COLLÈGE DE FRANCE
1530

CIFAR
CANADIAN INSTITUTE for ADVANCED RESEARCH

Lecture 4: Generalizations of Dynamical-Mean Field Theory and Improved Solvers

André-Marie Tremblay

UNIVERSITÉ DE SHERBROOKE

Collège de France, 30 mars 2015
17h00 à 18h30

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Outline

- Quantum cluster methods
  - Cluster Perturbation Theory
  - Self-energy functional
    - Variational cluster approximation
    - Cellular (cluster) Dynamical Mean-Field Theory
  - Dynamical Cluster Approximation
- Remark on other materials
  - Organics
  - Heavy fermions

Outline (continued)

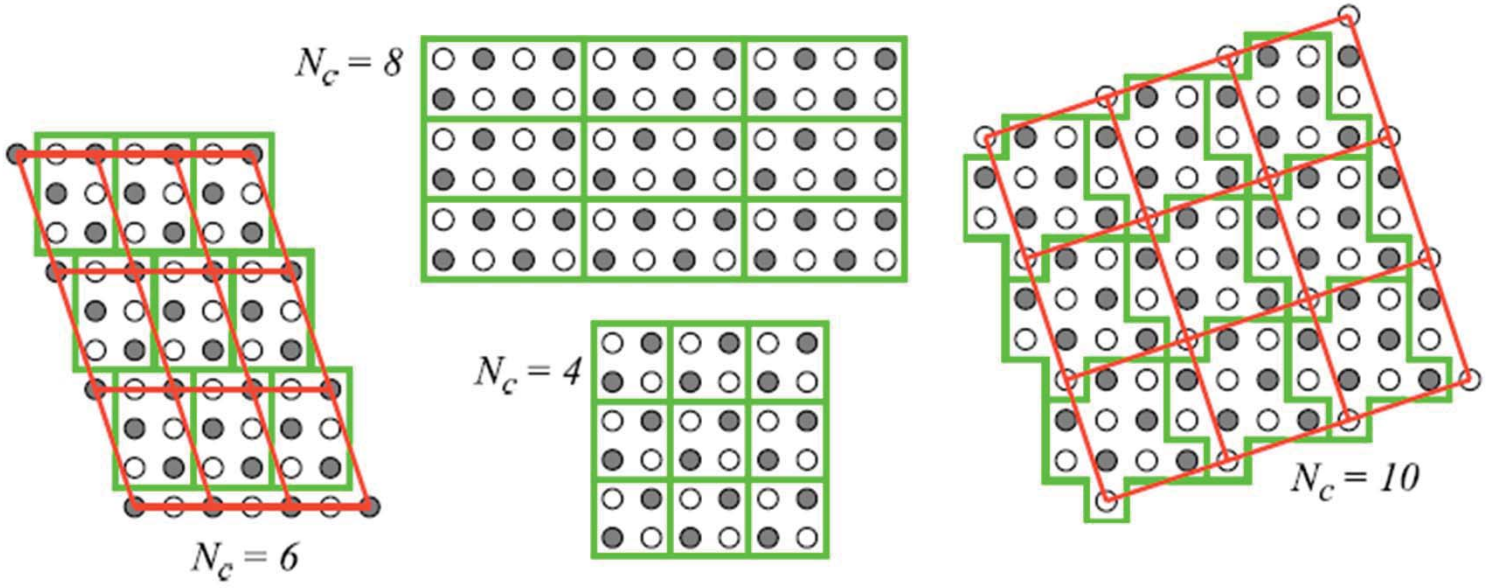
- Extensions: dual fermions
- Impurity solvers
  - Exact diagonalization
  - Quantum Monte Carlo
    - 3 improvements
- Maximum entropy analytic continuation
- Formal considerations with self-energy functional

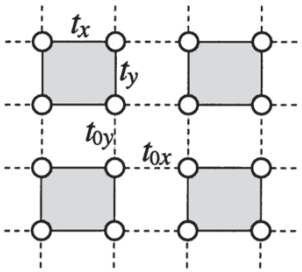
Some references

- Reviews
  - Maier, Jarrell et al., RMP. (2005)
  - Kotliar *et al.* RMP (2006)
  - A.-M.S. Tremblay, B. Kyung and D. Sénéchal Low Temperature Physics **32,** 424 (2006) (arXiv:cond-mat/0511334)

Cluster Perturbation Theory

Partitioning the infinite system





Perturbation theory in hopping (Hubbard I)

μ,ν Within cluster

$$t_{\mu\nu}^{mn} = t_{\mu\nu}^{(c)}\delta_{mn} + V_{\mu\nu}^{mn}$$

$$\left[\hat{G}^{-1}(\tilde{\mathbf{k}}, z)\right]_{\mu\nu} = \left[\hat{G}^{(c)-1}(z) - \hat{V}(\tilde{\mathbf{k}})\right]_{\mu\nu}$$

$$\hat{G}^{(c)-1}(z) = z + \mu - \hat{t}^{(c)} - \hat{\Sigma}^{(c)}$$

$$\hat{G}^{(0)-1}(\tilde{\mathbf{k}}, z) = z + \mu - \hat{t}^{(c)} - \hat{V}(\tilde{\mathbf{k}})$$

$$\hat{G}^{-1}(\tilde{\mathbf{k}}, z) = \hat{G}^{(0)-1}(\tilde{\mathbf{k}}, z) - \hat{\Sigma}^{(c)}(z)$$

Exact $t = 0$ and $U = 0$

C. Gros and R. Valenti, PRB 48, 418 (1993).
D. Sénéchal, D. Perez and M. Pioro-Ladriere, PRL **84**, 522 (2000).

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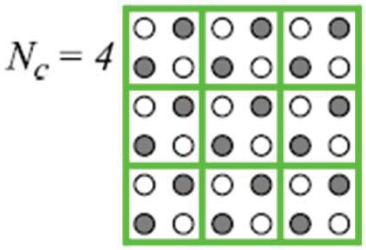
Periodization



$$\mathbf{k} = \tilde{\mathbf{k}} + \mathbf{K}$$

Four values of $\mathbf{K}$

$\tilde{\mathbf{k}}$ Runs over ¼ of the Brillouin zone

All the information is in $G\left(\tilde{\mathbf{k}}+\mathbf{K}, \tilde{\mathbf{k}}+\mathbf{K}'; i\omega_n\right)$

$$n = T\sum_n \sum_{\tilde{\mathbf{k}},\mathbf{K}} G\left(\tilde{\mathbf{k}}+\mathbf{K}, \tilde{\mathbf{k}}+\mathbf{K}; i\omega_n\right)$$

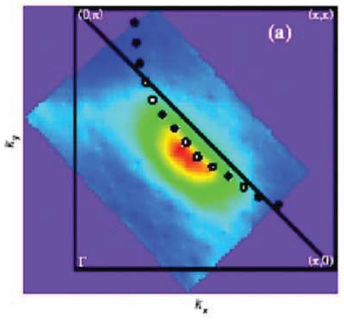
Periodization:

$$G\left(\tilde{\mathbf{k}}+\mathbf{K}, \tilde{\mathbf{k}}+\mathbf{K}'; i\omega_n\right) \rightarrow G\left(\tilde{\mathbf{k}}+\mathbf{K}, \tilde{\mathbf{k}}+\mathbf{K}; i\omega_n\right) \equiv G(\mathbf{k}; i\omega_n)$$

