SCES '19 OKAYAMA

23-28 September, 2019

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Spatial Correlations and Superconductivity in Dynamical Mean-Field Theory

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RIIS

科研費 KAKENHI

J-Physics：多極子伝導系の物理
J-Physics : Physics of Conductive Multipole Systems

Outline

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1. Heavy Fermion Superconductivity

- Dual fermion approach: beyond DMFT
- Role of incoherent part on superconductivities

2. Strong-coupling formula for $\chi(q)$

- Physically, easy to understand; Numerically, easy to compute
- Evaluation of Intersite interactions J_{ij} in DMFT

Collaborators

Dual fermion approach

- Hartmut Hafermann (Huawei)
- Alexander Lichtenstein (U Hamburg)

Strong-Coupling formula

- Hiroshi Shinaoka (Saitama U)
- Kazuyoshi Yoshimi (ISSP, U Tokyo)
- Yusuke Nomura (RIKEN)
- Masayuki Ohzeki (Tohoku U)

Special Thanks

- Yoshio Kuramoto (KEK)
- Hiroaki Kusunose (Meiji U)
- Dieter Vollhardt (U Augsburg)


Shinaoka


Yoshimi


Nomura


Ohzeki

Introduction

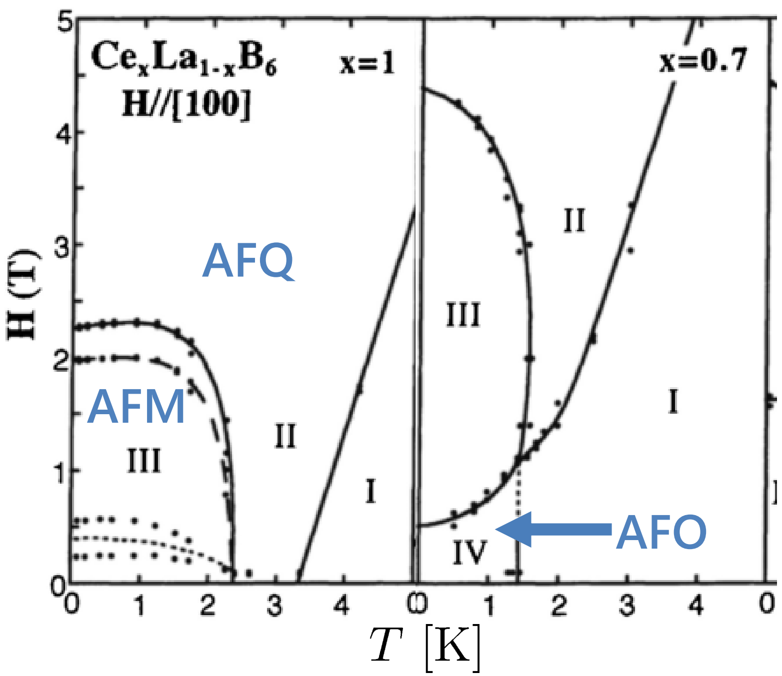
Heavy fermion systems

Itinerant and localized nature of f electrons

f-electron materials

Magnetism (multipole ordering)

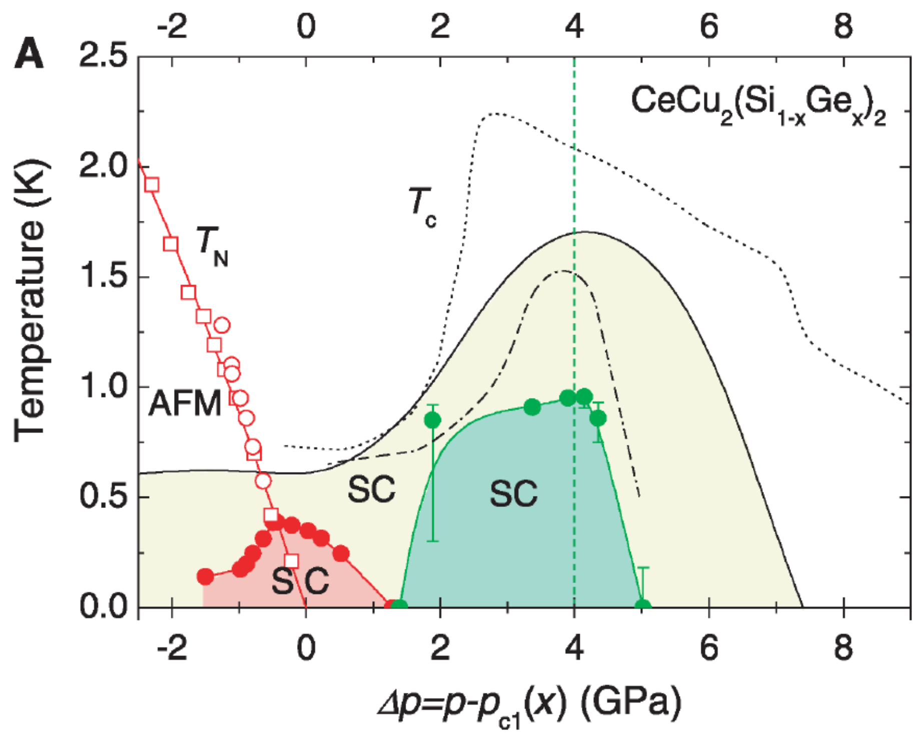
CeB_6 Tayama et al 1997



A lot of Ce, Pr, Nd, …, U compounds

Superconductivity

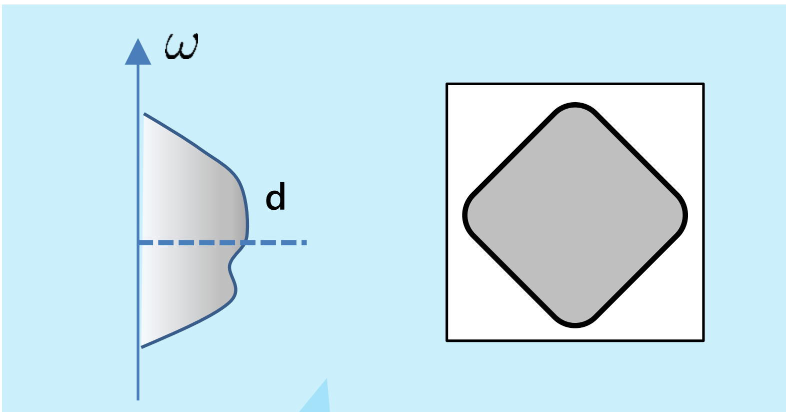
$CeCu_2Si_2$ Steglich 1979, Yuan et al. 2003



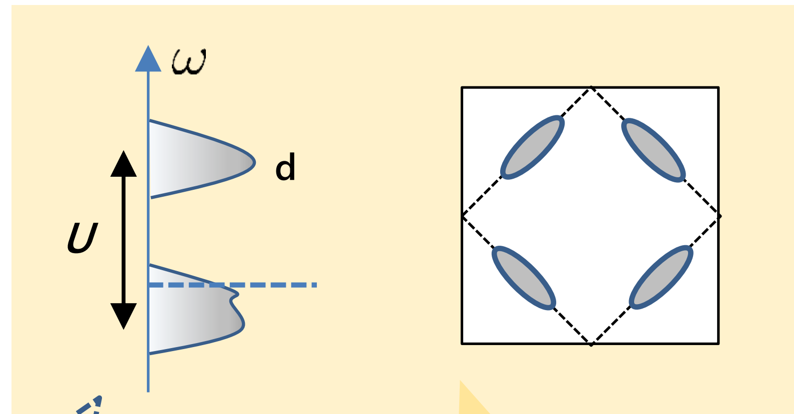
$CePd_2Si_2$, $CeCoIn_5$, URu_2Si_2, UGe_3, UCoGe, …

