東北大学大学院理学研究科
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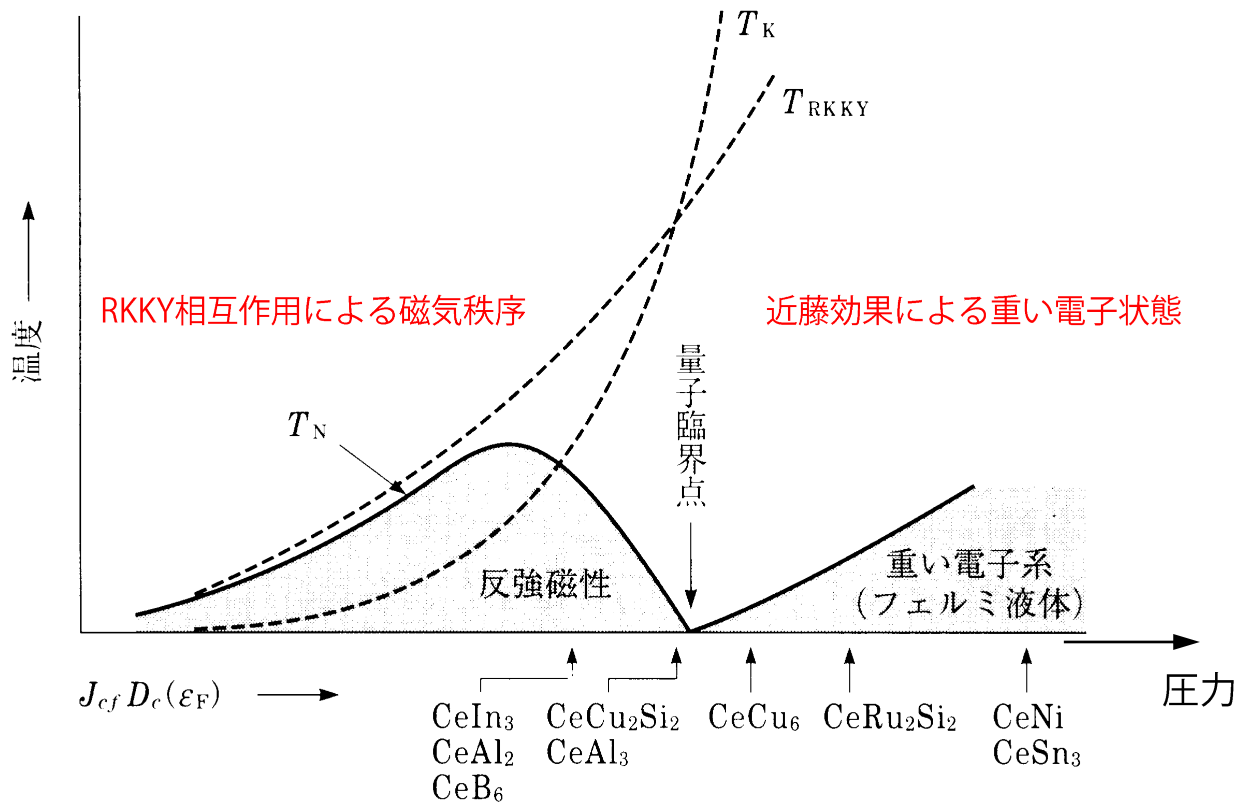
3.3. 動的平均場理論の応用例

RKKY相互作用による磁気秩序
重い電子の形成と大きいフェルミ面
混晶系
モット絶縁体

RKKY相互作用による磁気秩序

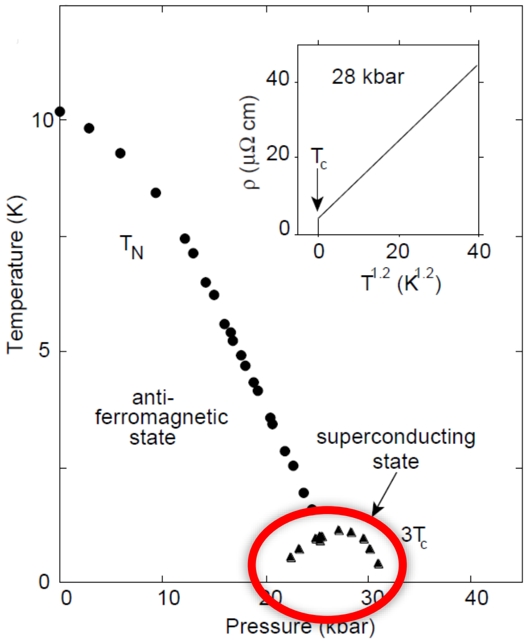
重い電子系



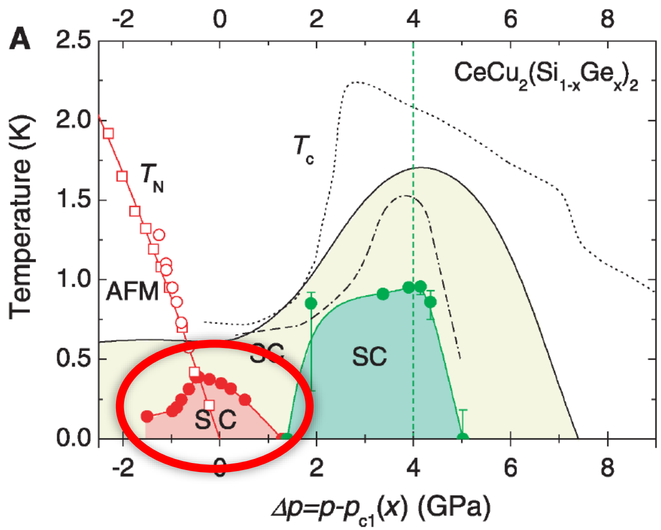
上田和夫・大貫惇睦「重い電子系の物理」

重い電子系超伝導

$CeIn_3$ Mathur et al. 1998



$CeCu_2Si_2$ Steglich et al. 1979, Yuan et al. 2003



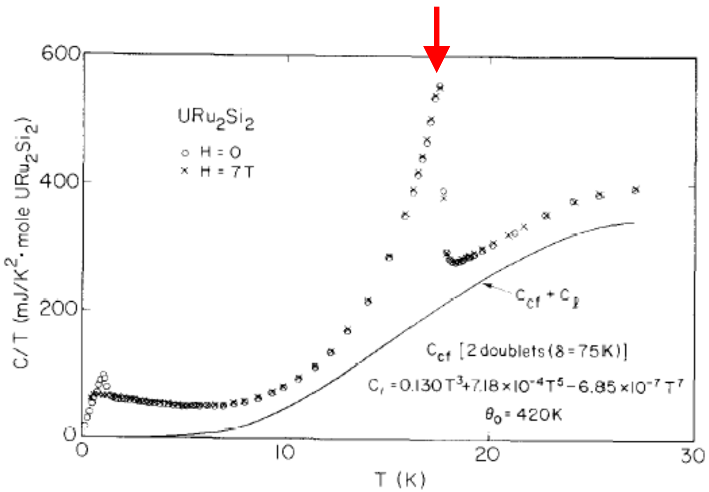
非従来型超伝導？
d波対称性？（銅酸化物との類推）
s波対称性？(Kittaka et al. 2014, Ikeda et al. 2015)

重い電子超伝導の微視的理論を発展させる必要

重い電子系における「隠れた秩序」

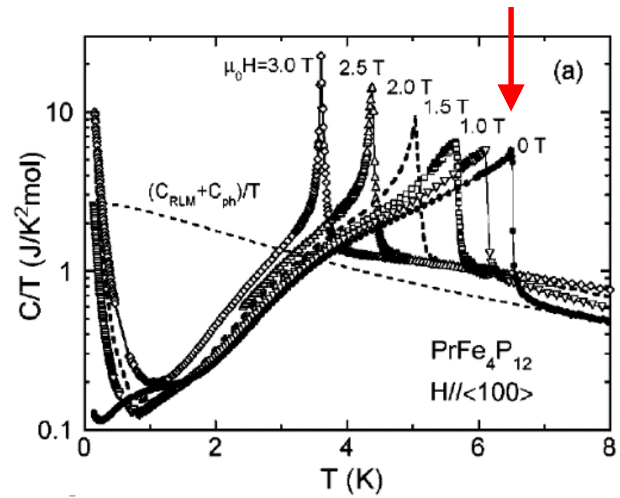
- 相転移（比熱の跳び etc）
- 未知の秩序変数

URu_2Si_2 since 1986 Palstra et al.



From Fisher et al. 1990

$PrFe_4P_{12}$ since 1987 Torikachvili et al.



From Aoki et al. 2002

反強的スカラー秩序変数

Kiss, Kuramoto 2006, Sakai et al. 2007

多極子秩序の枠組みを超えた理論が必要

Kondo lattice model

drop orbital deg. of freedom

7 orbitals in f shell (inter- and intra-orbital Coulomb, LS coupling⋯)

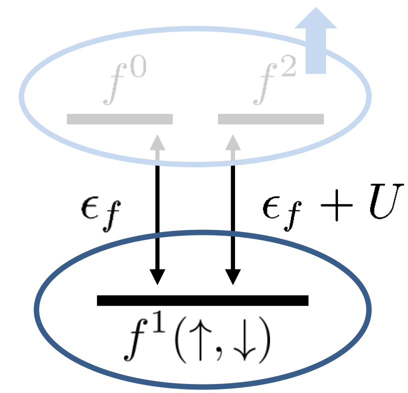
Periodic Anderson model

$$H_{\mathrm{PA}} = \sum_{\boldsymbol{k}\sigma} \epsilon_{\boldsymbol{k}} c^{\dagger}_{\boldsymbol{k}\sigma} c_{\boldsymbol{k}\sigma} + \epsilon_f \sum_{i\sigma} n^f_{i\sigma} + V \sum_{i\sigma} \left(f^{\dagger}_{i\sigma} c_{i\sigma} + c^{\dagger}_{i\sigma} f_{i\sigma} \right) + U \sum_{i} n^f_{i\uparrow} n^f_{i\downarrow}$$

remove valence fluctuations

Kondo limit

$$J = \frac{4V^2}{U} \quad \left(U \to \infty, \quad \epsilon_f = -\frac{U}{2}\right)$$



