Dynamical Mean Field Theory

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INSTITUT QUANTIQUE

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1 Introduction

2 Dynamical Mean Field Theory

3 Cluster Perturbation Theory

4 Cluster Dynamical Mean Field Theory

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1 Introduction

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The Hubbard model

Hamiltonian:

$$H = \sum_{r,r',\sigma} t_{r,r'} c^{\dagger}_{r\sigma} c_{r'\sigma} + U \sum_{r} n_{r\uparrow} n_{r\downarrow}$$

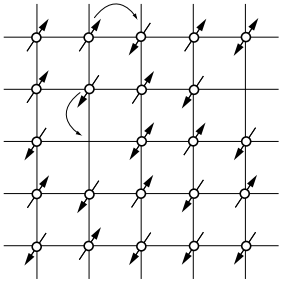
hopping amplitude ←

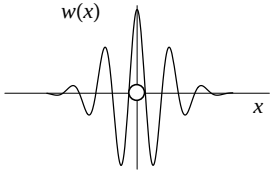
→ number of spin ↑ electrons at r

creation operator ←

→ local Coulomb repulsion

(chemical potential $\mu = -t_{rr}$)





The Green function

- Hilbert space of dimension $\sim 4^L$ (L: # of sites)
- The many-body ground state $|\Omega\rangle$ contains too much information
- A lot of useful information is contained in the one-particle Green function: (here at $T = 0$)

matrix $\boldsymbol{G}$

$$G_{\alpha\beta}(z) = \langle\Omega|c_\alpha \frac{1}{z - H + E_0} c_\beta^\dagger|\Omega\rangle + \langle\Omega|c_\beta^\dagger \frac{1}{z + H - E_0} c_\alpha|\Omega\rangle$$

G.S. energy

- Retarded Green function:

$$\boldsymbol{G}^R(t) = -i\Theta(t)\langle\Omega|\{c_\alpha(t), c_\beta^\dagger(0)\}|\Omega\rangle \implies \boldsymbol{G}^R(\omega) = \boldsymbol{G}(\omega + i0^+)$$

- Approximation schemes for $\boldsymbol{G}$ are easier to implement

Spectral representation

$$G_{\alpha\beta}(z) = \sum_{r>0} \langle \Omega | c_\alpha | r \rangle \frac{1}{z - E_r + E_0} \langle r | c_\beta^\dagger | \Omega \rangle + \sum_{r<0} \langle \Omega | c_\beta^\dagger | r \rangle \frac{1}{z + E_r - E_0} \langle r | c_\alpha | \Omega \rangle$$

$\rightarrow$ eigenstate with $N+1$ particles

eigenstate with $N-1$ particles $\leftarrow$

Q-matrix:

$$Q_{\alpha r} = \begin{cases} \langle \Omega | c_\alpha | r \rangle & (r > 0) \\ \langle r | c_\alpha | \Omega \rangle & (r < 0) \end{cases} \quad \text{and} \quad \omega_r = \begin{cases} E_r - E_0 & (r > 0) \\ E_0 - E_r & (r < 0) \end{cases}$$

Spectral representation:

$$G_{\alpha\beta}(z) = \sum_r \frac{Q_{\alpha r} Q_{\beta r}^*}{z - \omega_r}$$

(partial fractions)

Spectral representation (cont.)

Completeness relations:

$$\sum_r Q_{\alpha r} Q^*_{\beta r} = \langle \Omega | \left(c_\alpha c^\dagger_\beta + c^\dagger_\beta c_\alpha \right) | \Omega \rangle$$
$$= \delta_{\alpha\beta}$$

Asymptotic behavior:

$$\lim_{z \to \infty} G_{\alpha\beta}(z) = \frac{\delta_{\alpha\beta}}{z}$$

Spectral function

Spectral function:

$$A_{\alpha\beta}(\omega) = -2\,\mathrm{Im}G_{\alpha\beta}(\omega + i0^+)$$

Translation-invariant system:

$$G(\boldsymbol{k}, z) = \sum_{r>0} |\langle\Omega|c_{\boldsymbol{k}}|r\rangle|^2 \frac{1}{z - E_r + E_0} + \sum_{r<0} |\langle\Omega|c^\dagger_{\boldsymbol{k}}|r\rangle|^2 \frac{1}{z + E_r - E_0}$$

$$\begin{aligned} A(\boldsymbol{k}, \omega) &= -2\,\mathrm{Im}G(\boldsymbol{k}, \omega + i0^+) \\ &= \sum_{r>0} |\langle\Omega|c_{\boldsymbol{k}}|r\rangle|^2 2\pi\delta(\omega - E_r + E_0) \\ &\quad + \sum_{r<0} |\langle\Omega|c^\dagger_{\boldsymbol{k}}|r\rangle|^2 2\pi\delta(\omega + E_r - E_0) \end{aligned}$$

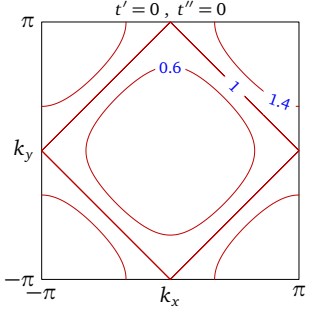
prob. of electron with $\varepsilon = E_r - E_0$

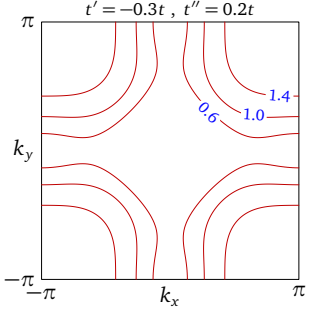
prob. of hole with $\varepsilon = E_r - E_0$

non-interacting limit ($U = 0$)

$$|\Omega\rangle = \prod_{\epsilon_k < 0} c_k^\dagger |0\rangle \qquad \text{(Fermi sea)}$$

$$G(z) = \frac{1}{z - t} \qquad G(z, k) = \frac{1}{z - \varepsilon_k} \qquad \varepsilon_k = \sum_r t_{0,r} e^{-ik\cdot r}$$

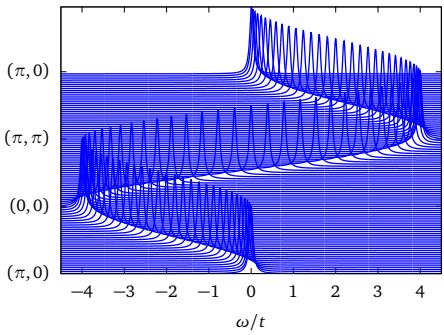




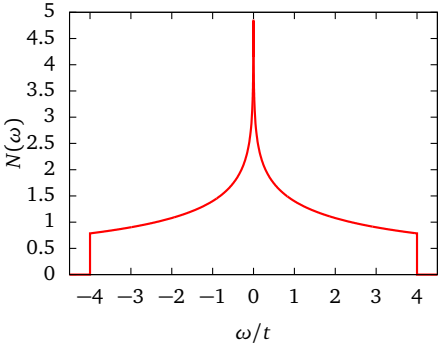
non-interacting limit (cont.)

Spectral function & density of states:

$$A(\boldsymbol{k},\omega) = 2\pi\delta(\omega - \varepsilon_{\boldsymbol{k}}) \qquad \rho(\omega) = \int_{\boldsymbol{k}} A(\boldsymbol{k},\omega)$$



Spectral function, half-filling, NN hopping



Associated density of states

Self-energy

Interacting Green function:

$$G(z) = \frac{1}{z - t - \Sigma(z)}$$

↳ self-energy

Local limit at half-filling ($t = -\frac{1}{2}U\mathbf{1}$):

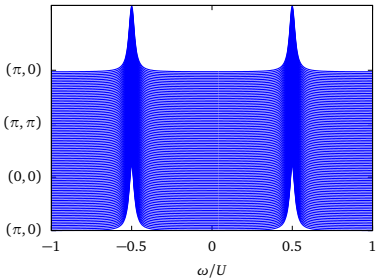
$$G(z) = \frac{1/2}{z + U/2} + \frac{1/2}{z - U/2} = \frac{1}{z - \dfrac{U^2}{4z}}$$

$$\Sigma(z) = \frac{U^2}{4z} + \frac{U}{2}$$

Analytic structure:

$$\Sigma_{\alpha\beta}(z) = \Sigma^{\infty}_{\alpha\beta} + \sum_r \frac{S_{\alpha r} S^*_{\beta r}}{z - \sigma_r}$$

Hartree-Fock ↵



Spectral function, half-filled HM ($t = 0$)

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1 Introduction

2 Dynamical Mean Field Theory
- Approximation schemes
- The cavity method
- The hybridization function
- The self-consistency condition
- Impurity solvers
- The Mott transition

3 Cluster Perturbation Theory

4 Cluster Dynamical Mean Field Theory

Approximation schemes

Hartree-Fock

- $\Sigma(\omega, \boldsymbol{k}) \to \Sigma(\infty, \boldsymbol{k})$ is frequency-independent
- Can be absorbed in new dispersion relation $\varepsilon'(\boldsymbol{k})$
- Approximation equivalent to new one-body Hamiltonian

DMFT

- $\Sigma(\omega, \boldsymbol{k}) \to \Sigma(\omega)$ is momentum-independent
- System still fundamentally interacting
- Approximated by single site with effective medium

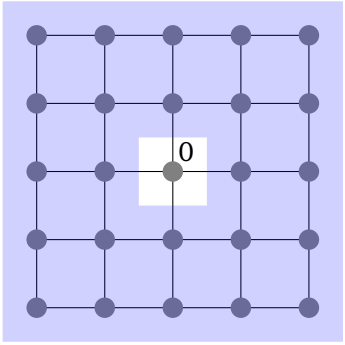
The cavity method

Action of the Hubbard model:

$$S[c_{r\sigma}, c^{\dagger}_{r\sigma}] = \int_0^{\beta} \mathrm{d}\tau \left\{ \sum_{r,\sigma} c^{\dagger}_{r\sigma} \partial_{\tau} c_{r\sigma} + \sum_{r,r',\sigma} t_{rr'} c^{\dagger}_{r\sigma} c_{r'\sigma} + U \sum_{r} n_{r\uparrow} n_{r\downarrow} \right\}$$

One-site effective action:

$$\frac{1}{Z_{\text{eff.}}} \mathrm{e}^{-S_{\text{eff.}}[c_{0\sigma}, c^{\dagger}_{0\sigma}]} = \frac{1}{Z} \int \prod_{r \neq 0, \sigma} \mathscr{D} c_{r\sigma} \mathscr{D} c^{\dagger}_{r\sigma} \mathrm{e}^{-S}$$



The cavity method (cont.)

