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TOHOKU UNIVERSITY

Review on theories beyond DMFT

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

目的

DMFT $\Sigma(\omega, \boldsymbol{k}) \to \Sigma(\omega)$

○		×	
	Mott insulator Heavy fermion Emergent ordered state Einstein phonon		Ordered state beyond MF Unconventional SC Fermi surface structure Transport

Beyond DMFT
$\Sigma(\omega, \boldsymbol{k})$

Model calculations

2次元格子
厳密な定理
(e.g. Mermin-Wagner)

Material calculations

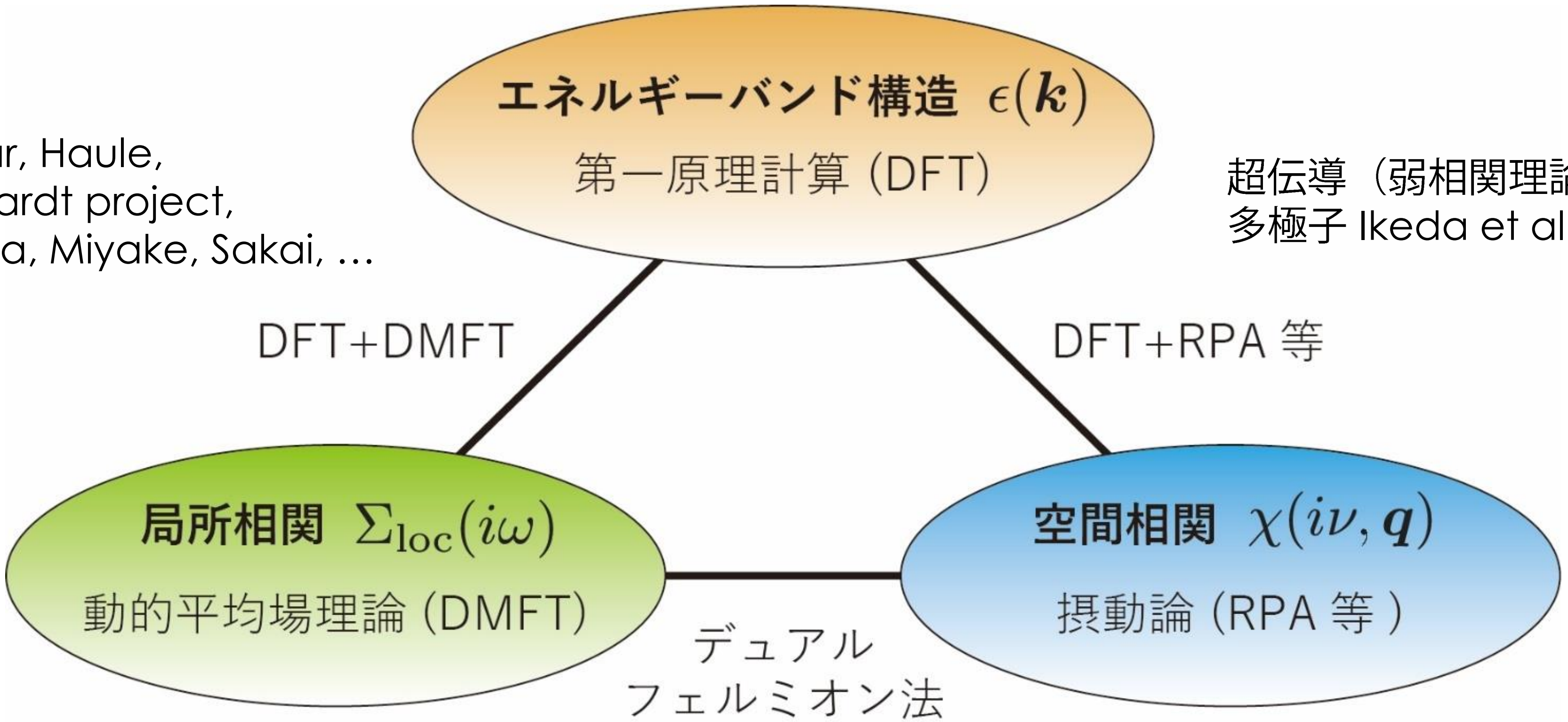
適度な計算量
時には大胆な近似

強相関化合物における磁性と超伝導の計算に向けて

大槻純也、楠瀬博明：固体物理 2016年4月号

Kotliar, Haule,
Vollhardt project,
Imada, Miyake, Sakai, …

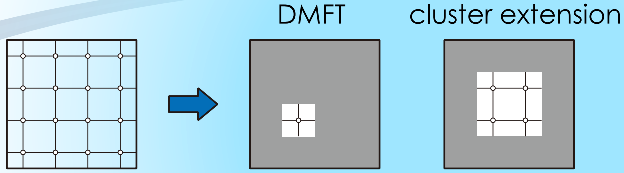
超伝導（弱相関理論）
多極子 Ikeda et al.



Kusunose, Toschi et al, Rubtsov et al, Hafermann et al.
JO et al, Taranto et al, Kitatani et al., …

Two roots of including non-local correlations

Finite-size cluster



Kotliar et al. 2001
Hettler et al. 1998
Potthoff 2003
Maier et al. 2005

Real space
Short-range correlations

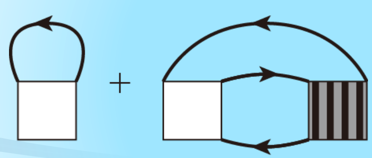
DMFT

$\Sigma(i\omega)$

Local correlations

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

Diagrammatic expansion



Kusunose 2006
Toschi et al. 2007
Slezak et al. 2009
Taranto et al. 2013
Kitatani et al. 2015

Momentum space
Long-range correlations

To avoid a double counting problem
→dual fermion approach
(Rubtsov et al. 2008
Hafermann et al. 2009)

