-SC
- charge instability (phase separation)
- staggered flux state / d-DW

("quasi-2D") Phase diagram

Half filling, n=1

➔ doping δ=1-n



Critical regime

$\chi \sim e^{c\beta},\ \lambda \sim 1 - e^{-c\beta}$

Real AFM transition

(Mermin, Wagner)

$\chi = \infty,\ \lambda = 1$

Mott transition in CDMFT
with paramagnetic bath
(e.g. Park et al. 2008)

Superconductivity I: formalism

Pairing correlation with q=(iν,**q**)=0

$$\tilde{P}^{\pm}_{kk'} = \tilde{P}_{kk'} \pm \tilde{P}_{k-k'} \qquad \tilde{P}_{kk'} = \langle f_{k\uparrow} f_{-k\downarrow} f^*_{-k'\downarrow} f^*_{k'\uparrow} \rangle$$

Linearized BS equation

$$\hat{K}^{\pm}\phi^{\pm} = \lambda^{\pm}\phi^{\pm}, \quad \hat{K}^{\pm} = \frac{T}{N}\hat{\tilde{P}}^{0}\hat{\Gamma}^{\mathrm{pp}\pm} \quad \Rightarrow \quad \lambda, \ \phi(i\omega, \boldsymbol{k})$$

$$k = (i\omega, \boldsymbol{k})$$

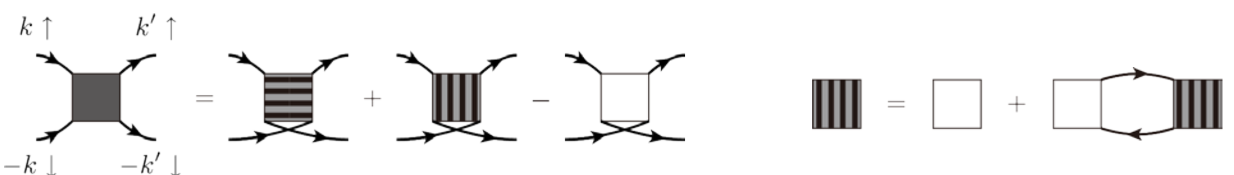
$$f_{k\uparrow} f_{-k\downarrow} \to \frac{1}{\sqrt{2}}(f_{k\uparrow} f_{-k\downarrow} \mp f_{k\downarrow} f_{-k\uparrow})$$

BS equation

$$\tilde{P}_{kk'} = \tilde{P}^0_k \delta_{kk'} + \frac{T}{N}\sum_{k''} \tilde{P}^0_k \Gamma^{\mathrm{pp}}_{kk''} \tilde{P}_{k''k'}$$