Effective action (exact form, spin indices suppressed):

$$S_{\text{eff.}} = S_0 + \sum_{n=1}^{\infty} \sum_{\boldsymbol{r}_1,\ldots,\boldsymbol{r}'_n} \int \mathrm{d}\tau \; \eta^{\dagger}_{\boldsymbol{r}_1} \cdots \eta^{\dagger}_{\boldsymbol{r}_n} \eta_{\boldsymbol{r}'_1} \ldots \eta_{\boldsymbol{r}'_n} G^{\text{env}}_{\boldsymbol{r}_1 \cdots \boldsymbol{r}'_n}(\tau_1 \cdots \tau_{\boldsymbol{r}_n}, \tau_1 \cdots \tau_n)$$

where $\eta_{\boldsymbol{r}} = t_{\boldsymbol{r}0} c_{\boldsymbol{r}0}$ acts like a source field and

$$S_0 = \int_0^{\beta} \mathrm{d}\tau \left\{ c_0 \partial_\tau c_0 - \mu n_0 + U n_{0\uparrow} n_{0\downarrow} \right\}$$

One can show that in the $d \to \infty$ limit, if $t \to t/\sqrt{2d}$, only $n = 1$ survives.
DMFT approximation:

$$S_{\text{eff.}} = S_0 + \sum_{\boldsymbol{r},\boldsymbol{r}'} t_{0\boldsymbol{r}} t_{0\boldsymbol{r}'} \int \mathrm{d}\tau \; \mathrm{d}\tau' \; c^{\dagger}_0(\tau) c_0(\tau') G^{\text{env}}_{\boldsymbol{r},\boldsymbol{r}'}(\tau, \tau')$$

The cavity method (cont.)

Effective action:

$$S_{\text{eff.}} = -\int \mathrm{d}\tau\, \mathrm{d}\tau'\, c_0^\dagger(\tau)\mathscr{G}_0^{-1}(\tau-\tau')c_0(\tau') + U\int_0^\beta \mathrm{d}\tau\, n_{0\uparrow}n_{0\downarrow}$$

$$\mathscr{G}_0^{-1}(i\omega_n) = i\omega_n + \mu - \sum_{r,r'} t_{0r}t_{0r'}G^{\text{env}}_{r,r'}(i\omega_n)$$

- $G^{\text{env}}_{r,r'}(i\omega_n)$ unknown.
  Rather, treat $\mathscr{G}_0^{-1}$ as an adjustable **dynamical mean field**
- Only single particles hop on and off the site
- The environment is uncorrelated
- Nonlocal in time: no Hamiltonian involving c_0 only

The hybridization function

- $\mathcal{G}_0$ has the analytic properties of a Green function: poles on the real axis and positive residues.
- Define the **hybridization function** $\Gamma(z)$:

$$\mathcal{G}_0^{-1}(z) = z + \mu - \Gamma(z)$$

- $\Gamma(z)$ has the analytic properties of a self-energy and can represented by a (quasi-infinite) set of poles:

$$\Gamma(z) = \sum_r \frac{\theta_r^2}{z - \epsilon_r}$$

- Interacting Green function of the effective theory for the 'single site:

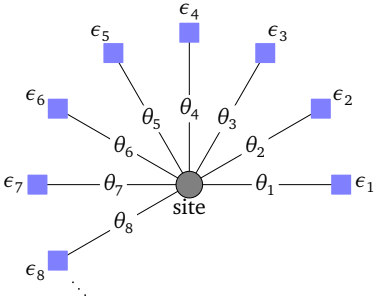
$$G_s(z) = \frac{1}{z + \mu - \Gamma(z) - \Sigma(z)}$$

Hamiltonian representation

G_s can be obtained from the following AIM Hamiltonian:

$$H_{\mathrm{AIM}} = \sum_{r=1}^{N_b} \theta_r \left(c_0^\dagger a_r + \mathrm{H.c} \right) + \sum_{r=1}^{N_b} \epsilon_r a_r^\dagger a_r - \mu c_0^\dagger c_0 + U n_{0\uparrow} n_{0\downarrow}$$

hyb. amplitude ← → bath orbital → bath energy



One-body matrix:

$$\boldsymbol{T} = \begin{pmatrix} -\mu & \boldsymbol{\theta}_{[1\times N_b]} \\ \boldsymbol{\theta}^\dagger_{[N_b\times 1]} & \boldsymbol{\varepsilon}_{[N_b\times N_b]} \end{pmatrix}$$

Proof ($U = 0$)

$$\boldsymbol{G}_{\text{full}}(z) = \begin{pmatrix} G_s & G_{sb} \\ G_{bs} & G_b \end{pmatrix} \qquad \boldsymbol{G}^{-1}_{\text{full}}(z) = z - \boldsymbol{T} = \begin{pmatrix} z+\mu & -\boldsymbol{\theta} \\ -\boldsymbol{\theta}^\dagger & z-\boldsymbol{\varepsilon} \end{pmatrix}$$

Need to invert a block matrix:

$$\begin{pmatrix} z+\mu & -\boldsymbol{\theta} \\ -\boldsymbol{\theta}^\dagger & z-\boldsymbol{\varepsilon} \end{pmatrix} \begin{pmatrix} G_s & G_{sb} \\ G_{bs} & G_b \end{pmatrix} = \mathbf{1}$$

block equations:

$$(z+\mu)G_s - \boldsymbol{\theta} G_{bs} = \mathbf{1} \quad \text{and} \quad -\boldsymbol{\theta}^\dagger G_s + (z-\boldsymbol{\varepsilon})G_{bs} = 0$$

$$G_{bs} = (z-\boldsymbol{\varepsilon})^{-1}\boldsymbol{\theta}^\dagger G_s \implies \left[(z+\mu) - \boldsymbol{\theta}\frac{1}{z-\boldsymbol{\varepsilon}}\boldsymbol{\theta}^\dagger\right] G_s = \mathbf{1}$$

therefore

$$G_s^{-1} = z + \mu - \boldsymbol{\theta}\frac{1}{z-\boldsymbol{\varepsilon}}\boldsymbol{\theta}^\dagger = z + \mu - \Gamma(z)$$

Proof (cont.)

where

$$\Gamma(z) = \boldsymbol{\theta} \frac{1}{z - \boldsymbol{\varepsilon}} \boldsymbol{\theta}^\dagger = \sum_{r=1}^{N_b} \frac{\theta_r^2}{z - \epsilon_r}$$

If $U \neq 0$, simply add the self-energy:

$$G_s(z) = \frac{1}{z + \mu - \Gamma(z) - \Sigma(z)}$$

The self-consistency condition

- Lattice model Green function in the DMFT approximation:

$$G(i\omega_n, \boldsymbol{k}) = \frac{1}{i\omega_n - \varepsilon(\boldsymbol{k}) - \Sigma(i\omega_n)}$$

- The local Green function

$$\bar{G}(i\omega_n) = \frac{1}{N}\sum_{\boldsymbol{k}} G(i\omega_n, \boldsymbol{k})$$

must coincide with $G_s(i\omega_n)$:

$$\begin{aligned}\bar{G}(i\omega_n)^{-1} &= i\omega_n + \mu - \Gamma(i\omega_n) - \Sigma(i\omega_n) \\ &= \mathscr{G}_0^{-1}(i\omega_n) - \Sigma(i\omega_n)\end{aligned}$$

Variant in terms of the density of states

- Noninteracting density of states: $\rho_0(\omega) = (1/N)\sum_k \delta(\omega - \varepsilon(\boldsymbol{k}))$
- Sum over wavevectors replaced by single integral over frequencies:

$$\frac{1}{N}\sum_{\boldsymbol{k}} F(\varepsilon(\boldsymbol{k})) = \int d\omega F(\omega)\rho_0(\omega)$$