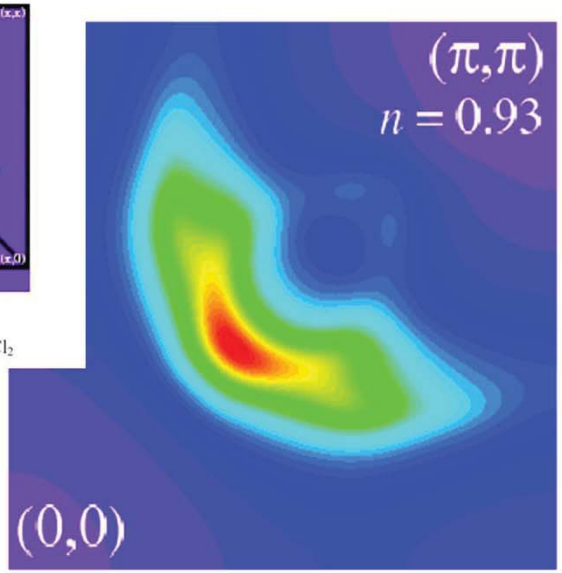
Fermi surface plots, $U = 8t$, $L = 8$

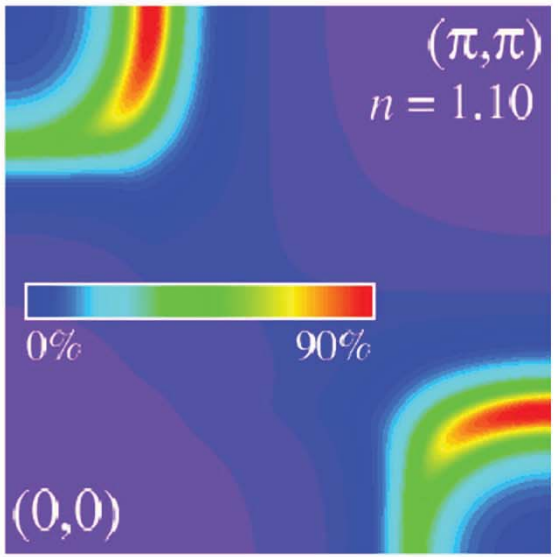
MDC at the Fermi energy

Hole-doped, 10%



F. Ronning et al. Jan. 2002, $Ca_{2-x}Na_xCuO_2Cl_2$





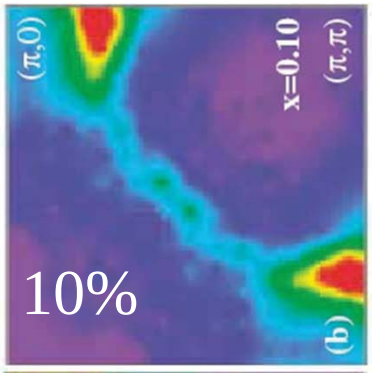


FIG. 3: Intensity plot of the spectral function at the Ferr
level, in the first quadrant of the Brillouin zone, for $U = 8t$ c
a $L = 8$ cluster. Left: Hole-doped system ($n = 0.93$). Righ
Electron-doped systems ($n = 1.10$). A Lorentzian broadenir
of $0.2t$ is used.

Wave-particle

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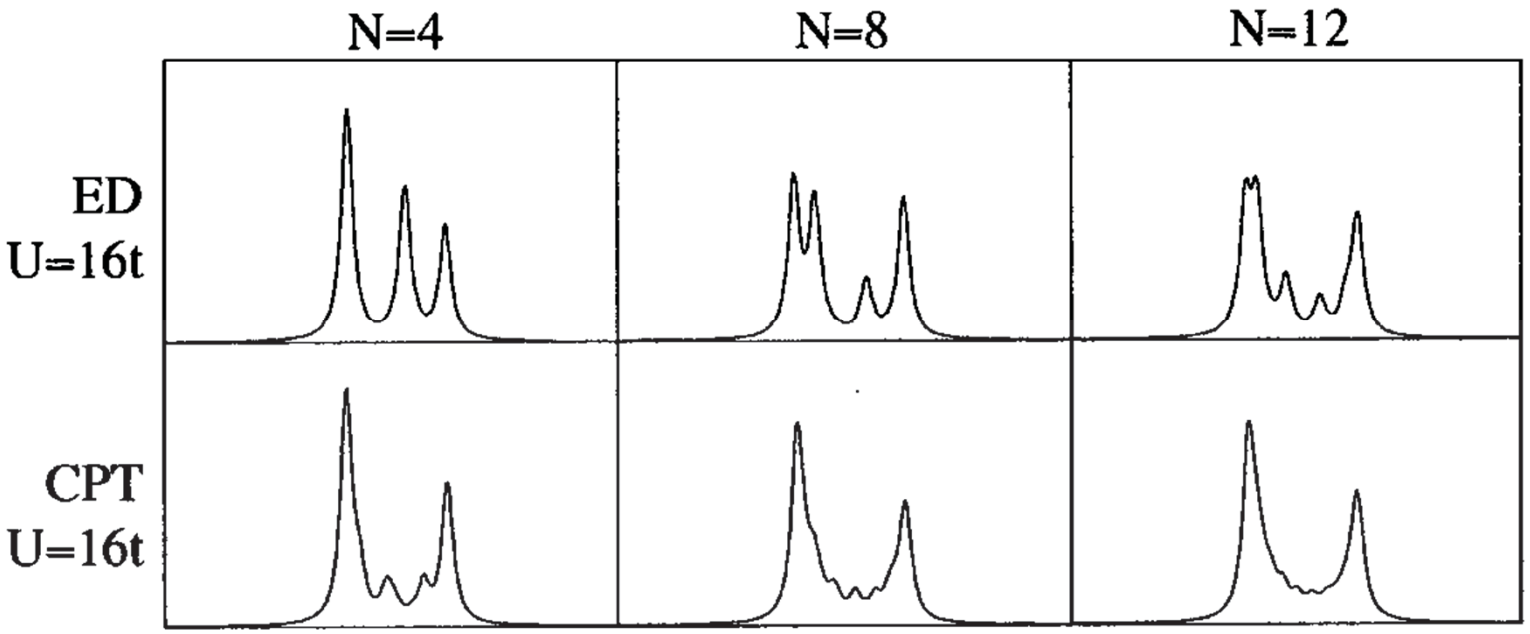
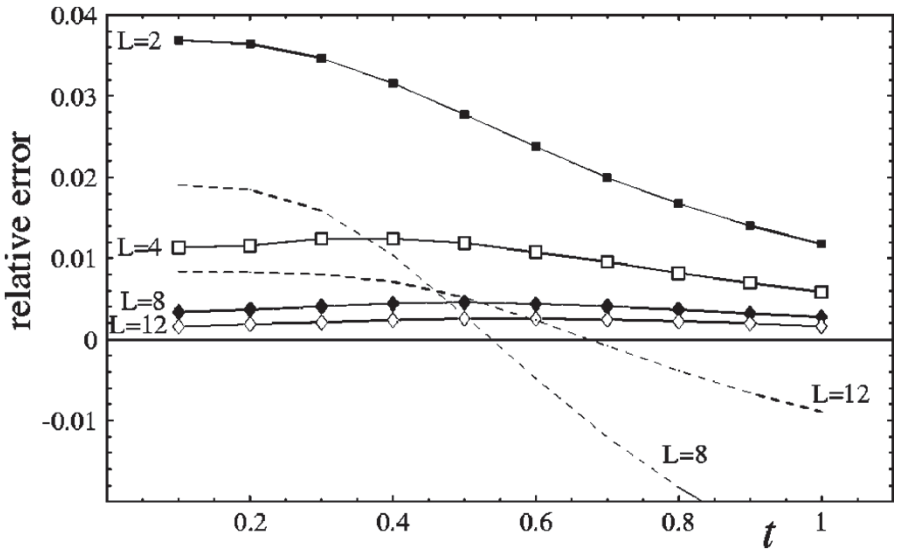
Cluster Perturbation Theory

Benchmarks

1d Hubbard





$U = 2$ vs Bethe ansatz

Sénéchal et al. PRL **84**, 522 (2000)
Sénéchal et al. PRB **66**, 075129 (2002)

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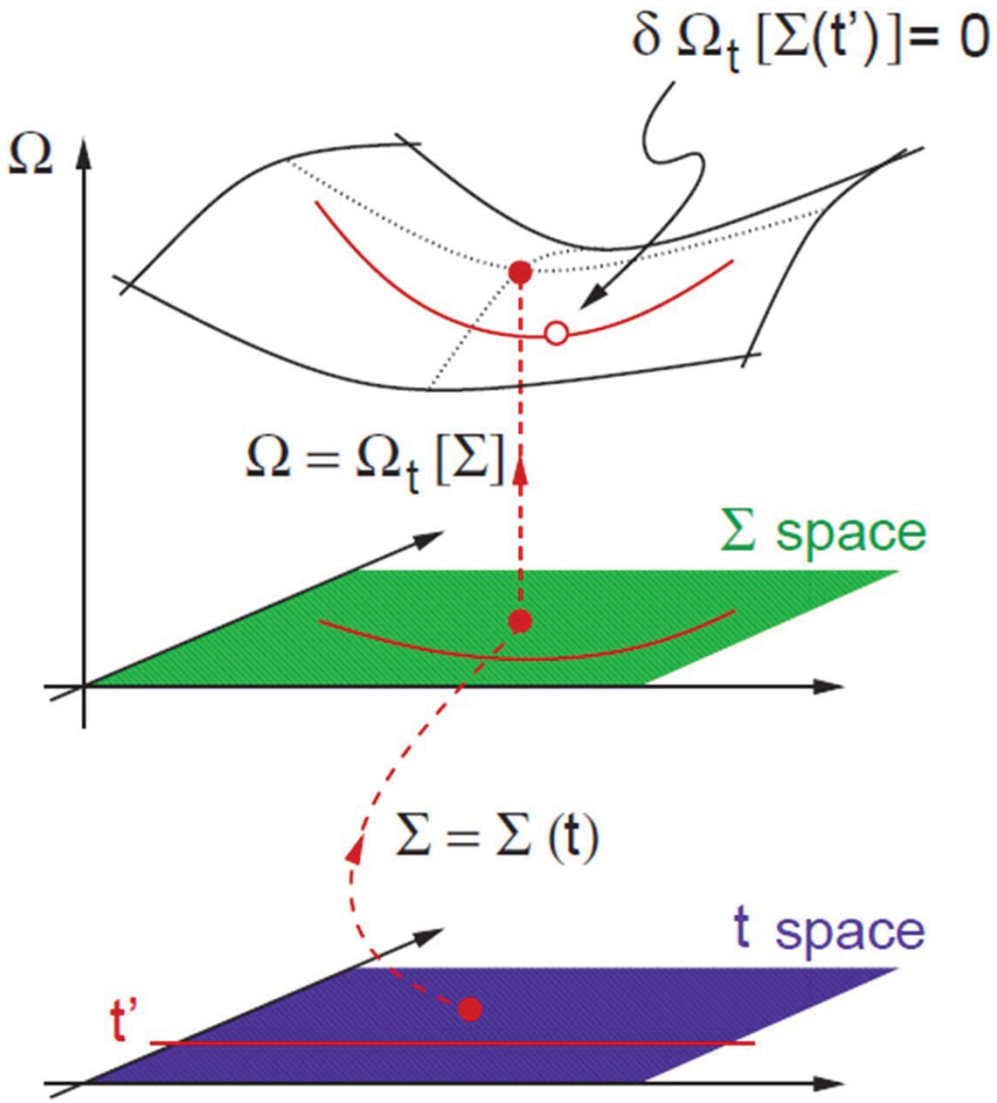
Self-energy functional