$$\tilde{P}^0_k = \tilde{G}_k \tilde{G}_{-k}$$

Irreducible vertex for superconductivity

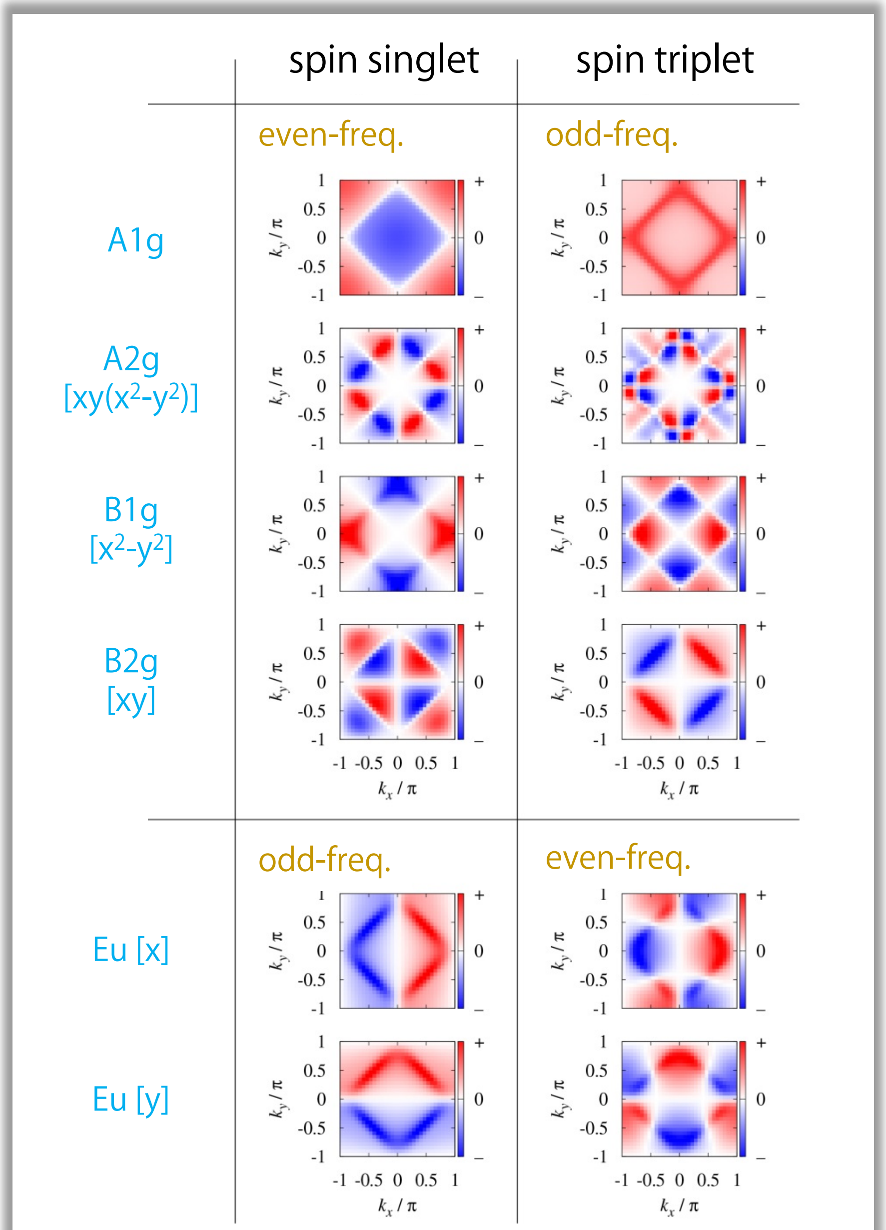


transverse spin fluctuations

charge & longitudinal spin fluctuations

Superconductivity II: Eigenfunctions

$\phi(i\pi T, \boldsymbol{k})$



U=8t, δ=0.14, T=0.1t

How to solve

$$\hat{K}^{\pm}\phi^{\pm} = \lambda^{\pm}\phi^{\pm}$$

-use the power method