Outline

i. Cluster extensions

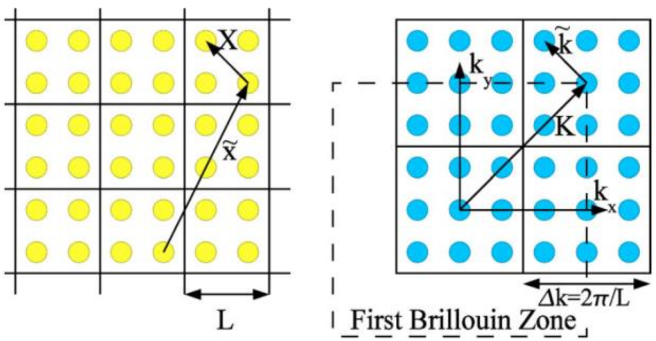
ii. Diagrammatic extensions

iii. Non-local interactions

Cluster extensions

Cluster extensions

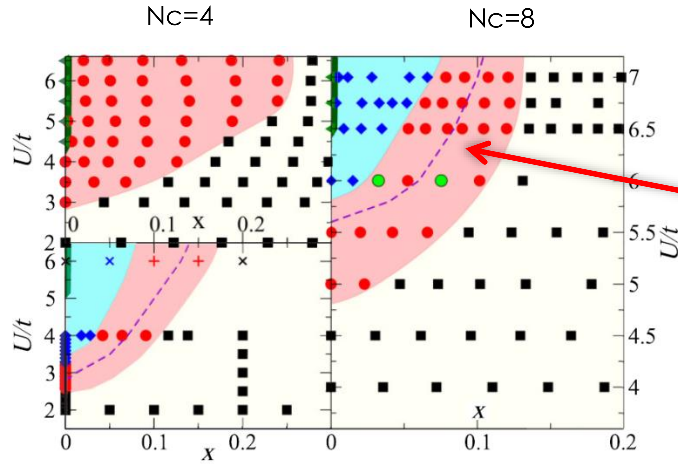
single impurity → cluster impurity



Self-consistency condition in
- r-space: Cellular DMFT (C-DMFT)
  Hettler et al. 1998
- k-space: Dynamical Cluster Approximation (DCA)
  Kotliar et al. 2001

T=t/40, t'=0 Gull et al. 2013

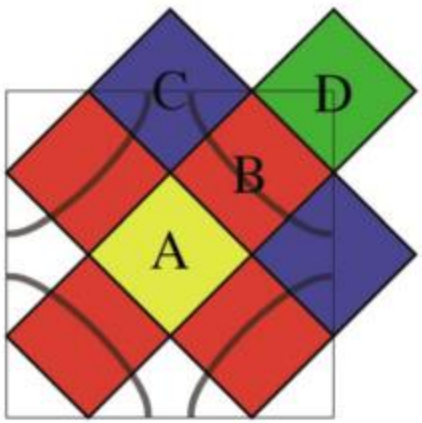
short-range correlation
- Dimer
- Plaquette singlet
- Frustration?
- d-wave superconductivity (Nc≧4)