Itinerant/Localized in d-electron systems

Fermi gas/liquid = Itinerant

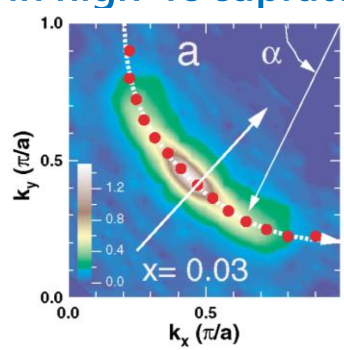


Mott insulator = Localized



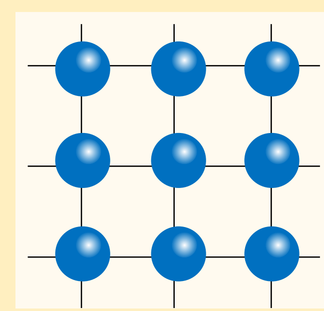
wave

Fermi arc in high-Tc cuprates



From Yoshida et al. 2003

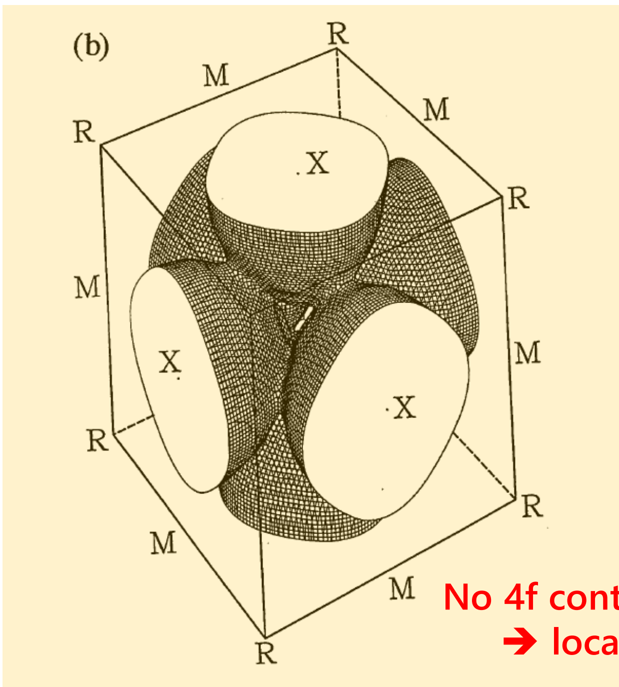
particle



Itinerant/Localized in f-electron systems

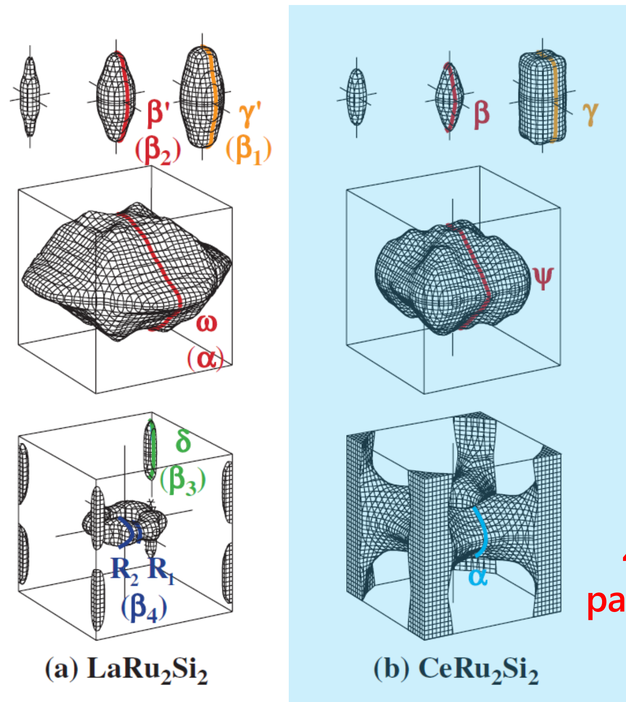
Fermi surface

CeB_6



No 4f contribution
➔ localized

$CeRu_2Si_2$



4f electrons
participate in FS
➔ itinerant

Similar to LaB_6

Onuki et a. 1989

Harima, Kasuya 1989, 1996

Different from $LaRu_2Si_2$

Yamagami, Hasegawa 1992

H. Aoki et al. 1993

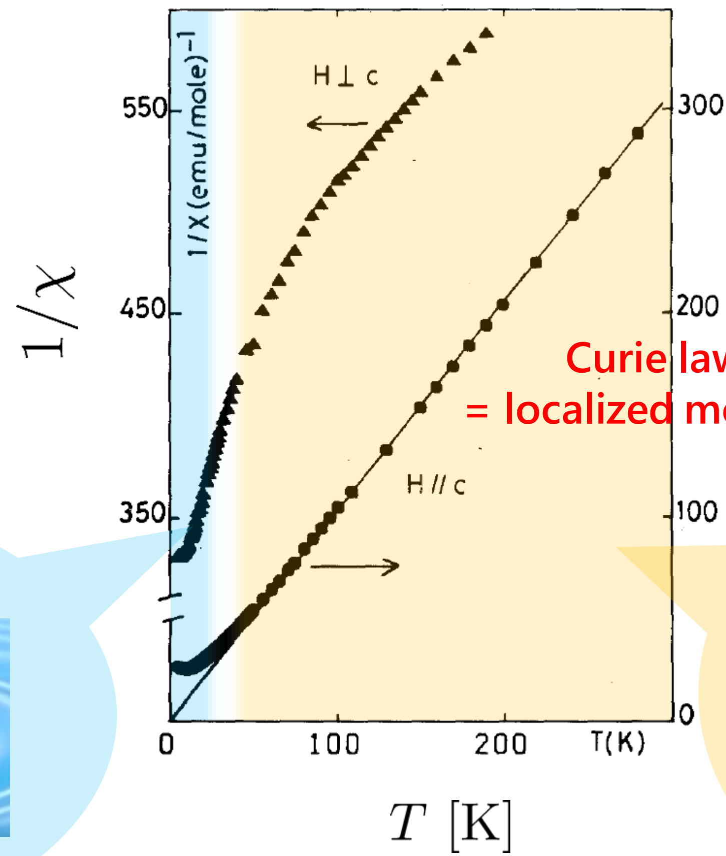
Matsumoto et al. 2010

Ce^{3+} : $4f^1$, La^{3+} : $4f^0$

Itinerant/Localized in f-electron systems

Magnetic susceptibility

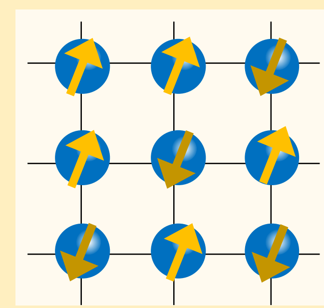
$CeRu_2Si_2$



Haen et al. 1987

wave

particle



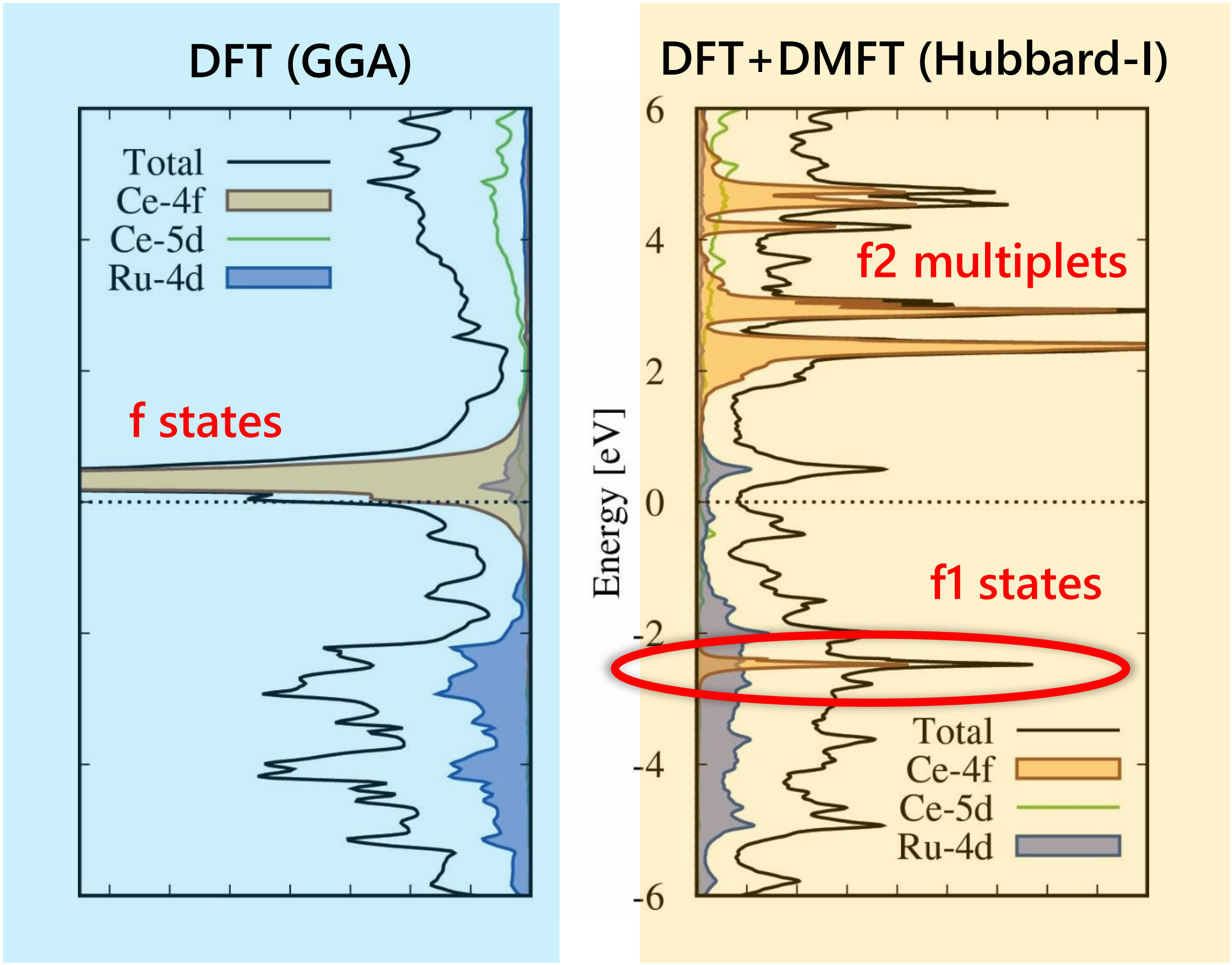
Itinerant/Localized in f-electron systems

$CeRh_2Si_2$

U (Slater type)

itinerant

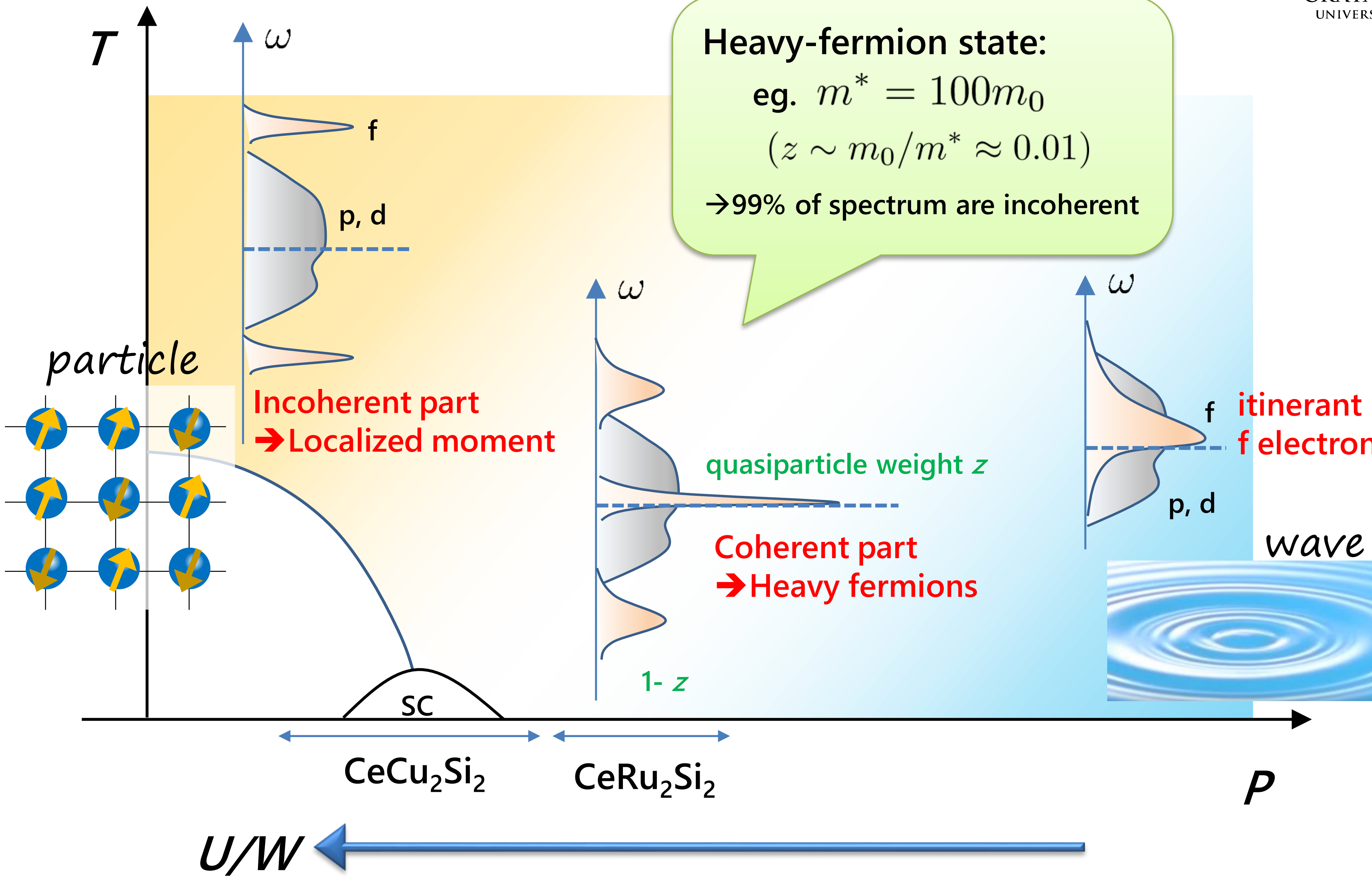
high pressure



localized

low pressure

Heavy fermions = itinerant + localized natures



Heavy-fermion state:

eg. $m^* = 100m_0$

$(z \sim m_0/m^* \approx 0.01)$

→99% of spectrum are incoherent

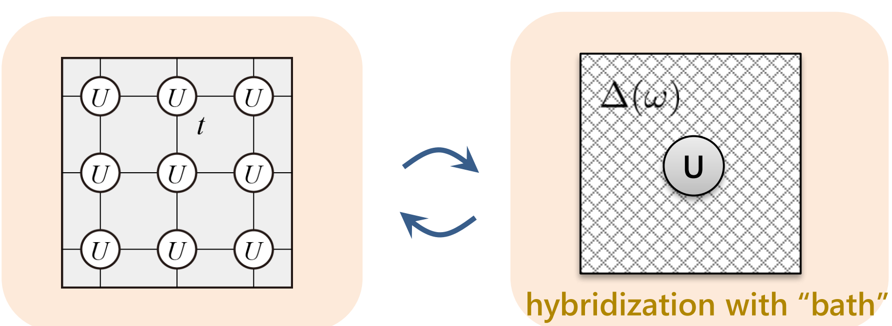
Dynamical Mean-Field Theory (DMFT)

Plenary talk by Dieter Vollhardt

Local approximation

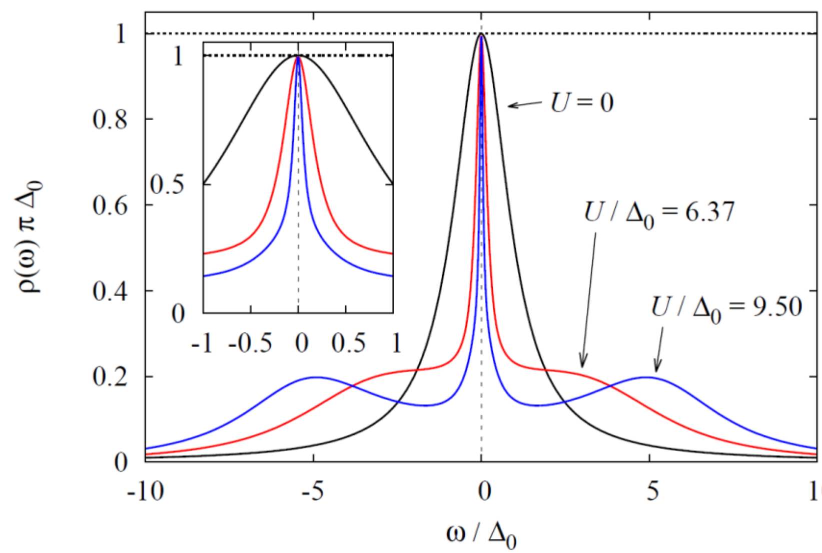
$$\Sigma(\omega, \boldsymbol{k}) \approx \Sigma^{\mathrm{DMFT}}(\omega)$$

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



Local correlations
exactly taken into account

Solution of the impurity Anderson model by continuous-time QMC (CT-QMC)



JO in summer school textbook 2016

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Heavy Fermion Superconductivity

PHYSICAL REVIEW B **90**, 235132 (2014)

Superconductivity, antiferromagnetism, and phase separation in the two-dimensional Hubbard model: A dual-fermion approach

Junya Otsuki,[1] Hartmut Hafermann,[2] and Alexander I. Lichtenstein[3]

PRL **115,** 036404 (2015) PHYSICAL REVIEW LETTERS week ending 17 JULY 2015

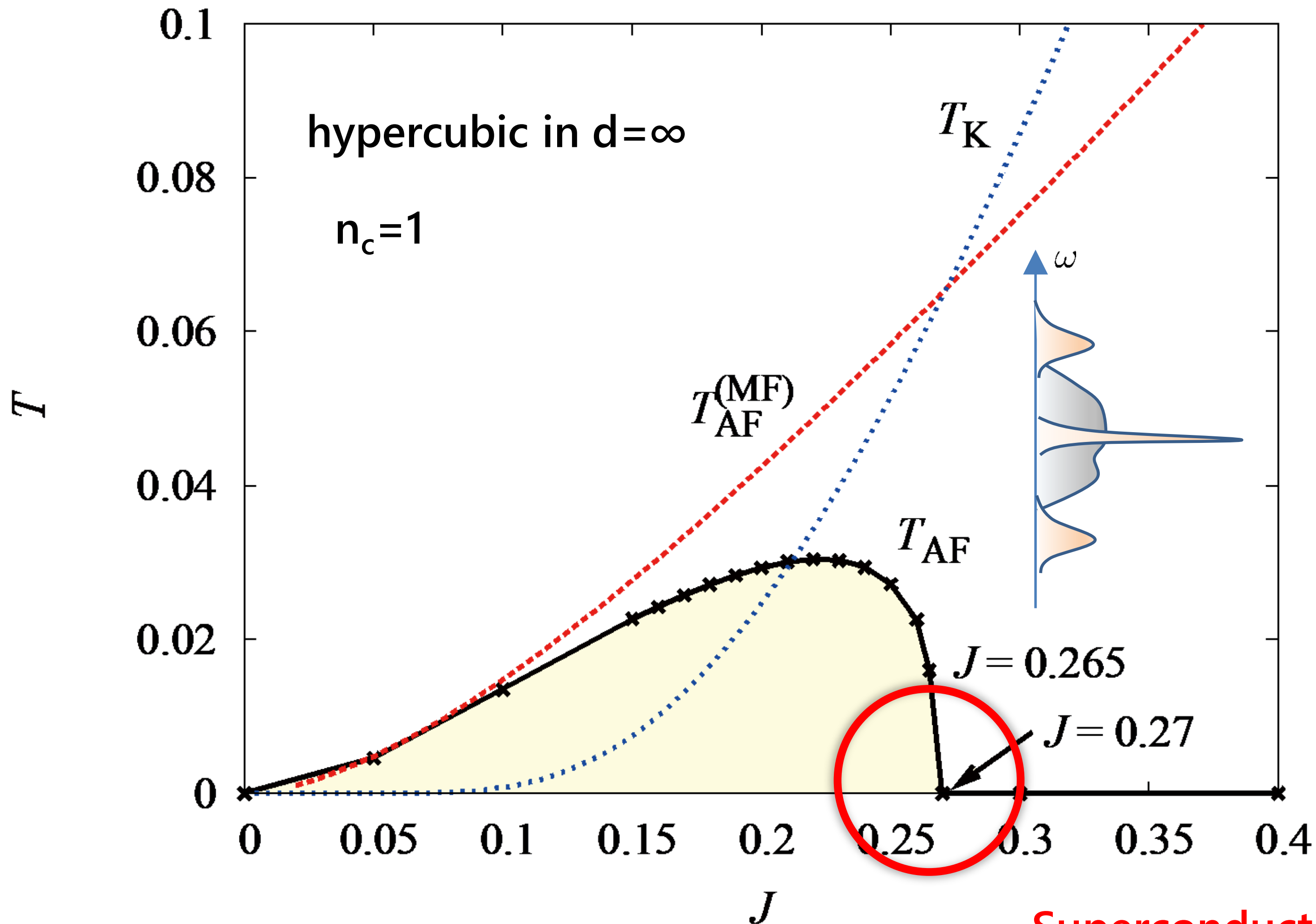
Competing *d*-Wave and *p*-Wave Spin-Singlet Superconductivities in the Two-Dimensional Kondo Lattice

Junya Otsuki
Department of Physics, Tohoku University, Sendai 980-8578, Japan
(Received 21 April 2015; published 15 July 2015)

AFM phase diagram in DMFT

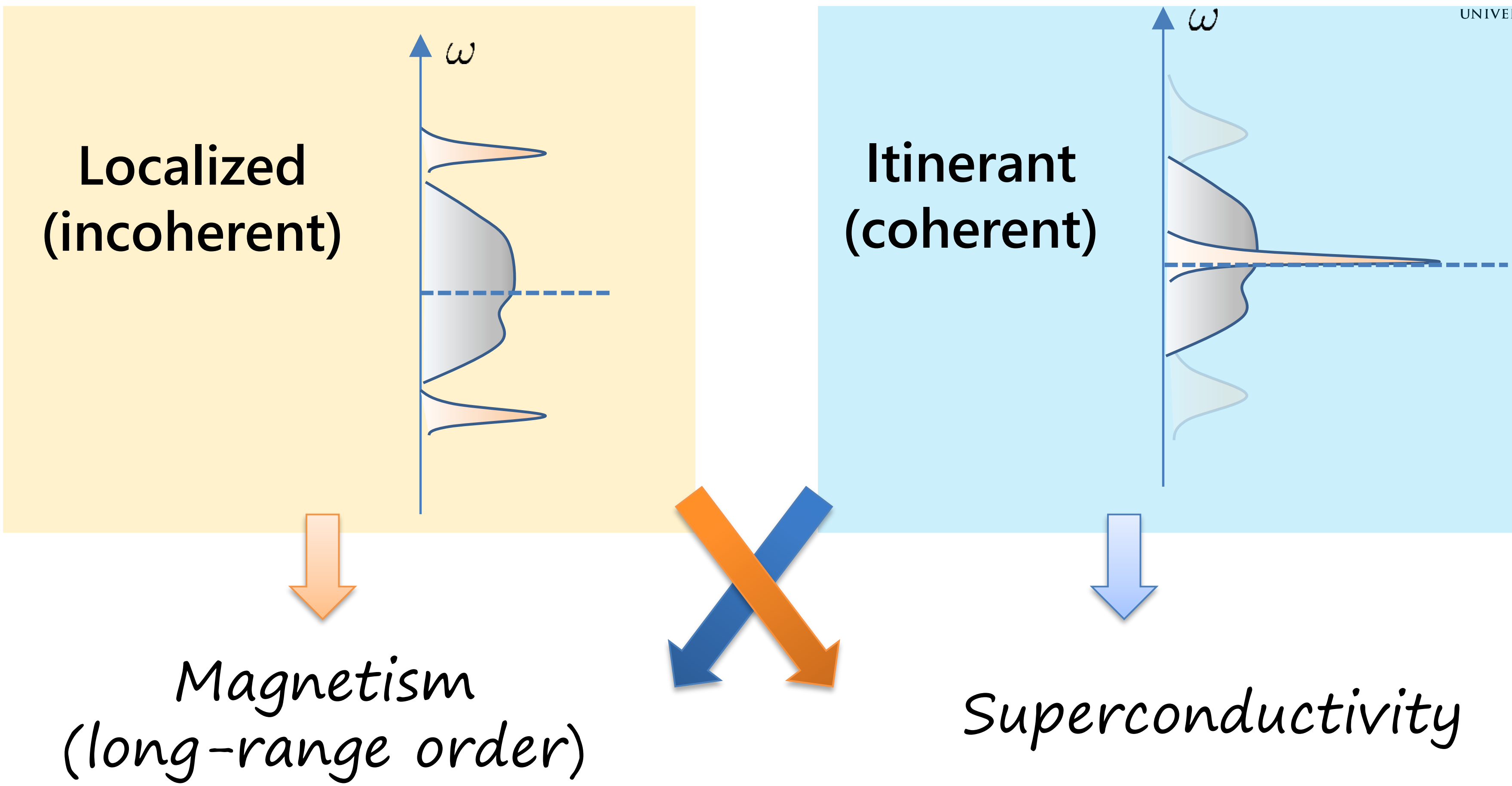
Kondo lattice solved with DMFT + CT-QMC(CT-J)