$$\phi^{\text{new}} = \mathcal{P}\hat{K}\phi^{\text{old}}$$

orbital projection

-multiply a phase factor, then

$$\text{Im}\phi(i\omega, \boldsymbol{k}) = 0$$

-Either even- or odd-freq. part finite

$$\phi(i\omega, \boldsymbol{k}) \pm \phi(-i\omega, \boldsymbol{k})$$

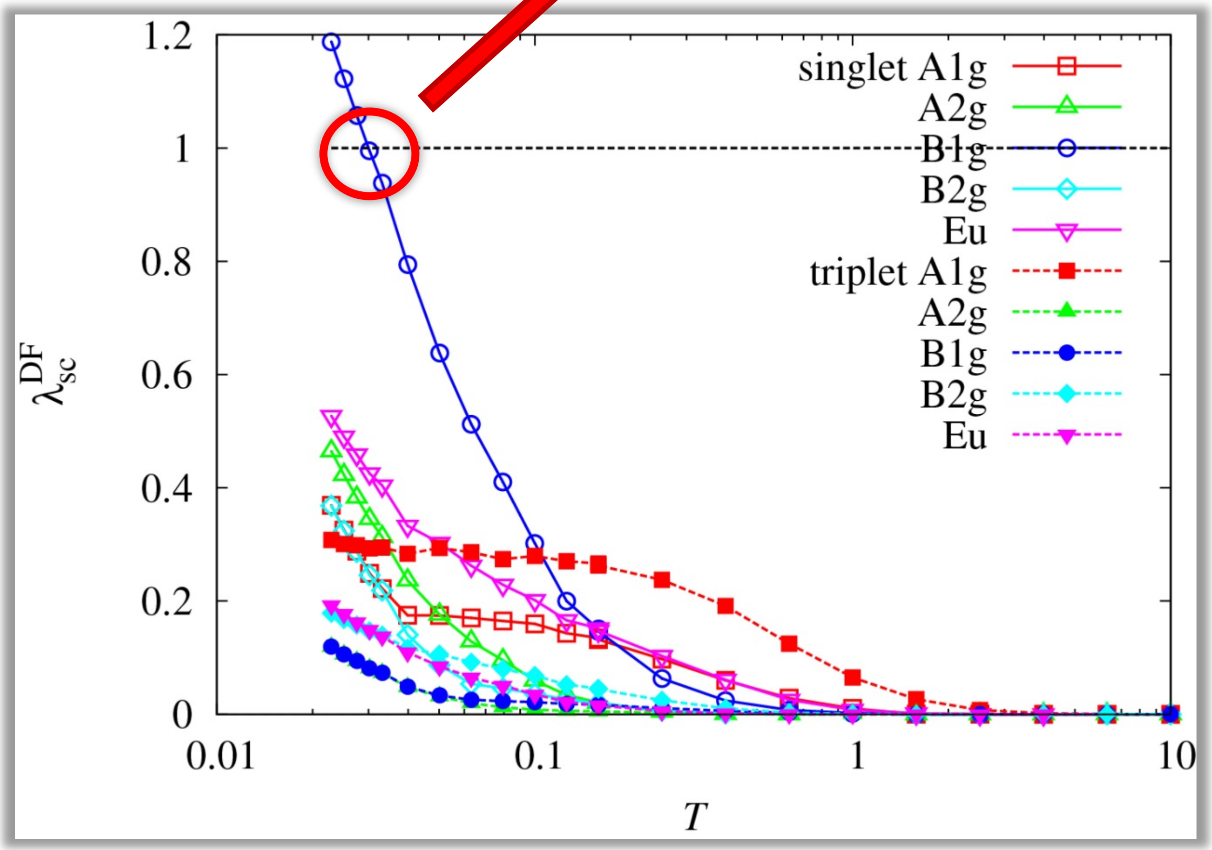
Pauli principle is fulfilled

(spin × parity × time-reversal)

