Quantum Cluster Methods (CPT/CDMFT)

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Outline

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The Hubbard model

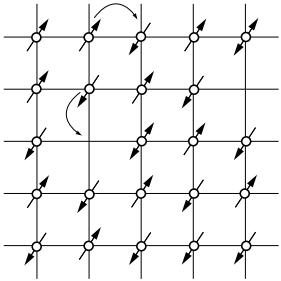
Hamiltonian:

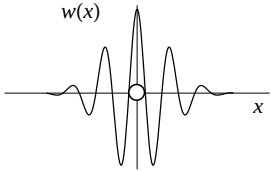
hopping amplitude ↙ ↘ number of spin ↑ electrons at r

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

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:

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

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

(eigenstate with $N+1$ particles)

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

(eigenstate with $N-1$ particles)

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:

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

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

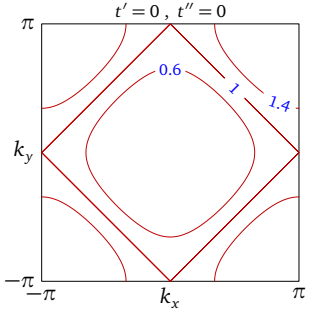
prob. of electron with $\varepsilon = E_r - E_0$

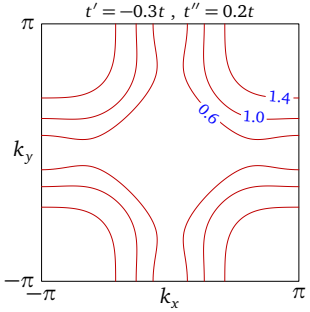
prob. of hole with $\varepsilon = E_r - E_0$

non-interacting limit ($U = 0$)

$$|\Omega\rangle = \prod_{\epsilon_{\boldsymbol{k}} < \mu} c^\dagger_{\boldsymbol{k}} |0\rangle \qquad \text{(Fermi sea)}$$

$$\boldsymbol{G}(z) = \frac{1}{z - \boldsymbol{t}} \qquad G(z, \boldsymbol{k}) = \frac{1}{z - \varepsilon_{\boldsymbol{k}}} \qquad \varepsilon_{\boldsymbol{k}} = \sum_{\boldsymbol{r}} t_{0,\boldsymbol{r}} e^{-i\boldsymbol{k}\cdot\boldsymbol{r}}$$

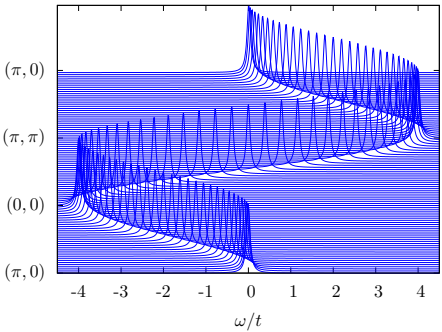




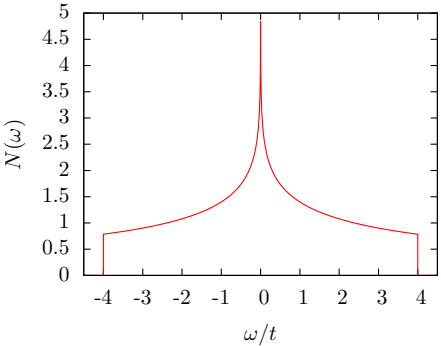
non-interacting limit (cont.)

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:

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

↳ self-energy

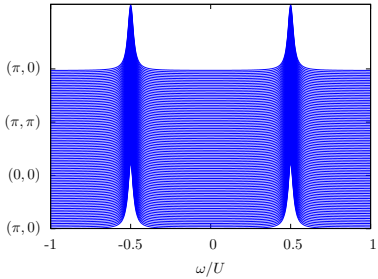
Local limit at half-filling ($\boldsymbol{t} = 0$, $\mu = U/2$):

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

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

Analytic structure:

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



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

Outline

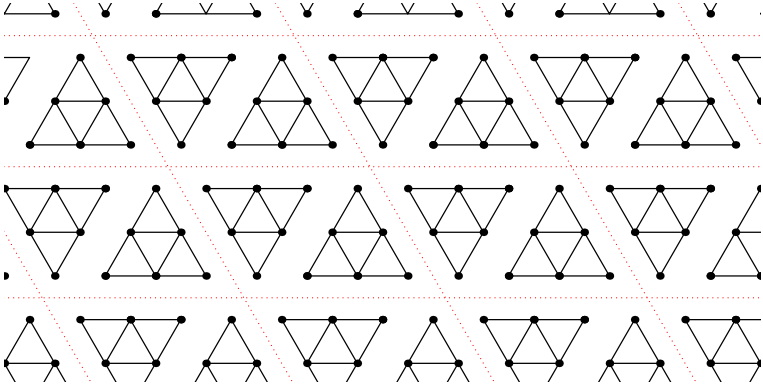
Real-space cluster methods: General idea