JO, Kusunose, Kuramoto, JPSJ 2009



Superconductivity?
→beyond DMFT

Motivations

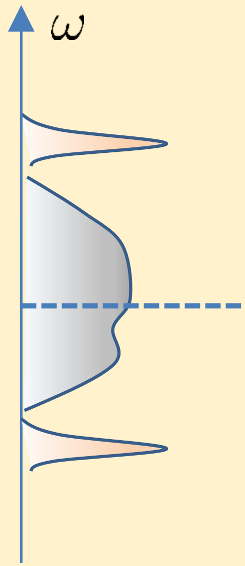


Both localized and itinerant nature should be taken into account

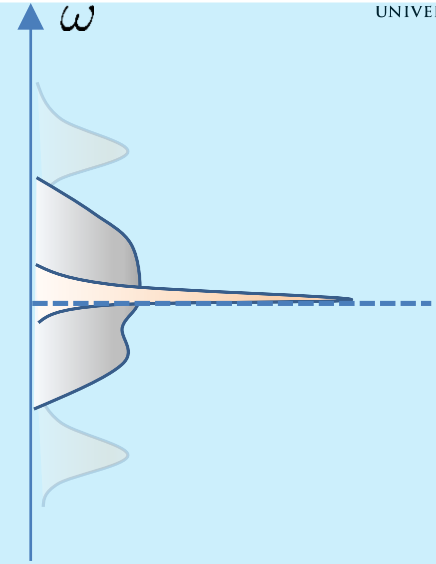
cf. Phenomenology: `duality model' (Kuramoto, Miyake, 1990)

Motivations

Localized
(incoherent)



Itinerant
(coherent)



Kondo resonance

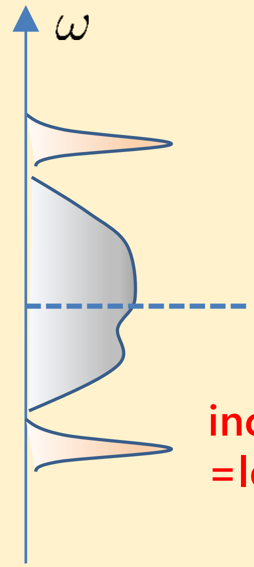
Magnetism
(long-range order)

Symmetry breaking
induced by Kondo effect

Kondo singlet-CEF singlet order in $PrFe_4P_{12}$
Hoshino, JO, Kuramoto, 2011

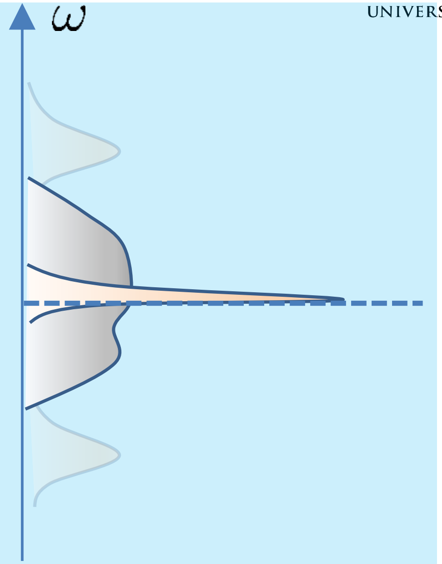
Motivations

Localized
(incoherent)



incoherent part
=localized moment

Itinerant
(coherent)

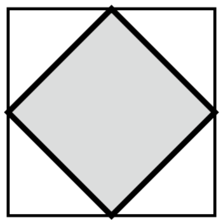


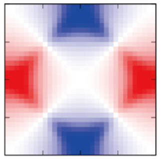
Superconductivity

heavy-fermion SC
exotic pairing state

Differences between d- and f-electron SCs ?

d = 2



+ U → AFM →  d-SC

+ J → AFM → ?

(Kondo) (RKKY)

Expansion around DMFT

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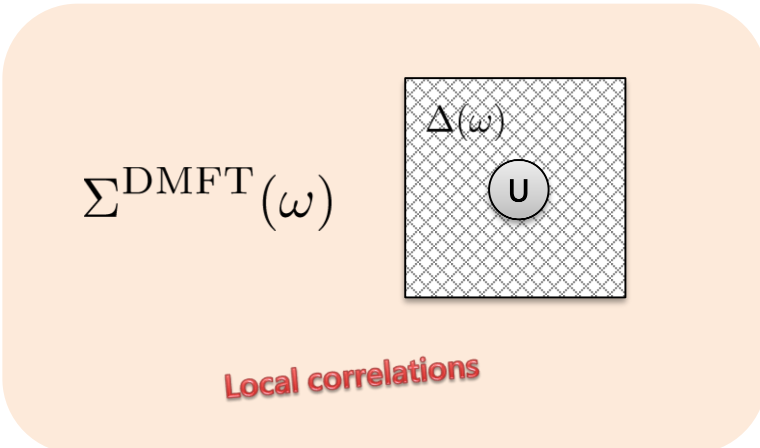
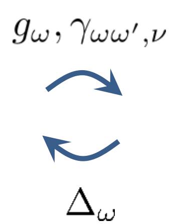
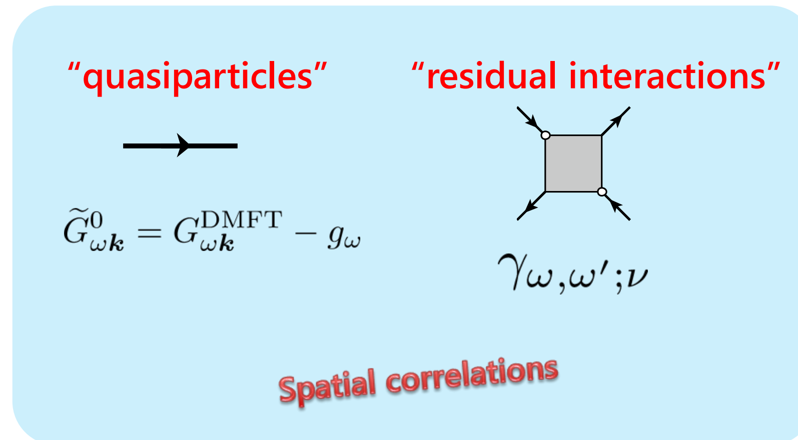
Rubtsov, Katsnelson, Lichtenstein 2008

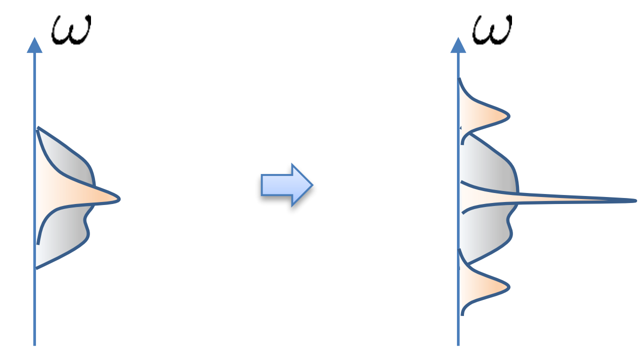
(1) Dynamical mean-field theory (DMFT)