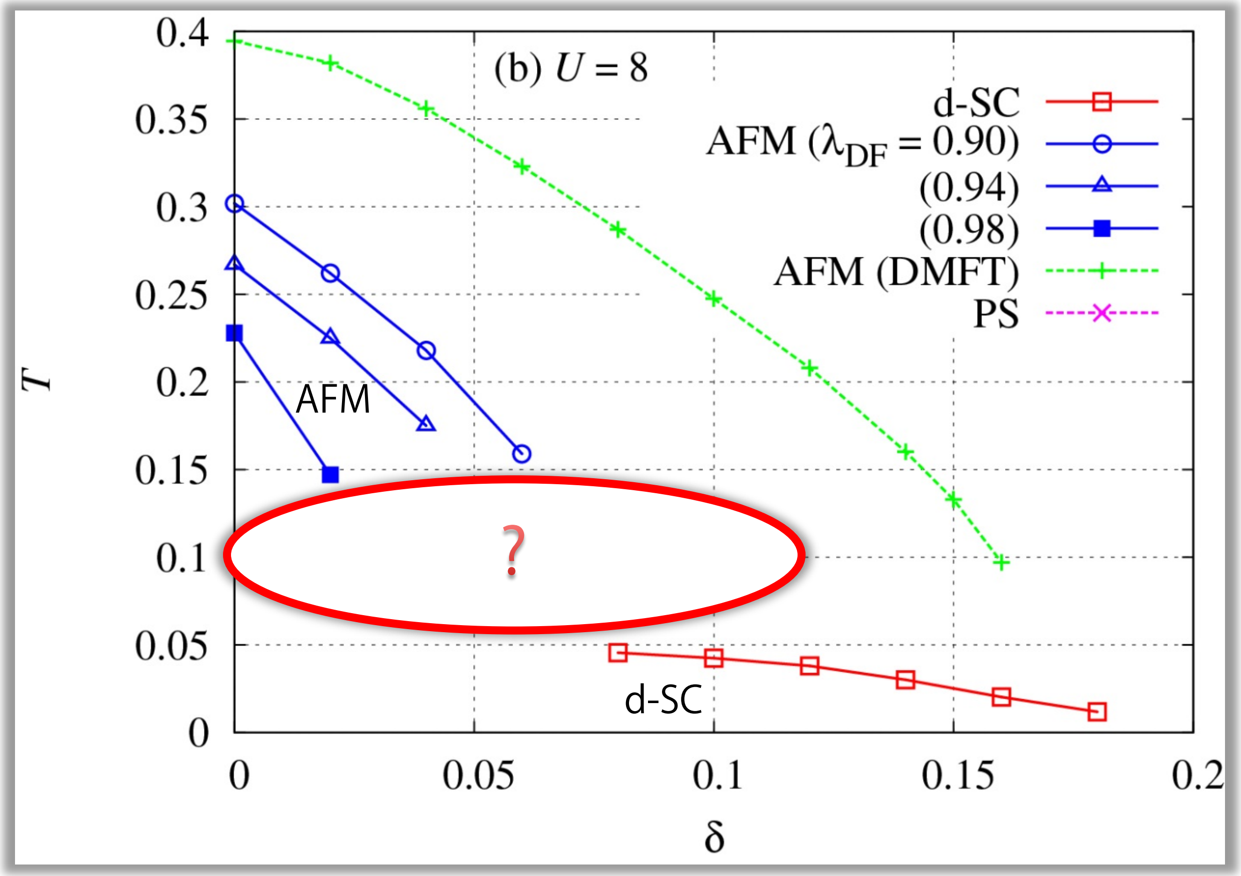
Superconductivity III: Eigenvalues

U=8t, δ=0.14

T_{dSC}



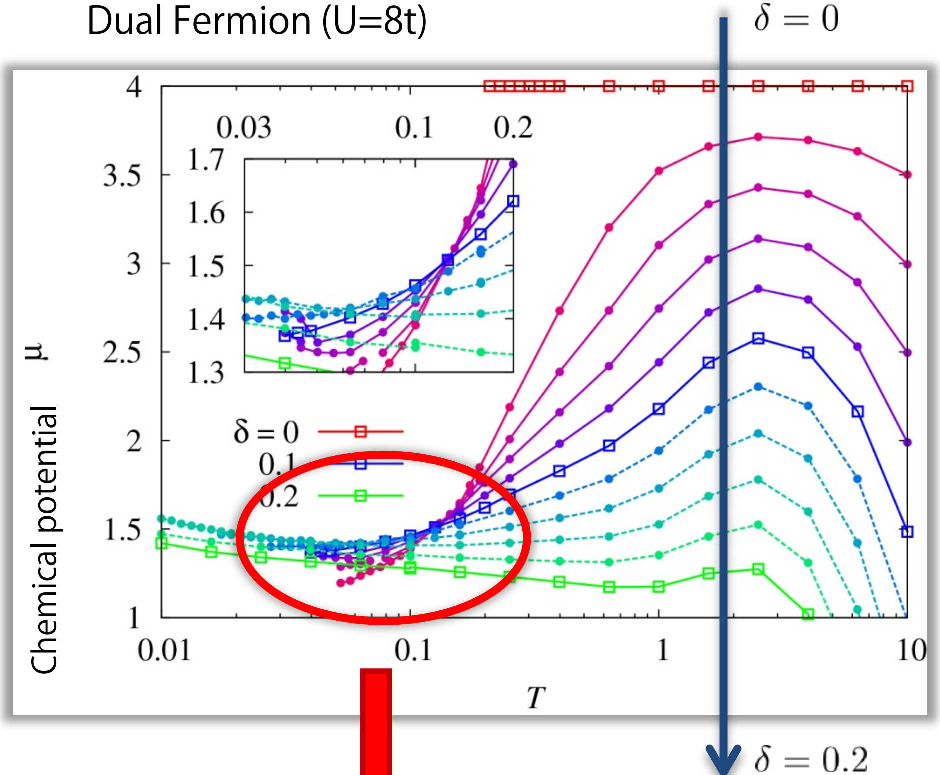
Phase diagram



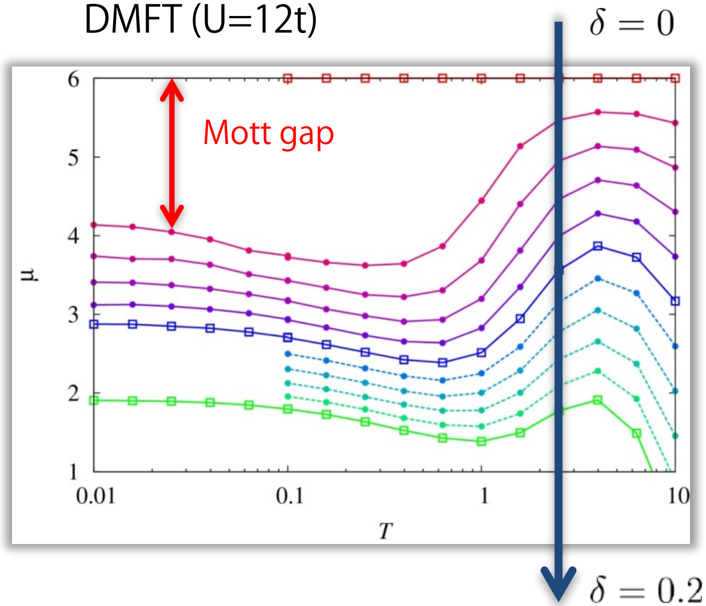
Phase transition? (charge instability, staggered flux state)
Or just a normal metal with strong spin fluctuations.