- 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:

$$\boldsymbol{t} = \begin{pmatrix} \boldsymbol{t}^{(1,1)} & \boldsymbol{t}^{(1,2)} & \cdots & \boldsymbol{t}^{(1,n)} \\ \boldsymbol{t}^{(2,1)} & \boldsymbol{t}^{(2,2)} & \cdots & \boldsymbol{t}^{(2,n)} \\ \vdots & \vdots & \ddots & \vdots \\ \boldsymbol{t}^{(n,1)} & \boldsymbol{t}^{(n,2)} & \cdots & \boldsymbol{t}^{(n,n)} \end{pmatrix}$$

$$\boldsymbol{t} = \boldsymbol{t}' + \boldsymbol{t}_{\mathrm{ic}}$$

→ 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:

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

→ inter-cluster blocks

Cluster Perturbation Theory (cont.)

lattice Hamiltonian ← → cluster Hamiltonian

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

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

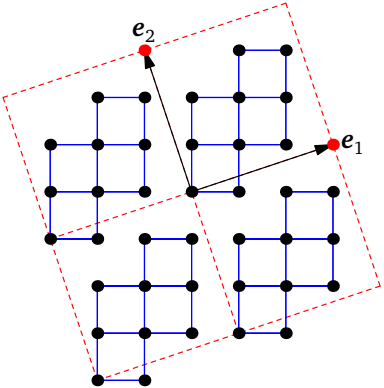
$$\boldsymbol{G}^{-1}(z) = \boldsymbol{G}'^{-1}(z) - \boldsymbol{t}_{\rm ic}$$

→ cluster Green function matrix

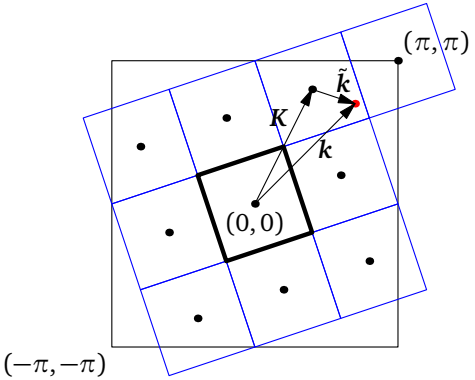
C. Gros and R. Valenti, Phys. Rev. B **48**, 418 (1993)

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

Green function and $\boldsymbol{t}_{\text{ic}}$ diagonal in $\tilde{\boldsymbol{k}}$.
$\boldsymbol{G}'$ independent of $\boldsymbol{k}$.
CPT formula 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:

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

complete superlattice cluster

Various representations of the annihilation operator

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

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

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 $\boldsymbol{k}$:

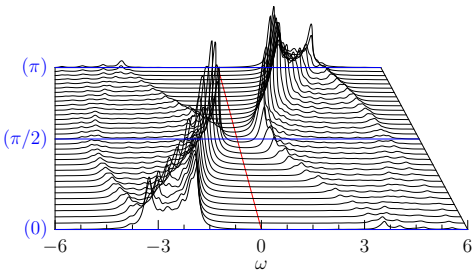
$$c(\tilde{\boldsymbol{k}} + \boldsymbol{K}) = \Lambda_{\boldsymbol{K},\boldsymbol{K}'}(\tilde{\boldsymbol{k}}) c_{\boldsymbol{K}'}(\tilde{\boldsymbol{k}})$$

Periodization

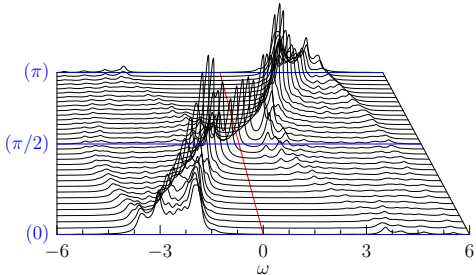
- CPT breaks translation invariance, which needs to be restored:

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

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



Green function periodization



Self-energy periodization

Periodization (2)

- Periodization as a change of basis:

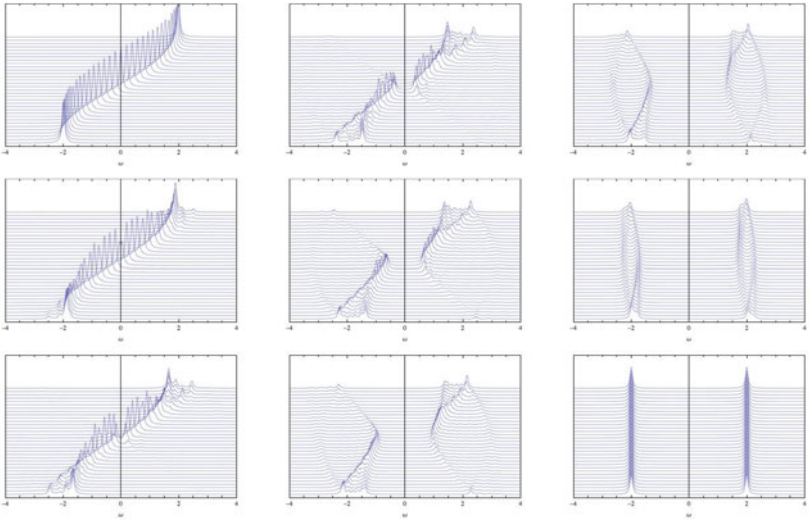
$$
\begin{aligned}
G(\tilde{\boldsymbol{k}}+\boldsymbol{K},\tilde{\boldsymbol{k}}+\boldsymbol{K}',z) &= \left(\boldsymbol{\Lambda}^{c}(\tilde{\boldsymbol{k}})\boldsymbol{G}(z)\boldsymbol{\Lambda}^{c\dagger}(\tilde{\boldsymbol{k}})\right)_{\boldsymbol{K}\boldsymbol{K}'} \\
&= \frac{1}{L^2}\sum_{\boldsymbol{R},\boldsymbol{R}',\boldsymbol{K}_1,\boldsymbol{K}_1'} e^{-i(\tilde{\boldsymbol{k}}+\boldsymbol{K}-\boldsymbol{K}_1)\cdot\boldsymbol{R}} e^{i(\tilde{\boldsymbol{k}}+\boldsymbol{K}'-\boldsymbol{K}_1')\cdot\boldsymbol{R}'} G_{\boldsymbol{K}_1\boldsymbol{K}_1'}(z) \\
&= \frac{1}{L}\sum_{\boldsymbol{R},\boldsymbol{R}'} e^{-i(\tilde{\boldsymbol{k}}+\boldsymbol{K})\cdot\boldsymbol{R}} e^{i(\tilde{\boldsymbol{k}}+\boldsymbol{K}')\cdot\boldsymbol{R}'} G_{\boldsymbol{R}\boldsymbol{R}'}(\tilde{\boldsymbol{k}},z)
\end{aligned}
$$

- Set $\boldsymbol{K}=\boldsymbol{K}'$: the spectral function is a partial trace and thus involves diagonal elements only
- Replace $\tilde{\boldsymbol{k}}$ by $\boldsymbol{k}=\tilde{\boldsymbol{k}}+\boldsymbol{K}$ in $G_{\boldsymbol{R}\boldsymbol{R}'}(\tilde{\boldsymbol{k}},z)$, which leaves $\boldsymbol{t}_{\rm ic}(\tilde{\boldsymbol{k}})$ unchanged
- Since this is a change of basis, analytic properties are still OK.