Kondo lattice model

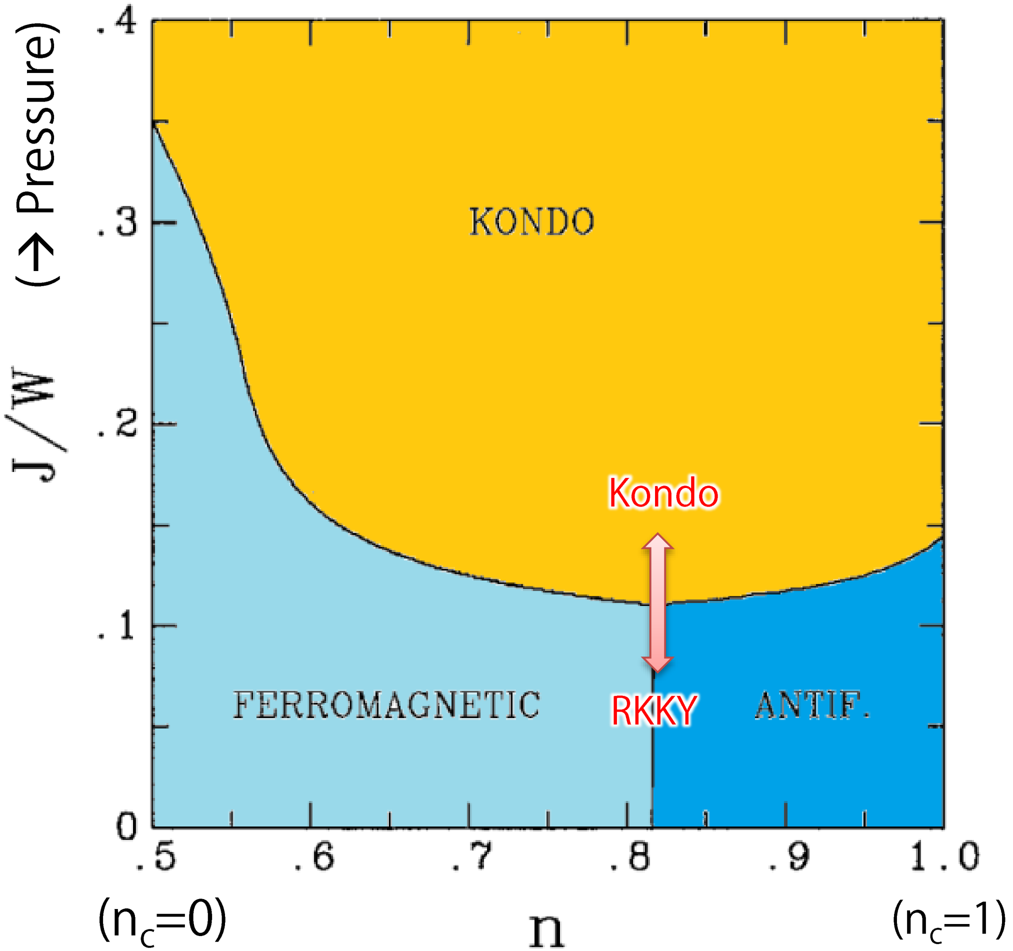
$$H_{\mathrm{K}} = \sum_{\boldsymbol{k}\sigma} \epsilon_{\boldsymbol{k}} c^{\dagger}_{\boldsymbol{k}\sigma} c_{\boldsymbol{k}\sigma} + J \sum_{i} \boldsymbol{S}_i \cdot \boldsymbol{\sigma}^{\mathrm{c}}_i$$

$$\boldsymbol{\sigma}^{\mathrm{c}}_i = \sum_{\sigma\sigma'} c^{\dagger}_{i\sigma} \boldsymbol{\sigma}_{\sigma\sigma'} c_{i\sigma'}$$

- Physically: Spin deg. of freedom (no valence fluc.)
  - Essential for formation of Kondo singlet (heavy fermions)
- Numerically: Fewer deg. of freedom
  - Lower-T are accessible
  - Fewer parameters (J, n)

Simple model is worth studying in detail !

Ground-state phase diagram of Kondo lattice

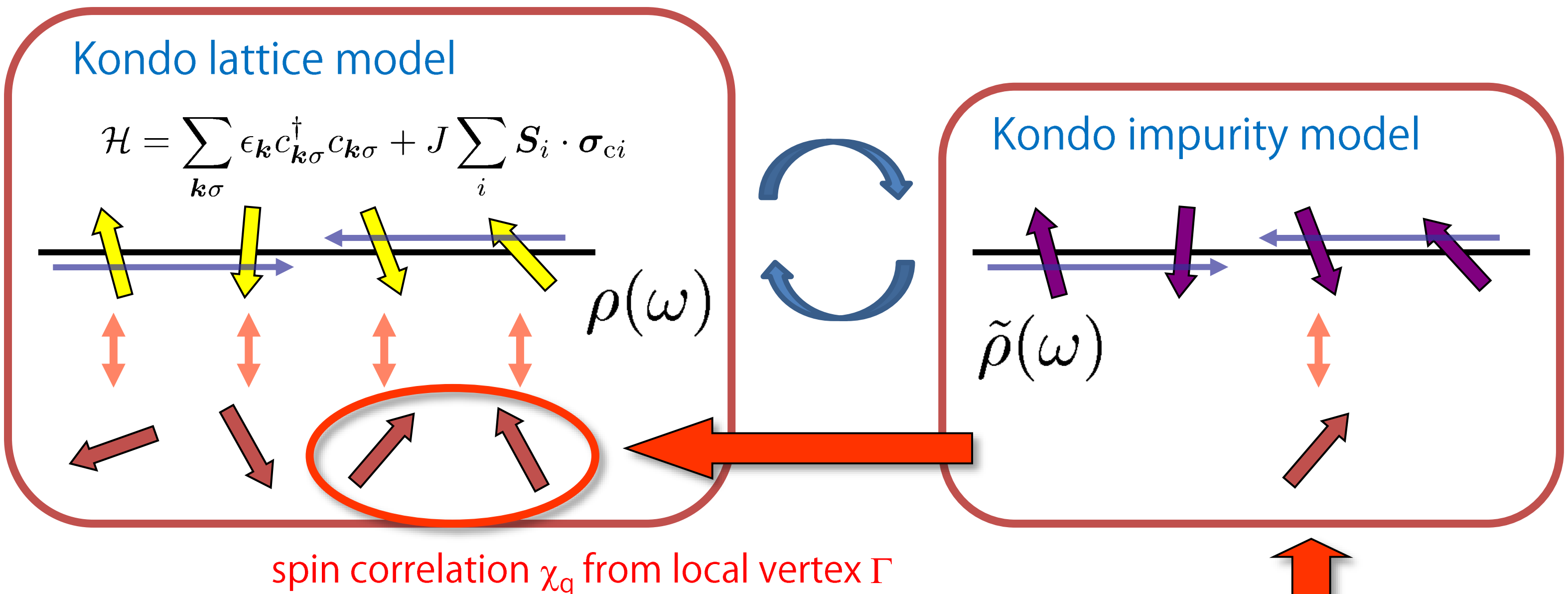


Variational approach
with mean-field calculations
Lacroix & Cyrot 1979
Fazekas & Muller-Hartmann 1991

DMFT + CT-QMC

Dynamical mean-field theory (DMFT): exact solution in d=1

Metzner & Vollhardt '87
Georges & Kotliar '92
Georges et al. RMP '96

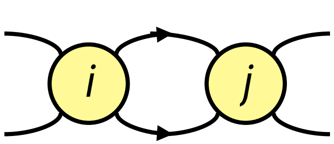


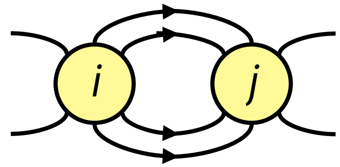
Treatment of localized spins in DMFT
JO, Kusunose, Kuramoto 2009

CT-QMC (CT-J) JO et al. 2007

Description including strong local correlations (Kondo physics)
→ Heavy fermion & magnetism (no anisotropic superconductivity)

Spatial dependent susceptibility





$\to 0 \quad (d \to \infty)$

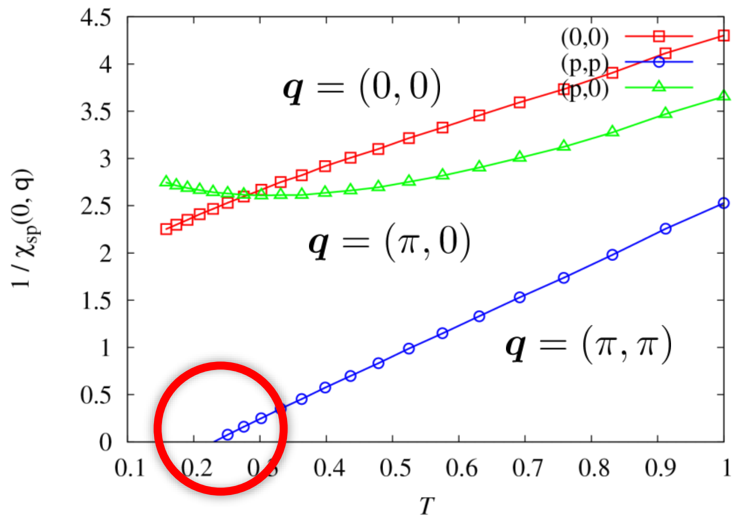
relevant in d→∞

Kuramoto, Watanabe 1988
Zlatic, Horvatic 1990
Jarrell 1992
「電子相関の物理」斯波弘行著

vertex becomes local

$\Gamma(i\omega, i\omega'; i\nu)$ ← computed in the effective impurity model

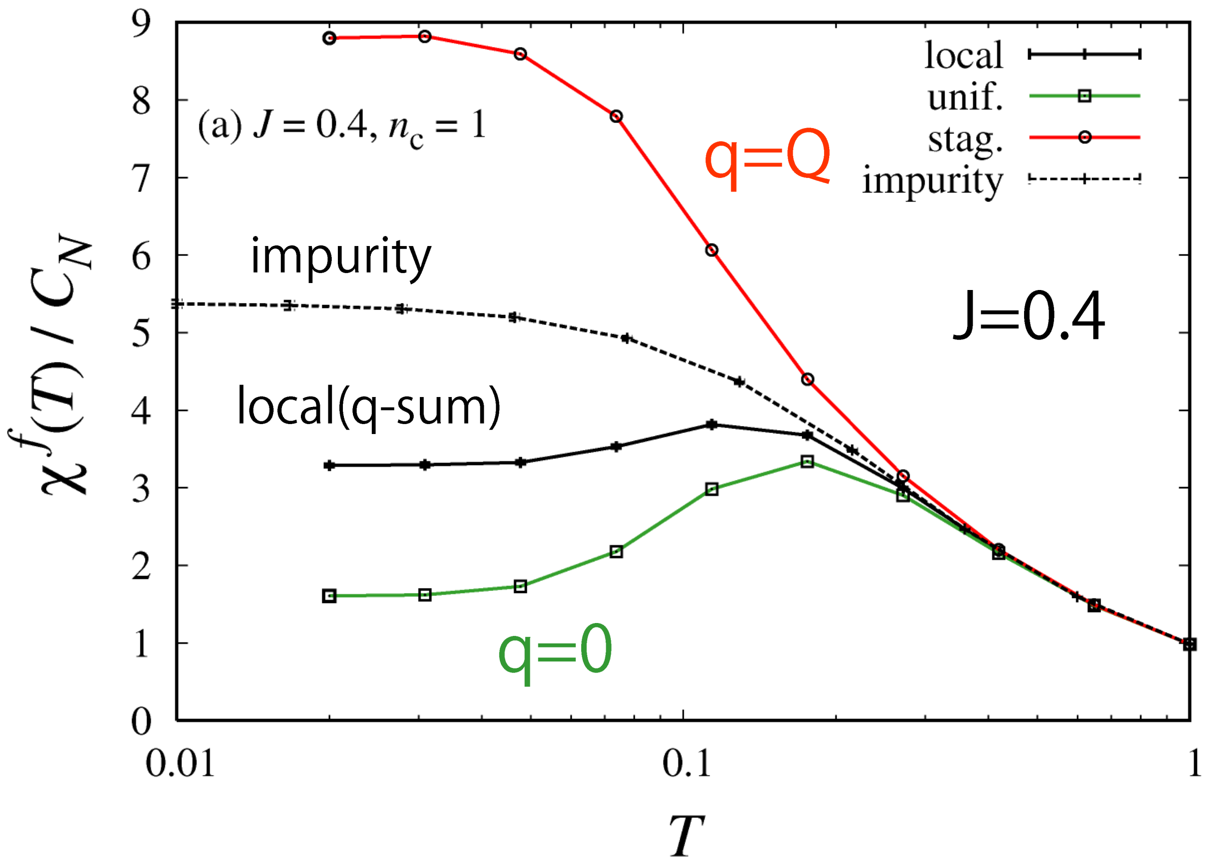
$1/\chi_{\boldsymbol{q}} \quad (\text{static } \nu = 0)$



mean-field level
concerning intersite corelations

Static susceptibility (half filling)