DMFT as a stationnary point



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Three diferent types of approximations

I. Approximate the Euler equations

II. Approximate the functional (finite set of diagrams or other method, analogy to DFT)

III. Take and the exact functional but for a limited set of possible functions (G, Σ...)

SFT : Self-energy Functional Theory

With $F[\Sigma]$ Legendre transform of Luttinger-Ward funct.

$$\Omega_{\mathbf{t}}[\Sigma] = F[\Sigma] + \mathrm{Tr}\ln(-(G_0^{-1} - \Sigma)^{-1})$$

is stationary with respect to Σ and equal to grand potential there.

$$\Omega_{\mathbf{t}}[\Sigma] = \Omega_{\mathbf{t}'}[\Sigma] - \mathrm{Tr}\ln(-(G_0'^{-1} - \Sigma)^{-1}) + \mathrm{Tr}\ln(-(G_0^{-1} - \Sigma)^{-1}).$$

Vary with respect to parameters of the cluster (including Weiss fields)

Variation of the self-energy, through parameters in H_0(**t'**)

M. Potthoff, Eur. Phys. J. B 32, 429 (2003).

Variational Cluster Approximation (Variational Cluster Perturbation Theory)

M. Potthoff, M. Aichhorn, and C. Dahnken
Phys. Rev. Lett. 91, 206402 (2003)

C. Dahnken, M. Aichhorn, W. Hanke, E. Arrigoni, and M. Potthoff
Phys. Rev. B **70**, 245110 (2004)

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Adding and subtracting Weiss fields

No mean-field factorization of interaction

$$H_0^{(\mathrm{intra})}(\mathbf{R}) \rightarrow H_0^{(\mathrm{intra})}(\mathbf{R}) + \Delta(\mathbf{R}),$$

$$H_0^{(\mathrm{inter})}(\mathbf{R},\mathbf{R}') \rightarrow H_0^{(\mathrm{inter})}(\mathbf{R},\mathbf{R}') - \delta_{\mathbf{R},\mathbf{R}'}\Delta(\mathbf{R})$$

$$\Delta(\mathbf{R}) = \sum_{a,b} \Delta_{a,b} c^{\dagger}_{\mathbf{R}a} c_{\mathbf{R}b}$$

e.g. antiferromagnétisme alternating field proportional to *h*

In the presence of interactions result depends on *h*: optimize

$$\Omega_{\mathbf{t}}(\mathbf{t}') = \Omega' - \int_C \frac{d\omega}{2\pi} \sum_{\mathbf{K}} \ln \det[1 + (G_0^{-1} - G_0'^{-1})G'],$$

VCA, consistency checks

D. Sénéchal, P. Sahebsara PRL **100,** 136402 (2008)

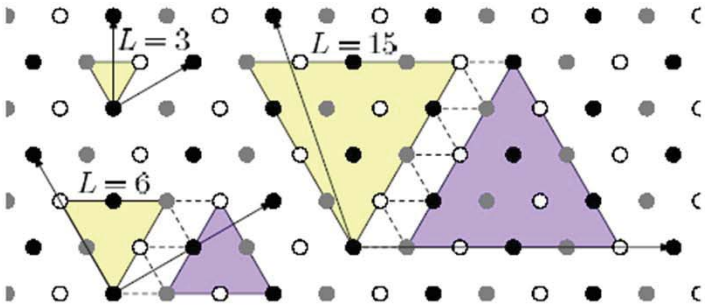

FIG. 1 (color online). clusters used in our study. The 6-site and 15-site clusters tile the lattice only when paired with identical, inverted clusters. Superlattice basis vectors are shown.

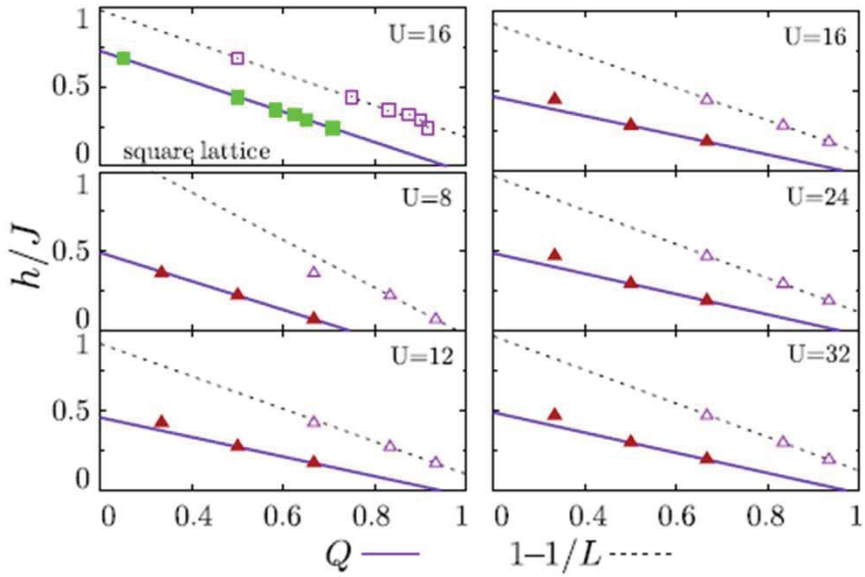

FIG. 4 (color online). Scaled Weiss field as a function of Q (solid lines) and $1 - 1/L$ (dashed lines) for various values of U. The data are obtained for 3-, 6-, and 15-sites triangular clusters. Top left panel: square-lattice results at $U = 16$ for the Néel Weiss field, with $L = 2$, 4, 8, 10, 12, and 16 sites.

Q = # of sites in cluster
/ # of sites/unit cell in infinite cluster

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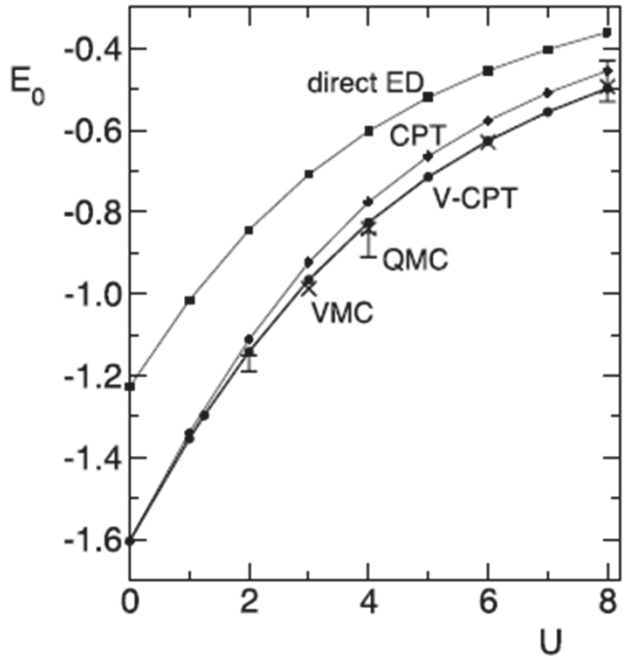
Ground state energy, $n = 1$, 2-d Hubbard



C. Dahnken, M. Aichhorn, W. Hanke, E. Arrigoni, and M. Potthoff
Phys. Rev. B **70**, 245110 (2004)

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Cellular Dynamical Mean-Field Theory
CDMFT

Gabriel Kotliar, Sergej Y. Savrasov, Gunnar Pálsson, and Giulio Biroli
Phys. Rev. Lett. 87, 186401 (2001)

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Methods of derivation for DMFT

- Cavity method
- Local nature of perturbation theory in infinite dimensions
- Expansion around the atomic limit
- Effective medium theory
- Local approximation for Luttinger Ward
- Potthoff self-energy functional