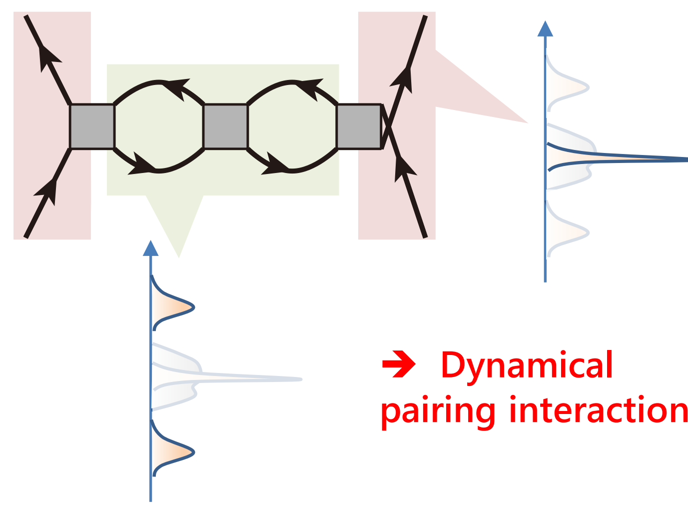


(2) Auxiliary fermion (dual fermion) lattice



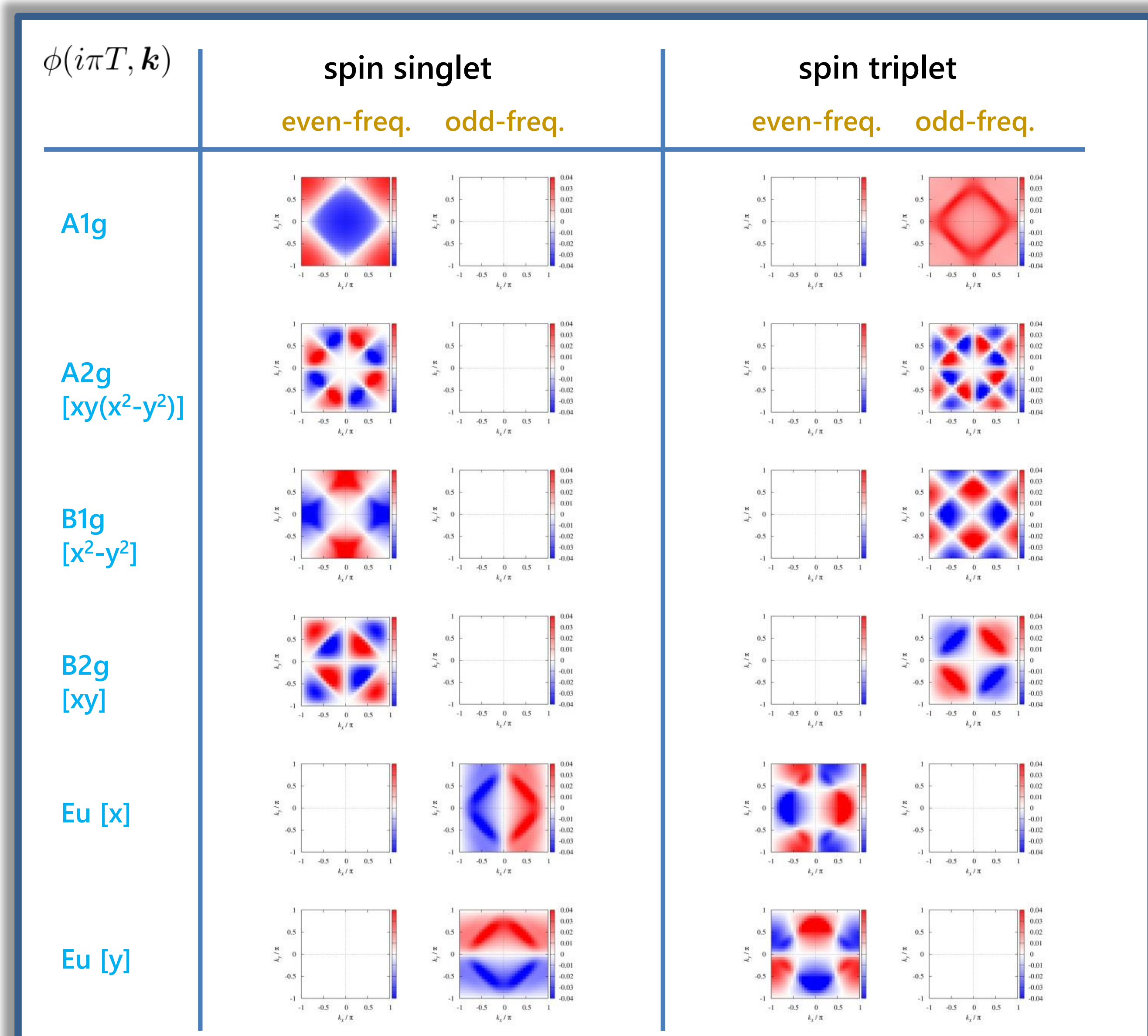


Heavy fermions
Mott insulator



➔ Dynamical pairing interactions

Superconductivity



U/t=8, n=0.9, T/t=0.1

Impurity solver:
CT-HYB (Werner et al. 2006)
Improved vertex calculation
(Hafermann et al. 2012)

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

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

-plot even- and odd-freq. parts

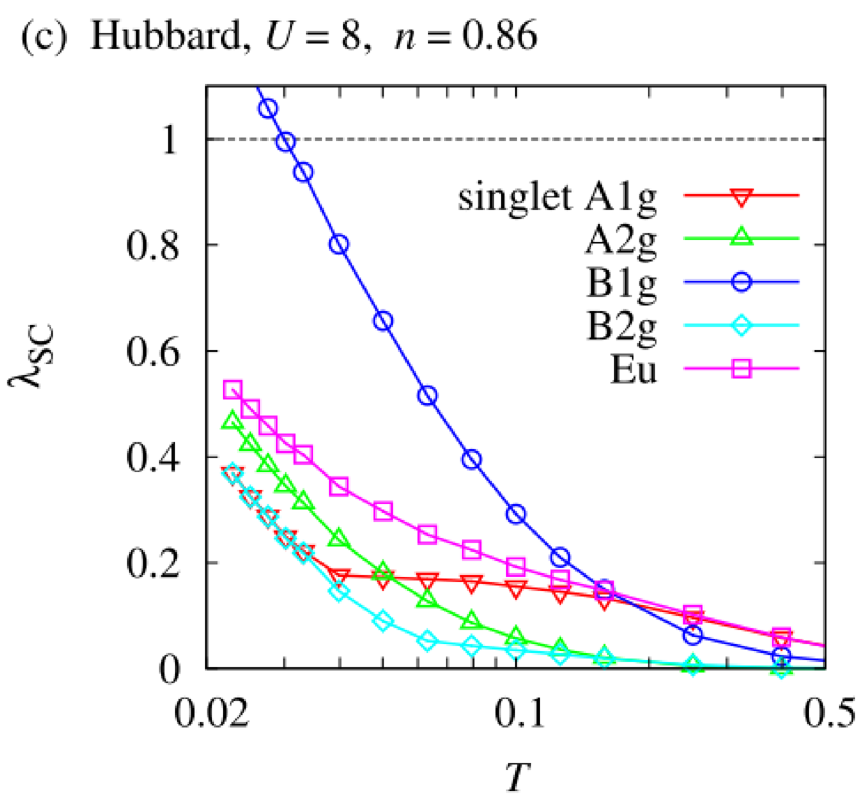
$$\phi(i\omega, \boldsymbol{k}) \pm \phi(-i\omega, \boldsymbol{k})$$

Pauli principle is fulfilled
(spin × parity × time-reversal)

Pairing instability

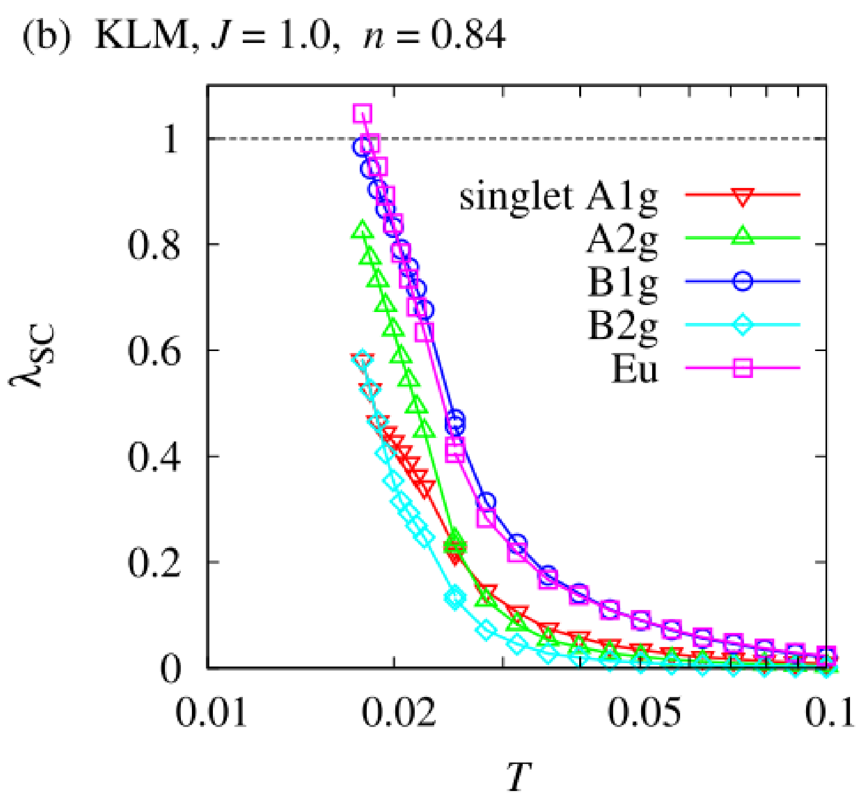
Hubbard model (square lattice)

JO, Hafermann, Lichtenstein, PRB 2014



Kondo lattice (square lattice)