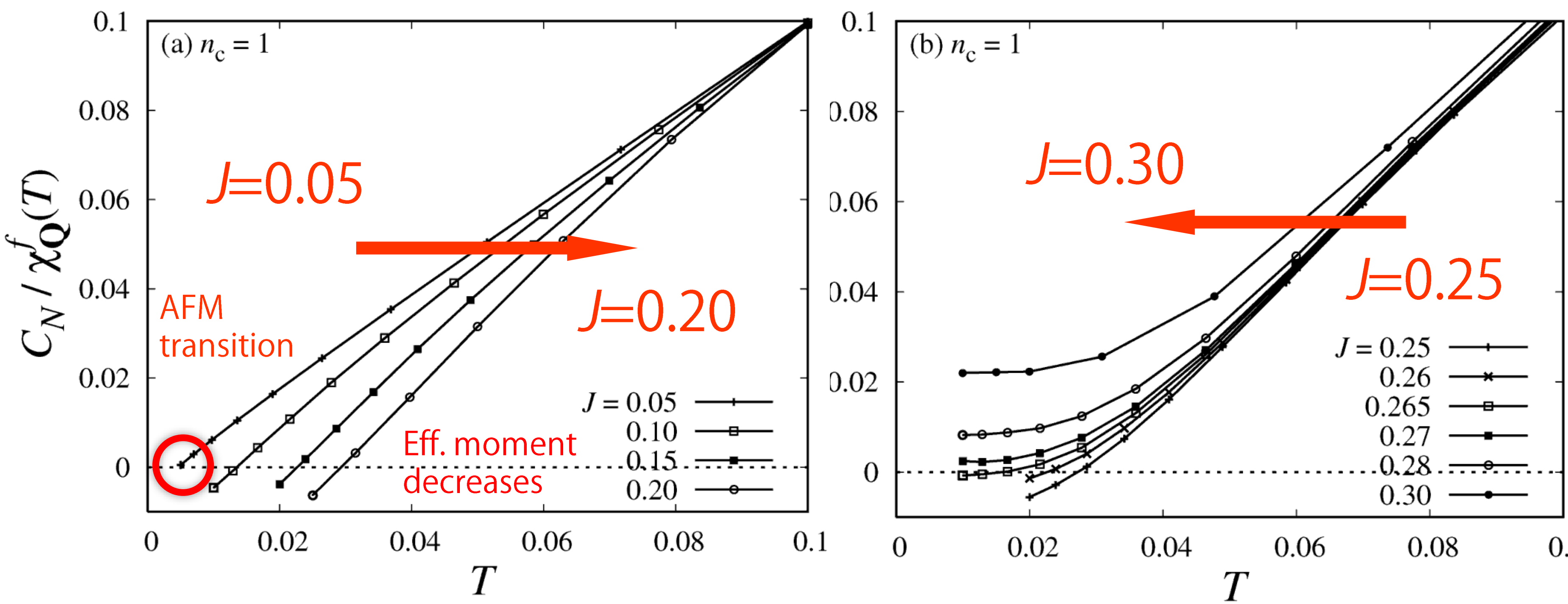
JPSJ 78, 034719 (2009)



AFM susceptibility (half filling)

JPSJ 78, 034719 (2009)

Inverse suscep. (q=Q)

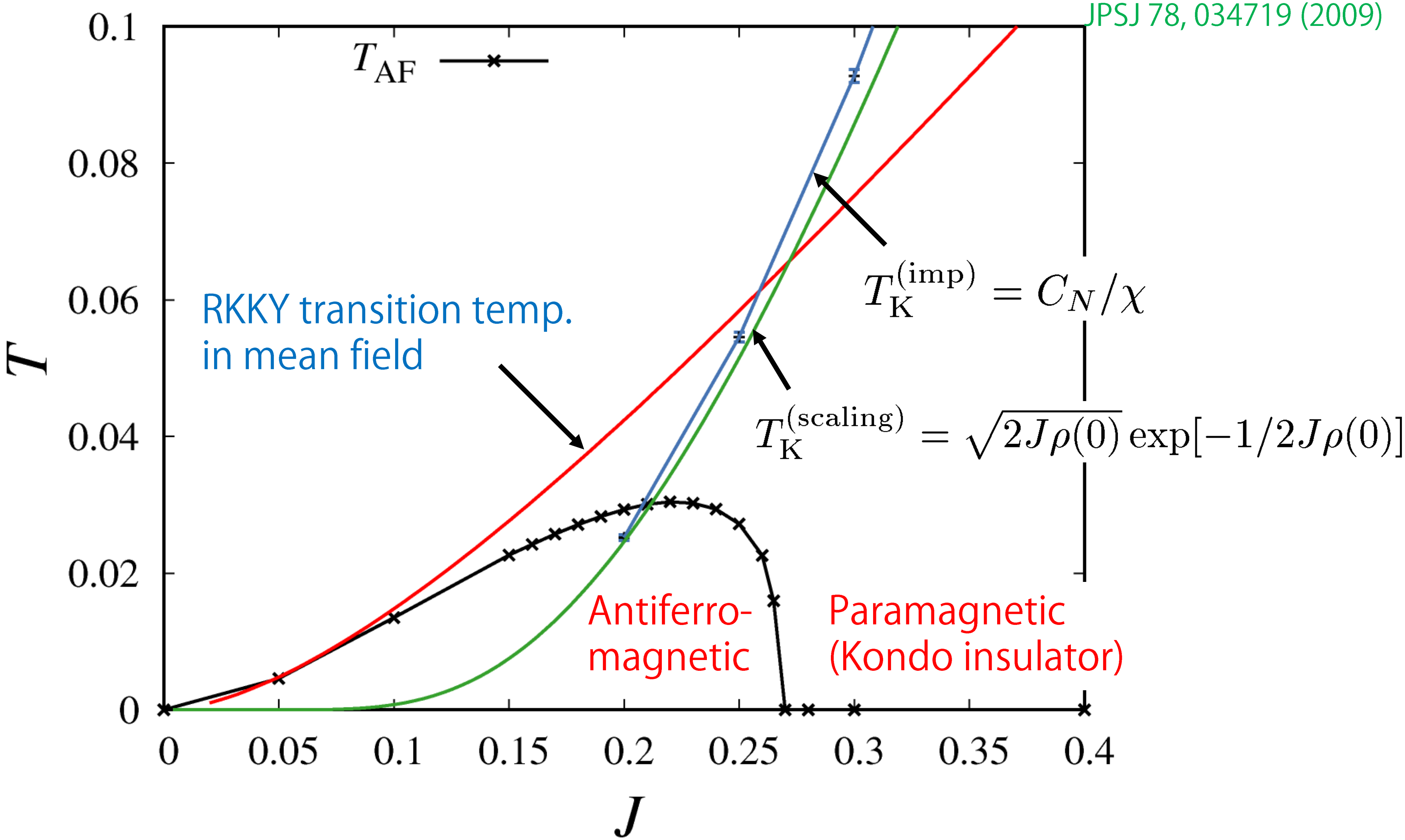


Ordering by RKKY interaction

Screening of spins (Kondo effect)

AFM phase diagram (half filling)

JPSJ 78, 034719 (2009)

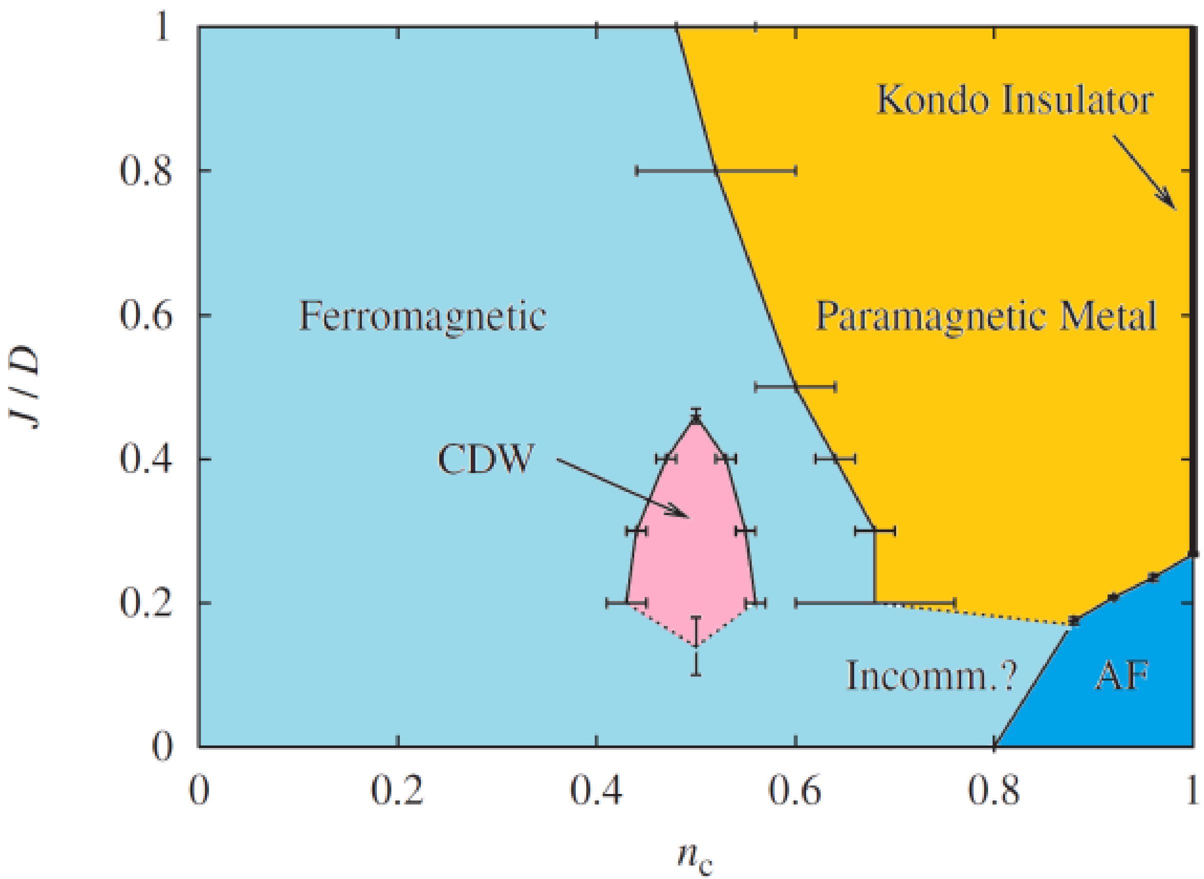


Competition between Kondo effect and RKKY
Doniach's picture ('77) is reproduced at $n_c \sim 1$

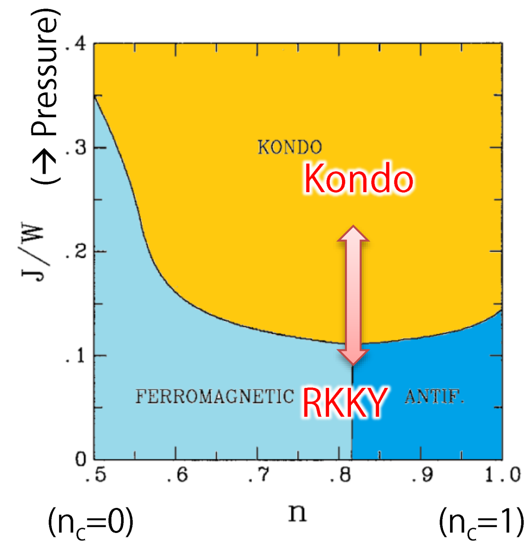
Phase diagram

JPSJ 78, 034719 (2009)