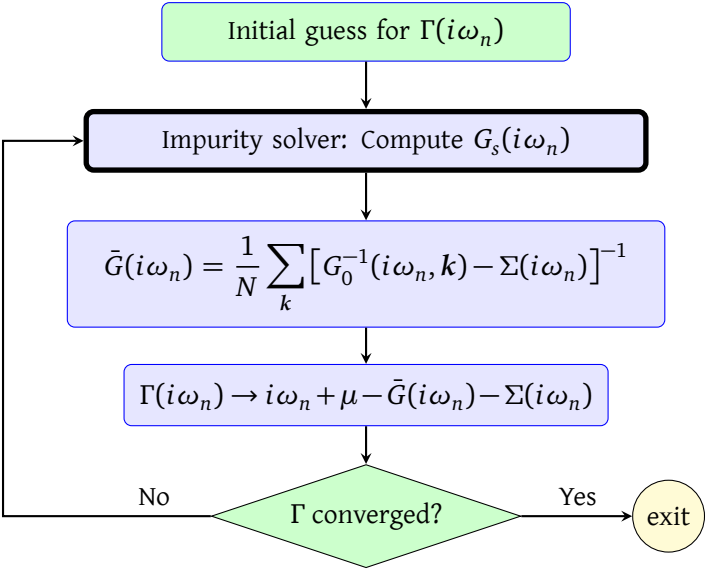
The local Green function is then

$$\bar{G}(i\omega_n) = \int d\omega \frac{\rho_0(\omega)}{i\omega_n - \omega - \Sigma(i\omega_n)} = R_0(i\omega_n - \Sigma(i\omega_n))$$

where

$$R_0(z) = \int d\omega \frac{\rho_0(\omega)}{z - \omega}$$

The DMFT self-consistency loop



The impurity solver

Methods for solving the impurity Hamiltonian:

- Perturbation theory (2nd order, NCA)
- Numerical Renormalization Group (NRG)
- Quantum Monte Carlo (QMC)
  - Infinite bath: only $\Gamma(i\omega_n)$ is needed.
  - Finite temperature
  - **Hirsch-Fye** (time grid) or **Continuous-time** (no discretization error)
  - But: sign problem
- Exact diagonalizations
  - restricted to small, discrete baths (explicit form of H_{AIM})
    Hence self-consistency relation only approximately satisfied
  - real-frequency information
  - zero temperature
- Other real frequency methods: CI, natural basis, DMRG & other tensor networks

The DMFT self-consistency loop (discrete bath version)

1. Start with a guess value of $(\theta_r, \varepsilon_r)$
2. Compute the impurity Green function $G_s(i\omega_n)$ (ED)
3. Compute the lattice-averaged (or local) Green function

$$\bar{G}(i\omega_n) = \frac{1}{N}\sum_{\boldsymbol{k}} \frac{1}{G_0^{-1}(\boldsymbol{k}) - \Sigma(i\omega_n)} \quad \text{and} \quad \mathcal{G}_0^{-1}(i\omega_n) = \bar{G}^{-1} + \Sigma(i\omega_n)$$

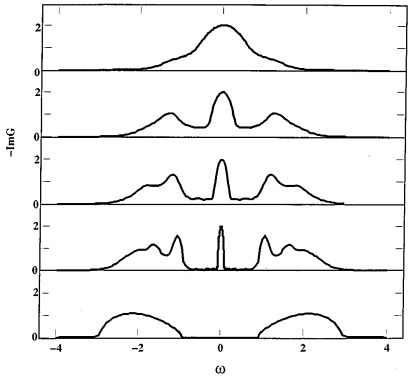
4. Minimize the following **distance function**:

$$d(\boldsymbol{\theta}, \boldsymbol{\varepsilon}) = \sum_{\omega_n} W(i\omega_n) \operatorname{tr} \left| G_s^{-1}(i\omega_n) - \bar{G}^{-1}(i\omega_n) \right|^2$$

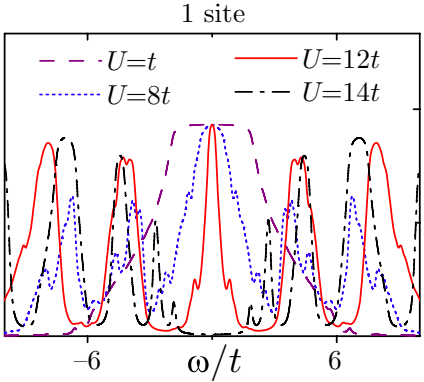
   ↳ weights

   over the set of bath parameters. Thus obtain a new set $(\theta_r, \varepsilon_r)$.
5. Go back to step (2) until convergence.

Application: The Mott transition

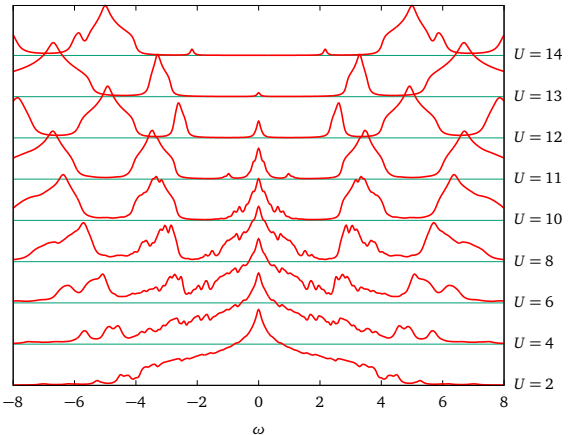


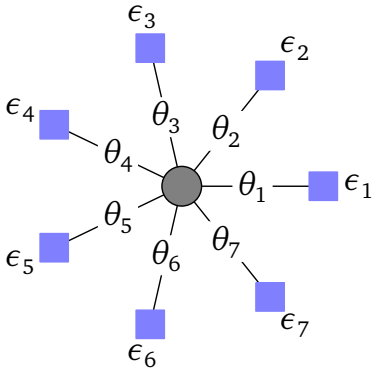
Density of states $N(\omega)$ for the half-filled Hubbard model on the Bethe lattice with interactions $U/D = 1, 2, 2.5, 3, 4$. Iterated perturbation theory. Zhang et al., Phys. Rev. Lett. **70**, 1666 (1993).



$N(\omega)$ for the half-filled 3D Hubbard model. Exact diagonalization solver. Zhang and Imada, Phys. Rev. B **76**, 045108 (2007).

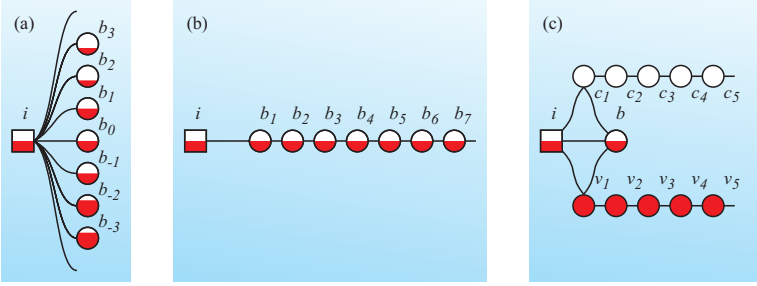
The Mott transition (cont.)





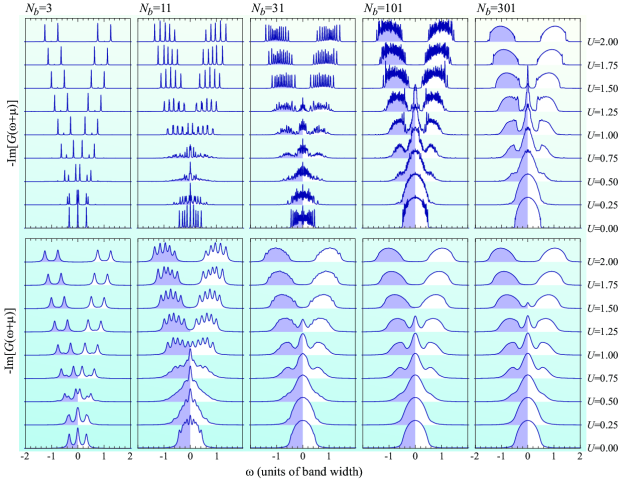
$N(\omega)$ in the 2D, half-filled Hubbard model. Exact diagonalization solver with $N_b = 7$.

Breaking the exponential barrier



Lu et al., Phys. Rev. B**90**, 085102 (2014).

Breaking the exponential barrier (cont.)

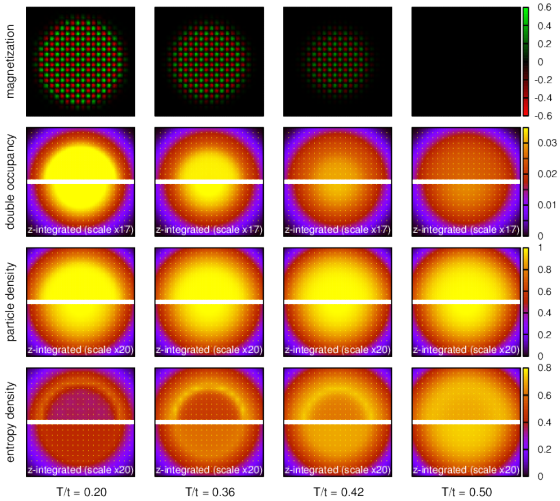


Lu et al., Phys. Rev. B**90**, 085102 (2014).