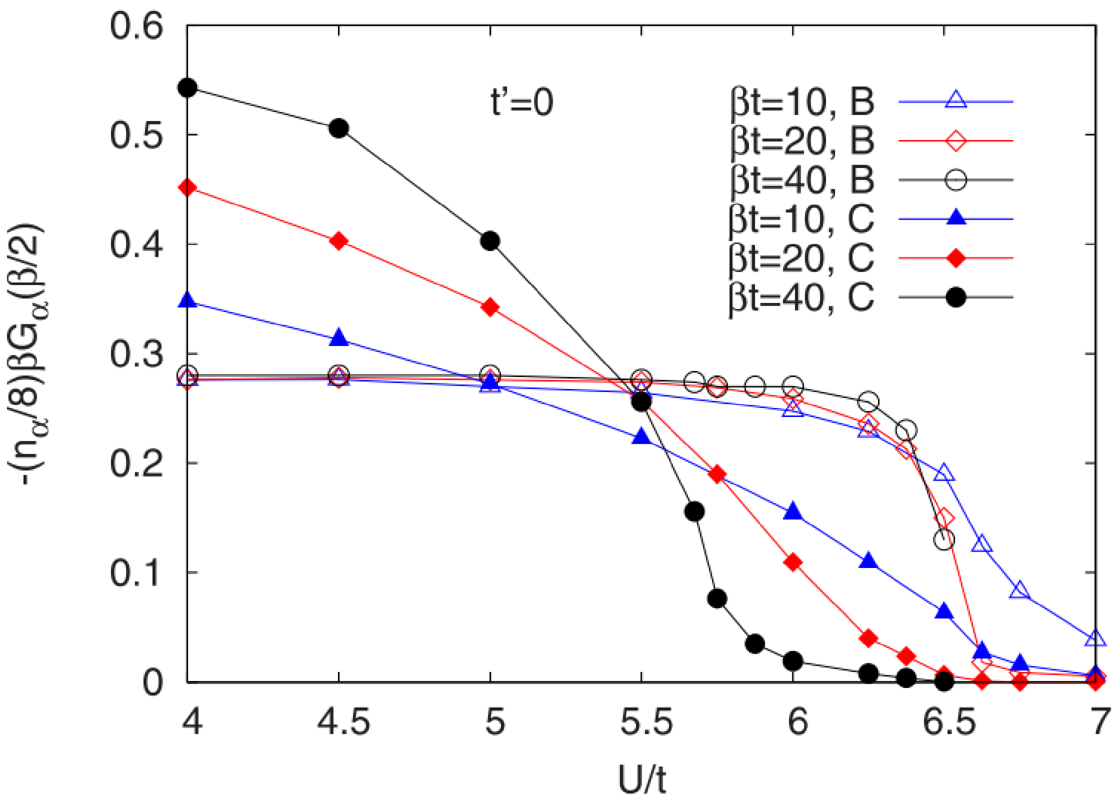


Momentum-selective Mott transition

Werner, Gull, Parcollet, Millis, 2009

DCA



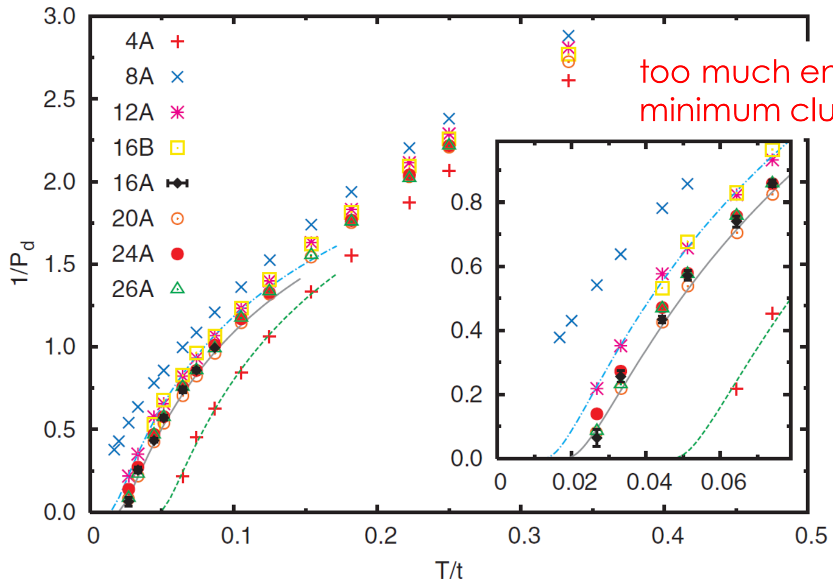


Problems in cluster DMFT

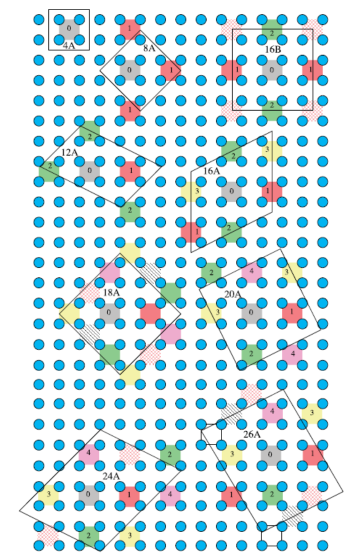
(i) Finite size effect

Maier et al., PRL **95,** 237001 (2005)

d-wave pairing susceptibility



too much enhanced in the minimum cluster size, Nc=4



(ii) Sign problem in QMC

$$\langle \text{sign} \rangle \sim e^{-\beta\Delta}$$

Sever sign problem for Nc>1

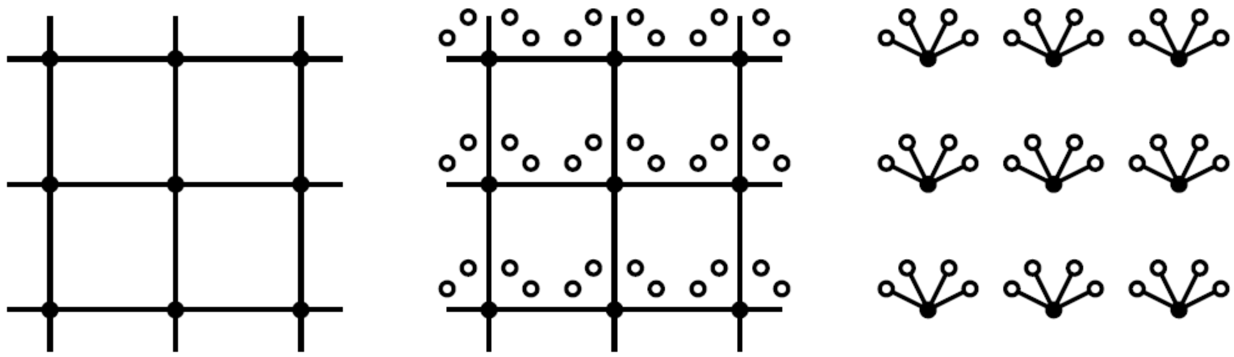
Very difficult to access low-T and thermodynamic limit

Self-energy Functional Theory (SFT)

Potthoff EPJB 32, 429 (2003)

Original system

"reference system" (solvable)



(a) (b) (c)