Outline

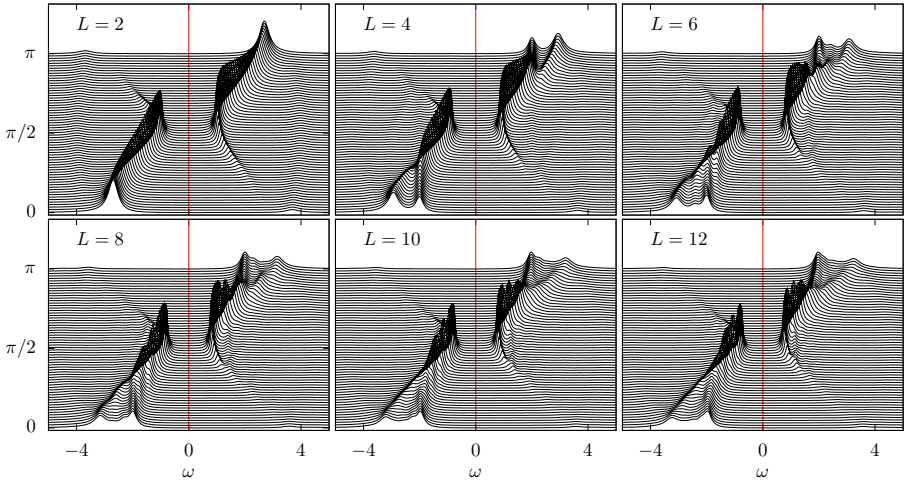
One-dimensional example

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



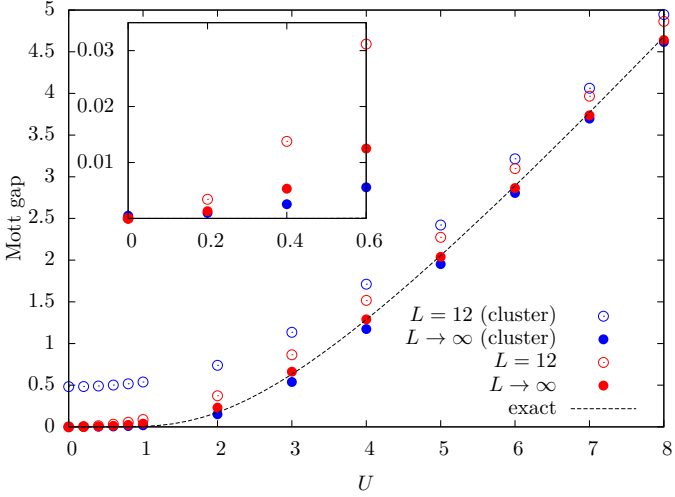
One-dimensional example (cont.)

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

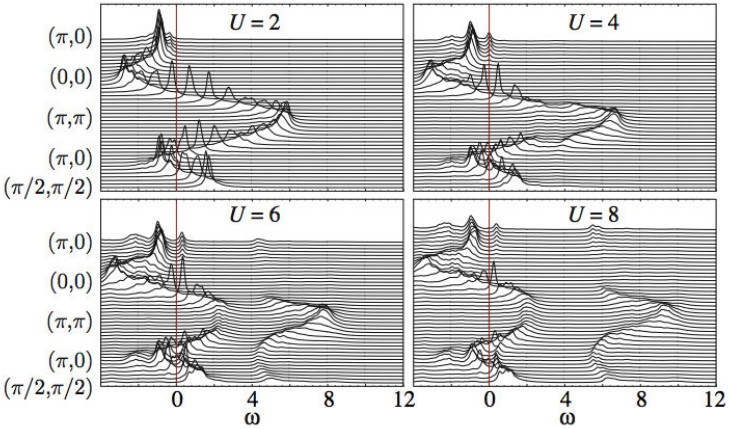


One-dimensional example (cont.)

Spectral gap at half-filling: periodic cluster vs CPT



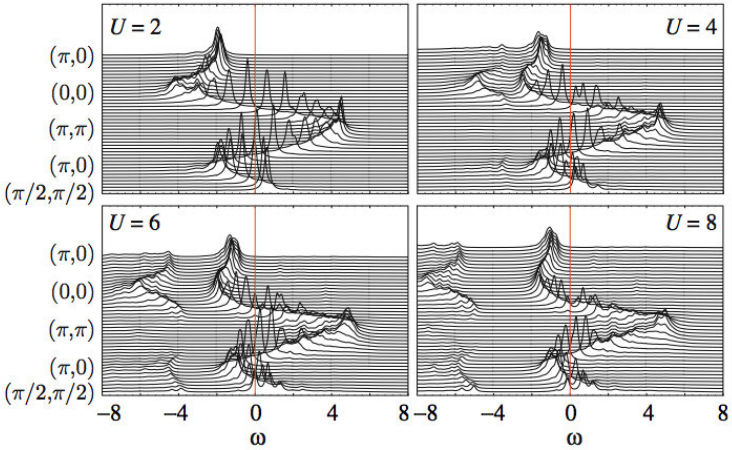
Application: Pseudogap in h-doped cuprates



2D Hubbard model, $t' = -0.3t$, $t'' = 0.2t$, 3×4 cluster, $n = 5/6$

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

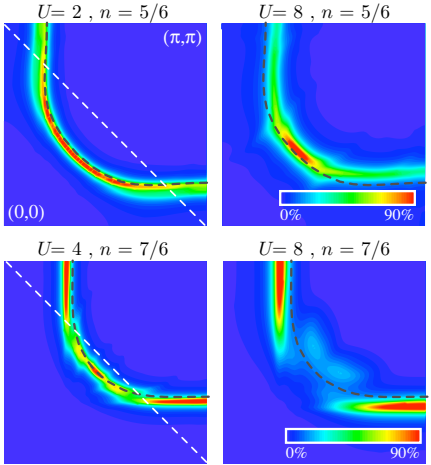
Application: Pseudogap in e-doped cuprates



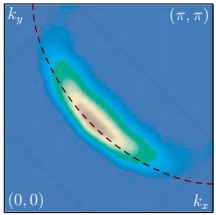
2D Hubbard model, $t' = -0.3t$, $t'' = 0.2t$, 3×4 cluster, $n = 7/6$