Phase separation (uniform charge instability)

Dual Fermion (U=8t)



DMFT (U=12t)

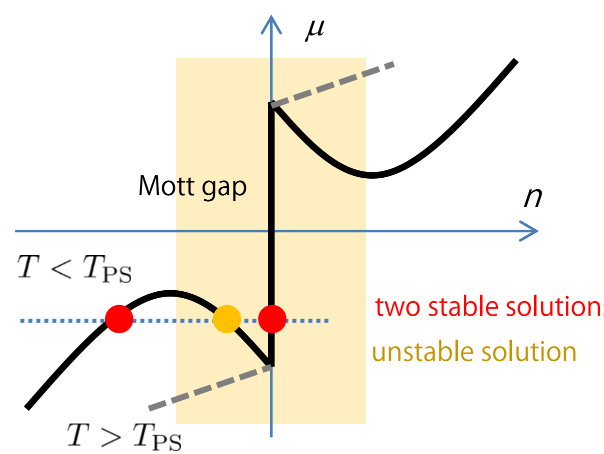


$$\chi^{\mathrm{ch}}_{\boldsymbol{q}=0} = \frac{\partial n}{\partial \mu} = \infty$$

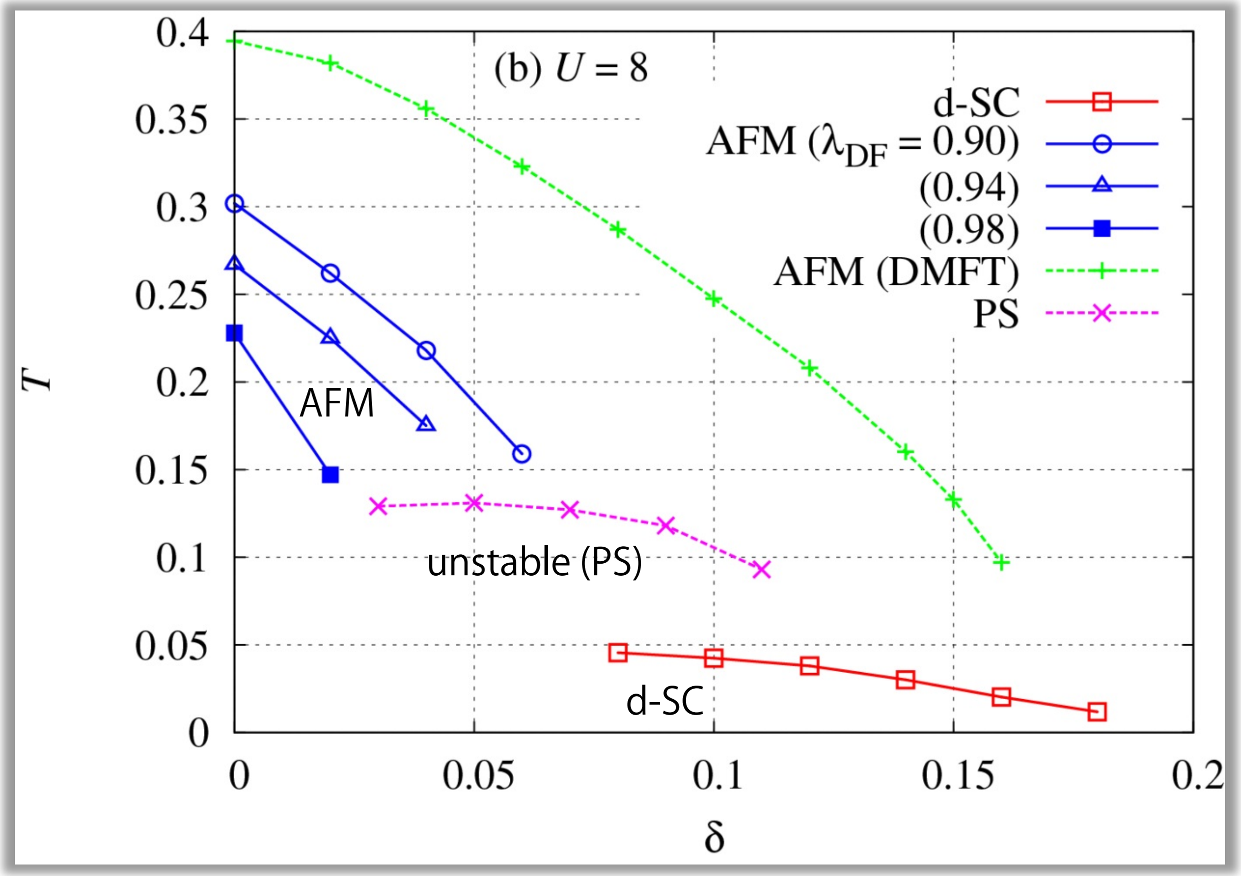
at $T = T_{\mathrm{PS}}$

$T < T_{\mathrm{PS}}$

Phase separation



Phase diagram



PS consistent with VMC (Misawa, Imada, arXiv)
Other possibilities? (staggered flux state)