Dynamical mean-field theory

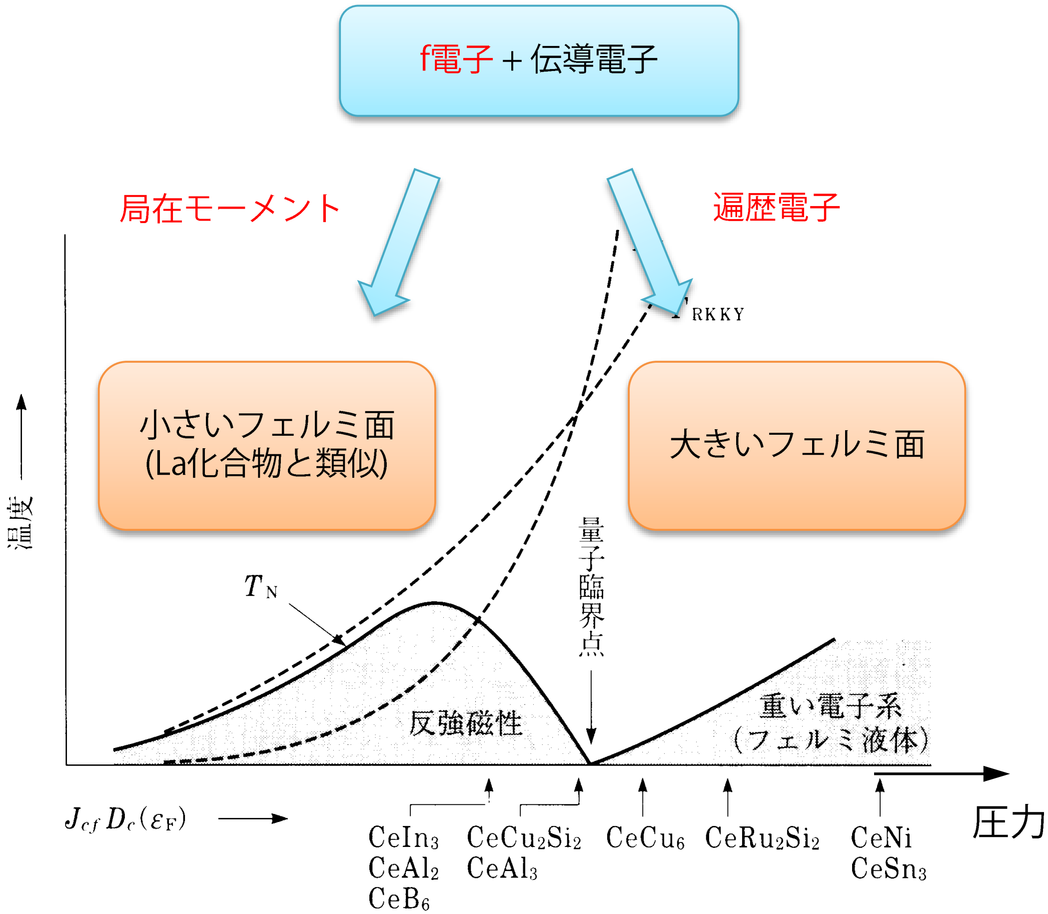


Variational approach
Lacroix & Cyrot 1979
Fazekas & Muller-Hartmann 1991



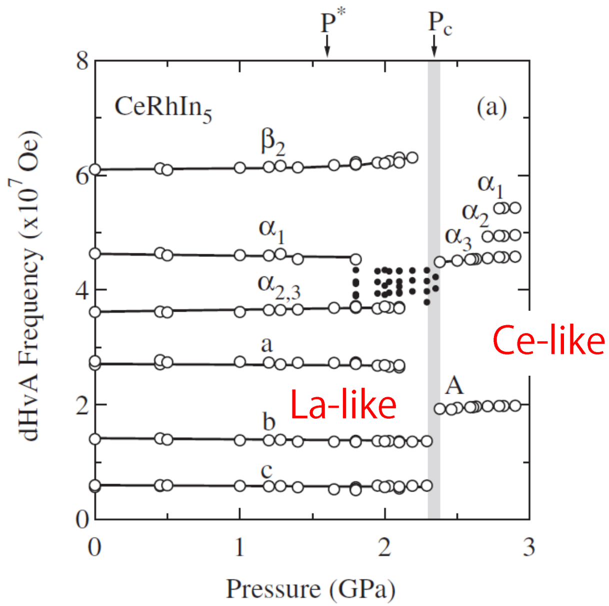
重い電子の形成と大きいフェルミ面

重い電子の遍歴・局在



上田和夫・大貫惇睦「重い電子系の物理」

$CeRhIn_5$



Shishido et al. 2005

f電子の遍歴・局在の定量的な議論が必要

Fermi surface in the Kondo lattice

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$$H_{\mathrm{K}} = \sum_{\boldsymbol{k}\sigma} \epsilon_{\boldsymbol{k}} c^{\dagger}_{\boldsymbol{k}\sigma} c_{\boldsymbol{k}\sigma} + J \sum_{i} \boldsymbol{S}_i \boldsymbol{\sigma}^{c}_{i}$$

$\boldsymbol{S}_i$: localized spin
completely localized (no charge deg. of free.)

Luttinger's theorem on FS volume

$$\Omega \equiv 2 \int_{\mathrm{FS}} \frac{d\boldsymbol{k}}{(2\pi)^3} = n_{\mathrm{band}}$$

even with interactions
(conserved quantity)

"small Fermi surface" or "large Fermi surface"

$$\Omega = n_{\mathrm{cond}}$$

(J=0) localized

$$\Omega = n_{\mathrm{cond}} + 1$$

(Anderson lattice) itinerant

Does the localized spin contribute to the FS volume?

Related studies

Numerical approaches (1D)
- Shiba & Fazekas 1990 (VMC)
- Tsunetsugu et al. 1997 (ED)
- Moukouri & Caron 1996 (DMRG)
- Shibata et al. 1996 (DMRG)

Large FS realizes

Approximations
- Coleman & Andrei 1989
- Burdin et al 2002
- Senthil et al. 2003

Non-perturbative approach (high dimensions)
- Oshikawa 2000: *If Fermi liquid*, then large FS realizes

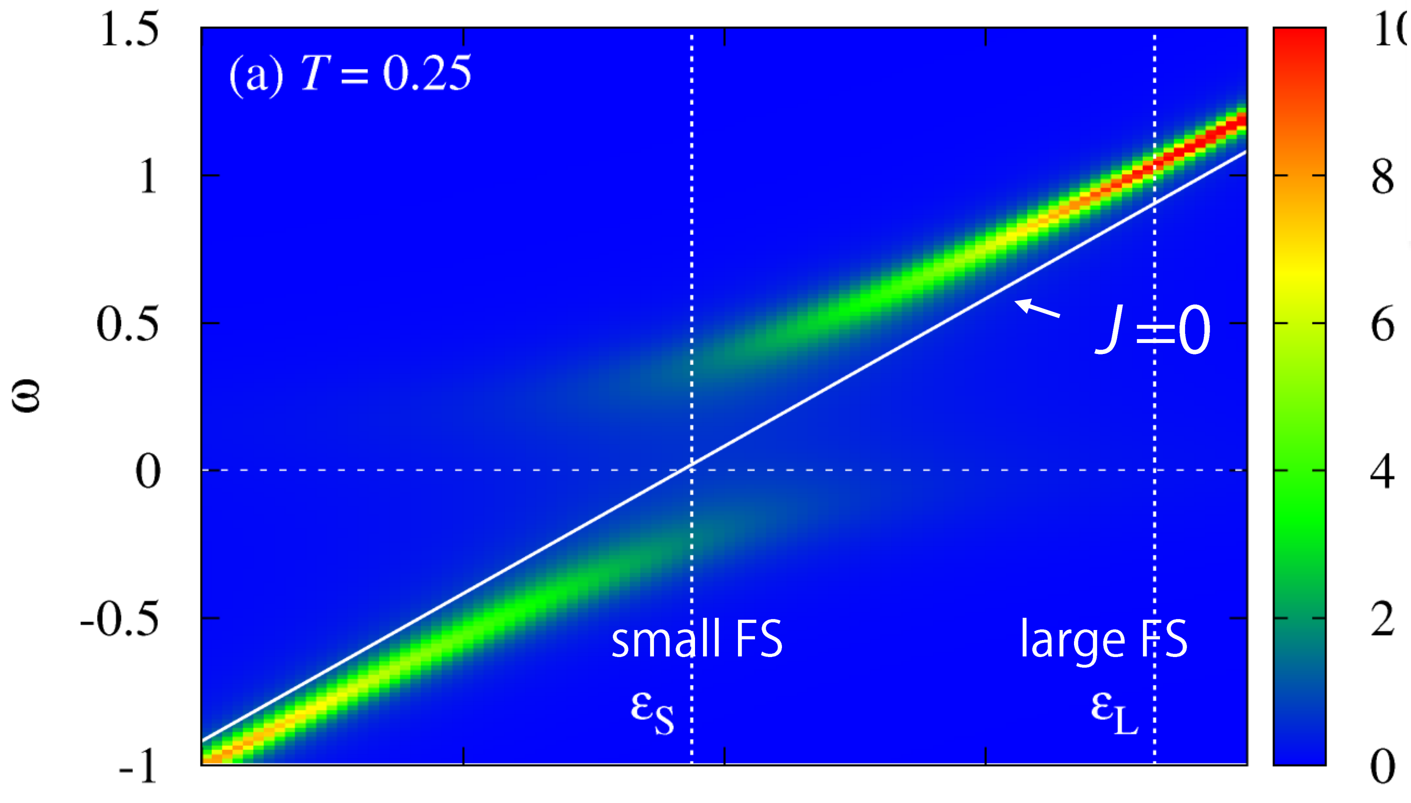
Our study

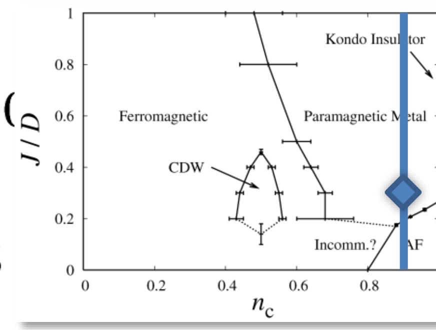
- High dimensions (DMFT)
- T-dependent evolution of the large Fermi surface

Crossover from local moment (localized) to the Fermi liquid (itinerant)

Single-particle excitation spectrum

$A(\epsilon,\omega) = -\mathrm{Im}G_c(\epsilon,\omega+i0)/\pi \qquad G_c(\epsilon_{\boldsymbol{k}}, i\epsilon_n) = \dfrac{1}{i\epsilon_n + \mu - \epsilon_{\boldsymbol{k}} - \Sigma_c(i\epsilon_n)}$