M. Potthoff, Eur. Phys. J. B **32**, 429 (2003).
A. Georges *et al.*, Rev. Mod. Phys. **68**, 13 (1996).

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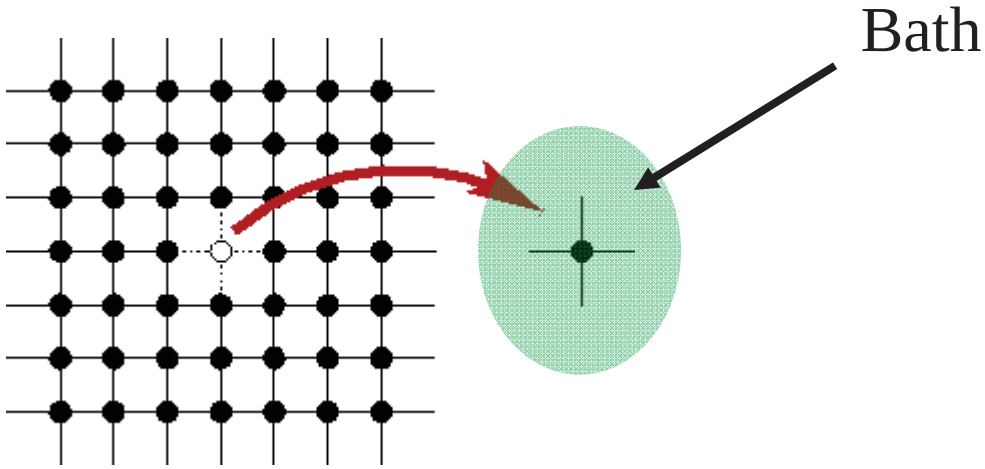
Mott transition and Dynamical Mean-Field Theory. The beginnings in *d = infinity*

- Compute scattering rate (self-energy) of impurity problem.
- Use that self-energy (ω dependent) for lattice.
- Project lattice on single-site and adjust bath so that single-site DOS obtained both ways be equal.



W. Metzner and D. Vollhardt, PRL (1989)
A. Georges and G. Kotliar, PRB (1992)
M. Jarrell PRB (1992)

DMFT, (*d = 3*)

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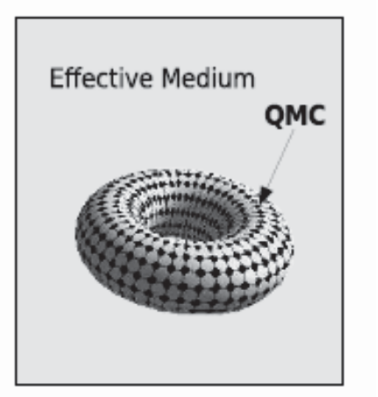
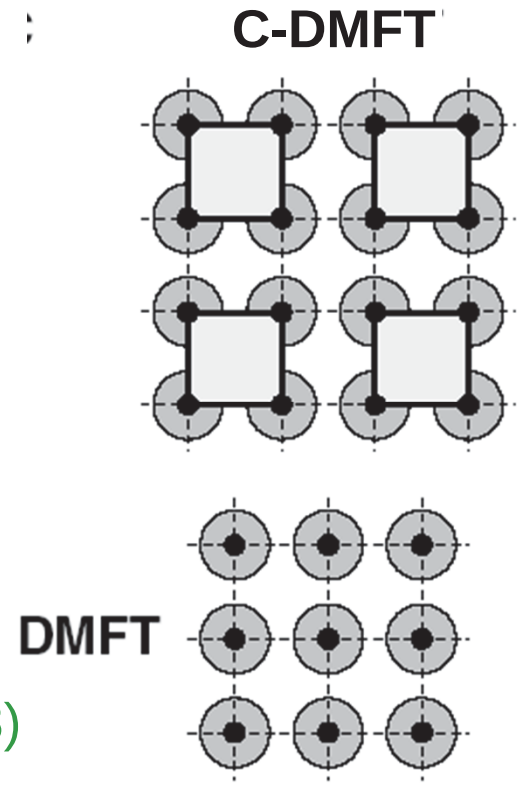
2d Hubbard: Quantum cluster method



DCA



Hettler …Jarrell…Krishnamurty PRB **58** (1998)
Kotliar et al. PRL **87** (2001)
M. Potthoff *et al.* PRL **91,** 206402 (2003).

REVIEWS
Maier, Jarrell et al., RMP. (2005)
Kotliar *et al.* RMP (2006)
AMST *et al.* LTP (2006)

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Hybridization function

$$\mathsf{G}^{-1}_{\text{full}}(\omega) = \frac{1}{\omega - \mathbf{T}} \qquad \mathbf{T} = \begin{pmatrix} -\mathsf{t} & \boldsymbol{\theta} \\ \boldsymbol{\theta}^{\dagger} & -\boldsymbol{\varepsilon} \end{pmatrix}$$

$$\mathsf{G}^{-1} = \omega - \mathsf{t} - \boldsymbol{\theta} \frac{1}{\omega - \boldsymbol{\varepsilon}} \boldsymbol{\theta}^{\dagger}$$

Self-consistency

$$\mathcal{G}_\sigma^{imp}(i\omega_n)^{-1} = \mathcal{G}_\sigma^{0-imp}(i\omega_n)^{-1} - \Sigma_\sigma(i\omega_n)$$

Impurity $\mathcal{G}^0$ depends on hybridization function

$$N_c \int \frac{d^d\tilde{\mathbf{k}}}{(2\pi)^d} \frac{1}{\mathcal{G}^0_{\tilde{\mathbf{k}}\sigma}(i\omega_n)^{-1} - \Sigma_\sigma(i\omega_n)} = \mathcal{G}_\sigma^{imp}(i\omega_n)$$

Modify the bath (hybridization) for the impurity
until this equality is satisfied

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Self-consistency condition

- Obtain Green's function for the « impurity » (cluster) in a bath
- Extract Σ
- Substitute Σ in lattice Green's function
- Project lattice Green's function on impurity (cluster).
- If the two Green's functions are not equal, modify the bath until they are.

+ and -

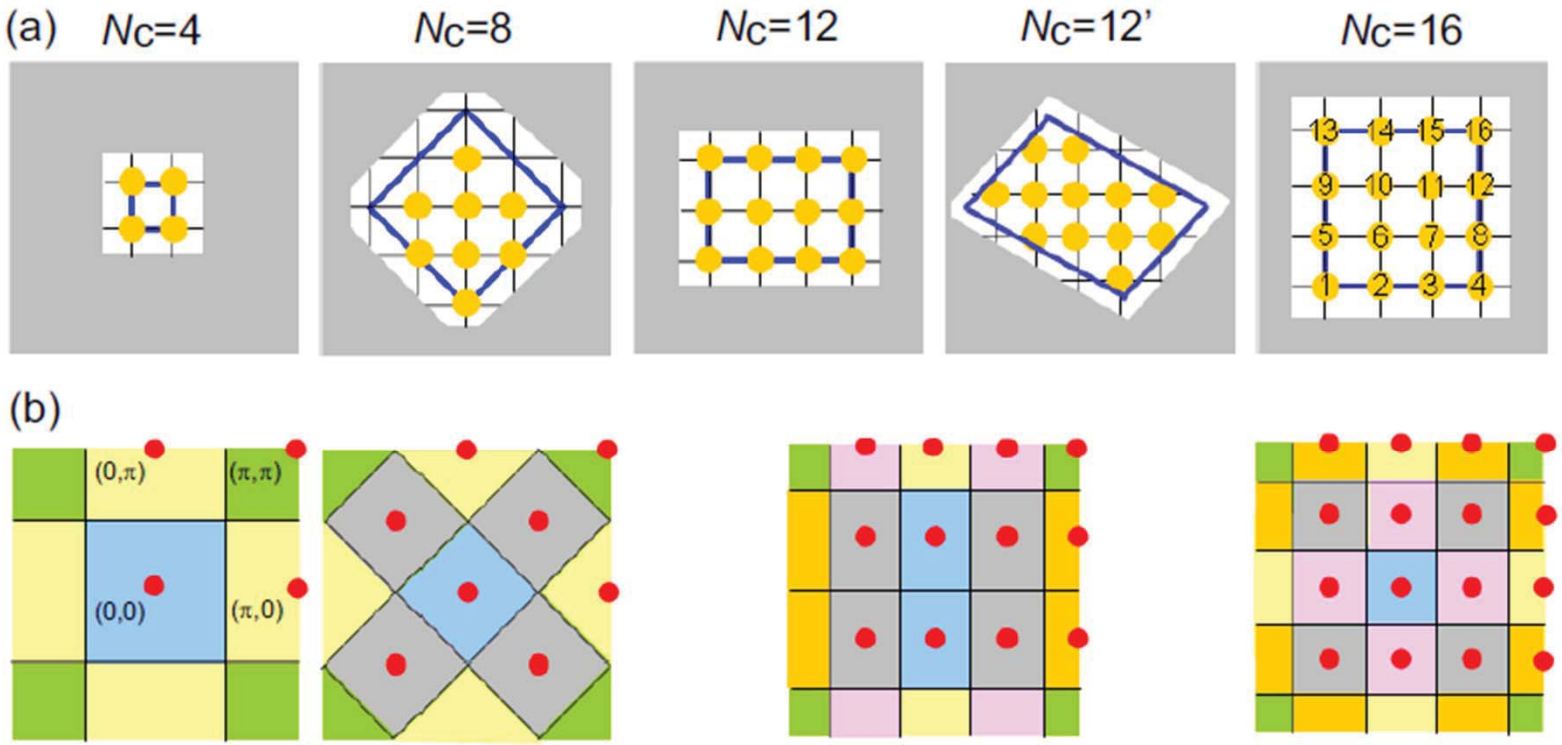
- Long range order:
  - Allow symmetry breaking in the bath (mean-field)
- Included:
  - Short-range dynamical and spatial correlations