Unconventional SDW/CDW

Unconventional DW $\quad \boldsymbol{Q} \equiv (\pi, \pi)$

$$M_{\pm}^{\alpha} = \sum_{\boldsymbol{k}} \phi_{\boldsymbol{k}}^{\alpha} \left(\langle c_{\boldsymbol{k}\uparrow}^{\dagger} c_{\boldsymbol{k}+\boldsymbol{Q}\uparrow} \rangle \pm \langle c_{\boldsymbol{k}\downarrow}^{\dagger} c_{\boldsymbol{k}+\boldsymbol{Q}\downarrow} \rangle \right)$$

$$\phi_{\boldsymbol{k}}^{\alpha} = 1,\ \underline{\cos k_x - \cos k_y},\ \cos k_x + \cos k_y, \cdots$$

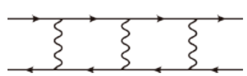
staggered flux state / d-DW

Kotliar 1988
Nayak 2000

Mean-field (RPA) analysis (Ozaki 92)

$$H = \sum_{\boldsymbol{k}\sigma} \epsilon_{\boldsymbol{k}} c_{\boldsymbol{k}\sigma}^{\dagger} c_{\boldsymbol{k}\sigma} + U \sum_{i} c_{i\uparrow}^{\dagger} c_{i\uparrow} c_{i\downarrow}^{\dagger} c_{i\downarrow} + \frac{1}{2} \sum_{\langle ij \rangle} \sum_{\sigma\sigma'} \left[V c_{i\sigma}^{\dagger} c_{i\sigma} c_{j\sigma'}^{\dagger} c_{j\sigma'} + J c_{i\sigma}^{\dagger} c_{i\sigma'} c_{j\sigma'}^{\dagger} c_{j\sigma} \right]$$

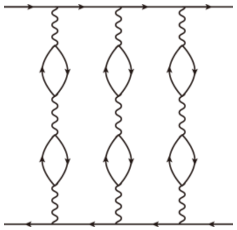
(A) (B)

		U	*V, J*	
(A)		Conventional DW (charge & longitudinal spin)	Conventional DW	$V_{\boldsymbol{q}} = V(\cos q_x + \cos q_y)$
(B)		Conventional DW (transverse spin)	Unconventional DW	$V_{\boldsymbol{k}-\boldsymbol{k}'} = \sum_{\alpha} I_{\alpha} \phi_{\boldsymbol{k}}^{\alpha} \phi_{\boldsymbol{k}'}^{\alpha}$

$$\chi_{\alpha\boldsymbol{Q}} = \frac{\chi_{\alpha\boldsymbol{Q}}^{0}}{1 - I_{\alpha}\chi_{\alpha\boldsymbol{Q}}^{0}} \qquad \chi_{\alpha\boldsymbol{Q}}^{0} = -\frac{T}{N} \sum_{\boldsymbol{k}\omega} |\phi_{\boldsymbol{k}}^{\alpha}|^{2} G_{\boldsymbol{k}\omega} G_{\boldsymbol{k}+\boldsymbol{Q},\omega}$$

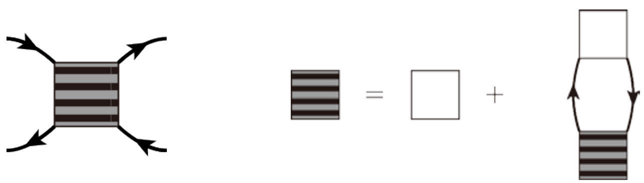
$I_{\alpha}(\boldsymbol{Q})$	Conventional	Unconventional
SDW	*U + 4J*	*V*
CDW	*- U + 4J + 8V*	*V + 2J*