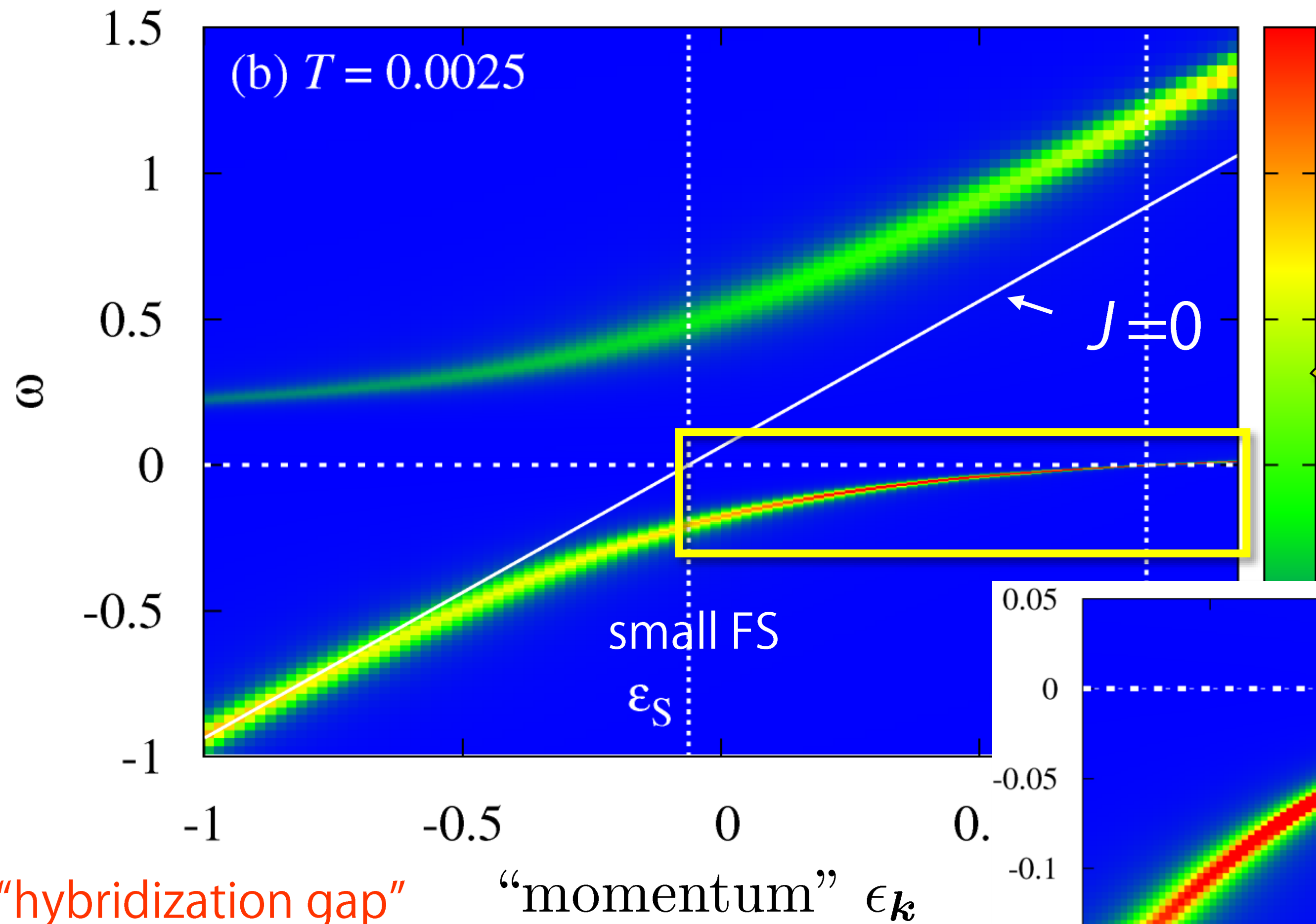
J=0.3, n_c=0.9
(T_K~0.1)

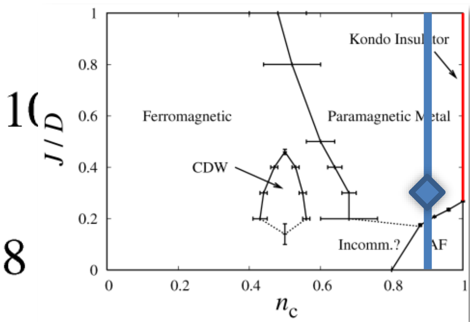
"hybridization gap"
by local spins
$\Delta_{gap} \sim T_K$

"momentum" $\epsilon_{\boldsymbol{k}}$

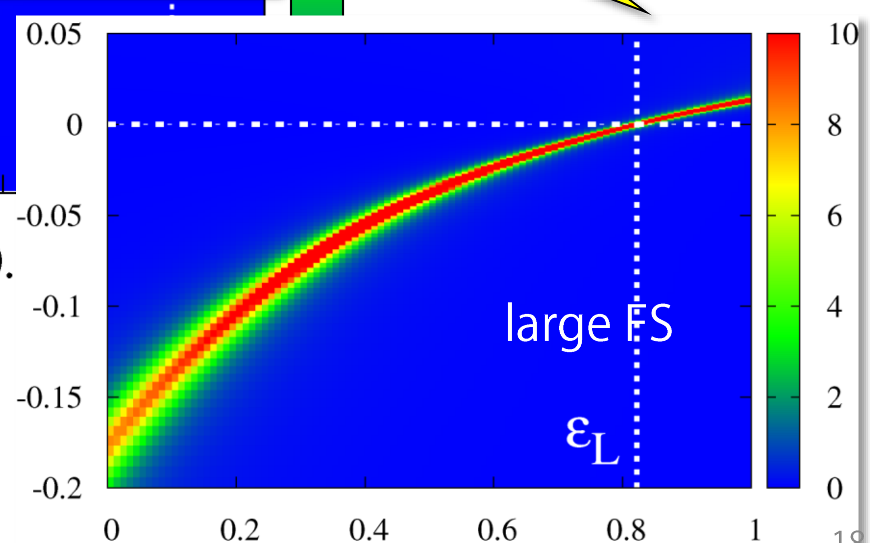
Single-particle excitation spectrum

$$A(\epsilon,\omega) = -\mathrm{Im}G_c(\epsilon,\omega+i0)/\pi \qquad G_c(\epsilon_{\boldsymbol{k}}, i\epsilon_n) = \frac{1}{i\epsilon_n + \mu - \epsilon_{\boldsymbol{k}} - \Sigma_c(i\epsilon_n)}$$





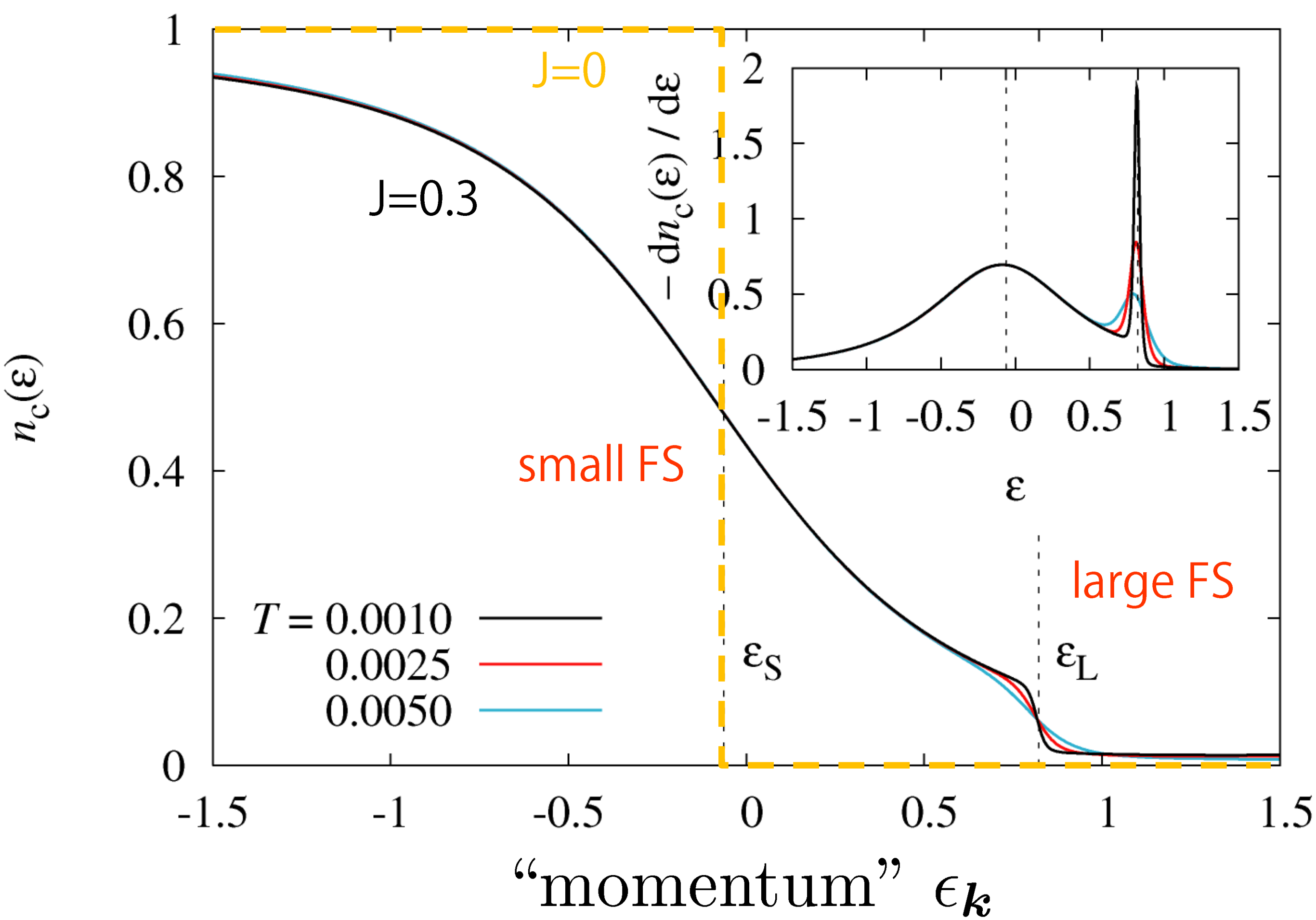
J=0.3, n_c=0.9
($T_K \sim 0.1$)

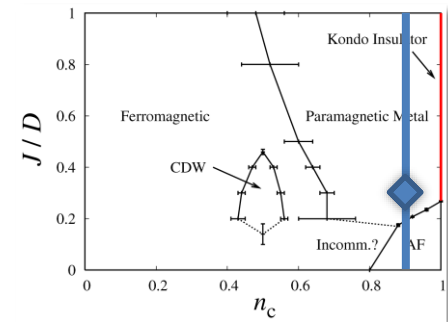


"hybridization gap"
by local spins
$\Delta_{gap} \sim T_K$

Momentum distribution function

$$n_c(\epsilon) = T \sum_n G_c(\epsilon, i\epsilon_n) e^{i\epsilon_n \delta}$$





J=0.3, n_c=0.9
($T_K \sim 0.1$)

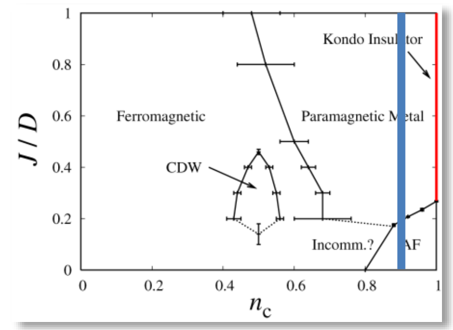
Temperature depend. of self-energy

$$G_c(\epsilon_{\boldsymbol{k}}, \omega = 0) = \frac{1}{\mu - \epsilon_{\boldsymbol{k}} - \Sigma_c(0)}$$ $= 0$