- Missing:
  - Long wavelength p-h and p-p fluctuations

CDMFT

Benchmarks

2d Hubbard: Size dependence of CDMFT

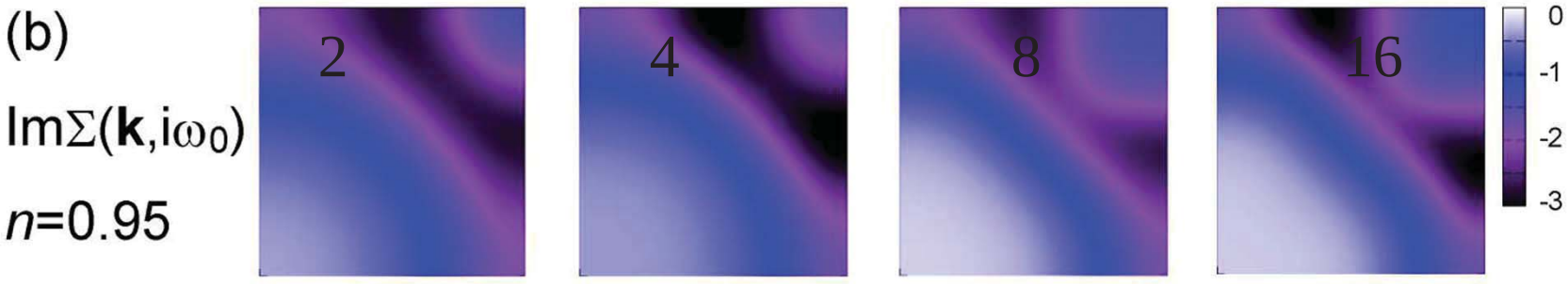


Systematic study on cluster-size dependence in the cellular dynamical mean-field theory

Shiro Sakai,[1,2] Giorgio Sangiovanni[1], Marcello Civelli[3], Yukitoshi Motome[2], Karsten Held[1], and Masatoshi Imada[2]

Sakai et al. Phys. Rev. B **85**, 035102 (2012)

Size dependence near FS



T = 0.06t, U=8t, t'=-0.2,
1%, 3%, 5% doping

Sakai et al. Phys. Rev. B **85**, 035102 (2012)

Main conclusions:

- 4 site close to 16 site
- (0,0) and (π/2, π/2) converge faster

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Their prefered periodization

M is irreducible with respect to all intersite terms in H

$$M_{\mu,\nu} = \left(\frac{1}{i\omega_n - \mu - \Sigma} \right)_{\mu,\nu}$$

$$M(\mathbf{k}) = \sum_{\mu,\nu} e^{i\left(\tilde{\mathbf{k}}+\mathbf{K}\right)\cdot(\mathbf{R}_\mu - \mathbf{R}_\nu)} M_{\mu,\nu}$$

$$G^{-1}(\mathbf{k}) = M^{-1}(\mathbf{k}) - t(\mathbf{k})$$

Periodizing the self-energy is bad! (Sénéchal)

Dynamical Cluster Approximation
DCA

M. H. Hettler, A. N. Tahvildar-Zadeh, M. Jarrell, T. Pruschke, and H. R. Krishnamurthy
Phys. Rev. B 58, R7475(R) (1998)

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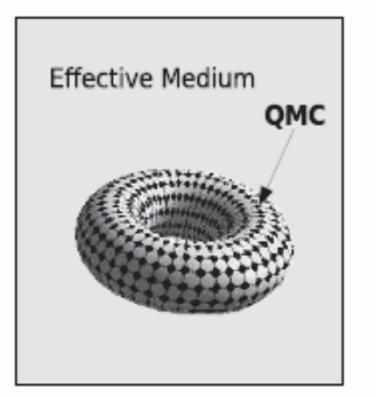
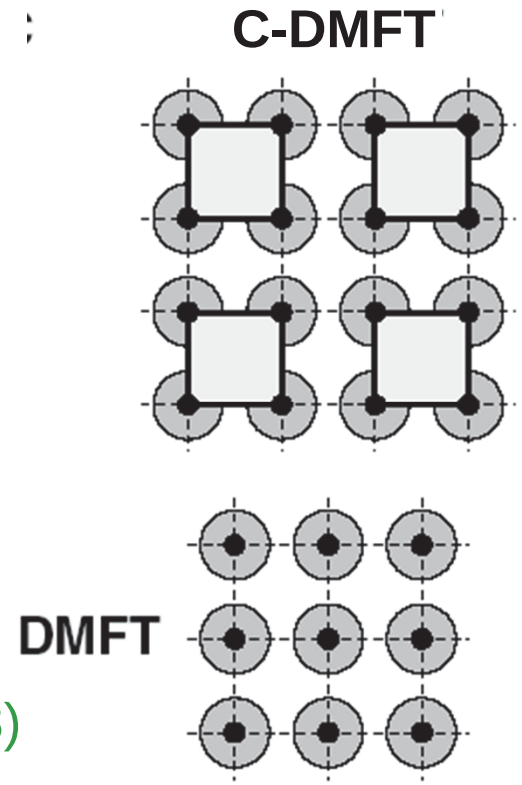
2d Hubbard: Quantum cluster method



DCA



Hettler …Jarrell…Krishnamurty PRB **58** (1998)
Kotliar et al. PRL **87** (2001)
M. Potthoff *et al.* PRL **91,** 206402 (2003).

REVIEWS
Maier, Jarrell et al., RMP. (2005)
Kotliar *et al.* RMP (2006)
AMST *et al.* LTP (2006)

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DCA

Cannot be derived from self-energy functional
Based on mapping on a translationally invariant cluster

$$t^{m,n}_{\mu,\nu} = \sum_{\tilde{\mathbf{k}},\mathbf{K}} e^{i\left(\tilde{\mathbf{k}}+\mathbf{K}\right)\cdot\left(\mathbf{r}^{m,n}+\mathbf{R}_{\mu,\nu}\right)} t\left(\tilde{\mathbf{k}}+\mathbf{K}\right)$$

$$t_{\mu,\nu}\left(\tilde{\mathbf{k}}\right) = \sum_{\mathbf{K}} e^{i\mathbf{K}\cdot\mathbf{R}_{\mu,\nu}} t\left(\tilde{\mathbf{k}}+\mathbf{K}\right); \quad \mathbf{K}\cdot\mathbf{r}^{m,n} = 0 \text{ (Modulo } 2\pi)$$

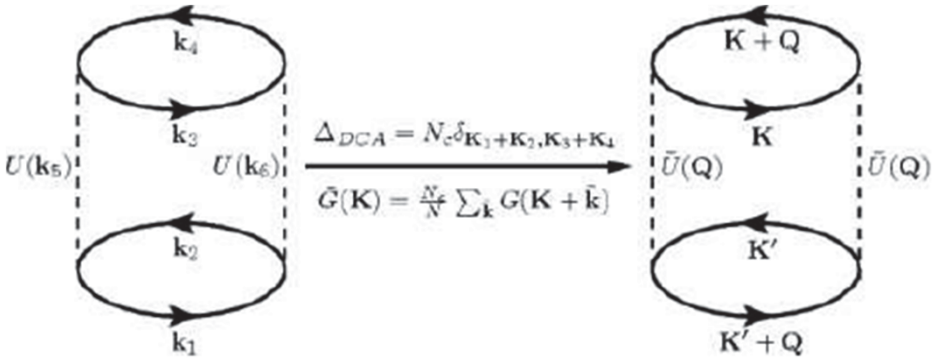
$$t^{m,n}(\mathbf{K}) = \sum_{\tilde{\mathbf{k}}} e^{i\tilde{\mathbf{k}}\cdot\left(\mathbf{r}^{m,n}+\mathbf{R}_{\mu,\nu}\right)} t\left(\tilde{\mathbf{k}}+\mathbf{K}\right)$$

$$t^{DCA}(\mathbf{K}) = \sum_{\tilde{\mathbf{k}}} e^{i\tilde{\mathbf{k}}\cdot\mathbf{R}_{\mu,\nu}} t\left(\tilde{\mathbf{k}}+\mathbf{K}\right)$$