JO, PRL 2015

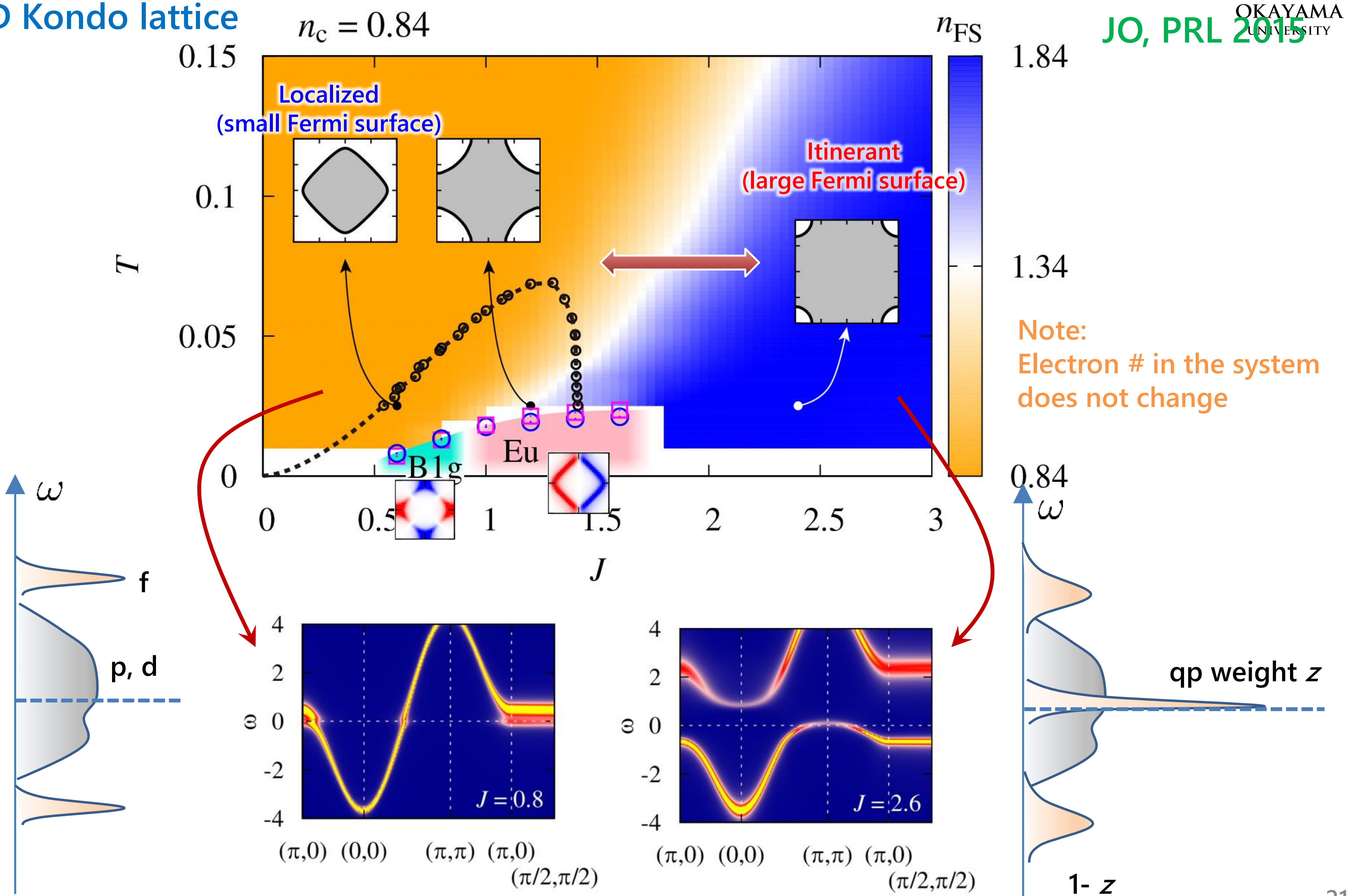


Competing d-wave and p-wave SC

Superconductivity in 2D Kondo lattice

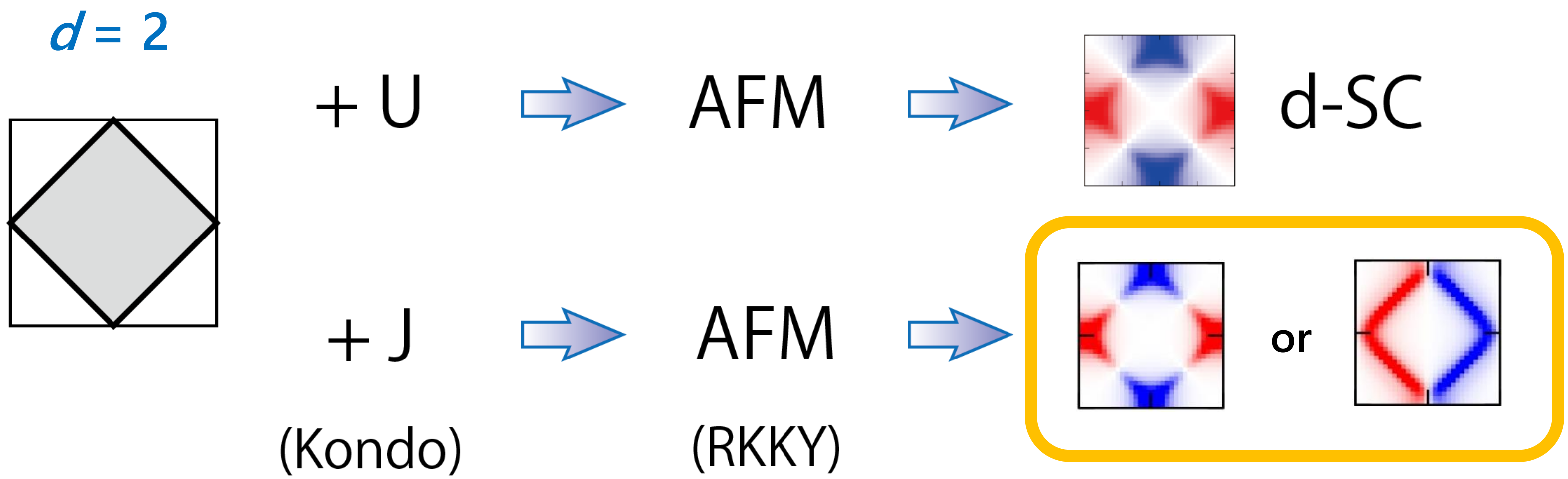
2D Kondo lattice

JO, PRL 2015



Note:
Electron # in the system does not change

Differences between d- and f-electron SC ?



- Formation of large Fermi surface
- Dynamical qp interactions

Odd-frequency SCs:
$CeCu_2Si_2$, $CeRhIn_5$, Fuseya, Kohno, Miyake, 2003
Thermodynamic stability, Solenov 2009, Kusunose et al., 2011

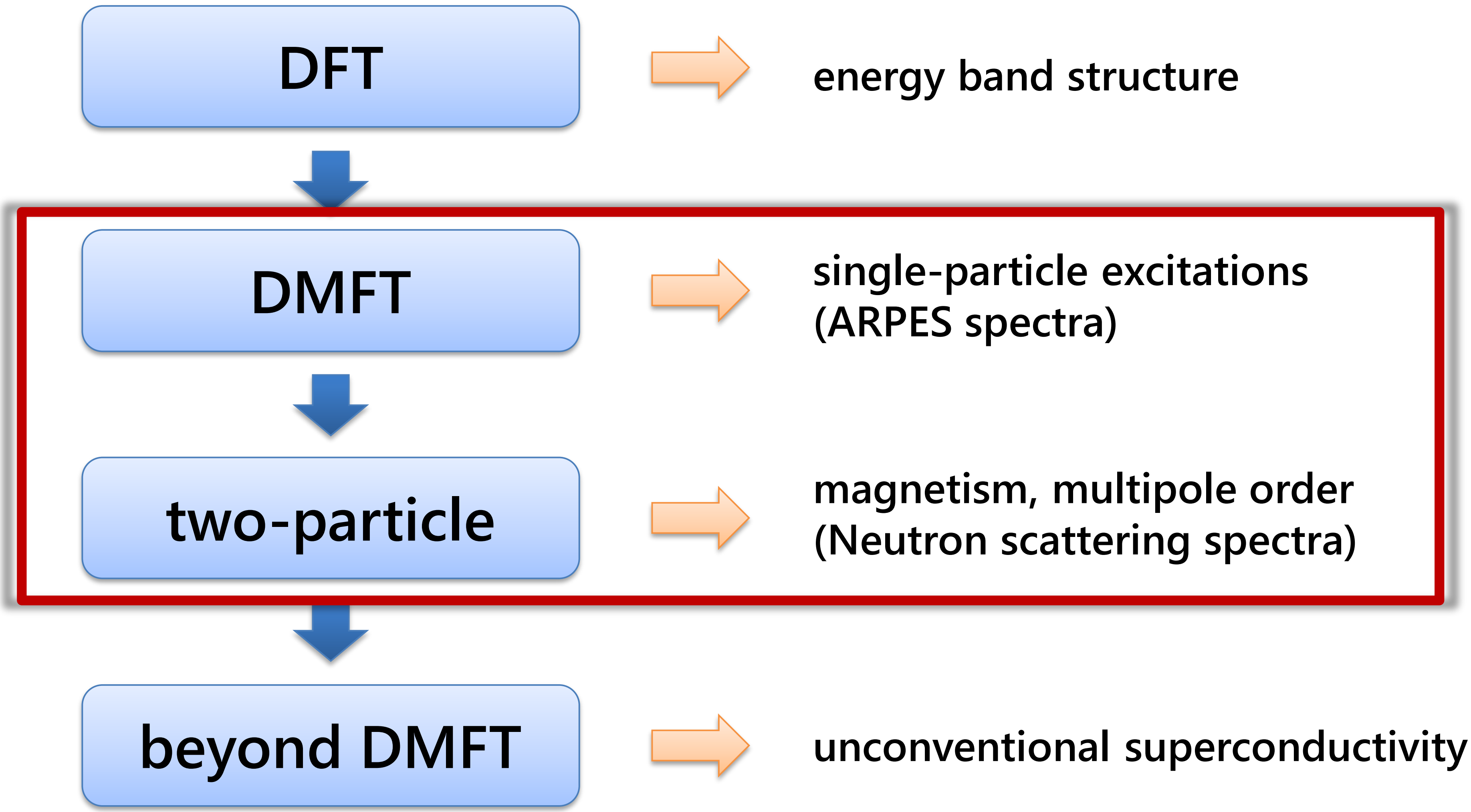
$\chi(q)$ in DMFT

PHYSICAL REVIEW B **99**, 165134 (2019)

Strong-coupling formula for momentum-dependent susceptibilities in dynamical mean-field theory

Junya Otsuki,[1,*] Kazuyoshi Yoshimi,[2] Hiroshi Shinaoka,[3] and Yusuke Nomura[4]

DFT+DMFT calculation flow



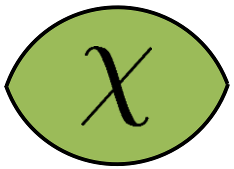
Momentum-dependent susceptibilities in DMFT

Susceptibility matrix

$$[\boldsymbol{\chi}(\boldsymbol{q}, i\Omega)]_{12,34} = \int_0^\beta d\tau \langle O_{12}(\boldsymbol{q}, \tau) O_{43}(-\boldsymbol{q})\rangle e^{i\Omega\tau}$$

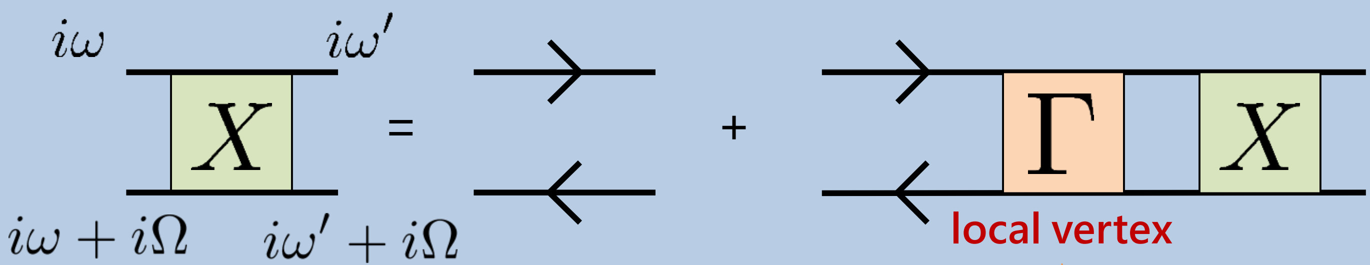
$$O_{m\sigma,m'\sigma'}(i) = c^\dagger_{im\sigma} c_{im'\sigma'}$$

$$1 \equiv (m, \sigma)$$



$$\chi_{12,34}(\boldsymbol{q}, i\Omega) = T \sum_{\omega\omega'} X_{12,34}(i\omega, i\omega'; \boldsymbol{q}, i\Omega)$$