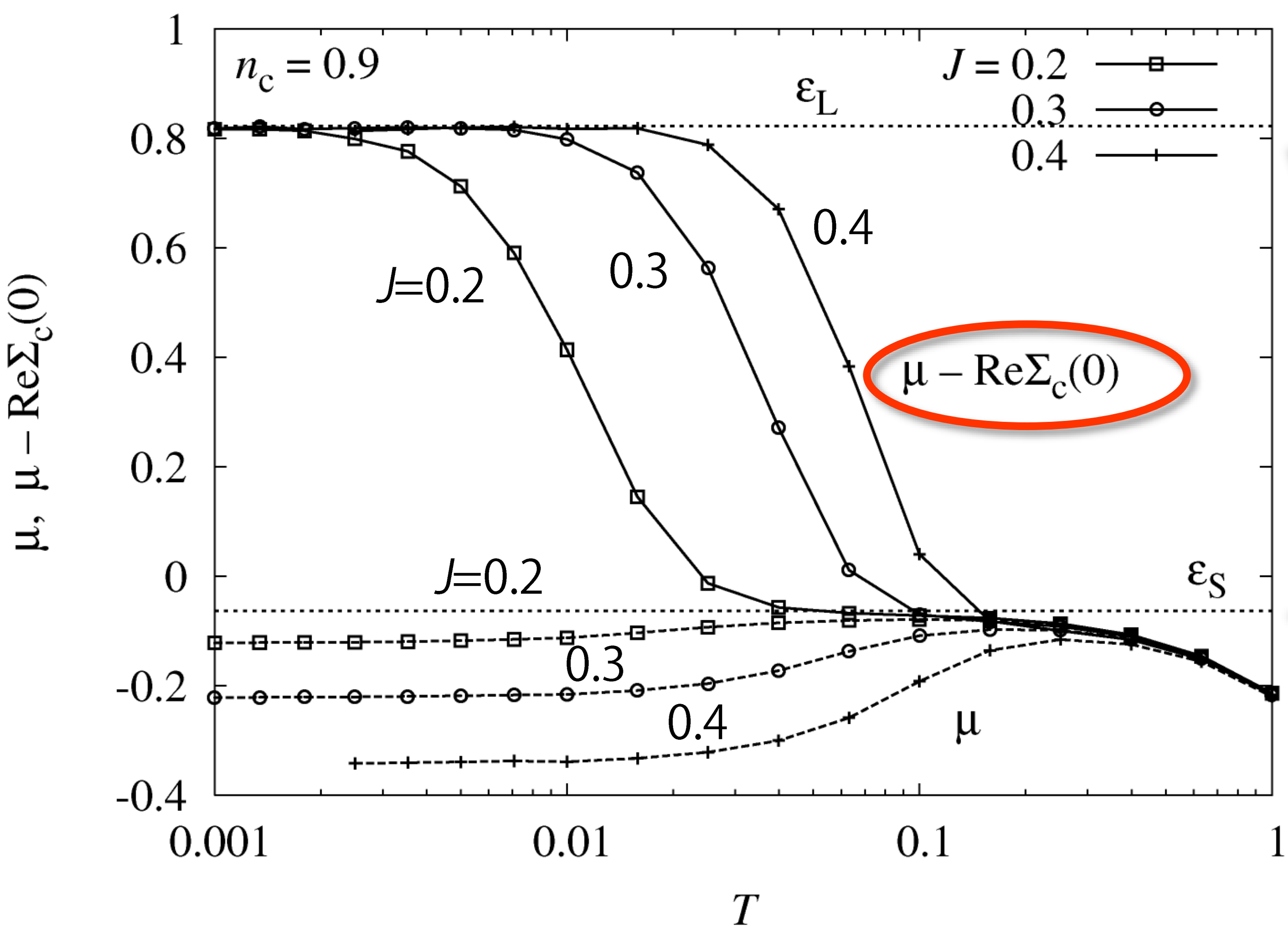
Fermi momentum

$$\epsilon_{\boldsymbol{k}_F} = \mu - \mathrm{Re}\Sigma_c(0)$$

Renormalized chemical potential



n_c=0.9



large FS
"itinerant"

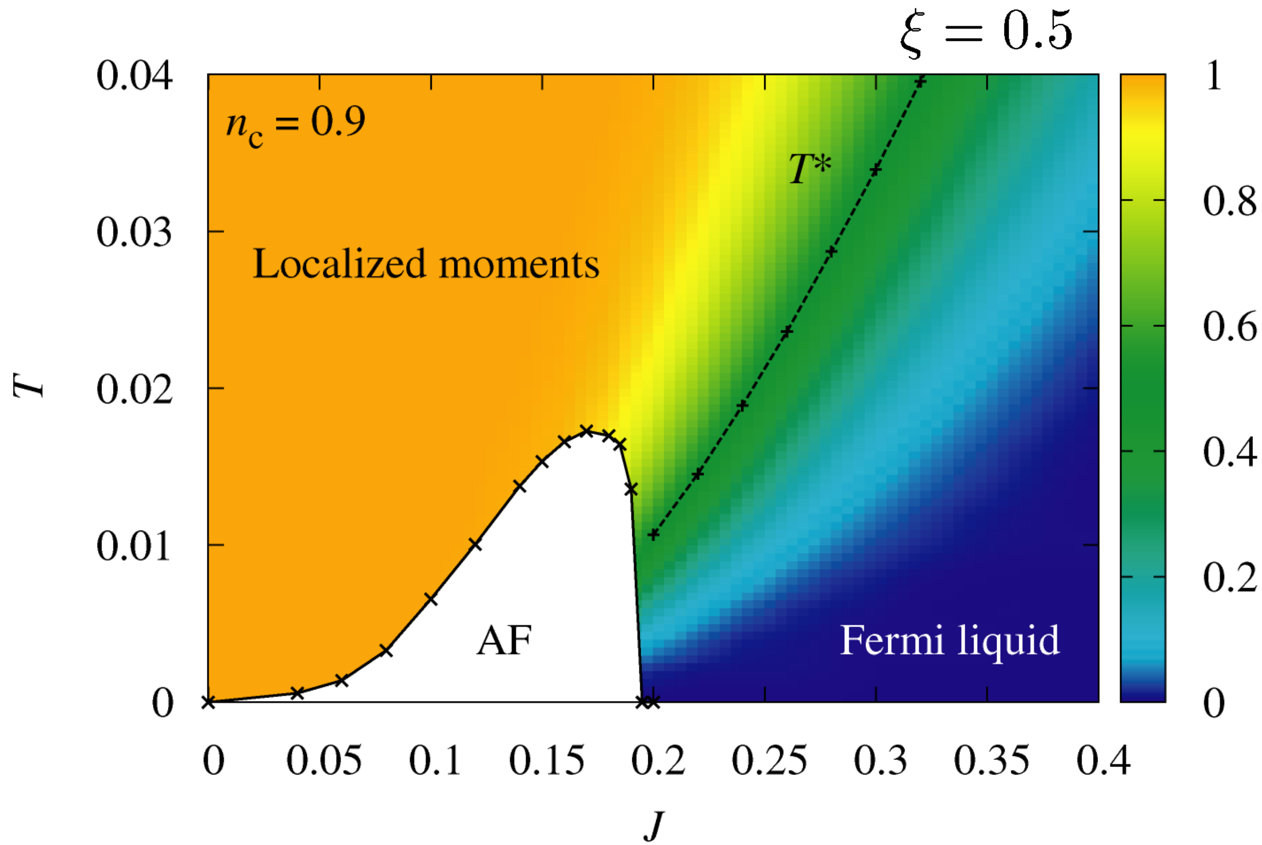
small FS
"localized"

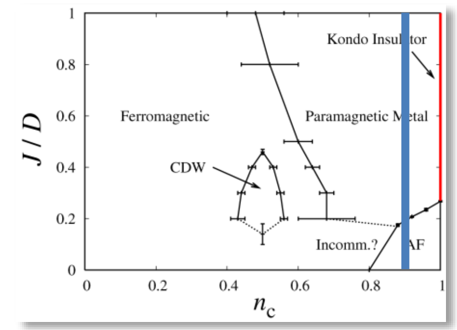
T–J phase diagram

“itinerancy” ξ

$$\xi = \frac{\mu - \mathrm{Re}\Sigma_c(0) - \epsilon_L}{\epsilon_S - \epsilon_L}$$

$\xi = 0$: large FS ($\Omega = n_{cond} + 1$)
$\xi = 1$: small FS ($\Omega = n_{cond}$)





n_c=0.9

Coherence temperature T^*

$$T^* < T_K$$

No criticality in single-particle quantities at QCP
(only in two-particle quantities)

混晶系

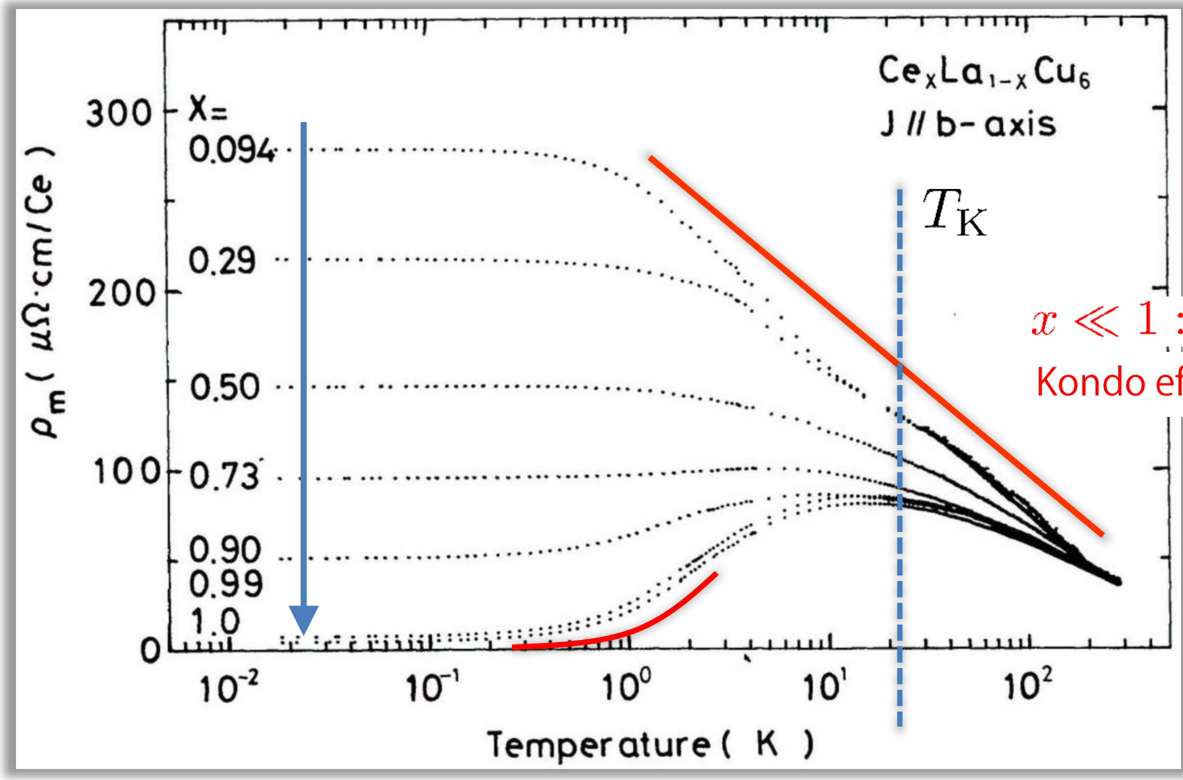
近藤効果から重い電子へ

Sumiyama et al. (1986)

Electric resistivity in $Ce_xLa_{1-x}Cu_6$

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

$$\rho_{\mathrm{m}} = (\rho_x - \rho_0)/x$$



$x \ll 1: \ \rho(T) \sim -\log T$

Kondo effect (local Fermi liquid)