DCA self-consistency

$$\bar{\mathbf{G}}(z) = \frac{N_c}{N} \sum_{\tilde{\mathbf{k}}} [\mathbf{G}_0^{-1}(\tilde{\mathbf{k}}, z) - \mathbf{\Sigma}_c(z)]^{-1}$$ CDMFT

$$\bar{G}(\mathbf{K}, z) = \frac{N_c}{N} \sum_{\tilde{\mathbf{k}}} [G_0^{-1}(\mathbf{K} + \tilde{\mathbf{k}}) - \Sigma_c(\mathbf{K}, z)]^{-1}$$ DCA



Matrix vs scalar

For large systems, fewer terms in DC self-consistency

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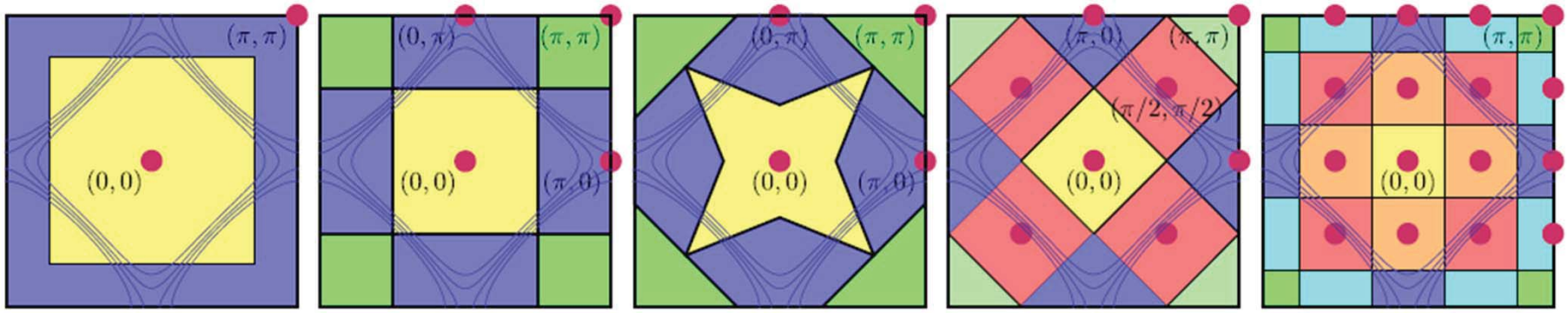
Dynamical Cluster Approximation
DCA

Benchmarks

Taking advantage of liberty in choice of patch



E. Gull, M. Ferrero, O. Parcollet, A. Georges, and A. J. Millis
Phys. Rev. B **82**, 155101 (2010)

T = 0.05t, U=7t, t'=-0.15,
Many dopings

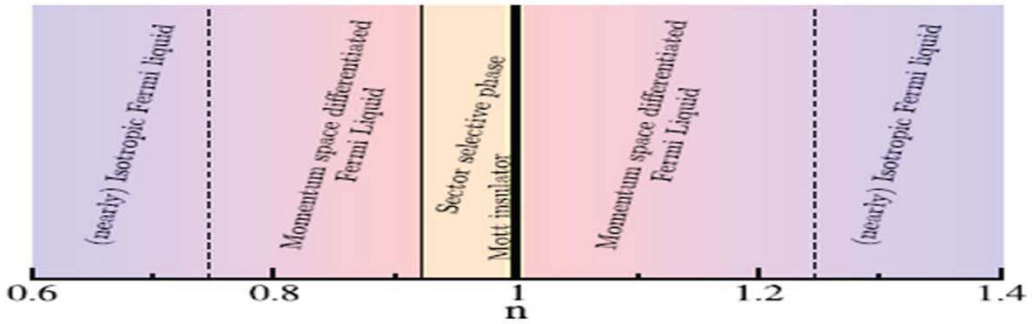


FIG. 1: Qualitative sketch of doping regimes for parameters considered in this paper.

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Comparison of DMFT, CDMFT and DCA

Annalen der Physik, 23 December 2011

Thinking locally: reflections on Dynamical Mean-Field Theory from a high-temperature/high energy perspective.

Antoine Georges[1,2] *

[1] Collège de France, 11 place Marcelin Berthelot, 75005 Paris
[2] Centre de Physique Théorique, Ecole Polytechnique, CNRS, 91128 Palaiseau Cedex, France

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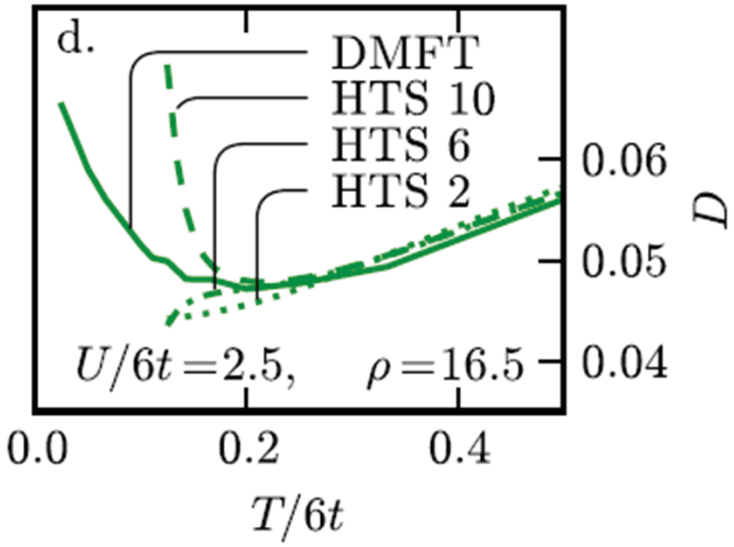
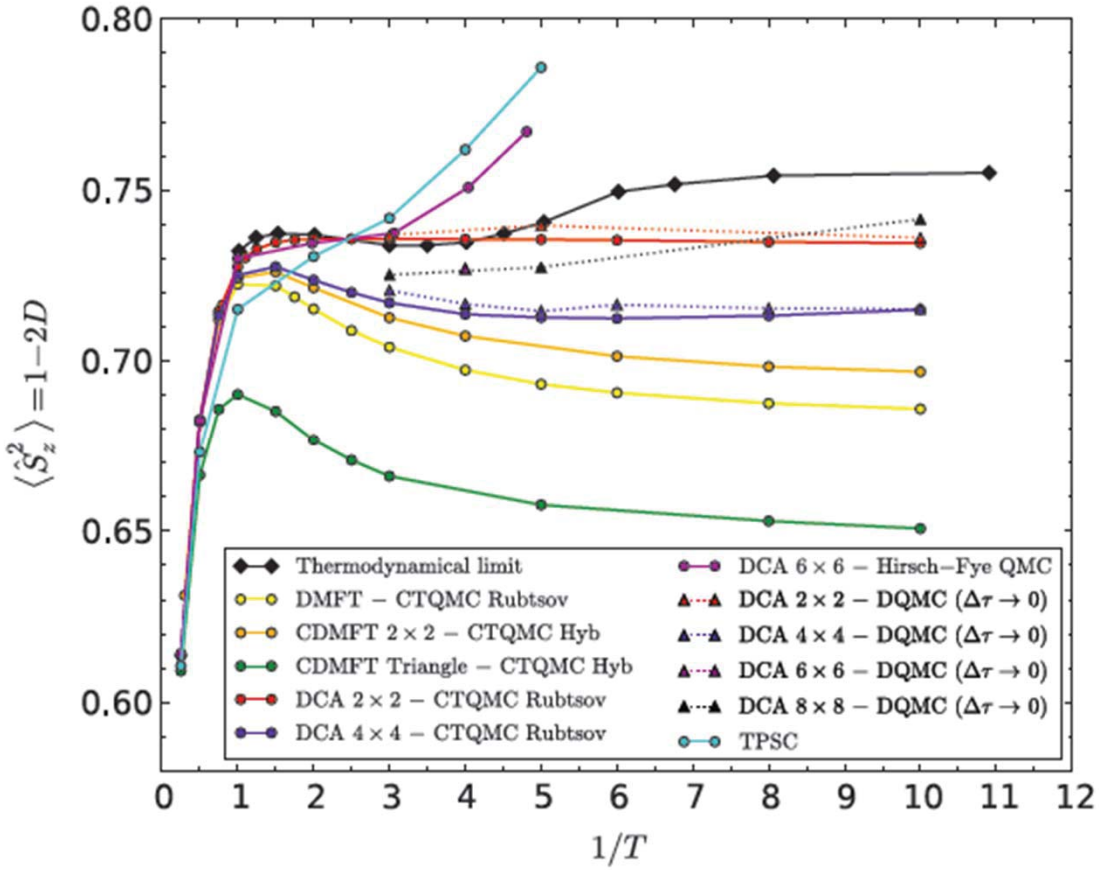
DMFT vs High temperature series: 3-d Hubbard