Real-space DMFT : Ultra-cold atoms

Antiferromagnetic order in cold atom systems with harmonic trap

$$H = \sum_{r,r',\sigma} t_{r,r'} c^{\dagger}_{r\sigma} c_{r'\sigma} + U \sum_{r} n_{r\uparrow} n_{r\downarrow} - \sum_{r,\sigma} (V_r - \mu) n_{r,\sigma}$$



Gorelik et al., Phys. Rev. Lett. **105**, 065301 (2010)

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3 Cluster Perturbation Theory
- kinematics
- CPT : examples

4 Cluster Dynamical Mean Field Theory

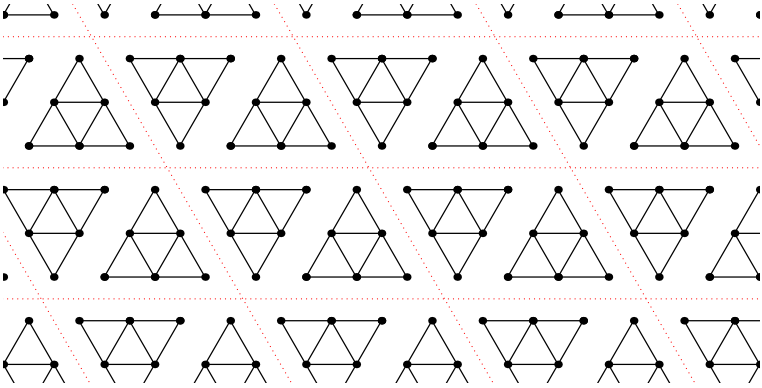
Real-space cluster methods: General idea

- Tile the lattice with small units (clusters)
- Solve an approximate, effective problem on each cluster
- Use the self-energies $\mathbf{\Sigma}^{(j)}(z)$ to approximate the full self-energy:

$$\mathbf{\Sigma} = \begin{pmatrix} \mathbf{\Sigma}^{(1)} & 0 & \cdots & 0 \\ 0 & \mathbf{\Sigma}^{(2)} & \cdots & 0 \\ \vdots & \vdots & \ddots & \vdots \\ 0 & 0 & \cdots & \mathbf{\Sigma}^{(n)} \end{pmatrix}$$

- Varieties:
  - CPT : Cluster Perturbation Theory
  - VCA : Variational Cluster Approximation
  - CDMFT : Cluster Dynamical Mean Field Theory
  - CDIA : Cluster Dynamical Impurity Approximation

Tiling the lattice into clusters



Tiling of the triangular lattice with 6-site clusters

Cluster Perturbation Theory

Cluster decomposition of the one-body matrix:

$$\boldsymbol{t} = \begin{pmatrix} \boldsymbol{t}^{(1,1)} & \boldsymbol{t}^{(1,2)} & \dots & \boldsymbol{t}^{(1,n)} \\ \boldsymbol{t}^{(2,1)} & \boldsymbol{t}^{(2,2)} & \dots & \boldsymbol{t}^{(2,n)} \\ \vdots & \vdots & \ddots & \vdots \\ \boldsymbol{t}^{(n,1)} & \boldsymbol{t}^{(n,2)} & \dots & \boldsymbol{t}^{(n,n)} \end{pmatrix} \qquad \boldsymbol{t} = \boldsymbol{t}' + \boldsymbol{t}_{\mathrm{ic}}$$

↳ diagonal blocks

Cluster Green function:

$$\boldsymbol{G}^{(j)-1}(z) = z - \boldsymbol{t}^{(j,j)} - \boldsymbol{\Sigma}^{(j)}(z)$$

CPT Green function for the full system:

$$\boldsymbol{G}^{-1}_{\mathrm{cpt}}(z) = \bigoplus_j \boldsymbol{G}^{(j)-1}(z) - \boldsymbol{t}_{\mathrm{ic}}$$

↳ inter-cluster blocks

Cluster Perturbation Theory (cont.)

lattice Hamiltonian ← → cluster Hamiltonian

$$H = H' + H_{\mathrm{ic}} \qquad H_{\mathrm{ic}} = \sum_{\alpha,\beta} (t_{\mathrm{ic}})_{\alpha\beta} c_\alpha^\dagger c_\beta$$

- Treat H_{ic} at lowest order in Perturbation theory
- At this order, the Green function is

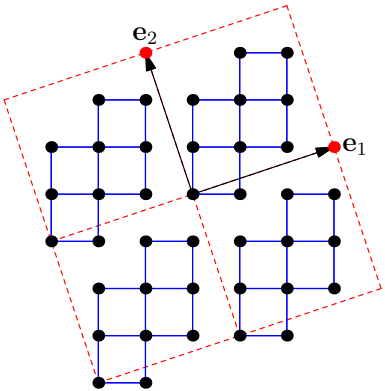
$$\boldsymbol{G}^{-1}(z) = \boldsymbol{G}'^{-1}(z) - \boldsymbol{t}_{\mathrm{ic}}$$

↳ cluster Green function matrix

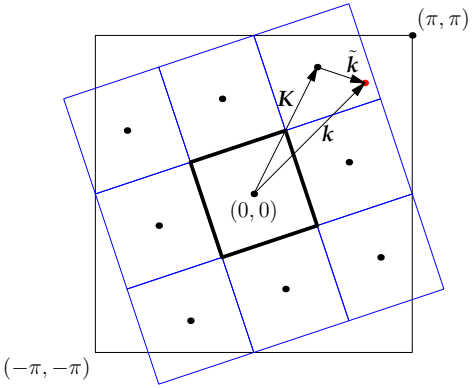
C. Gros and R. Valenti, Phys. Rev. B **48**, 418 (1993)

D. Sénéchal, D. Perez, and M. Pioro-Ladrière. Phys. Rev. Lett. **84**, 522 (2000)

Superlattices and reduced Brillouin zones



10-site cluster



Brillouin zones

CPT for translation invariant tilings

site within cluster ← → reduced wavevector

$$\text{one-body index} = (\boldsymbol{R}, \tilde{\boldsymbol{k}}, \sigma)$$

↳ spin (or band)

Green function and $\boldsymbol{t}_{\text{ic}}$ are diagonal in $\tilde{\boldsymbol{k}}$.
$\boldsymbol{G}'$ is independent of $\boldsymbol{k}$.
The CPT formula may be written as

$$\boldsymbol{G}^{-1}(z, \tilde{\boldsymbol{k}}) = \boldsymbol{G}'^{-1}(z) - \boldsymbol{t}_{\text{ic}}(\tilde{\boldsymbol{k}})$$

where matrices are now in $(\boldsymbol{R}, \sigma)$ space.

Interlude : Fourier transforms

Unitary matrices performing Fourier transforms:

$$U^{\gamma}_{k,r} = \frac{1}{\sqrt{N}} e^{-ik\cdot r} \qquad U^{\Gamma}_{\tilde{k}\tilde{r}} = \sqrt{\frac{L}{N}} e^{-i\tilde{k}\cdot\tilde{r}} \qquad U^{c}_{K,R} = \frac{1}{\sqrt{L}} e^{-iK\cdot R}$$

complete superlattice cluster

Various representations of the annihilation operator

$$c(k) = \sum_{r} U^{\gamma}_{kr}\, c_r \qquad c_K(\tilde{k}) = \sum_{\tilde{r},R} U^{\Gamma}_{\tilde{k}\tilde{r}} U^{c}_{KR}\, c_{\tilde{r}+R}$$

$$c_R(\tilde{k}) = \sum_{\tilde{r}} U^{\Gamma}_{\tilde{k}\tilde{r}}\, c_{\tilde{r}+R} \qquad c_{\tilde{r},K} = \sum_{R} U^{c}_{KR}\, c_{\tilde{r}+R}$$

Caveat: $\boldsymbol{U}^{\gamma} \neq \boldsymbol{U}^{\Gamma} \otimes \boldsymbol{U}^{c}$
The matrix $\boldsymbol{\Lambda} = \boldsymbol{U}^{\gamma}(\boldsymbol{U}^{\Gamma} \otimes \boldsymbol{U}^{c})^{-1}$ relates $(\boldsymbol{K}, \tilde{\boldsymbol{k}})$ to $\boldsymbol{k}$:

$$c(\tilde{\boldsymbol{k}} + \boldsymbol{K}) = \Lambda_{K,K'}(\tilde{k}) c_{K'}(\tilde{k})$$

Fourier transforms (cont.)

$$c_{\tilde{\mathbf{r}}+\mathbf{R}} = \frac{\sqrt{N_c}}{\sqrt{N}} \sum_{\tilde{\mathbf{k}}} e^{i\tilde{\mathbf{k}}\cdot\mathbf{R}} e^{i\tilde{\mathbf{k}}\cdot\tilde{\mathbf{r}}} \frac{1}{\sqrt{N_c}} \sum_{\mathbf{K}} e^{i\mathbf{K}\cdot\mathbf{R}} c_{\tilde{\mathbf{k}}+\mathbf{K}}$$

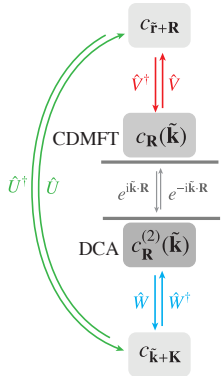
CDMFT $c_{\mathbf{R}}(\tilde{\mathbf{k}})$ DCA $c^{(2)}_{\mathbf{R}}(\tilde{\mathbf{k}})$

$$c_{\tilde{\mathbf{k}}+\mathbf{K}} = \frac{1}{\sqrt{N_c}} \sum_{\tilde{\mathbf{r}}} e^{-i\mathbf{K}\cdot\mathbf{R}} e^{-i\tilde{\mathbf{k}}\cdot\mathbf{R}} \frac{\sqrt{N_c}}{\sqrt{N}} \sum_{\mathbf{R}} e^{-i\tilde{\mathbf{k}}\cdot\tilde{\mathbf{r}}} c_{\tilde{\mathbf{r}}+\mathbf{R}}$$

$$[\hat{U}]_{\mathbf{r},\mathbf{k}} = \frac{1}{\sqrt{N}} e^{i\mathbf{k}\cdot\mathbf{r}}$$

$$[\hat{V}]_{\tilde{\mathbf{r}},\tilde{\mathbf{k}}} = \frac{\sqrt{N_c}}{\sqrt{N}} e^{i\tilde{\mathbf{r}}\cdot\tilde{\mathbf{k}}}$$

$$[\hat{W}]_{\mathbf{R},\mathbf{K}} = \frac{1}{\sqrt{N_c}} e^{i\mathbf{R}\cdot\mathbf{K}}$$