Unconventional DW mediated by spin fluctuations



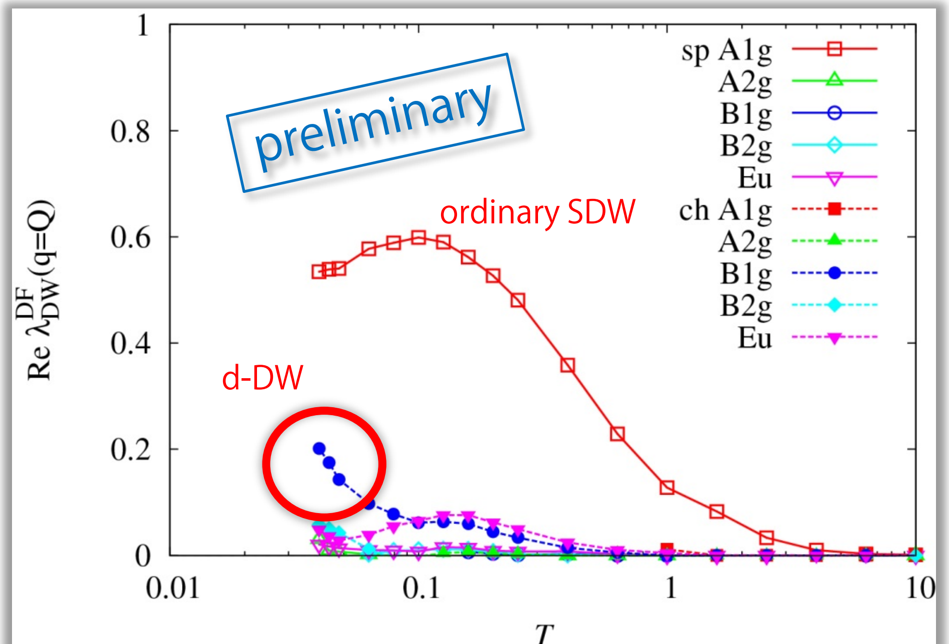
Unconventional SDW/CDW

irreducible vertex for unconventional DW



Linearized BS equation

$$\hat{L}_{\boldsymbol{Q}}\psi = \lambda\psi, \quad (\hat{L}_{\boldsymbol{Q}})_{kk'} = \frac{T}{N} G_{\omega\boldsymbol{k}} G_{\omega,\boldsymbol{k}+\boldsymbol{Q}} \Gamma'_{kk}$$



U=8t, δ=0.1

No transition to d-DW was found

$$\lambda_{\mathrm{dSC}} > \mathrm{Re}\lambda_{\mathrm{dDW}}$$

Technical difficulty:
treatment of complex eigenvalues in the power method
(λ consists of pure real and complex ones)

i. Introduction

ii. Extension of DMFT: Dual fermion approach

local correlation + long-range correlation

iii. Demonstrative results for 2D Hubbard model:

- AFM
- Unconventional superconductivity
- Charge instability (phase separation)
- Unconventional SDW/CDW

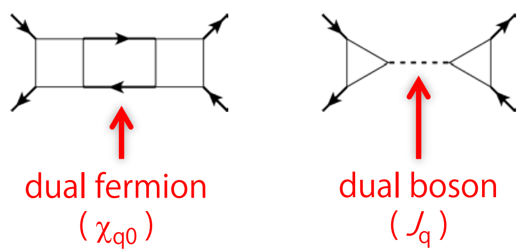
iv. Further development: dual boson

short-range correlation

Further development

- DMFT: Local correlation
- Dual fermion: Long-range correlation, collective modes
- How to deal with **short-range correlation**?
  - ➔ DMFT for spin systems
  - ➔ dual boson approach

vicinity of Mott-I, frustration, spin glass, ...



Dual boson approach... (Rubtsov et al. 2012)

(i) treats χ_{q0} and J_q on equal footing
(ii) takes into account feedback from spin fluctuations to the effective impurity (short-range correlation)

Effective impurity coupled with fermionic and bosonic baths

$$S_{\rm imp} = \int d\tau d\tau' \left\{ \sum_\sigma c_\sigma^\dagger(\tau)[\partial_{\tau'} - \mu + \Delta(\tau-\tau')]c_\sigma(\tau') - \frac{1}{2}\sum_{\alpha=0,x,y,z} S_\alpha(\tau)\mathcal{J}_\alpha(\tau-\tau')S_\alpha(\tau') \right\} + U\int d\tau n_\uparrow(\tau)n_\downarrow(\tau).$$

Hybridization expansion (CT-HYB) Werner et al. 2006
+charge-boson coupling Werner, Millis 2007, 2010
+spin-boson coupling JO 2013
no sign problem

Intersite interaction in DMFT → dual boson approach

Dynamical local interaction (dynamical MF)

$$S_{\mathrm{int}} = -\frac{1}{2}\int d\tau d\tau' \boldsymbol{S}_i(\tau)\mathcal{J}(\tau-\tau')\boldsymbol{S}_i(\tau')$$

self-consistently determined

DMFT for quantum spins

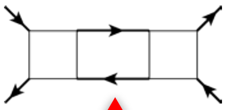
- Quantum spin glass
  Bray, Moore 1980, Sachdev, Ye 1993,
  Grempel, Rozenberg 1998, Georges et al. 2000
- 1/d fluctuations around MF
  Kuramoto, Fukushima 1998, JO, Kuramoto 2013
- Impurity embedded in AFM
  Vojta et al. 2000

For electrons systems...