$$H = H_0(\boldsymbol{t}) + H_1(\boldsymbol{U})$$

$$H' = H_0(\boldsymbol{t}') + H_1(\boldsymbol{U})$$

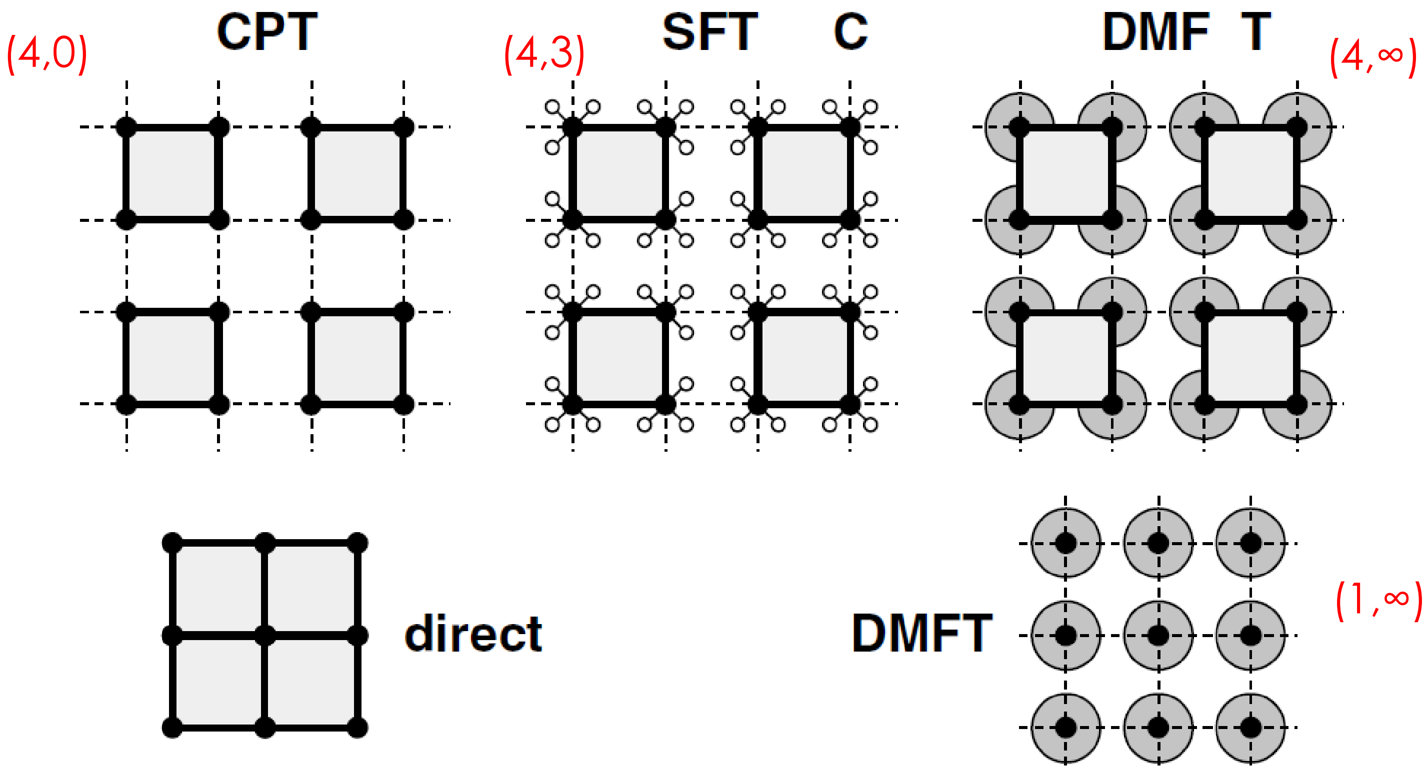
SFT

Ω Ω'

Choices of reference systems

Potthoff et al. PRL (2003)

$(N_{\mathrm{c}}, n_{\mathrm{b}})$

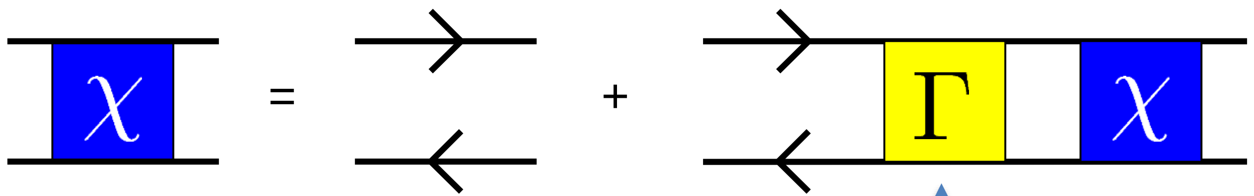


additional symmetry breaking field
→ VCA (Variational Cluster Approximation)

Diagrammatic extensions

Two-particle correlations in DMFT

Bethe-Salpeter equation



?

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

$\Gamma(\boldsymbol{k}, \omega, \boldsymbol{k}', \omega'; \boldsymbol{q}, \nu)$

irreducible vertex

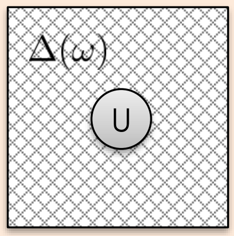
DMFT
(local approx.)

$\Gamma_{\rm loc}(\omega, \omega'; \nu)$

Expansion around DMFT: General idea

(1) Dynamical mean-field theory (DMFT)

$\Sigma^{\mathrm{DMFT}}(\omega)$



Local correlations
localized

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

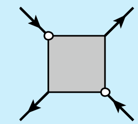
Δ_ω

(2) Auxiliary fermion lattice

"quasiparticles"

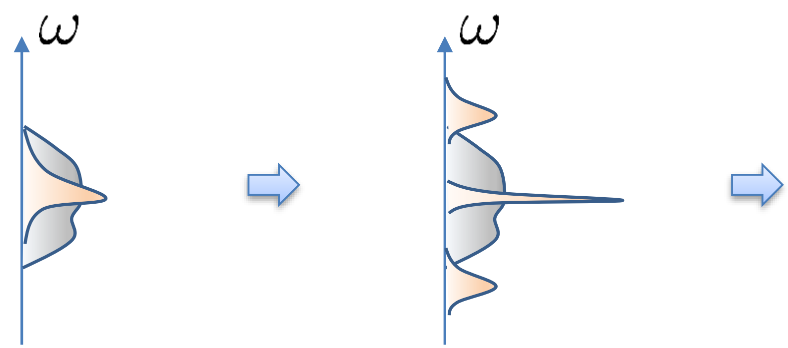
$\sim G^{\mathrm{DMFT}}_{\omega \boldsymbol{k}}$

"residual interactions"