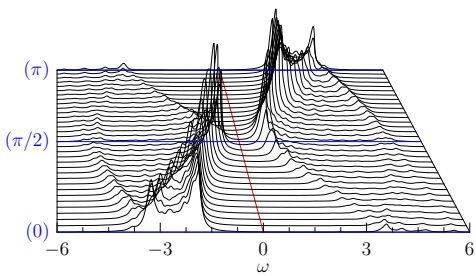
Simon Verret (unpublished)

Periodization

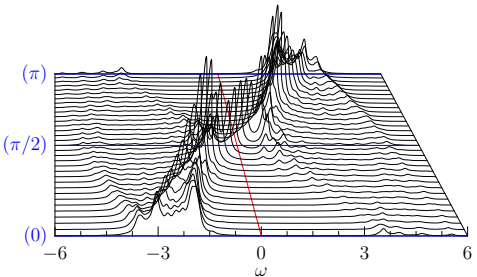
- CPT breaks translation invariance, which needs to be restored:

$$G_{\text{per.}}(\boldsymbol{k}, z) = \frac{1}{L} \sum_{\boldsymbol{R},\boldsymbol{R}'} \mathrm{e}^{-i\boldsymbol{k}\cdot(\boldsymbol{R}-\boldsymbol{R}')} G_{\boldsymbol{R}\boldsymbol{R}'}(\tilde{\boldsymbol{k}}, z)$$

- Periodizing (1D half-filled HM, 12-site cluster):



Green function periodization



Self-energy periodization

Periodization (2)

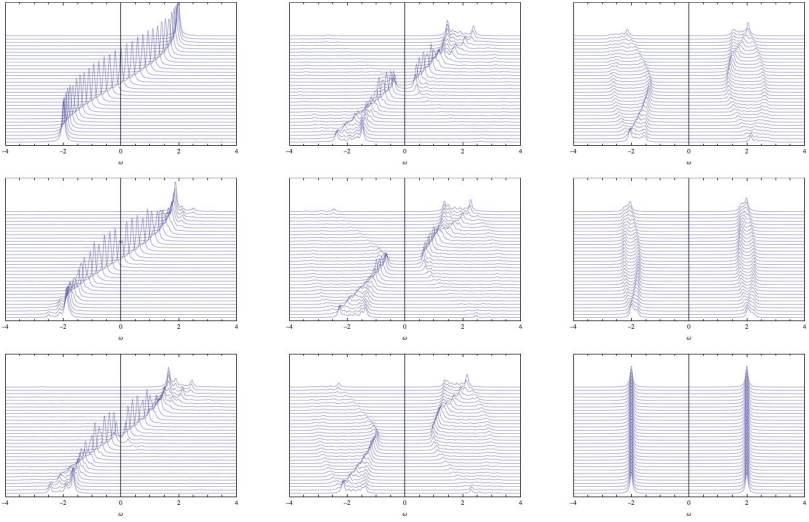
- Periodization as a change of basis:

$$
\begin{aligned}
G(\tilde{k}+K,\tilde{k}+K',z) &= \left(\Lambda^{c}(\tilde{k})G(z)\Lambda^{c\dagger}(\tilde{k})\right)_{KK'} \\
&= \frac{1}{L^2}\sum_{R,R',K_1,K_1'} \mathrm{e}^{-i(\tilde{k}+K-K_1)\cdot R}\mathrm{e}^{i(\tilde{k}+K'-K_1')\cdot R'}G_{K_1K_1'}(z) \\
&= \frac{1}{L}\sum_{R,R'} \mathrm{e}^{-i(\tilde{k}+K)\cdot R}\mathrm{e}^{i(\tilde{k}+K')\cdot R'}G_{RR'}(\tilde{k},z)
\end{aligned}
$$

- Set $K = K'$: the spectral function is a partial trace and thus involves diagonal elements only
- Replace $\tilde{k}$ by $k = \tilde{k} + K$ in $G_{RR'}(\tilde{k},z)$, which leaves $t_{\mathrm{ic}}(\tilde{k})$ unchanged
- Since this is a change of basis, analytic properties are still OK.

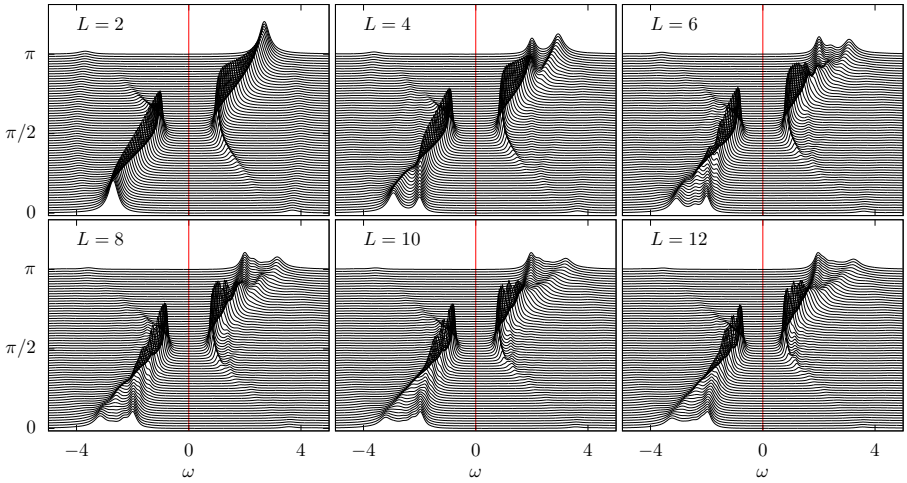
One-dimensional example

Spectral function of the half-filled HM with increasing U/t:



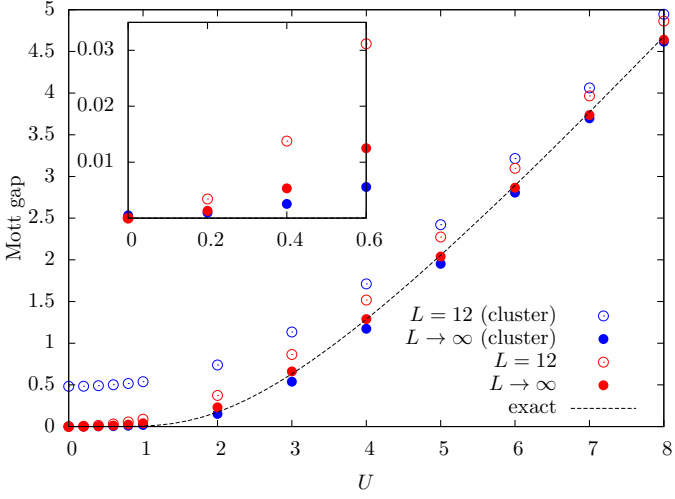
One-dimensional example (cont.)

Spectral function of the half-filled HM with increasing L at $U = 4t$:

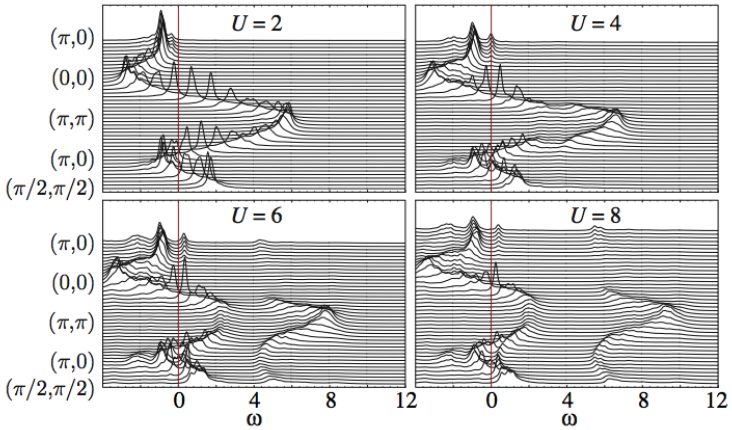


One-dimensional example (cont.)