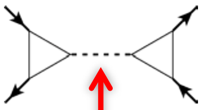
- Random coupling model
  Parcollet, Georges 1999, JO, Vollhardt 2013
- Non-random coupling model (Extended-DMFT)
  Smith, Si 2000, Haule et al. 2002,
  Sun, Kotliar 2002 GW+extendedDMFT

Dual boson approach... Rubtsov et al. 2012

- takes into account feedback from spin fluctuations to the effective impurity (short-range correlation)
- treats χ_{q0} and J_q on equal footing



dual fermion
(χ_{q0})



dual boson
(J_q)

Impurity coupled with fermionic and bosonic baths

$$S_{\rm imp} = \int d\tau d\tau' \left\{ \sum_{\sigma} c^{\dagger}_{\sigma}(\tau)[\partial_{\tau'} - \mu + \Delta(\tau-\tau')]c_{\sigma}(\tau') - \frac{1}{2}\sum_{\alpha=0,x,y,z} S_{\alpha}(\tau)\mathcal{J}_{\alpha}(\tau-\tau')S_{\alpha}(\tau') \right\} + U\int d\tau n_{\uparrow}(\tau)n_{\downarrow}(\tau).$$

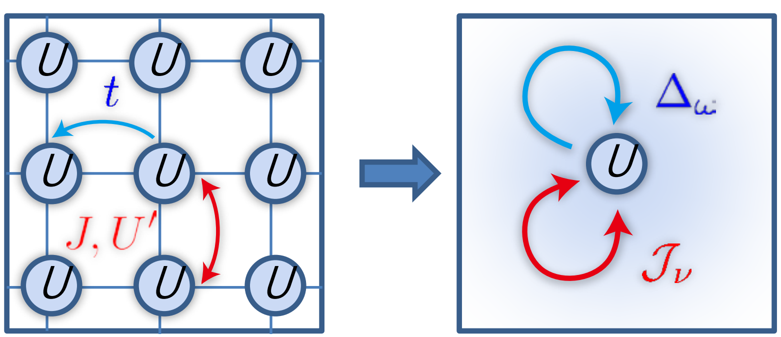
an equivalent Hamiltonian

fermionic bath

bosonic bath

$$H_{\rm imp} = -\mu n + U n_{\uparrow} n_{\downarrow} + \sum_{\boldsymbol{k}\sigma} \epsilon_{\boldsymbol{k}} a^{\dagger}_{\boldsymbol{k}\sigma} a_{\boldsymbol{k}\sigma} + V\sum_{\sigma}(c^{\dagger}_{\sigma}a_{\sigma} + a^{\dagger}_{\sigma}c_{\sigma}) + \sum_{\boldsymbol{q}\alpha} \omega_{\boldsymbol{q}\alpha} b^{\dagger}_{\boldsymbol{q}\alpha} b_{\boldsymbol{q}\alpha} + \sum_{\alpha} g_{\alpha} S_{\alpha}(b_{\alpha} + b^{\dagger}_{\alpha})$$

$$\Delta(i\omega_n) = \frac{V^2}{N}\sum_{\boldsymbol{k}} \frac{1}{i\omega_n - \epsilon_{\boldsymbol{k}}}, \qquad \mathcal{J}_{\alpha}(i\nu_n) = \frac{g_{\alpha}^2}{N}\sum_{\boldsymbol{q}} \frac{2\omega_{\boldsymbol{q}\alpha}}{\nu_n^2 + \omega_{\boldsymbol{q}\alpha}^2}$$



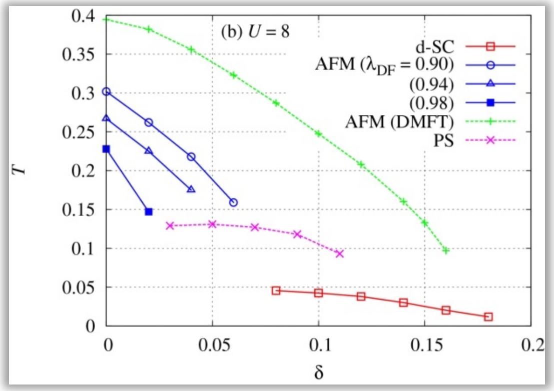
Continuous-time quantum Monte Carlo (CT-QMC)

Hybridization expansion (CT-HYB) Werner et al. 2006
+charge-boson coupling Werner, Millis 2007, 2010
+spin-boson coupling JO 2013
no sign problem

Interaction expansion (CT-INT) Rubtsov et al. 2005
sign problem for spin-boson coupling

Summary

- Extension of DMFT
  - Local correlation by DMFT
  - Long-range correlation by FLEX-type diagrams in dual fermion
  - Short-range correlation by spin-boson coupling in dual boson (future investigation)
- Demonstrative results
  - AFM: Mermin-Wager theorem fulfilled
  - d-SC
  - Phase separation near Mott insulator
  - d-DW was not found (preliminary)



- Issues
  - Improving numerical stability
  - Reasonable approximation to the vertices (low-energy behavior of gamma)
- Possible future investigations
  - Exotic orders in other models: triplet s-wave SC, unconventional SDW/CDW
  - Frequency dependence of the d-wave gap function
  - Heavy-fermion superconductivity: Kondo lattice