$x = 1: \ \rho(T) = AT^2$

Fermi liquid

$$\frac{m^*}{m} \sim \frac{E_{\mathrm{F}}}{T_{\mathrm{K}}} \sim 10^2, 10^3$$

Heavy fermions

Coherent Potential Approximation (CPA) + DMFT

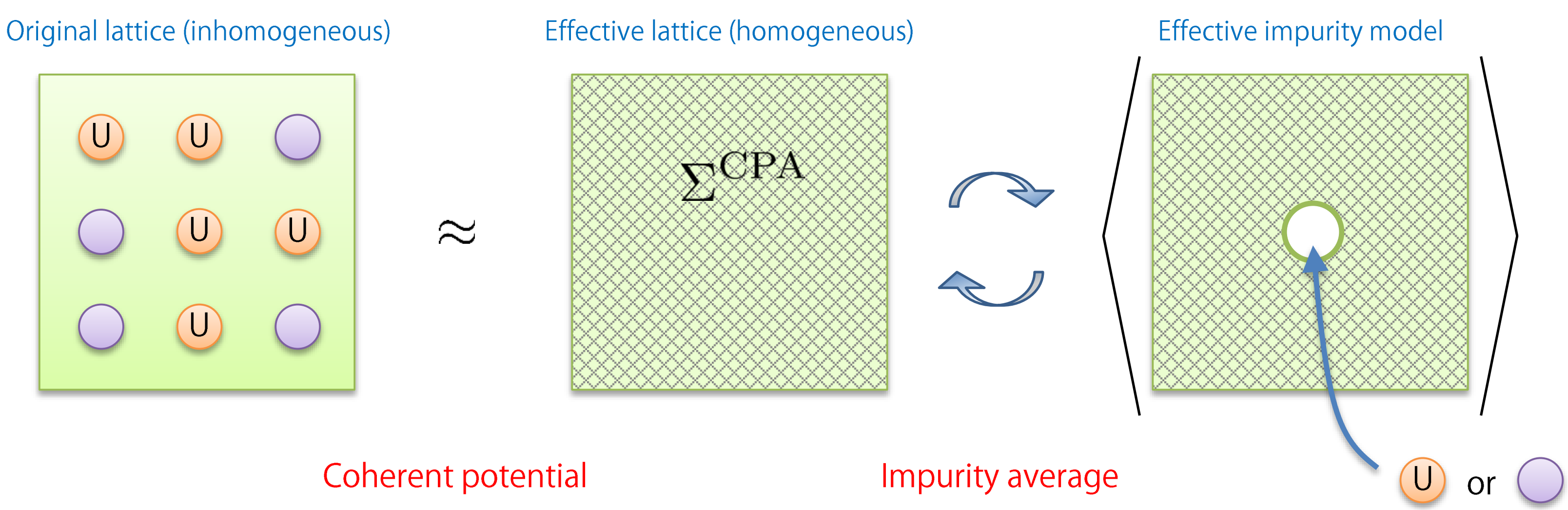
二元合金

$$H = \sum_{\boldsymbol{k}\sigma} \left(\epsilon_{\boldsymbol{k}} c^{\dagger}_{\boldsymbol{k}\sigma} c_{\boldsymbol{k}\sigma} + V_{\boldsymbol{k}} f^{\dagger}_{\boldsymbol{k}\sigma} c_{\boldsymbol{k}\sigma} + V^{*}_{\boldsymbol{k}} c^{\dagger}_{\boldsymbol{k}\sigma} f_{\boldsymbol{k}\sigma} \right) + \sum_{i \in \mathrm{Ce}} \left(\epsilon_f^{(\mathrm{Ce})} n_i^f + U n^f_{i\uparrow} n^f_{i\downarrow} \right) + \sum_{i \in \mathrm{La}} \left(\epsilon_f^{(\mathrm{La})} n_i^f \right)$$

CPAグリーン関数

$$G_{\mathrm{c}}(i\omega, \boldsymbol{k}) = \frac{1}{i\omega - \epsilon_{\boldsymbol{k}} + \mu - \Sigma^{\mathrm{CPA}}(i\omega)}$$

Yoshimori, Kasai 1986
Shiina 1995
Miranda et al. 1997 Hybridization disorder
Mutou 2001 transport
Grenzebach et al. 2008 transport
Otsuki et al. 2010 Fermi surface



Coherent potential

Impurity average

$$G_f = x G_f^{(\mathrm{Ce})} + (1 - x) G_f^{(\mathrm{La})}$$

(Ce,La)混晶系の理論計算

希釈された周期アンダーソン模型

Mutou, Phys. Rev. B 64, 245102 (2001)

Also in Grenzebach et al. 2008

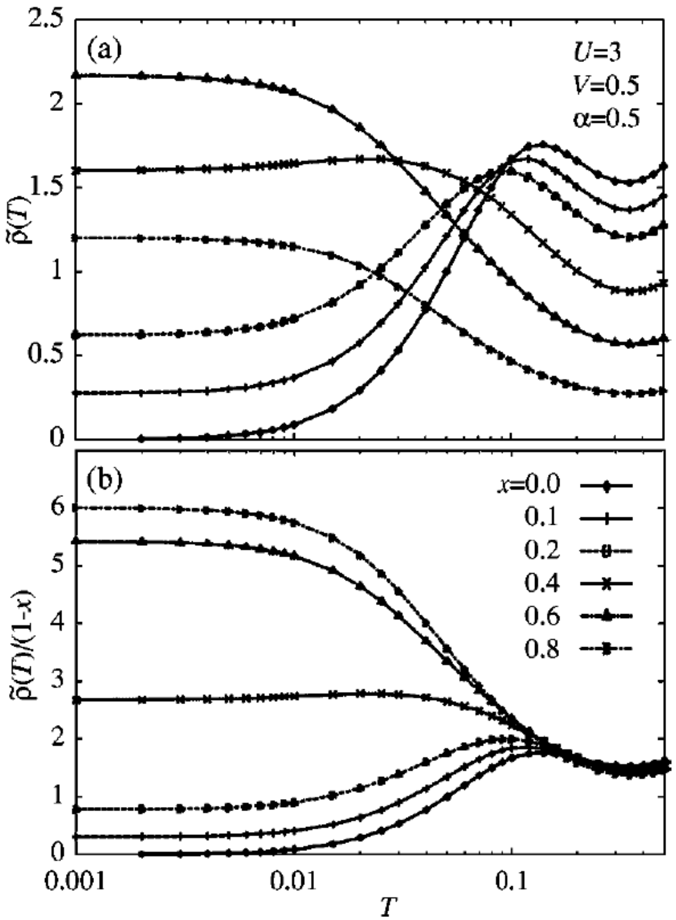


FIG. 1. (a) Temperature dependence of the resistivity for several values of x: $x=0.0$, 0.1, 0.2, 0.4, 0.6, and 0.8 ($U=3$, $V=0.5$, and $\alpha=0.5$). (b) Data divided by $1-x$ for same parameters.

Anderson絶縁体

相加平均 (CPA)

$$G_f(i\omega) = \langle G_f(i\omega) \rangle$$

相乗(幾何)平均

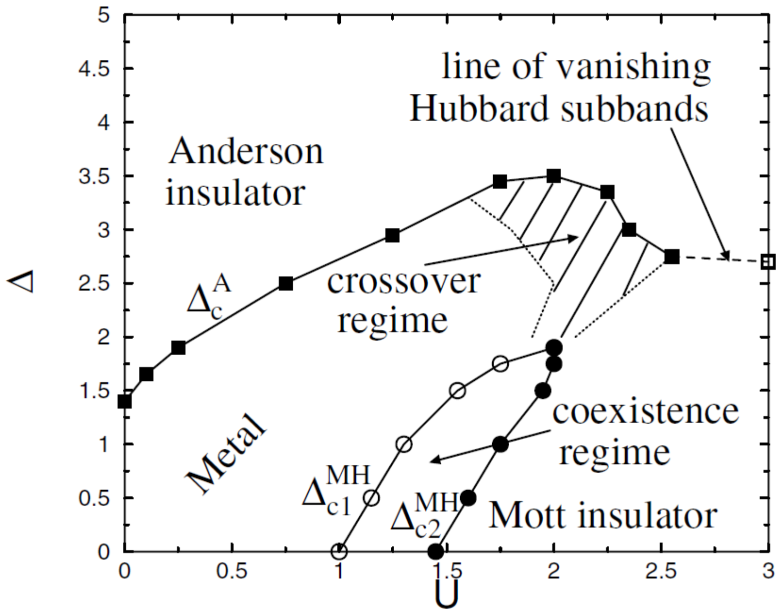
$$\rho(\omega) = \exp[\langle \ln \rho_f(\omega) \rangle]$$

$$\rho_f(\omega) = -\frac{1}{\pi}\mathrm{Im}G_f(\omega + i0)$$

Anderson-Hubbard model (Byczuk et al. 2005)

$$H_{\mathrm{AH}} = -t\sum_{\langle ij\rangle\sigma} a_{i\sigma}^\dagger a_{j\sigma} + \sum_{i\sigma}\epsilon_i n_{i\sigma} + U\sum_i n_{i\uparrow}n_{i\downarrow},$$

$$\mathcal{P}(\epsilon_i) = \Theta(\Delta/2 - |\epsilon_i|)/\Delta$$

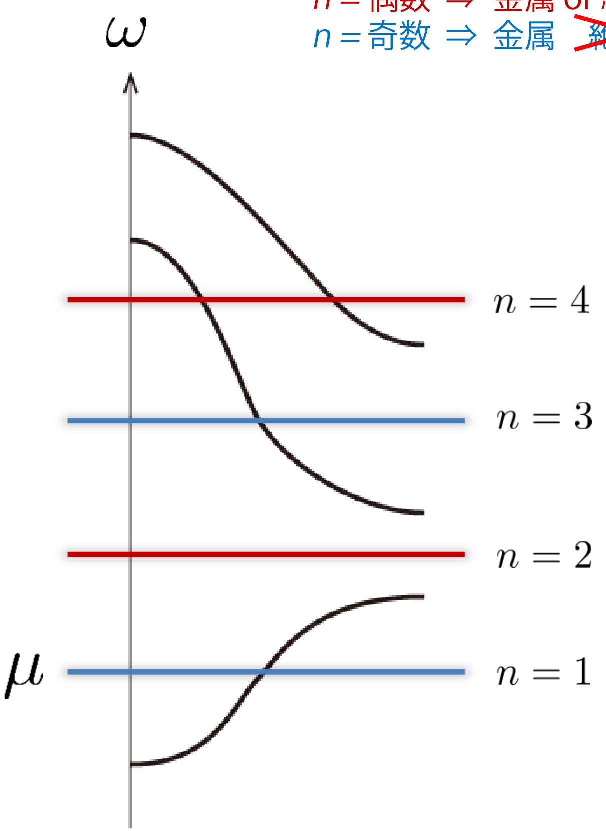


モット転移

強相関電子系：*Mott*絶縁体

バンド理論

単位胞あたりの電子数*n*
n＝偶数 ⇒ 金属 or 絶縁体
n＝奇数 ⇒ 金属 ~~絶縁体~~



バンド理論では説明できない絶縁体

MnO, FeO, CoO, NiO, CuO, ⋯

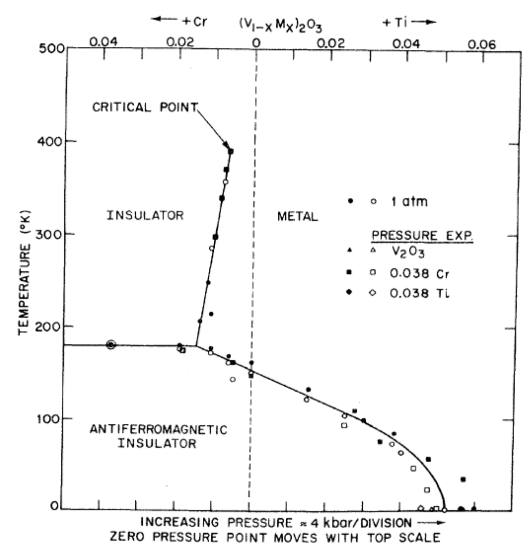
4	5	6	7	8	9	10	11
22 Ti	23 V	24 Cr	25 Mn	26 Fe	27 Co	28 Ni	29 Cu

from Wikipedia

電子間相互作用による絶縁体：モット絶縁体

Mott, Peierls, 1937

V_2O_3 under pressure



McWhan et al. 1973

Hubbard模型

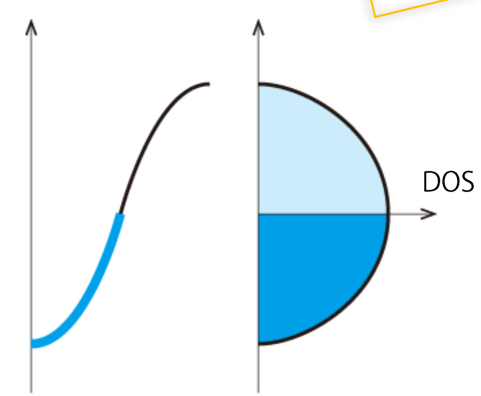
$$H = \sum_{\boldsymbol{k}\sigma} (\epsilon_{\boldsymbol{k}} - \mu) c^\dagger_{\boldsymbol{k}\sigma} c_{\boldsymbol{k}\sigma} + U \sum_i c^\dagger_{i\uparrow} c_{i\uparrow} c^\dagger_{i\downarrow} c_{i\downarrow}$$

$$c_{i\sigma} = \frac{1}{\sqrt{N}} \sum_{\boldsymbol{k}} c_{\boldsymbol{k}\sigma} e^{i\boldsymbol{k}\cdot\boldsymbol{R}_i}$$