Spectral gap at half-filling: periodic cluster vs CPT

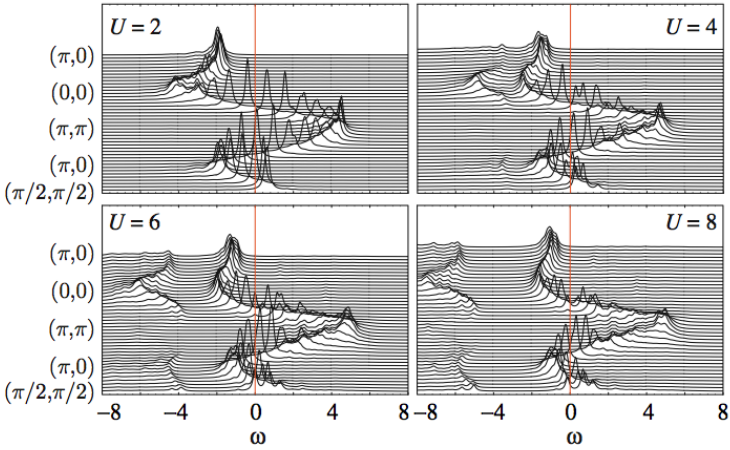


Application: Pseudogap in h-doped cuprates



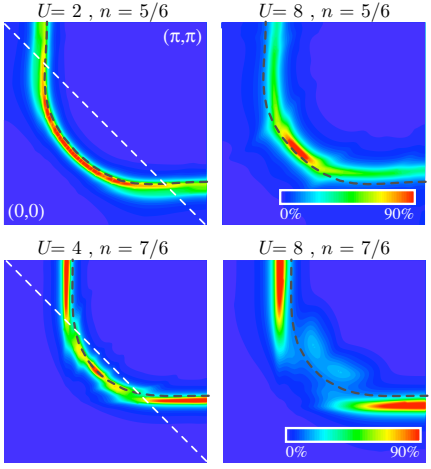
2D Hubbard model, $t' = -0.3t$, $t'' = 0.2t$, 3×4 cluster, $n = 5/6$
Sénéchal and Tremblay, PRL **92**, 126401 (2004)

Application: Pseudogap in e-doped cuprates

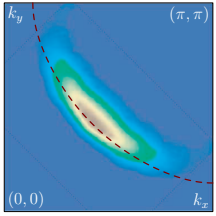


2D Hubbard model, $t' = -0.3t$, $t'' = 0.2t$, 3×4 cluster, $n = 7/6$
Sénéchal and Tremblay, PRL **92**, 126401 (2004)

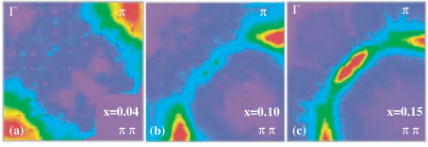
Application: Fermi surface maps



Sénéchal and Tremblay, PRL **92**, 126401 (2004)



F. Ronning et al., PRB **67**, 165101 (2003)



N.P. Armitage et al., PRL **88**, 257001 (2002)

CPT : Conclusion

- Approximation scheme for the one-body Green function
  - Yields approximate values for the averages of one-body operators
- Exact at $U = 0$
- Exact at $t_{ij} = 0$
- Exact short-range correlations
- Allows all values of the wavevector
- Controlled by the size of the cluster
- But :
  - No long-range order, no self-consistency
  - Higher Green functions still confined to the cluster

$\Longrightarrow$ A first step towards CDMFT or VCA

Outline

1 Introduction

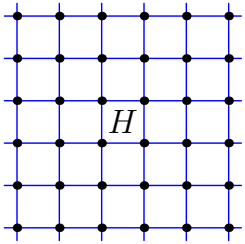
2 Dynamical Mean Field Theory

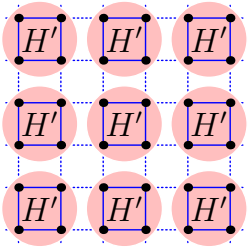
3 Cluster Perturbation Theory

4 Cluster Dynamical Mean Field Theory
- The hybridization function
- The CDMFT self-consistency condition
- Applications
- The Dynamical Cluster Approximation (DCA)

Generalization of DMFT to small clusters

- $H_{\mathrm{AIM}} \to H'$
- Simple adaptation of DMFT
- Scalar equations
  $\to$ matrix equations





Dynamical mean field $\mathscr{G}_0$:

$$S_{\mathrm{eff}}[c, c^*] = -\int_0^\beta \mathrm{d}\tau \mathrm{d}\tau' \sum_{\alpha,\beta} c^*_\alpha(\tau) \mathscr{G}^{-1}_{0,\alpha\beta}(\tau - \tau') c_\beta(\tau') + \int_0^\beta \mathrm{d}\tau\, H_1(c, c^*)$$

The hybridization function

In the frequency domain:

$$\mathscr{G}_0^{-1}(i\omega_n) = i\omega_n - \boldsymbol{t}' - \boldsymbol{\Gamma}(i\omega_n) \quad \text{where} \quad \mathscr{G}_0(i\omega_n) = \int_0^\beta \mathrm{e}^{i\omega_n\tau}\mathscr{G}_0(\tau)$$

→ hybridization function

Spectral representation of $\boldsymbol{\Gamma}$:

$$\Gamma_{\alpha\beta}(i\omega_n) = \sum_r^{N_b} \frac{\theta_{\alpha r}\theta^*_{\beta r}}{i\omega_n - \varepsilon_r} = \boldsymbol{\theta}\frac{1}{i\omega_n - \boldsymbol{\varepsilon}}\boldsymbol{\theta}^\dagger$$

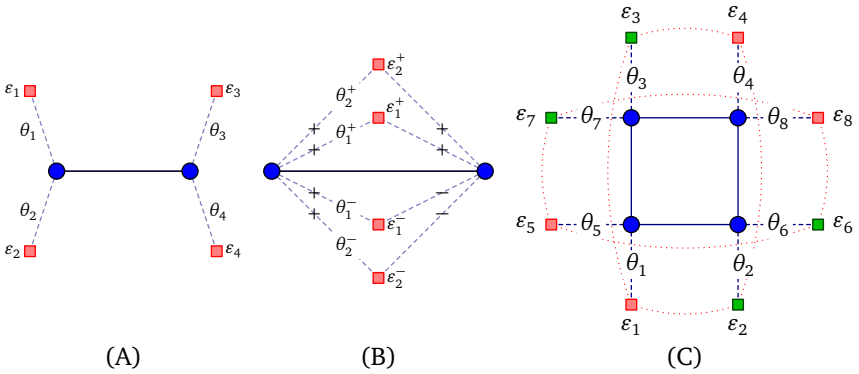
Corresponding Hamiltonian:

$$H' = \sum_{\alpha,\beta} t'_{\alpha\beta}c^\dagger_\alpha c_\beta + U\sum_i n_{i\uparrow}n_{i\downarrow} + \sum_{r,\alpha}\theta_{r\alpha}(c^\dagger_\alpha a_r + \text{H.c.}) + \sum_r \varepsilon_r a^\dagger_r a_r$$

hybridization matrix ← → bath orbital

bath energies ←

Discrete bath systems



(B) : Liebsch and Ishida, Journal of Physics: Condensed Matter 24 (2012), no. 5, 053201.

The CDMFT Procedure (discrete bath)

1. Start with a guess value of $(\theta_{\alpha r}, \varepsilon_r)$.
2. Calculate the cluster Green function $\boldsymbol{G}'(\omega)$ (ED).
3. Calculate the superlattice-averaged Green function

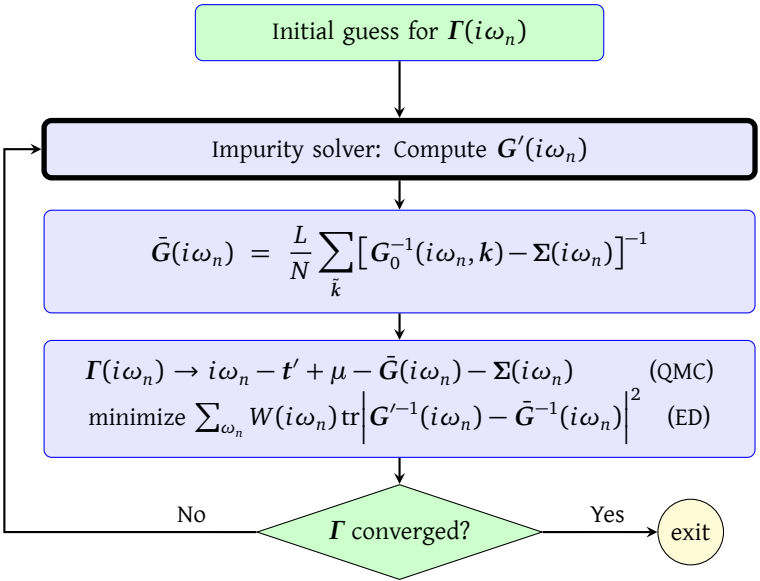
$$\bar{\boldsymbol{G}}(\omega) = \sum_{\tilde{\boldsymbol{k}}} \frac{1}{\boldsymbol{G}_0^{-1}(\tilde{\boldsymbol{k}}) - \boldsymbol{\Sigma}(\omega)} \quad \text{and} \quad \mathscr{G}_0^{-1}(\omega) = \bar{\boldsymbol{G}}^{-1} + \boldsymbol{\Sigma}(\omega)$$

4. Minimize the following distance function:

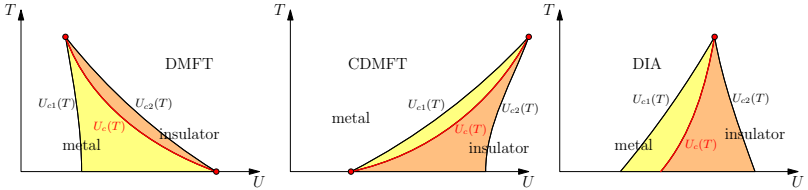
$$d(\boldsymbol{\theta}, \boldsymbol{\varepsilon}) = \sum_{\omega_n} W(i\omega_n) \operatorname{tr} \left| \boldsymbol{G}'^{-1}(i\omega_n) - \bar{\boldsymbol{G}}^{-1}(i\omega_n) \right|^2$$

   over the set of bath parameters. Thus obtain a new set $(\theta_{\alpha r}, \varepsilon_r)$.
5. Go back to step (2) until convergence.