Bethe-Salpeter equations



Jarrell 1992
Georges et al 1996

$$[\boldsymbol{X}_{\mathrm{loc}}(i\omega, i\omega'; i\Omega)]_{12,34}$$

$$\mathcal{O}(N^4_{\mathrm{orb}} N^2_\omega)$$

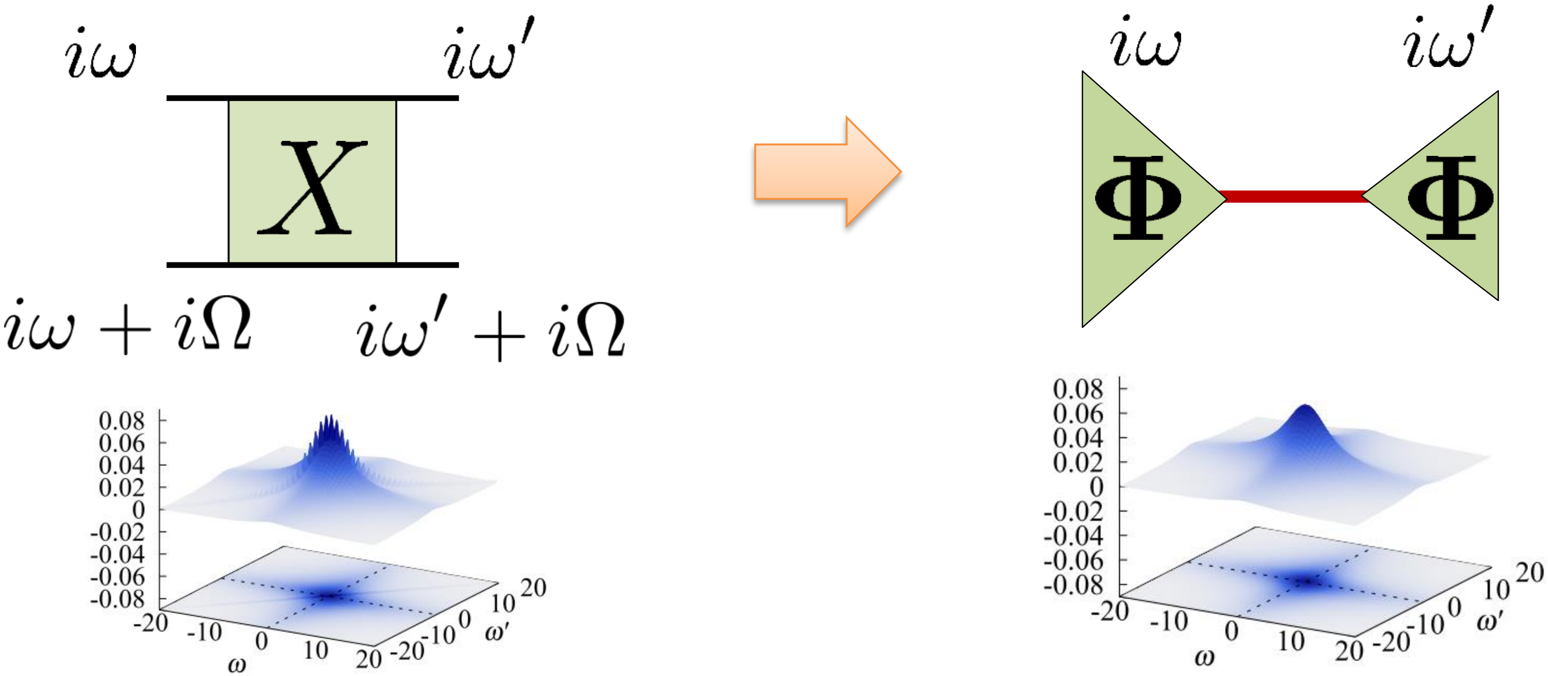
calculated in the effective impurity model (very heavy!)

Decoupling

$$X_{\mathrm{loc}}(i\omega, i\omega') \simeq \Phi(i\omega)\Phi(i\omega')$$

$\Omega = 0$

dynamical local interactions



Similar approximation was addressed by...

- **dual-boson approach:** Stepanov et al. 2016
- **diagrama analysis:** F. Krien, arXiv:1901.02832

Mathematical justification of the decoupling

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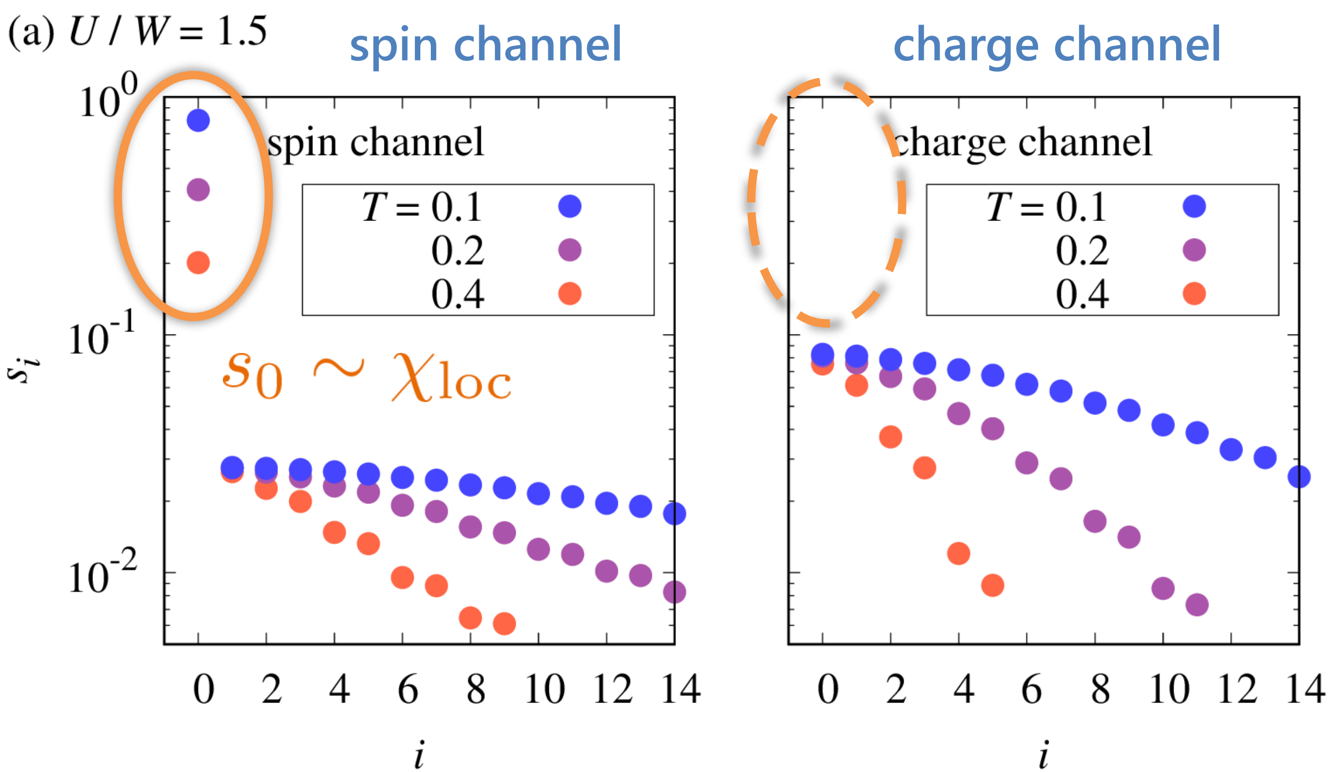
Singular Value Decomposition (SVD)

$$X_{\mathrm{loc}}(i\omega, i\omega') = \sum_{i\geq 0} s_i u_i(i\omega) v_i^*(i\omega') \simeq s_0 u_0(i\omega) v_0^*(i\omega')$$



Strong-Coupling-Limit (SCL) formula

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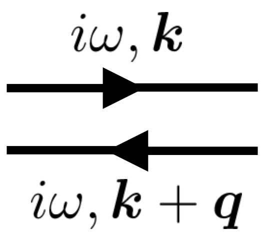
$$\chi_{\boldsymbol{q}}^{\mathrm{SCL}} = (\chi_{\mathrm{loc}}^{-1} - \boldsymbol{I}_{\boldsymbol{q}})^{-1}, \boldsymbol{I}_{\boldsymbol{q}} \simeq T \sum_{\omega} \boxed{\phi(i\omega)} \boxed{\boldsymbol{\Lambda}_{\boldsymbol{q}}(i\omega)} \boxed{\phi(i\omega)}$$

(i) Lattice information

$$\boldsymbol{\Lambda}_{\boldsymbol{q}}(i\omega) = \boldsymbol{X}_{0,\mathrm{loc}}^{-1}(i\omega) - \boldsymbol{X}_{0,\boldsymbol{q}}^{-1}(i\omega)$$



(ii) Local information

in general $\quad \phi(i\omega) \propto \boldsymbol{\Phi}(i\omega) \qquad \boldsymbol{X}_{\mathrm{loc}}(i\omega, i\omega') \simeq \boldsymbol{\Phi}(i\omega)\boldsymbol{\Phi}(i\omega')$

in the atomic limit $\quad \phi(i\omega) \propto \frac{1}{2}\left(\frac{1}{i\omega+\mu} - \frac{1}{i\omega+\mu-U}\right)$