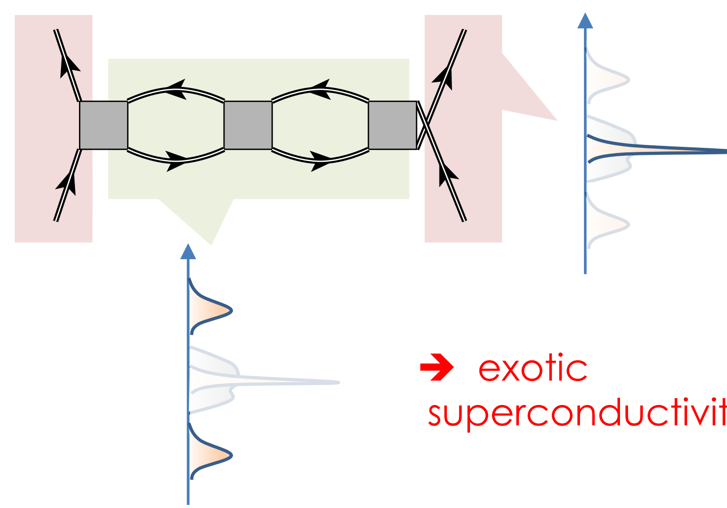


$\gamma_{\omega,\omega';\nu}$

Spatial correlations
itinerant



Heavy fermions
Mott insulator



➔ exotic superconductivity?

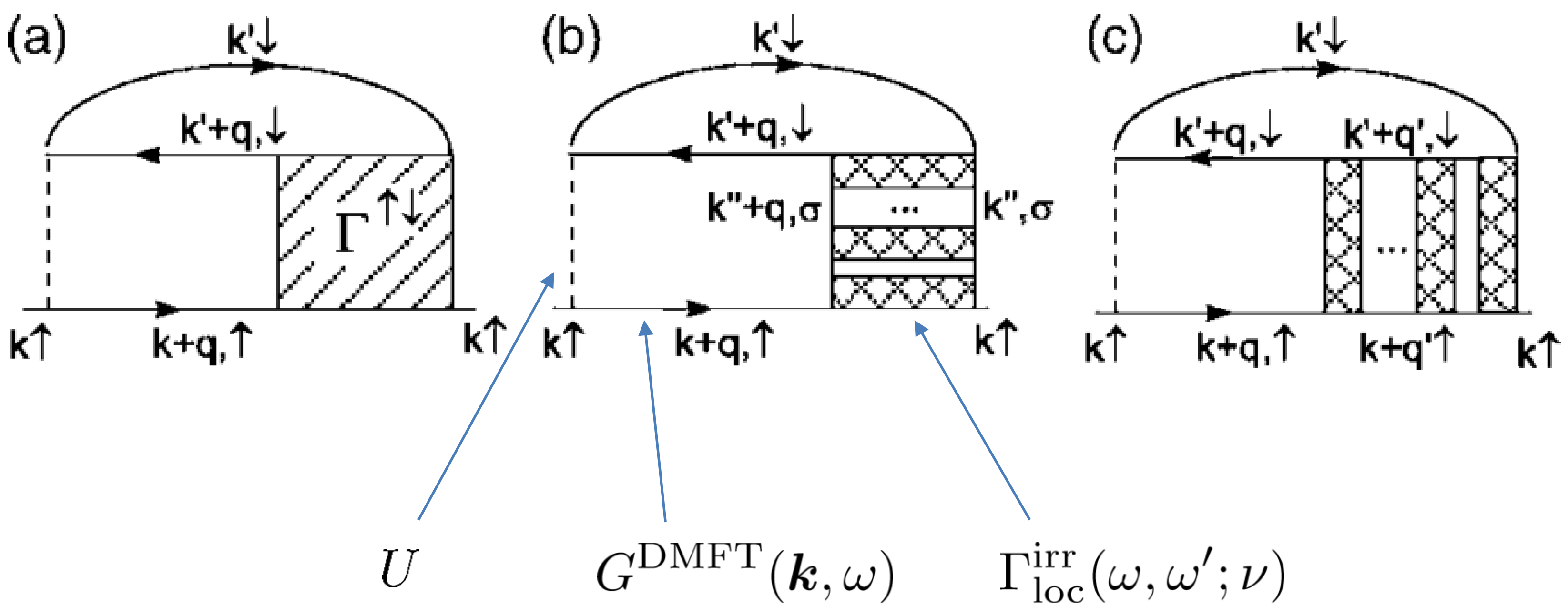
Comparison in terms of quantities used

Name	Authors	Input to effective lattice	Input to effective impurity
DΓA	Kusunose 2006 Toschi et al. 2007	G, U, Γ	μ, U, Δ(ω)
Dual fermion	Rubstov et al. 2008	G, Γ	μ, U, Δ(ω)
DMF^{2}RG	Taranto et al. 2014	G, U	μ, U, Δ(ω)
FLEX+DMFT	Kitatani et al. 2015	G, U	μ, U, Δ(ω)
TRILEX	Ayral, Parcollet 2015	G, U, Λ	μ, U, Δ(ω), U(ω), J(ω)

Dynamical vertex approximation (DΓA)