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

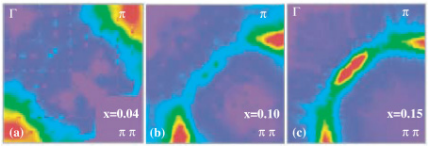
Application: Fermi surface maps



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



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



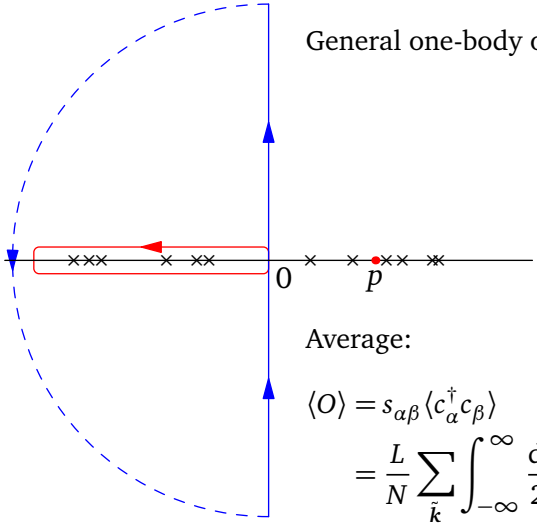
N.P. Armitage et al., PRL **88**, 257001 (2002)

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

Averages of one-body operators



General one-body operator:

$$O = \sum_{\alpha,\beta} s_{\alpha\beta} c_\alpha^\dagger c_\beta$$

$$s^\dagger = s$$

Average:

$$\langle O \rangle = s_{\alpha\beta} \langle c_\alpha^\dagger c_\beta \rangle$$

$$= \frac{L}{N} \sum_{\tilde{\boldsymbol{k}}} \int_{-\infty}^{\infty} \frac{\mathrm{d}\omega}{2\pi} \,\mathrm{Re}\left\{ \mathrm{tr}\big[\boldsymbol{s}(\tilde{\boldsymbol{k}}) \boldsymbol{G}(\tilde{\boldsymbol{k}}, i\omega)\big] - \frac{\mathrm{tr}\boldsymbol{s}(\tilde{\boldsymbol{k}})}{i\omega - p} \right\}$$

Outline

The dynamical mean field

Action formalism: $Z = \int \prod_\alpha [\mathrm{d}c_\alpha \mathrm{d}\bar{c}_\alpha] e^{iS[c,\bar{c}]}$

interaction

$$S[c,\bar{c}] = \int dt \left\{ \sum_{\alpha,\beta} \bar{c}_\alpha(t)(i\delta_{\alpha\beta}\partial_t - t_{\alpha\beta})c_\beta(t) - H_1(c,\bar{c}) \right\}$$

$$= \int dt\, dt' \left\{ \sum_{\alpha,\beta} \bar{c}_\alpha(t) G^{-1}_{0,\alpha\beta}(t-t')c_\beta(t') - H_1(c,\bar{c})\delta(t-t') \right\}$$

intra cluster ← → inter cluster

$$S = \sum_j S^{(j)} + \sum_{i,j} S^{(i,j)} \qquad \sum_{i\in\Gamma} S^{(i,j)} \to S^{(j)}_{\text{env.}}$$

The hybridization function

$$S_{\rm eff}[c,\bar{c}] = \int d\,t\,d\,t' \sum_{\alpha,\beta} \bar{c}_\alpha(t) \mathscr{G}^{-1}_{0,\alpha\beta}(t-t') c_\beta(t') + \int d\,t\, H_1(c,\bar{c})$$

$$\mathscr{G}_0^{-1}(\omega) = \omega - \boldsymbol{t}_c - \boldsymbol{\Gamma}(\omega)$$

The hybridization function has the analytic structure of a self-energy:

$$\Gamma_{\alpha\beta}(z) = \sum_r^{N_b} \frac{\theta_{\alpha r}\theta^*_{\beta r}}{z-\varepsilon_r}$$

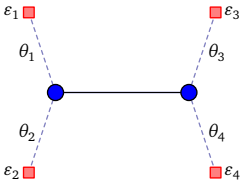
(the constant piece $\boldsymbol{\Gamma}^\infty$ is dropped in CDMFT)
N_b is potentially infinite.

The Anderson impurity model

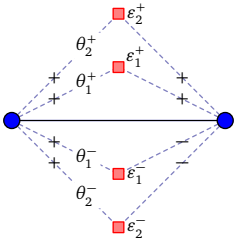
hybridization ↩ ↪ bath energy

$$H_{\mathrm{AIM}} = \sum_{\alpha,\beta} t_{c,\alpha\beta} c_\alpha^\dagger c_\beta + \sum_{\alpha,r} \left(\theta_{\alpha r} c_\alpha^\dagger a_r + \mathrm{H.c.} \right) + \sum_{r}^{N_b} \varepsilon_r a_r^\dagger a_r + H_1$$

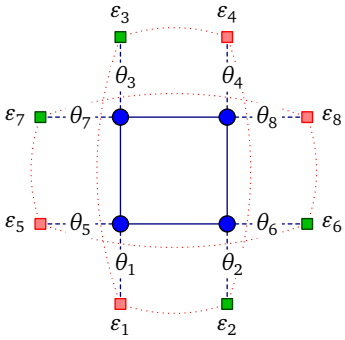
↪ bath annihilation operator



(A)



(B)



(C)

The Anderson impurity model (cont.)