R. Jördens, et al. PRL **104**, 180401 (2010)

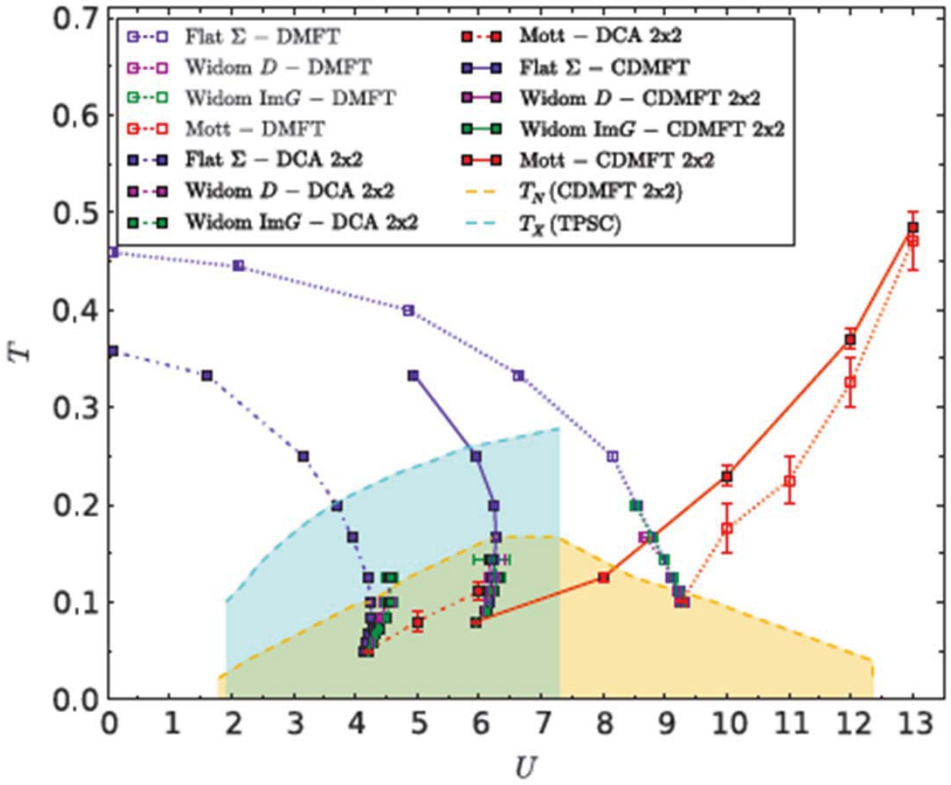
Double occupancy, square lattice various methods



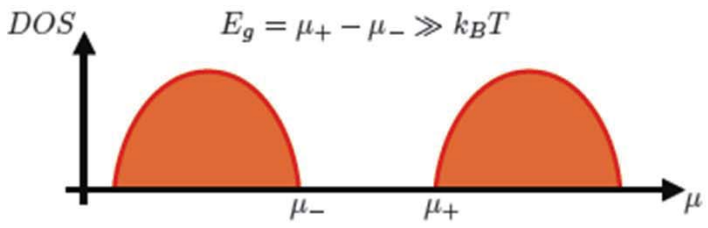
$U = 4t$

A. Reymbaut et al. unpublished

Crossovers square lattice: DCA, CDMFT, DMFT



A. Reymbaut et al. unpublished



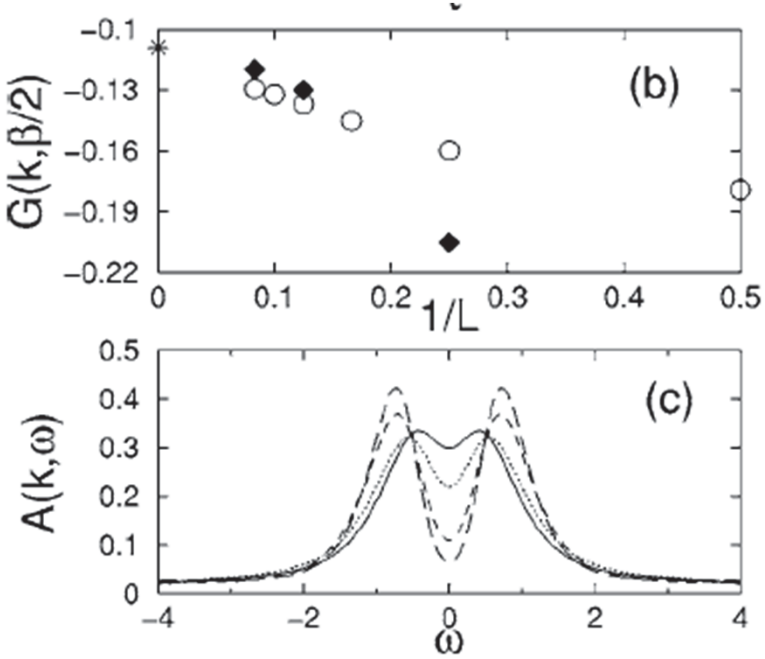
- ***Non particle-hole symmetric system :***

$$n = 1 + T\left[N(\mu_+)\, e^{\beta(\mu-\mu_+)} - N(\mu_-)\, e^{-\beta(\mu-\mu_-)}\right]$$

- ***Particle-hole symmetric system :***

$$n = 1 + 2T\, N\left(\frac{E_g}{2}\right)\, e^{-\beta\frac{E_g}{2}}\, \sinh\left(\beta\left[\mu - \frac{U}{2}\right]\right)$$

CDMFT vs DCA, 1-d Hubbard model



Kyung, Kotliar, AMST, PRB **73**, 205106 (2006)

$U = 4t$, $T = 1/5$, $n = 1$ (strong correlations)

Filled symbols from DCA. Pseudogap at $L = 8$ only

S. Moukouri, C. Huscroft, and M. Jarrell, in
Computer Simulations in Condensed Matter Physics VII,
ed. D. P. Landau et al. Springer-Verlag, Heidelberg, Berlin, 2000.

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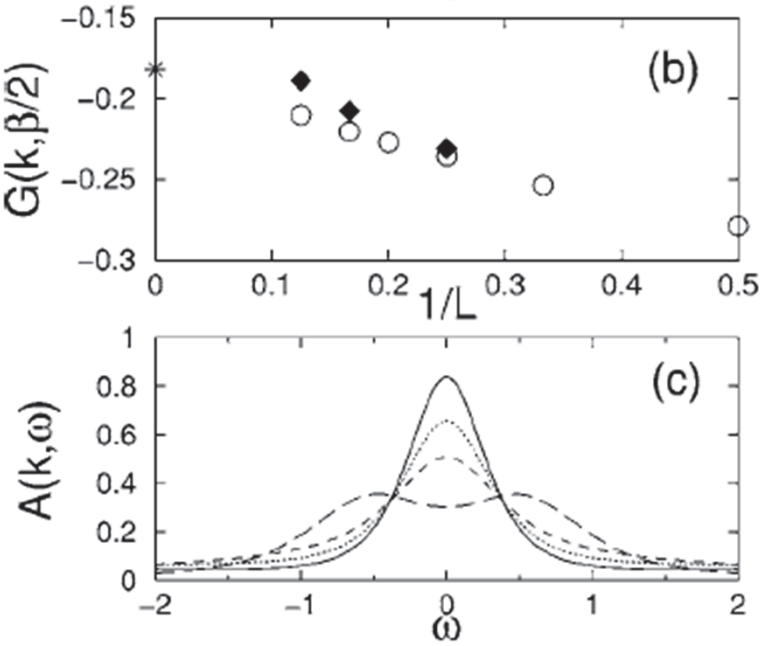
CDMFT vs DCA, 2-d Hubbard model

Pseudogap from long-wavelengths takęs large system sizes to converge

$N = L \times L$

$L = 2,3,4,6$



Kyung, Kotliar, AMST, PRB **73**, 205106 (2006)

$U = 4.4t$, $T = 1/4$, $n = 1$ (weak correlations)

Filled symbols from DCA. Pseudogap at $L = 8$ only

Jarrell et al. PRB **64**, 195130 (2001)

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Comparisons DCA-CDMFT with a large *N* model