Kusunose 2006
Tosch et al. 2007

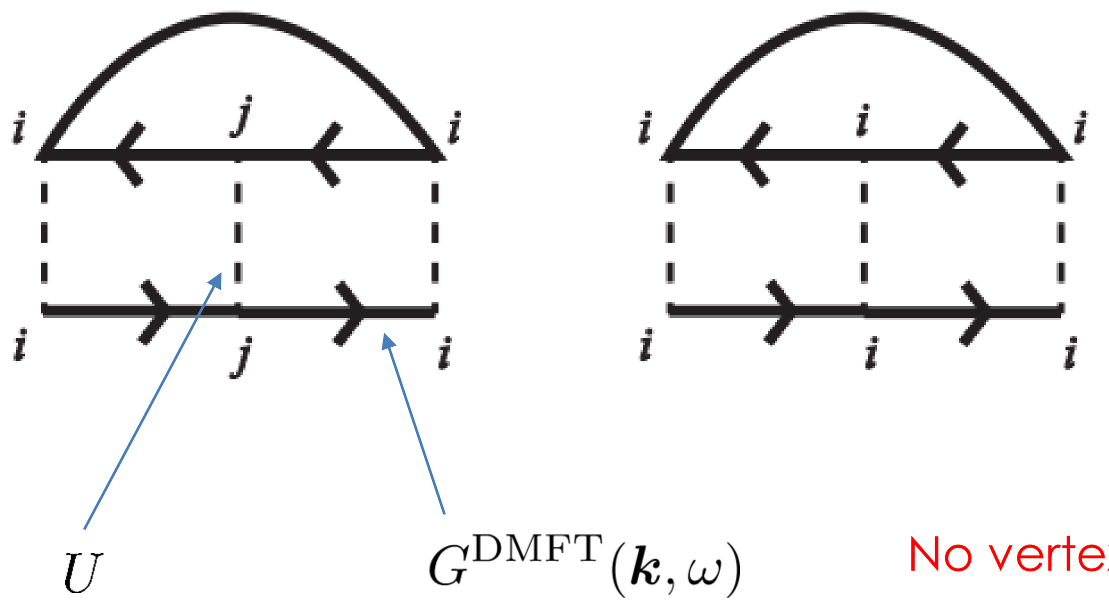
$$\Sigma(\omega, \boldsymbol{k})$$



FLEX+DMFT

Kitatani, Tsuji, Aoki 2015

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

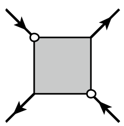


No vertex used

Dual fermion approach

Rubtsov, Katsnelson, Lichtenstein 2008
Hafermann et al. 2009

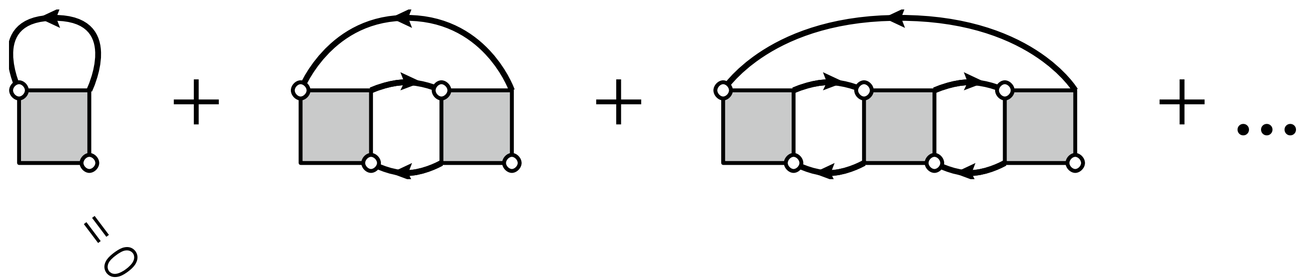
$= \widetilde{G}^{0}_{\omega\boldsymbol{k}} \equiv G^{\mathrm{DMFT}}_{\omega\boldsymbol{k}} - g_{\omega}$



$= \gamma_{\omega,\omega';\nu}$ (full vertex)

No bare interaction enters

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

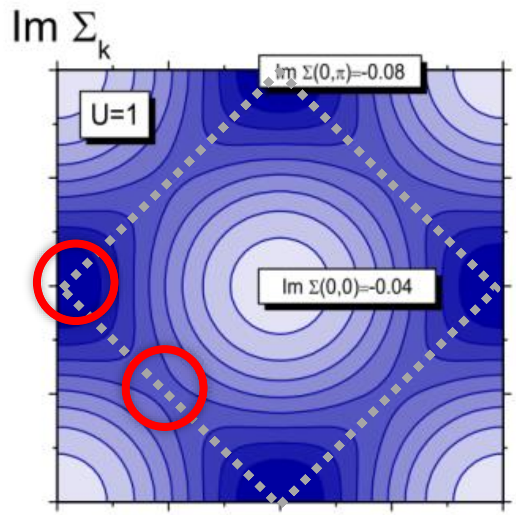


Example: Self-energy

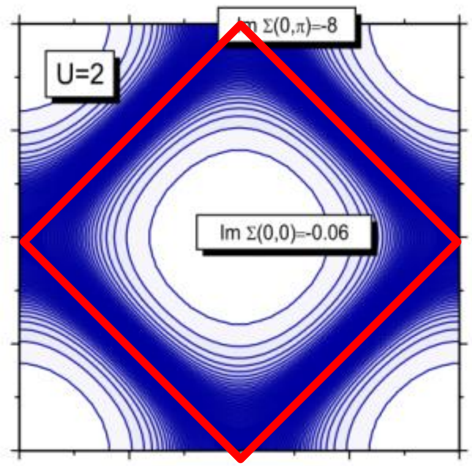
Rubtsov, Katsnelson, Lichtenstein 2008

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

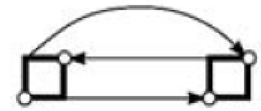
U/t=4 (metal)



U/t=8 (Mott Ins.)



n=1, T/t=0.2

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

k-dependent
renormalization

Energy gap
on the Fermi level

cf. Mott gap in DMFT

$$\mathrm{Im}\Sigma^{\mathrm{DMFT}}(\omega) \sim -\delta(\omega)$$

Fermi-surface structure + Strong local correlations

Applications and development of DF approach

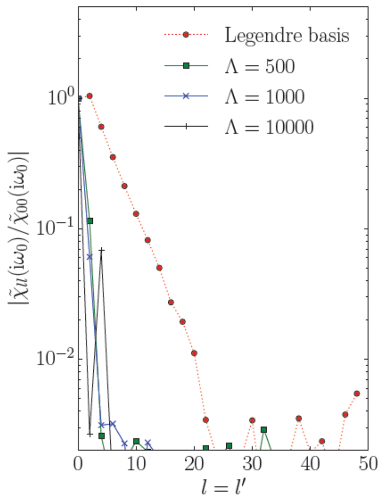
- Dual fermion + Ladder approximation
  - Hafermann et al. 2009, Paramagnon spectra
  - Li 2013, Kondo lattice
  - Antipov et al. 2014, Falikov-Kimball model
  - JO et al. 2014, Superconductivity in Hubbard model
  - JO 2015, Superconductivity in Kondo lattice
  - Tanaka, next talk
  - Takemori et al., Quasiperiodic lattice (2nd order)
- DΓA