Non interacting Green function (cluster+bath): $\boldsymbol{G}_0^{\text{full}}(z) = \dfrac{1}{z - \boldsymbol{T}}$

where $\boldsymbol{T} = \begin{pmatrix} \boldsymbol{t}_c & \boldsymbol{\theta} \\ \boldsymbol{\theta}^\dagger & \boldsymbol{\varepsilon} \end{pmatrix}$

$$\left(\boldsymbol{G}_0^{\text{full}}(z)\right)^{-1} = \begin{pmatrix} z - \boldsymbol{t}_c & -\boldsymbol{\theta} \\ -\boldsymbol{\theta}^\dagger & z - \boldsymbol{\varepsilon} \end{pmatrix} = \begin{pmatrix} A_{11} & A_{12} \\ A_{21} & A_{22} \end{pmatrix} = \begin{pmatrix} B_{11} & B_{12} \\ B_{21} & B_{22} \end{pmatrix}^{-1}$$

Need to extract the cluster component of $\boldsymbol{G}_0^{\text{full}}(z)$, i.e. B_{11}:

$$A_{11}B_{11} + A_{12}B_{21} = \mathbf{1} \qquad B_{21} = -A_{22}^{-1}A_{21}B_{11}$$

$$\left(A_{11} - A_{12}A_{22}^{-1}A_{21}\right)B_{11} = \mathbf{1}$$

$$\boldsymbol{G}_{0c}^{-1} = z - \boldsymbol{t}_c - \boldsymbol{\Gamma}(z) \qquad \boldsymbol{\Gamma}(z) = \boldsymbol{\theta}\,\frac{1}{z - \boldsymbol{\varepsilon}}\,\boldsymbol{\theta}^\dagger$$

The Anderson impurity model (cont.)

Interacting case: one must simply add the cluster self-energy (no self-energy on the bath). The cluster Green function is then

$$\begin{aligned} \boldsymbol{G}_c^{-1}(z) &= z - \boldsymbol{t}_c - \boldsymbol{\Gamma}(z) - \boldsymbol{\Sigma}(z) \\ &= \boldsymbol{\mathscr{G}}_0^{-1}(z) - \boldsymbol{\Sigma}(z) \end{aligned}$$

The self-consistency condition

The local, cluster Green function $\boldsymbol{G}_c$ must be consistent with the projection $\bar{\boldsymbol{G}}$ to the cluster of the lattice Green function:

$$\bar{\boldsymbol{G}}(z) = \frac{L}{N} \sum_{\tilde{\boldsymbol{k}}} \left[z - \boldsymbol{t}(\tilde{\boldsymbol{k}}) - \boldsymbol{\Sigma}(z) \right]^{-1}$$

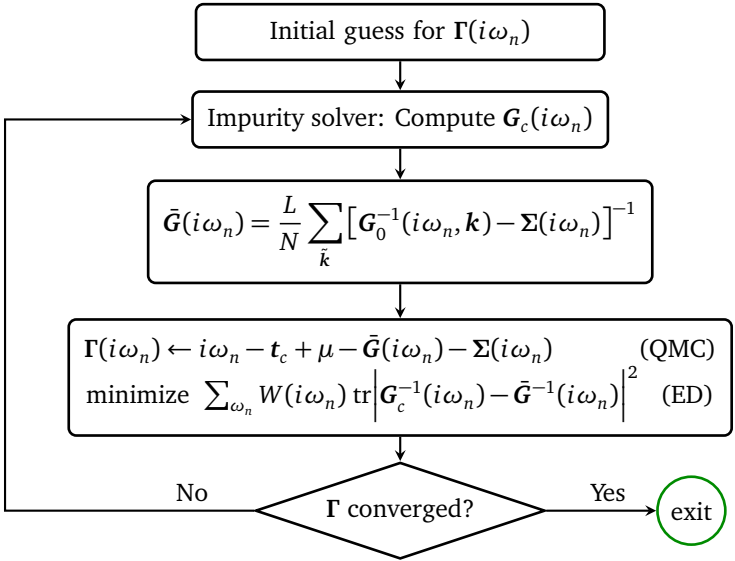
This condition may be statisfied (up to statistical errors) in QMC.
It can only be satisfied approximately in ED (i.e. with a finite bath).
Instead, one minimizes the distance function:

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

weight

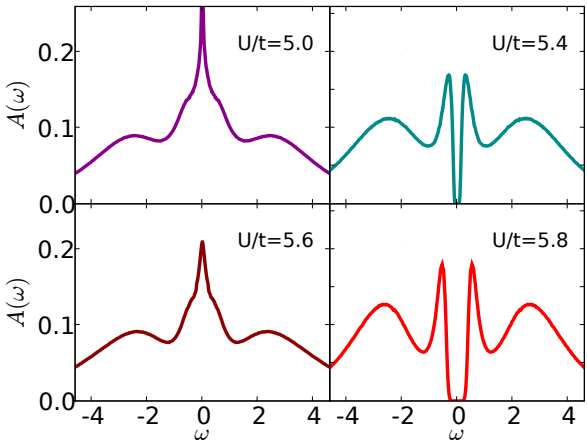
Matsubara freqs from a fictitious temperature β^{-1}

The CDMFT algorithm



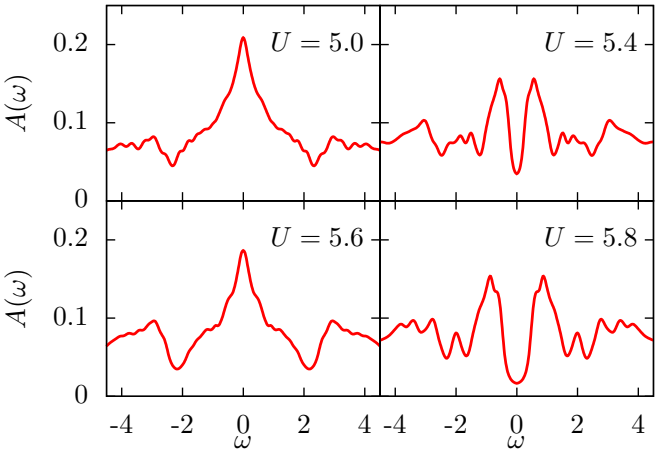
Outline

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)

Superconductivity

Pairing operator:

$$\hat{\Psi} = \frac{1}{N} \sum_{r,r'} g_{rr'} \left[c_{r\uparrow} c_{r'\downarrow} - c_{r\downarrow} c_{r'\uparrow} \right] \ .$$

In momentum space:

$$\hat{\Psi} = \frac{1}{N} \sum_{\boldsymbol{k}} g(\boldsymbol{k}) \left[c_\uparrow(\boldsymbol{k}) c_\downarrow(-\boldsymbol{k}) - c_\downarrow(\boldsymbol{k}) c_\uparrow(-\boldsymbol{k}) \right]$$

with the correspondence

$$g(\boldsymbol{k}) = \sum_{\boldsymbol{r}} g_{\boldsymbol{r},0} \ e^{-i\boldsymbol{k}\cdot\boldsymbol{r}}$$

Gorkov function:

$$F_{rr'}(z) = \langle \Omega | c_{r\uparrow} \frac{1}{z - H + E_0} c_{r'\downarrow} | \Omega \rangle + \langle \Omega | c_{r'\downarrow} \frac{1}{z + H - E_0} c_{r\uparrow} | \Omega \rangle$$

Trick: The Nambu formalism

Particle-hole transformation on the down spin: $d_{\boldsymbol{r}\sigma} = (c_{\boldsymbol{r}\uparrow}, c^\dagger_{\boldsymbol{r}\downarrow})$

Anticommutation relations OK : $\{d_{\boldsymbol{r}\sigma}, d^\dagger_{\boldsymbol{r}'\sigma'}\} = \delta_{\boldsymbol{r}\boldsymbol{r}'}\delta_{\sigma\sigma'}$

Pairing operator:

$$\hat{\Psi} = \frac{1}{N}\sum_{\boldsymbol{r},\boldsymbol{r}'} g_{\boldsymbol{r}\boldsymbol{r}'}\left[d_{\boldsymbol{r}\uparrow}d^\dagger_{\boldsymbol{r}'\downarrow} - d^\dagger_{\boldsymbol{r}\downarrow}d_{\boldsymbol{r}'\uparrow}\right]$$

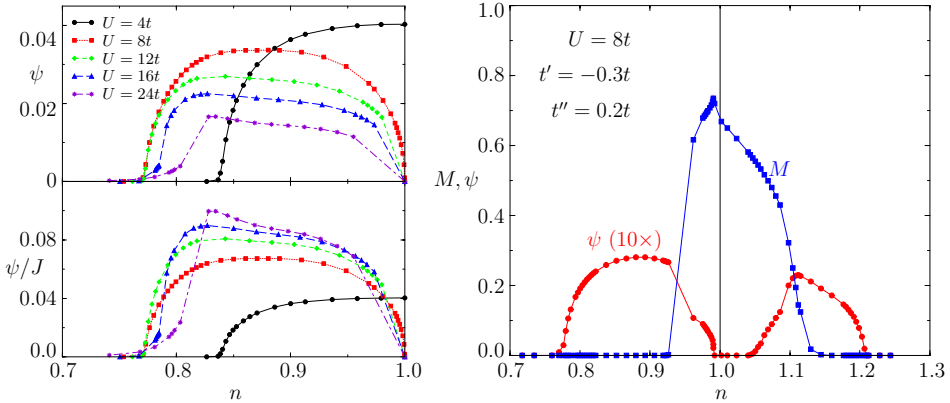
Gorkov function is off-diagonal block of Green function:

$$\boldsymbol{G}(z) = \begin{pmatrix} \boldsymbol{G}_\uparrow(z) & \boldsymbol{F}(z) \\ \boldsymbol{F}^\dagger(z) & -\boldsymbol{G}_\downarrow(z) \end{pmatrix}$$