非相互作用極限

$$|\Psi_0\rangle = \prod_{|\boldsymbol{k}|<k_{\rm F},\sigma} c^\dagger_{\boldsymbol{k}\sigma} |0\rangle$$

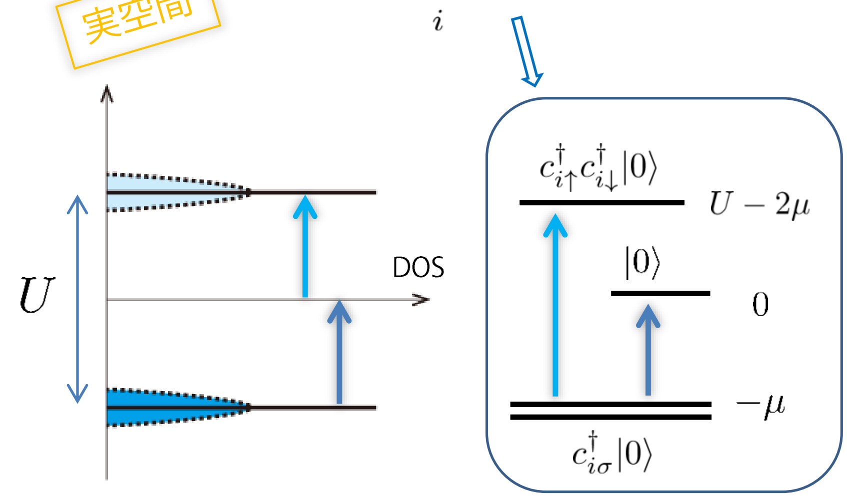
波数空間



強相関極限、原子極限

$$|\Psi_{\rm at}\rangle = \prod_i |\psi_i\rangle$$

実空間

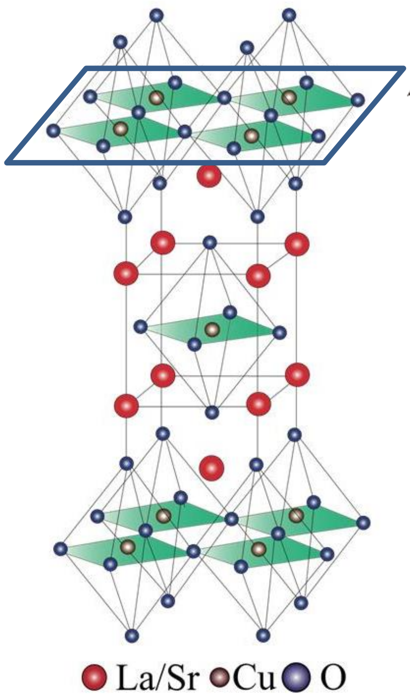


金属

絶縁体

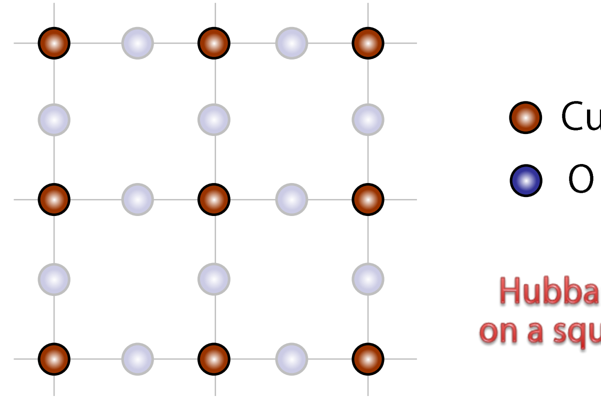
高温超伝導体

$La_{2-x}Sr_xCuO_4$



東大藤森研HPより
http://wyvern.phys.s.u-tokyo.ac.jp/f/Research/hts.htm

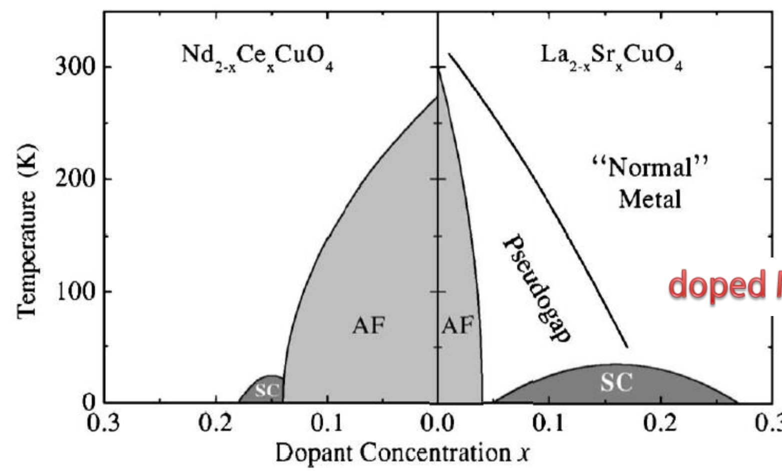
CuO_2面



Hubbard model
on a square lattice

La_2CuO_4
反強磁性絶縁体

電子ドープ← →ホールドープ



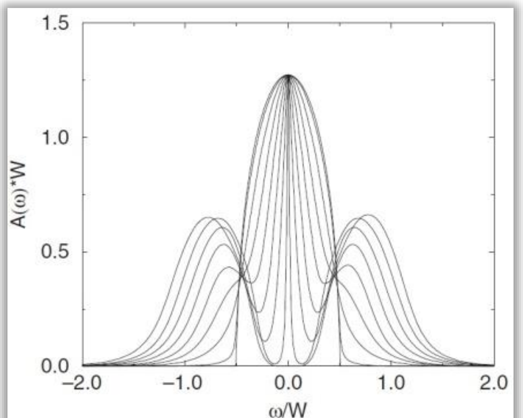
doped Mott insulator

From Damascelli et al. 2003

Mott transition

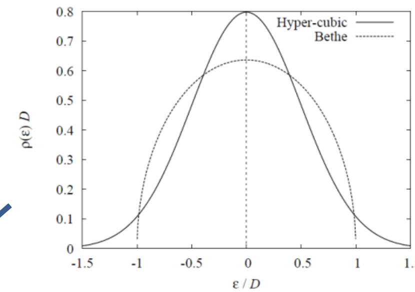
Hubbard model
at n=1 (half-filling)

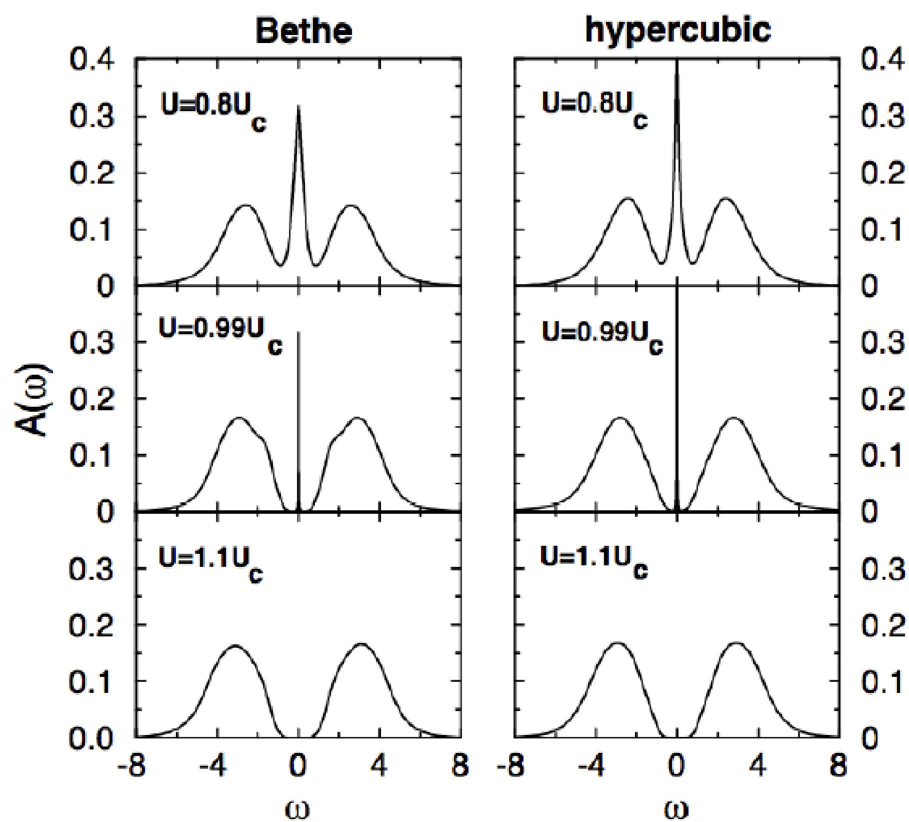
Bethe lattice



Vollhardt et al. 2005

Bulla 1999



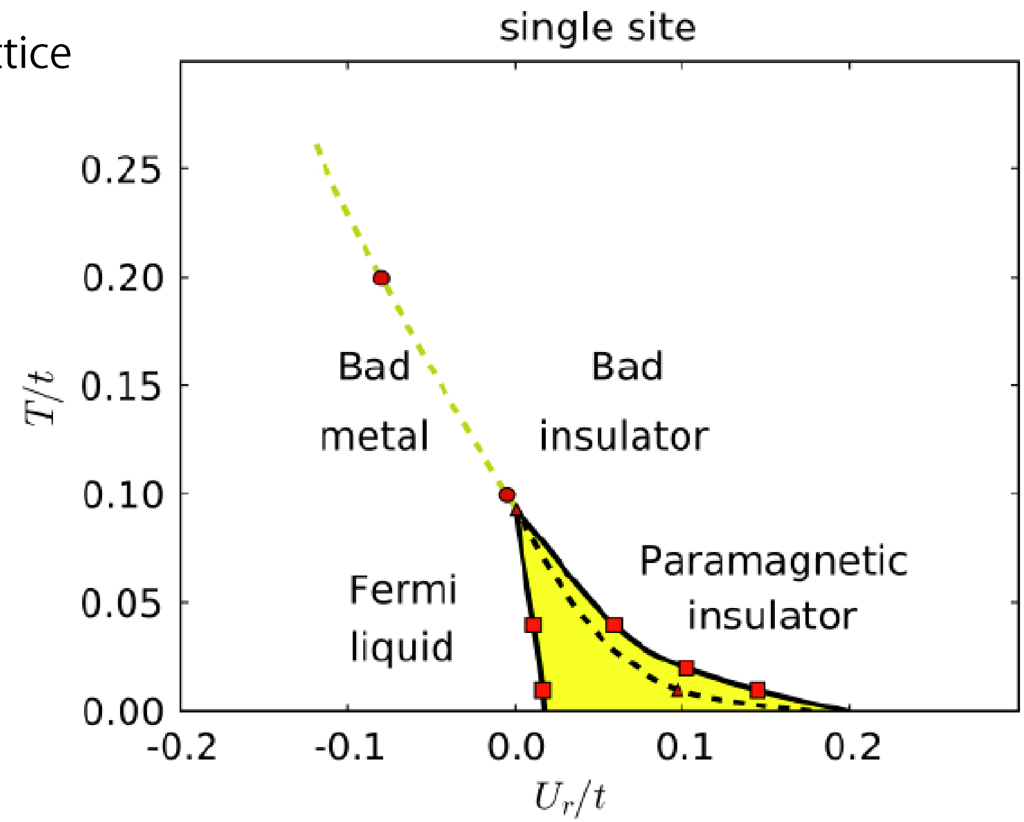


Phase diagram

Hubbard model
at n=1 (half-filling)

square lattice

Gull et al. 2007



Paramagnetism is assumed
→Antiferromagnetism?

$$U_{\mathrm{r}} = (U - U_{\mathrm{c}})/U_{\mathrm{c}}$$

$$U_{\mathrm{c}} = 9.35t$$

Phase diagram (including AFM)

Hubbard model
at n=1 (half-filling)

square lattice