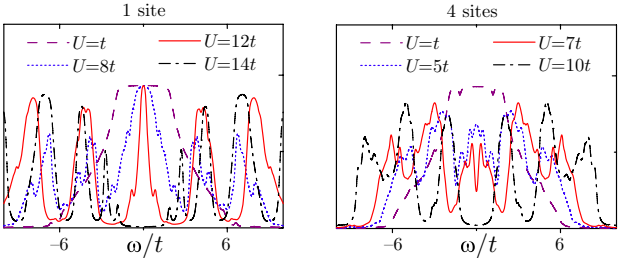
The CDMFT self-consistency loop



Application: The Mott transition

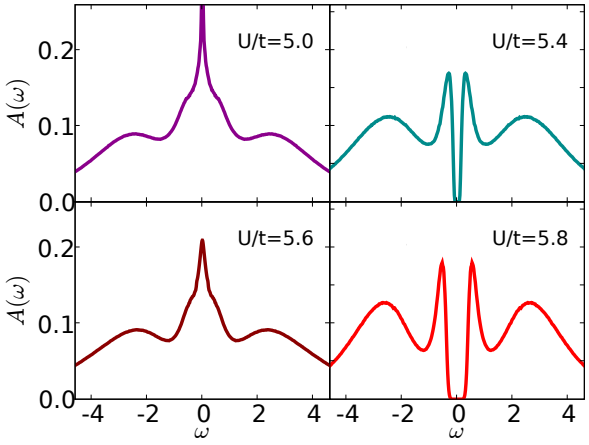


M. Balzer et al., Europhys. Lett. **85**, 17002 (2009)



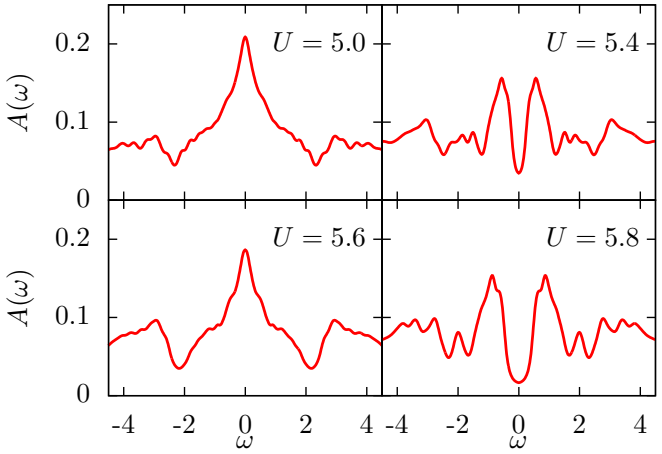
Y.Z. Zhang, M. Imada, Phys. Rev. B **76**, 045108 (2007)

Application: the Mott transition (QMC)



H. Park et al, PRL 101, 186403 (2008)

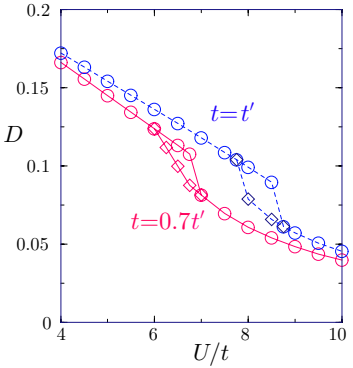
Application: the Mott transition (ED)

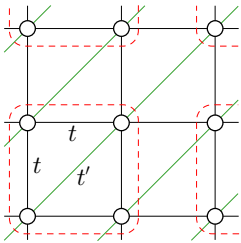


solutions from M. Balzer et al., Europhys. Lett. 85, 17002 (2009)

First-order character of the Mott transition (CDMFT)

- The Mott transition is seen in CDMFT as a hysteresis of the double occupancy
- This shows up nicely in a simulation of BEDT organic superconductors





B. Kyung, A.M.S. Tremblay, Phys. Rev. Lett. **97**, 046402 (2006)

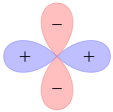
Digression: Superconductivity

- Superconductivity is described by pairing fields:

$$\Delta = \sum_{r,r'} \Delta_{rr'} c_{r\uparrow} c_{r'\downarrow} + \text{H.c}$$

- s-wave pairing: $\Delta_{rr'} = \delta_{rr'}$
- $d_{x^2-y^2}$ pairing:

$$\Delta_{rr'} = \begin{cases} 1 & \text{if} \quad r - r' = \pm x \\ -1 & \text{if} \quad r - r' = \pm y \end{cases}$$



- d_{xy} pairing:

$$\Delta_{rr'} = \begin{cases} 1 & \text{if} \quad r - r' = \pm(x + y) \\ -1 & \text{if} \quad r - r' = \pm(x - y) \end{cases}$$

- Pairing fields are introduced in the bath, and measured on the cluster

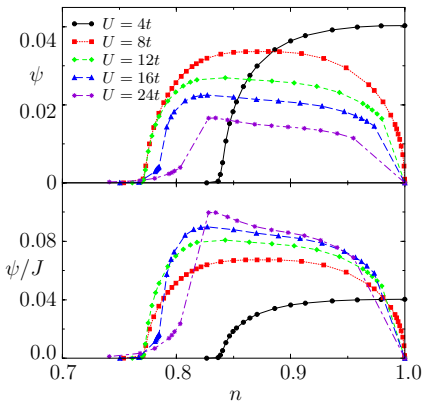
Digression: Superconductivity (cont.)

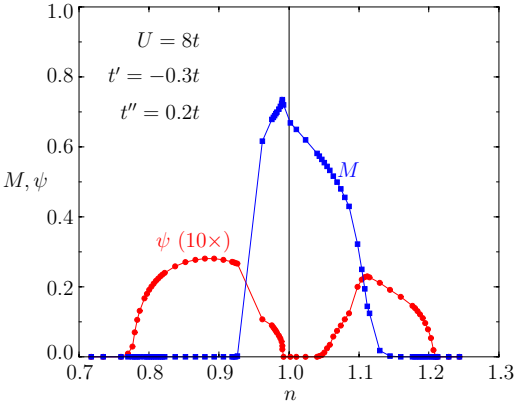
- Pairing fields violate particle number conservation
- The Hilbert space is enlarged to encompass all particle numbers with a given total spin
- Use the **Nambu formalism**: a particle-hole transformation on the spin-down sector: $c_{\alpha\downarrow} \rightarrow c^{\dagger}_{\alpha\downarrow}$ and $a_{r\downarrow} \rightarrow a^{\dagger}_{r\downarrow}$
- Structure of the one-body matrix:

$$\begin{array}{c} \\ c_\uparrow \\ a_\uparrow \\ c^\dagger_\downarrow \\ a^\dagger_\downarrow \end{array} \begin{pmatrix} \boldsymbol{t}_\uparrow & \boldsymbol{\theta}_\uparrow & 0 & 0 \\ \boldsymbol{\theta}^\dagger_\uparrow & \boldsymbol{\varepsilon}_\uparrow & 0 & \Delta_b \\ 0 & 0 & -\boldsymbol{t}_\downarrow & -\boldsymbol{\theta}_\downarrow \\ 0 & \Delta^\dagger_b & -\boldsymbol{\theta}^\dagger_\downarrow & -\boldsymbol{\varepsilon}_\downarrow \end{pmatrix}$$

Application: dSC and AF in the 2D Hubbard model

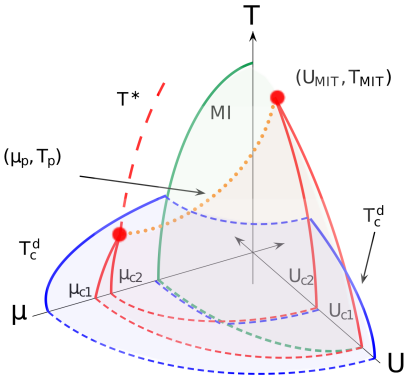
- Nine bath parameters
- Homogeneous coexistence of $d_{x^2-y^2}$ SC and Néel AF

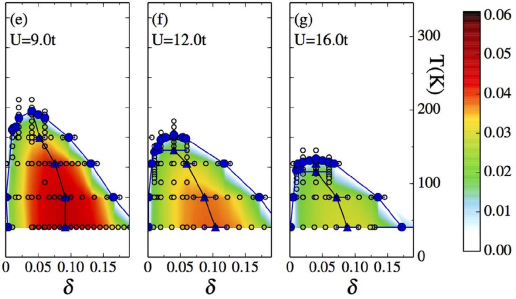




Kancharla et al., Phys. Rev. B 77 184516 (2008).

Mott transition and superconductivity





Fratino et al, Scientific Reports **6**, 22715 (2016)

Sordi et al., Phys. Rev. Lett. **108** (2012), 216401

Mott transition and superconductivity (cont.)