実用上の課題

バーテックスをどうやって計算するか、どうやって近似するか

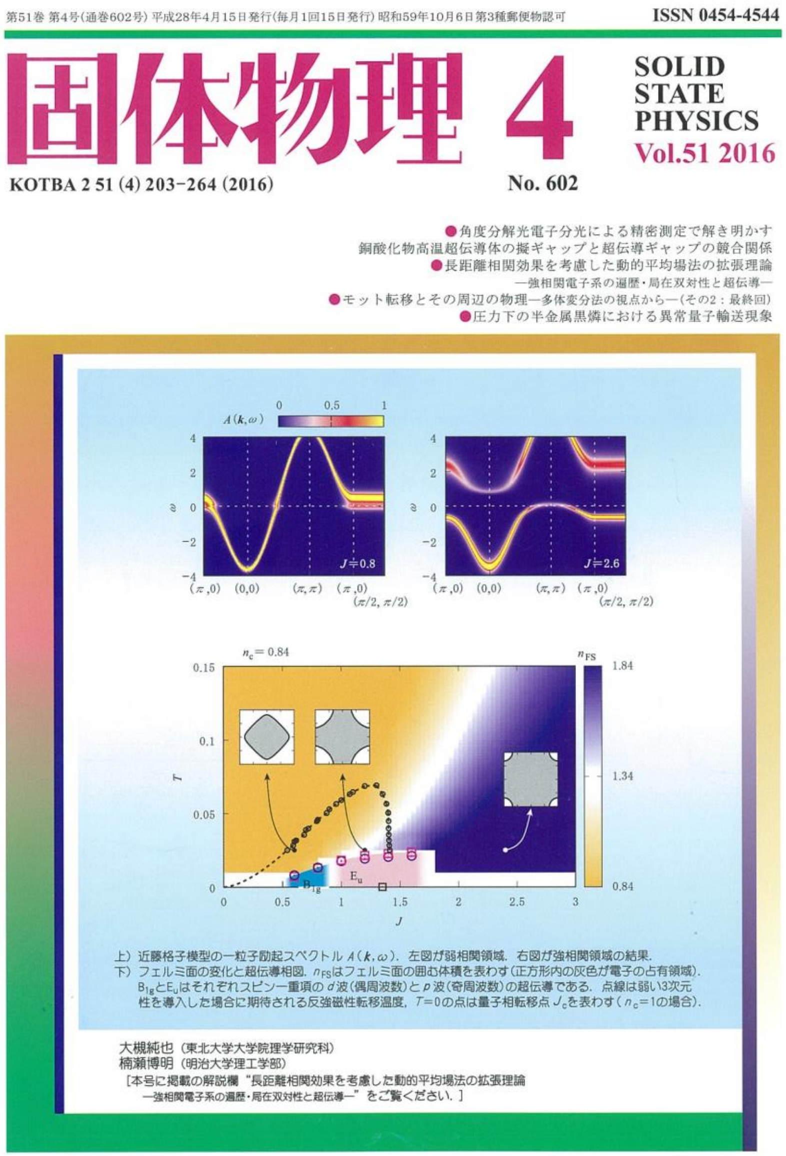
$$\gamma(i\omega, i\omega'; i\nu)$$

- 重要な要素のみ残す。ω=ω', ω+ω=ν
- Intermediate representation bw iω and ω
  Shinaoka et al., arXiv:1702.03054



$$\Gamma(i\omega, \boldsymbol{k}, i\omega', \boldsymbol{k}'; i\nu, \boldsymbol{q})$$

- diagrammatic Monte Carlo, Iskakov et al. 2016
- Parquet equation, Li et al. 2016
- fRG, Taranto et al. 2014