Numerical verification of the SCL formula

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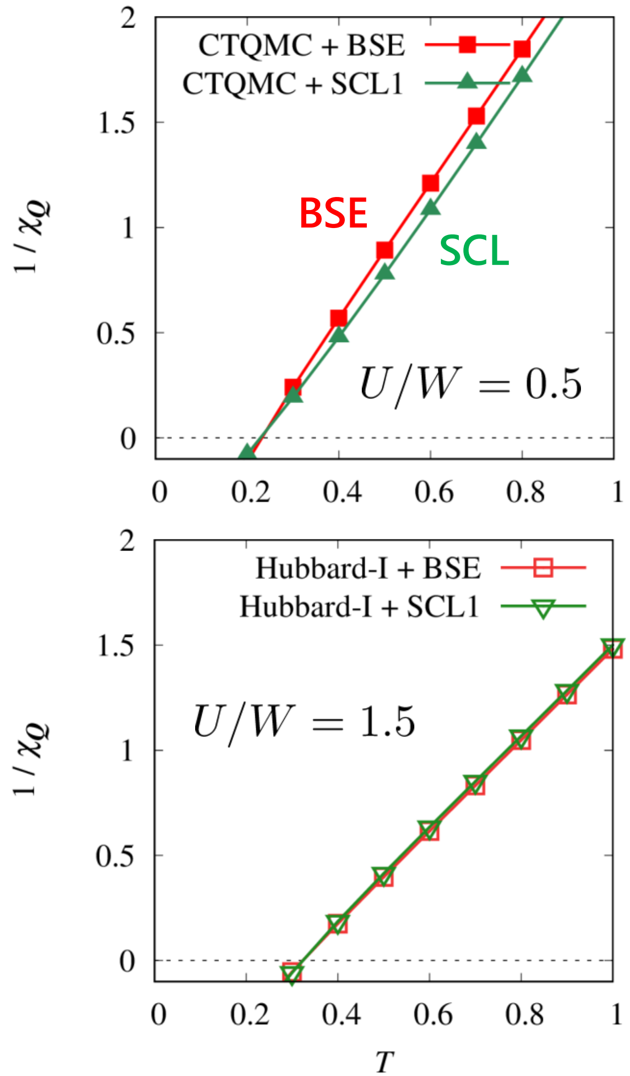
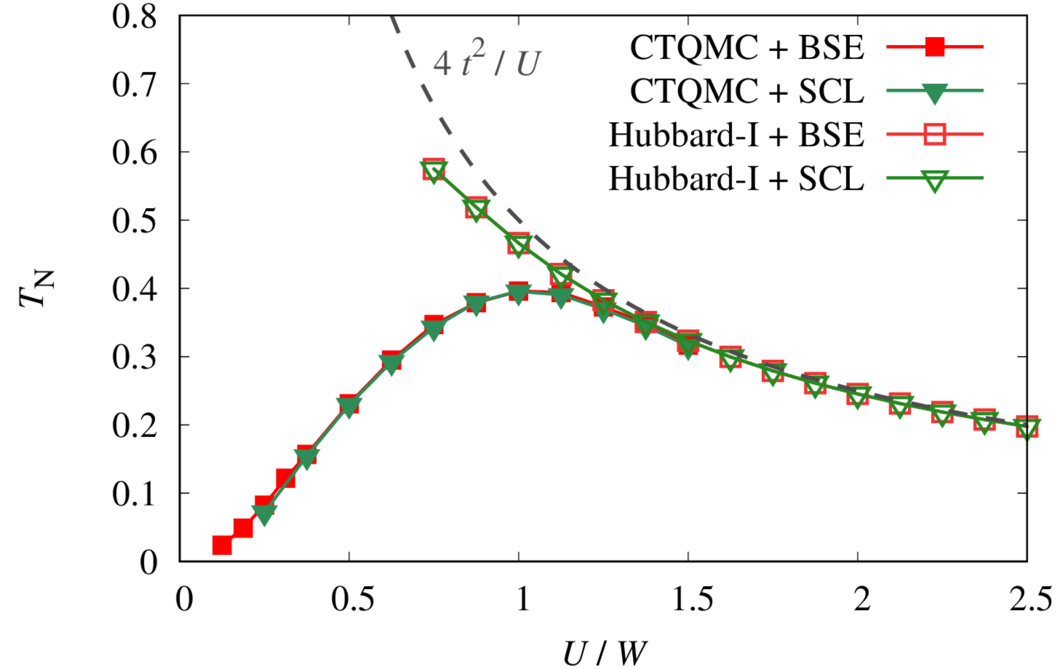
Inverse susceptibility



Phase diagram



perfect agreement
even in the weak-coupling regime

Validity has been confirmed also in a two-orbital model

Effective intersite interactions

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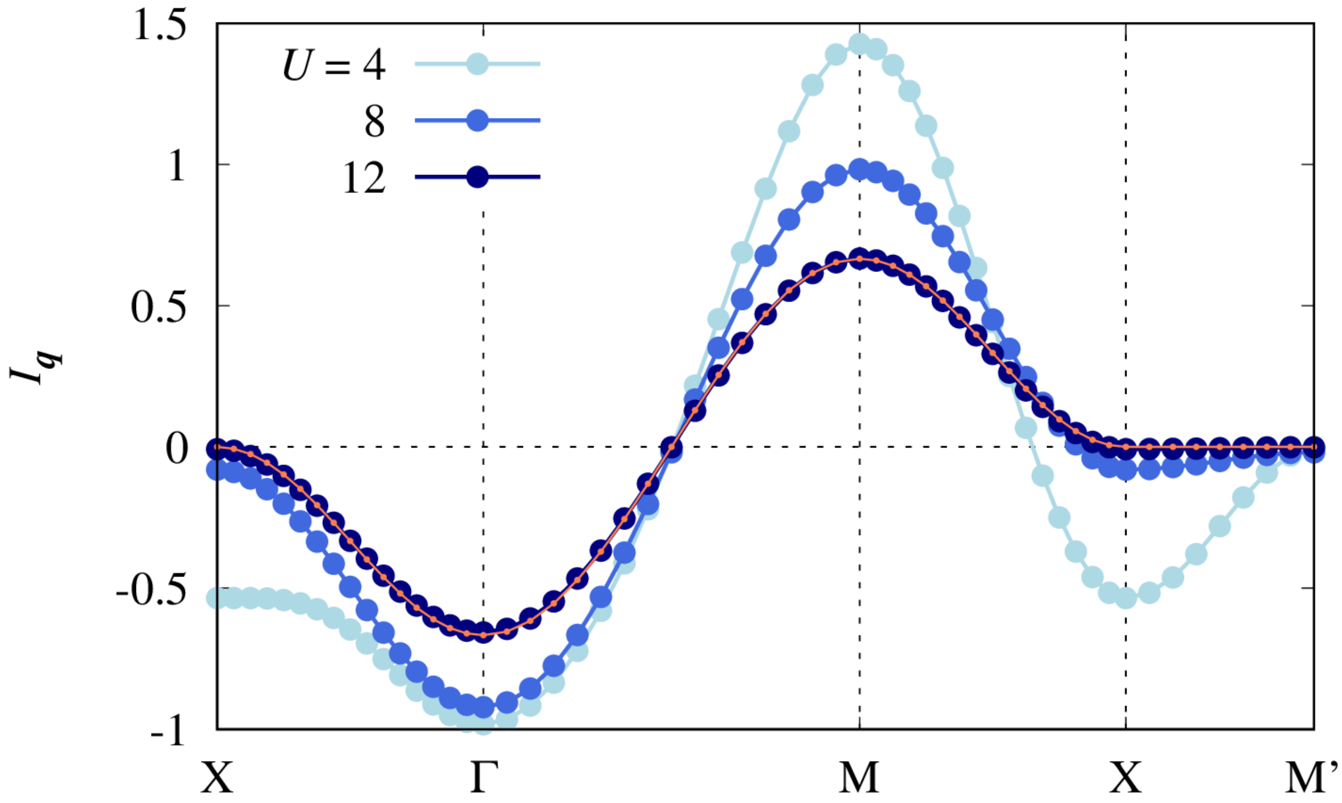
$$I_{\boldsymbol{q}} \simeq T \sum_{\omega} \phi(i\omega)\Lambda_{\boldsymbol{q}}(i\omega)\phi(i\omega)$$



strong-coupling limit

$$I_{\boldsymbol{q}} = -\frac{4t^2}{U}(\cos k_x + \cos k_y)$$

square-lattice Hubbard model

Effective intersite interactions in the atomic limit

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$$I_{\boldsymbol{q}} \simeq T \sum_{\omega} \phi(i\omega) \Lambda_{\boldsymbol{q}}(i\omega) \phi(i\omega)$$

Hubbard model

$$\Lambda_{\boldsymbol{q}}(i\omega) \simeq -2t^2 \gamma_{\boldsymbol{q}}$$

in the atomic limit

$$I_{\boldsymbol{q}} \simeq -\frac{4t^2 \gamma_{\boldsymbol{q}}}{U}$$

kinetic exchange interaction

Periodic Anderson model

in the atomic limit

$$I_{\boldsymbol{q}} \simeq J_{\mathrm{K}}^2 \chi_{\mathrm{c},\boldsymbol{q}}$$

Kondo coupling

$J_{\mathrm{K}} = 4V^2/U$

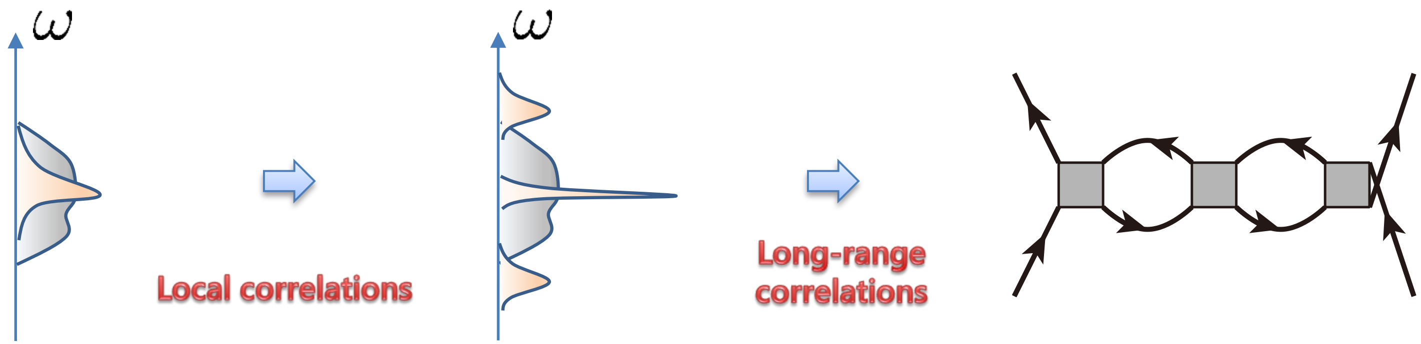
RKKY interaction

Modern derivation by means of Green functions (alternative to the effective Hamiltonian approach)

"Modern" derivation of effective intersite interactions

Summary

Microscopic derivation of heavy-fermion superconductivity



- Dual fermion approach: Spatial correlations beyond DMFT
- Itinerant-Localized crossovers can lead to an exotic pairing state

Strong-coupling formula on χ(q) within DMFT

This new formula has advantages…

- physically, easy to understand
- Effective intersite interactions
- numerically, easy to compute

$$\chi_{\boldsymbol{q}}^{\mathrm{SCL}} = (\chi_{\mathrm{loc}}^{-1} - I_{\boldsymbol{q}})^{-1}$$

$$I_{\boldsymbol{q}} \simeq T \sum_{\omega} \phi(i\omega)\Lambda_{\boldsymbol{q}}(i\omega)\phi(i\omega)$$