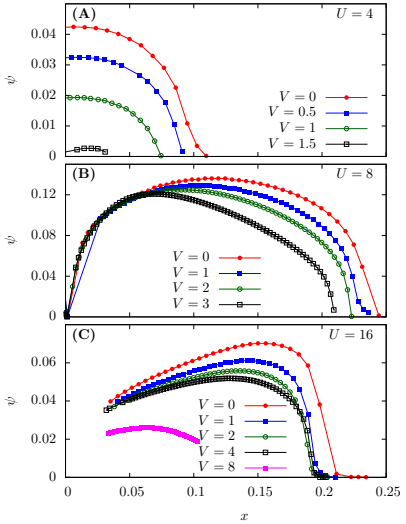
- First-order, finite-doping transition with finite-T critical point: correlated metal vs pseudogap phase.
- The pseudogap phenomenon is related to the Widom line in first-order transitions
- Even though the SC order parameter is suppressed by the Mott transition, T_c isn't
- Results obtained with an efficient CT-QCM-HYB solver.

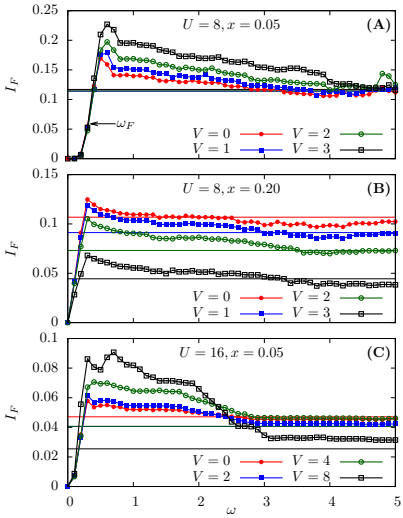
Application: Resilience of dSC to extended interactions

$$H = \sum_{r,r',\sigma} t_{r,r'} c^{\dagger}_{r\sigma} c_{r'\sigma} + U \sum_{r} n_{r\uparrow} n_{r\downarrow} + \sum_{r \neq r'} V_{rr'} n_r n_{r'} - \mu \sum_{r,\sigma} n_{r,\sigma}$$

- Question: effect of NN repulsion V on dSC in the 2D Hubbard model?
  - V is a priori detrimental to dSC (pair breaking effect), and larger than J.
  - But: V increases J.
- Exact treatment of V within the cluster; Hartree approximation between clusters.
- Result: a moderate V has no effect on dSC at low doping.
- The retarded nature of the effective pairing interaction is important.

Resilience of dSC to extended interactions (cont.)

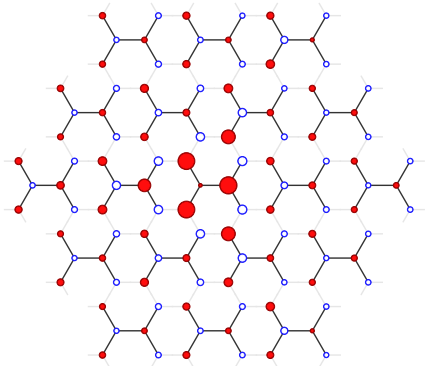


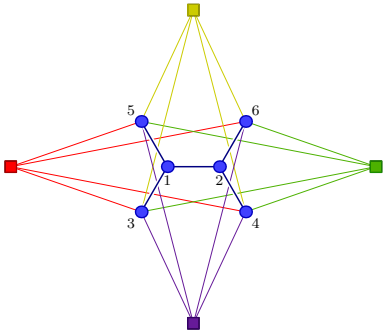


Sénéchal et al., Phys. Rev. B **87**, 075123 (2013).

Non-magnetic impurity in graphene

$$\mathbb{G}^{-1}(\tilde{k},z) = z - \mathbb{t}(\tilde{k}) - (z) = \begin{pmatrix} z - \boldsymbol{t}_{11}(\tilde{k}) - \boldsymbol{\Sigma}_1(z) & -\boldsymbol{t}_{12}(\tilde{k}) & -\boldsymbol{t}_{13}(\tilde{k}) & \dots & -\boldsymbol{t}_{1M}(\tilde{k}) \\ -\boldsymbol{t}_{21}(\tilde{k}) & z - \boldsymbol{t}_{22}(\tilde{k}) - \boldsymbol{\Sigma}_2(z) & -\boldsymbol{t}_{23}(\tilde{k}) & \dots & -\boldsymbol{t}_{2M}(\tilde{k}) \\ -\boldsymbol{t}_{31}(\tilde{k}) & -\boldsymbol{t}_{32}(\tilde{k}) & z - \boldsymbol{t}_{33}(\tilde{k}) - \boldsymbol{\Sigma}_3(z) & \dots & -\boldsymbol{t}_{3M}(\tilde{k}) \\ \vdots & \vdots & \vdots & \ddots & \vdots \\ -\boldsymbol{t}_{M1}(\tilde{k}) & -\boldsymbol{t}_{M2}(\tilde{k}) & -\boldsymbol{t}_{M3}(\tilde{k}) & \dots & z - \boldsymbol{t}_{MM}(\tilde{k}) - \boldsymbol{\Sigma}_M(z) \end{pmatrix}$$





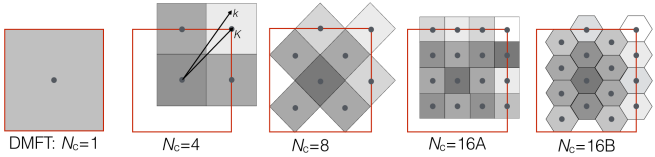
M. Charlebois et al., Phys. Rev. B**91**, 35132 (2015).

The Dynamical Cluster Approximation

- Based on periodic clusters
- The hybridization function is diagonal in $\boldsymbol{K}$ (cluster momentum):

$$\Gamma_K(i\omega_n) = \sum_r^{N_b} \frac{|\theta_{Kr}|^2}{i\omega_n - \varepsilon_r}$$

- The Brillouin zone may be tiled into patches:



Th. Maier, in `http://www.cond-mat.de/events/correl15`

Th. Maier et al., Rev. Mod. Phys. **77**, 1027 (2005).

The Dynamical Cluster Approximation (cont.)

- self-consistency condition:

$$\frac{1}{i\omega_n - \bar{t}_{\boldsymbol{K}} - \Gamma_{\boldsymbol{K}}(\omega) - \Sigma_{\boldsymbol{K}}(\omega)} = \frac{L}{N}\sum_{\tilde{\boldsymbol{k}}} \frac{1}{i\omega_n - \varepsilon(\tilde{\boldsymbol{k}} + \boldsymbol{K}) - \Sigma_{\boldsymbol{K}}(\omega)}$$

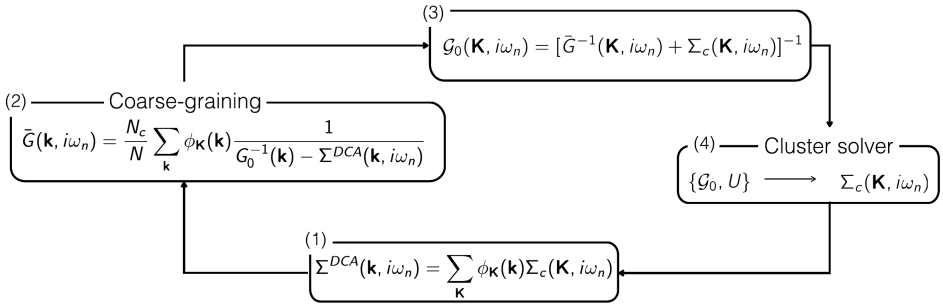
  where

$$\bar{t}_{\boldsymbol{K}} = \frac{L}{N}\sum_{\tilde{\boldsymbol{k}}} \varepsilon(\tilde{\boldsymbol{k}} + \boldsymbol{K})$$

- Not derivable from the Self-energy functional approach
- For large clusters:
  - DCA converges better for $\boldsymbol{k} = 0$ (average) quantities
  - CDMFT converges better for $\boldsymbol{r} = 0$ (local) quantities

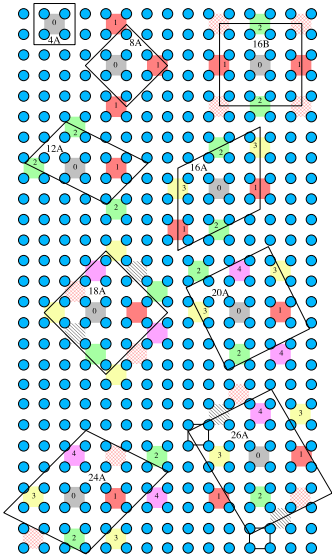
The DCA procedure

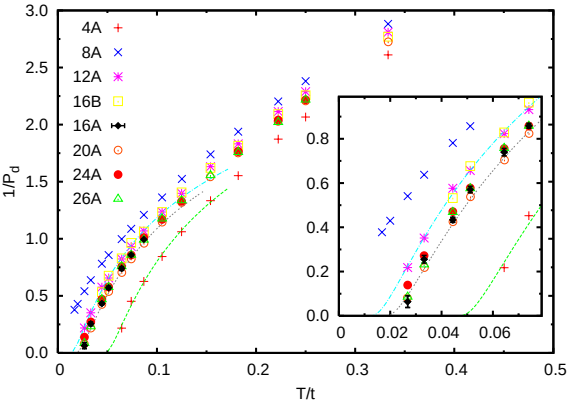
Patch function $\phi_{\mathbf{K}}(\mathbf{k}) = 1$ if $\mathbf{k}$ is in patch around $\mathbf{K}$, zero otherwise.



Th. Maier, in http://www.cond-mat.de/events/correl15

DCA on superconductivity





Maier et al., Phys. Rev. Lett. **95**, 237001 (2005).

QUESTIONS ?