長距離相関効果を考慮した動的平均場法の拡張理論　—強相関電子系の遍歴・局在双対性と超伝導—

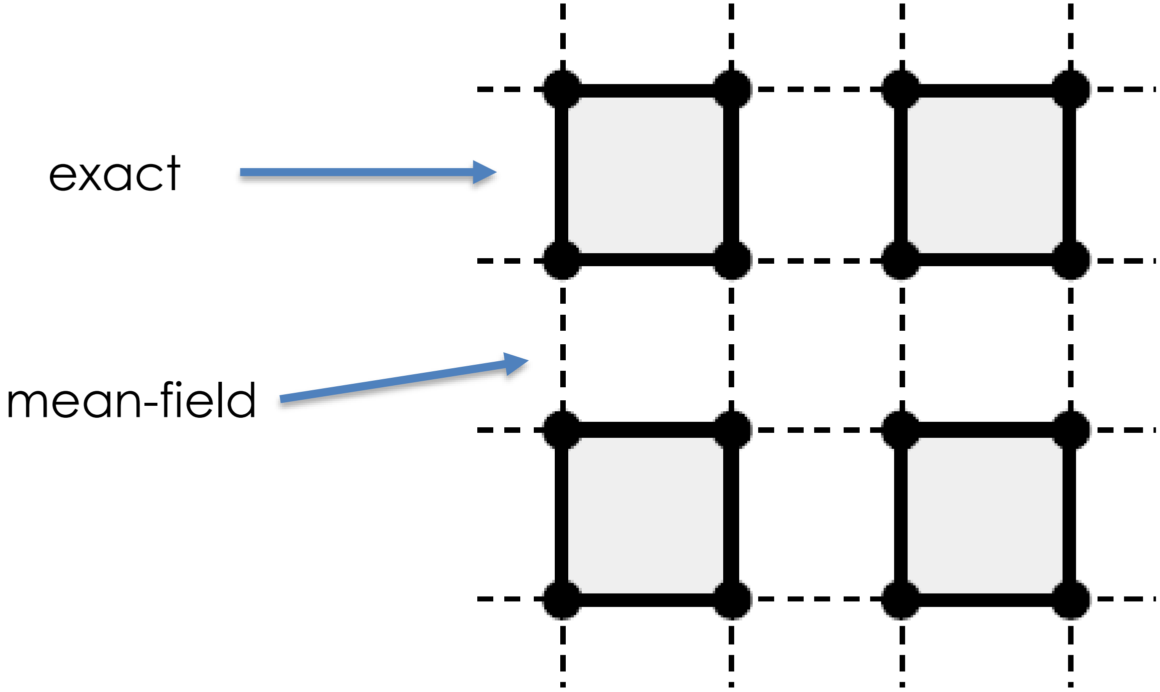
大槻純也、楠瀬博明

available online

デュアルフェルミオン法を数式なしで解説

Non-local interactions

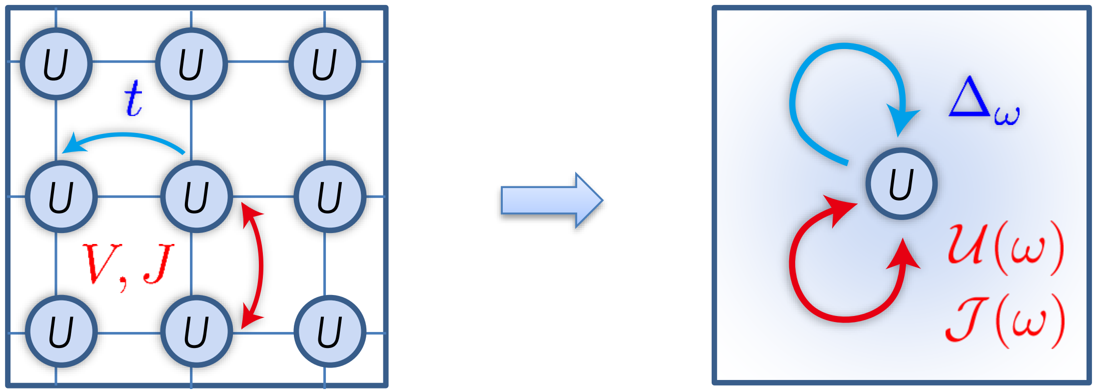
Non-local interactions in cluster DMFT



Non-local interactions in DMFT beyond MF

$$H = \sum_{ij} t_{ij} c_i^\dagger c_j + \sum_i H_{\mathrm{loc}}(i) + \sum_{ij} V_{ij} n_i n_j + \sum_{ij} J_{ij} \boldsymbol{S}_i \cdot \boldsymbol{S}_j$$

decoupling with auxiliary bosons
→ bosonic DMFT



Retarded interactions

CT-QMC:
Werner, Millis 2007, 2011
JO 2013, Steiner, Nomura, Werner, 2015

Extended DMFT in several contexts

- 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

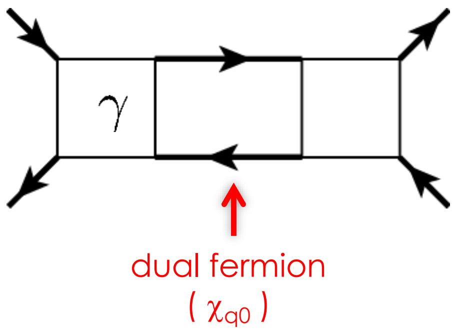
- For electrons systems...
  - Random coupling model
    Parcollet, Georges 1999, JO, Vollhardt 2013
  - Non-random coupling model (Extended-DMFT)
    Smith, Si 2000, Haule et al. 2002,
    Sun, Kotliar 2002 GW+extendedDMFT

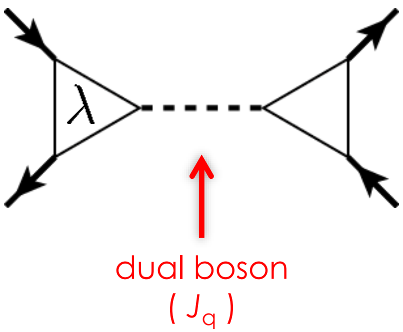
dual boson

$$H = \sum_{ij} t_{ij} c_i^\dagger c_j + \sum_i H_{\rm loc}(i) + \sum_{ij} V_{ij} n_i n_j + \sum_{ij} J_{ij} \boldsymbol{S}_i \cdot \boldsymbol{S}_j$$

decoupling → dual fermion

decoupling → dual boson





treats χ_{q0} and J_q on equal footing

Perturbation theory around (E-)DMFT solution

Comparison in terms of quantities used

Name	Authors	Input to effective lattice	Input to effective impurity
Dual boson w/ dual fermion	Rubtsov et al. 2012	G, Γ; D, Λ	μ, U, $\Delta(\omega)$; $U(\omega)$, $J(\omega)$
DMFT + GW	Sun, Kotliar 2002 Biermann et al. 2003	G, U; V, J	μ, U, $\Delta(\omega)$
TRILEX	Ayral, Parcollet 2015	G, U; Λ	μ, U, $\Delta(\omega)$; $U(\omega)$

まとめ

i. Cluster extensions

- short-range correlations
- key: finite-size effect, sign problem

ii. Diagrammatic extensions

- long-range correlations
- key: local vertex calculations, cross-channel fluctuations

iii. Non-local interactions

- treating χ_0 and V, J on equal footing
- key: retarded interaction, electron-phonon-like diagrams