Structure of the one-body matrix:

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

Superconductivity in the square-lattice Hubbard model



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

Inhomogeneous systems (many distinct clusters)

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

$$= \begin{pmatrix} z - \boldsymbol{t}^{(11)}(\tilde{\boldsymbol{k}}) - \boldsymbol{\Sigma}_1(z) & -\boldsymbol{t}^{(12)}(\tilde{\boldsymbol{k}}) & \dots & -\boldsymbol{t}^{(1n)}(\tilde{\boldsymbol{k}}) \\ -\boldsymbol{t}^{(21)}(\tilde{\boldsymbol{k}}) & z - \boldsymbol{t}^{(22)}(\tilde{\boldsymbol{k}}) - \boldsymbol{\Sigma}_2(z) & \dots & -\boldsymbol{t}^{(2n)}(\tilde{\boldsymbol{k}}) \\ \vdots & \vdots & \ddots & \vdots \\ -\boldsymbol{t}^{(n1)}(\tilde{\boldsymbol{k}}) & -\boldsymbol{t}^{(n2)}(\tilde{\boldsymbol{k}}) & \dots & z - \boldsymbol{t}^{(nn)}(\tilde{\boldsymbol{k}}) - \boldsymbol{\Sigma}_n(z) \end{pmatrix}$$

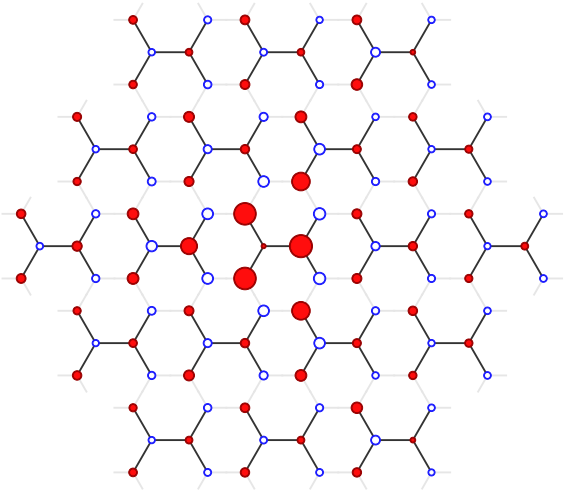
Distance function in that case:

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

→ G.F. of the j^{th} cluster

↳ j^{th} diagonal block of $\bar{\boldsymbol{G}}$

Non-magnetic impurity in graphene



$U = 12t$, $\epsilon_0 = 11t$

M. Charlebois et al., Phys. Rev. B 91, 035132 (2015)

Extended interactions: Dynamical Hartree Approximation

Extended interaction:

$$H_V = \frac{1}{2}\sum_{r,r'} V_{r'r} n_{r'} n_r = \frac{1}{2}\sum_{r,r'} V^{\mathrm{c}}_{r,r'} n_r n_{r'} + \frac{1}{2}\sum_{r,r'} V^{\mathrm{ic}}_{r,r'} n_r n_{r'}$$

V^{c}: intra cluster; V^{ic}: inter cluster

Dynamical Hartree Approximation:

$$\frac{1}{2}\sum_{r,r'} V^{\mathrm{ic}}_{r,r'} n_r n_{r'} \to \hat{V}^{\mathrm{ic}} = \frac{1}{2}\sum_{r,r'} V^{\mathrm{ic}}_{r,r'} (\bar{n}_r n_{r'} + n_r \bar{n}_{r'} - \bar{n}_r \bar{n}_{r'})$$

Set $n_r = \bar{n}_r + \delta n_r$, then neglect the term quadratic in fluctuations $\delta n_r \delta n_{r'}$

CDMFT : Conclusion

- Approximation scheme for the one-body Green function with exact short-range correlations and self-consistency
- Allows for broken symmetry phases (magnetism, superconductivity)
- Takes into account time-domain fluctuations better than spatial fluctuations
- Controlled by the size of the cluster (and size of the bath, in ED).
- But:
  - Restricted to small clusters for practical reasons
  - Clusters are not practical for incommensurate order
  - Two-body operators and fluctuations not well described (cluster only)

THANK YOU!

QUESTIONS ?