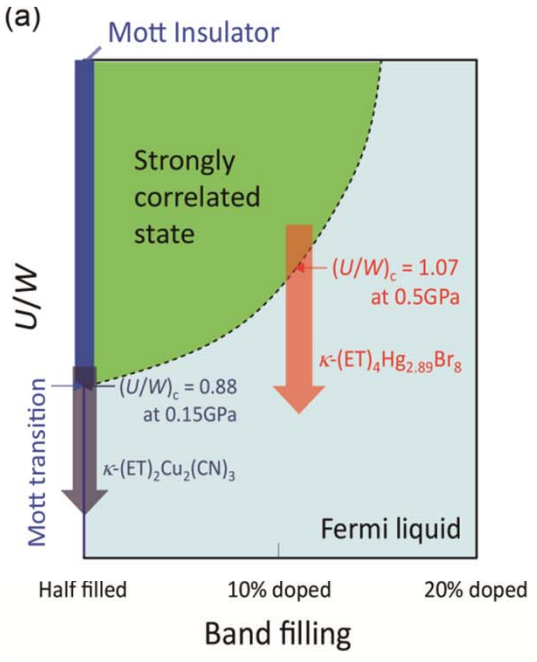
Local quantities (double occupancy etc…)
converge exponentially fast with CDMFT
(Take center of cluster)
Otherwise *1/L*

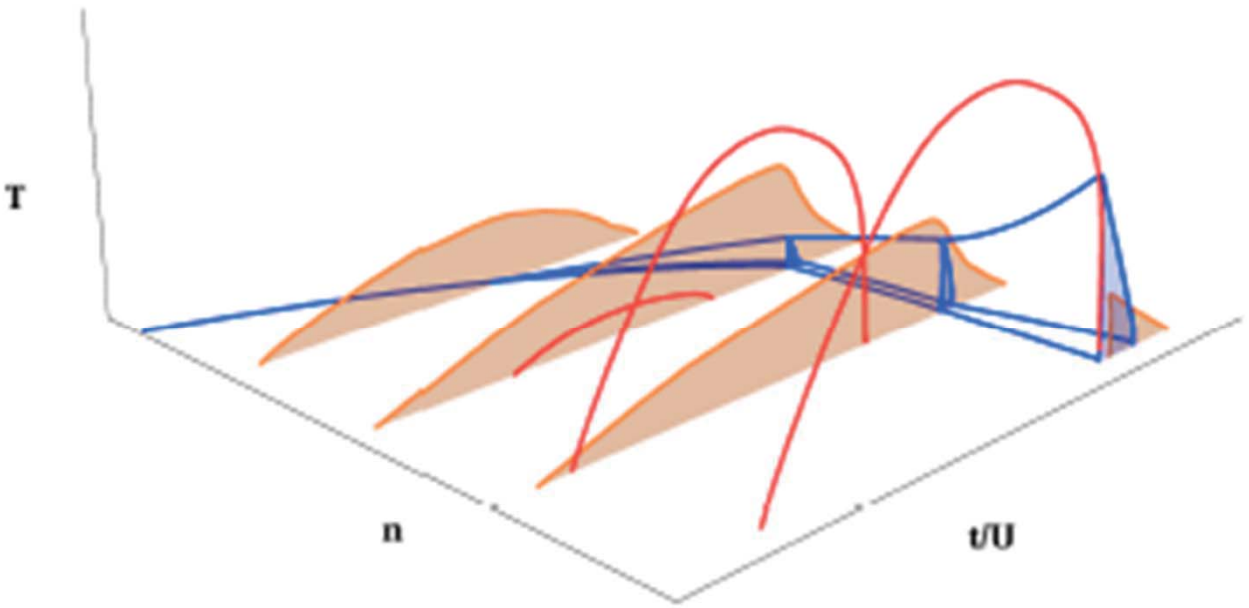
DCA faster for long wavelength quantities

G. Biroli and G. Kotliar, Phys. Rev. B **65**, 155112 2002.
T. A. Maier and M. Jarrell, Phys. Rev. B **65**, 041104R 2002.
K. Aryanpour, T. A. Maier, and M. Jarrell, Phys. Rev. B **71**, 037101 2005

Other materials

Generic case highly frustrated case





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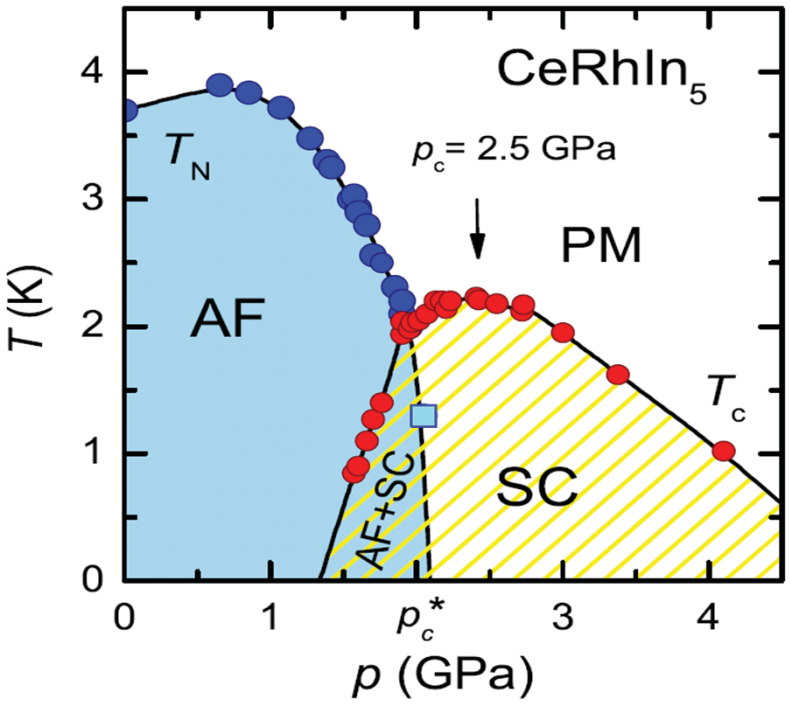
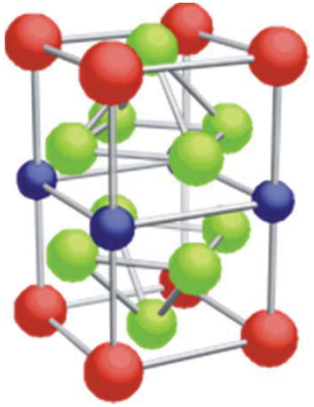
Heavy fermions

Heavy fermions **3D metals tuned by pressure, field or concentration**



Knebel et al. (2009)

CeRhIn$_5$



Magnetic superconductivity

Quantum criticality

Mathur et al., Nature 1998

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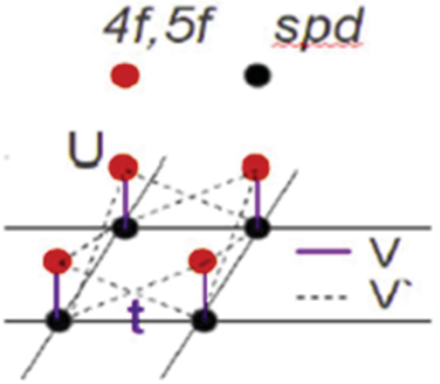
Heavy fermions

$$H = \sum_{k,\sigma} \epsilon_k c^\dagger_{k,\sigma} c_{k,\sigma} + \sum_{k,\sigma} \epsilon^f f^\dagger_{k,\sigma} f_{k,\sigma}$$
$$+ \sum_{k,\sigma} V_k (f^\dagger_{k,\sigma} c_{k,\sigma} + h.c.)$$
$$+ \sum_i U (n^\uparrow_f - \frac{1}{2})(n^\downarrow_f - \frac{1}{2})$$

$$V_k = V + 2V'[cos(k_x) + cos(k_y)]$$

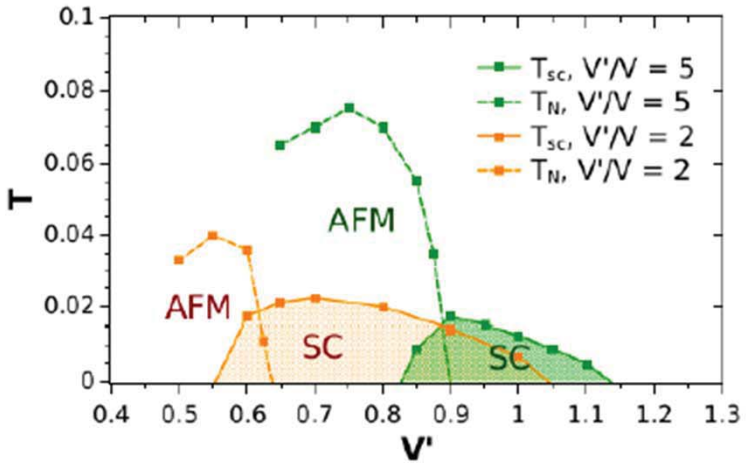


Phase diagram

U=4

AFM: antiferro-magnetism
SC: superconducting

V'/V = 2 : more frustrated case
V'/V = 5 : less frustrated case



W. Wu A.-M.S.T. Phys. Rev. X, 2015

Challenges

Challenges

- Weak to intermediate coupling (TPSC)
  - Generalize to broken symmetry states
  - Multiband states
  - Use in realistic calculations
- Strong coupling
  - Include long-wavelength fluctuations (vertex)
  - Feedback observable on double occupancy

Bio break