Dynamical Mean Field Theory
and
Quantum Cluster Methods

David Sénéchal

Département de physique
Université de Sherbrooke

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Outline

Introduction
Dynamical Mean Field Theory
Cluster Perturbation Theory
Cluster Dynamical Mean Field Theory
The self-energy functional approach
Exact Diagonalizations
Outline

Introduction
Dynamical Mean Field Theory
Cluster Perturbation Theory
Cluster Dynamical Mean Field Theory
The self-energy functional approach
Exact Diagonalizations
Strong correlations

- DFT fails to correctly describe ground state
- Failure of band theory or, more generally, the Fermi liquid picture
- Interactions lead to broken symmetry states
- Time fluctuations are important
  → frequency dependence of self-energy.
- Physics of Mott insulators and phases close to them
The Hubbard model

\[ H = \sum_{r, r', \sigma} t_{r, r'} c_{r\sigma}^{\dagger} c_{r'\sigma} + U \sum_{r} n_{r\uparrow} n_{r\downarrow} - \mu \sum_{r, \sigma} n_{r, \sigma} \]

- Hopping amplitude \( \leftarrow \)
- Creation operator \( \leftarrow \)
- Number of spin up electrons at \( r \) \( \rightarrow \)
- Repulsion \( \rightarrow \)
- Chemical potential \( \rightarrow \)
non-interacting limit \((U = 0)\)

\[
G(\omega, k) = \frac{1}{\omega - \epsilon_k + \mu}
\]

\[
\epsilon_k = \sum_r t_{0,r} e^{-i \mathbf{k} \cdot \mathbf{r}}
\]
non-interacting limit (cont.)

spectral function, half-filling, NN hopping only.

associated density of states
scaling: $t_{ij} = t/\sqrt{2d}$

$$\varepsilon_k = -\frac{t}{\sqrt{2d}} \sum_{i=1}^{d} \cos k_i$$

Each cosine term has standard deviation $1/\sqrt{2}$. Density of states (central limit theorem) is $d$-independent:

$$N(\omega) = \frac{1}{t\sqrt{2\pi}} e^{-\omega^2/2t}$$
Local limit \((t = 0)\)

\[
G(\omega) = \frac{1/2}{\omega + U/2} + \frac{1/2}{\omega - U/2} = \frac{1}{\omega - \frac{U^2}{4\omega}}
\]

\[
\Sigma(\omega) = \frac{U^2}{4\omega} + \frac{U}{2}
\]

Spectral function of the half-filled HM at \(t = 0\).
Outline

Introduction

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

**Cluster Perturbation Theory**

**Cluster Dynamical Mean Field Theory**

**The self-energy functional approach**

**Exact Diagonalizations**
## Approximation schemes

<table>
<thead>
<tr>
<th>Hartree-Fock</th>
<th>DMFT</th>
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<tbody>
<tr>
<td>▶ $\Sigma(\omega, k) \to \Sigma(\infty, k)$ is frequency-independent</td>
<td>▶ $\Sigma(\omega, k) \to \Sigma(\omega)$ is momentum-independent</td>
</tr>
<tr>
<td>▶ Can be absorbed in new dispersion relation $\epsilon'(k)$</td>
<td>▶ System still fundamentally interacting</td>
</tr>
<tr>
<td>▶ Approximation equivalent to new one-body Hamiltonian</td>
<td>▶ Approximated by single site with effective medium</td>
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The cavity method

\[ S[c_{i\sigma}, c_{i\sigma}^\dagger] = \int_0^\beta d\tau \left\{ \sum_{i,\sigma} c_{i\sigma}^\dagger \partial_\tau c_{i\sigma} - \sum_{i,j,\sigma} t_{ij} c_{i\sigma}^\dagger c_{j\sigma} - \mu \sum_{i,\sigma} n_{i\sigma} + U \sum_i n_{i\uparrow} n_{i\downarrow} \right\} \]

\[ \frac{1}{Z_{\text{eff.}}} e^{-S_{\text{eff.}}[c_{0\sigma}, c_{0\sigma}^\dagger]} = \frac{1}{Z} \int \prod_{i \neq 0,\sigma} \mathcal{D}c_{i\sigma} \mathcal{D}c_{i\sigma}^\dagger e^{-S} \] (1)
The cavity method (cont.)

Effective action (exact form, spin indices suppressed):

\[
S_{\text{eff.}} = S_0 + \sum_{n=1}^{\infty} \sum_{i_1,\ldots,i_n} \int d\tau \eta_{i_1}^\dagger \cdots \eta_{i_n}^\dagger \eta_{j_1} \cdots \eta_{j_n} G_{i_1 \cdots j_n}^{\text{env.}}(\tau_{i_1} \cdots \tau_{i_n}, \tau_{j_1} \cdots \tau_{j_n})
\]

where \( \eta_i = t_{i0}c_{i0} \) acts like a source field and

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

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

DMFT approximation:

\[
S_{\text{eff.}} = S_0 + \sum_{i,j} t_{0i} t_{0j} \int d\tau \ d\tau' c_0^\dagger(\tau)c_0(\tau')G_{i,j}^{\text{env.}}(\tau, \tau')
\]
The cavity method (cont.)

Effective action:

\[ S_{\text{eff.}} = \int d\tau\ d\tau' \ c_0^\dagger(\tau) G_0^{-1}(\tau - \tau') c_0(\tau') + U \int_0^\beta d\tau\ n_0^\uparrow n_0^\downarrow \]

\[ G_0^{-1}(i\omega_n) = i\omega_n + \mu - \sum_{i,j} t_{0i} t_{0j} G_{i,j}^\text{env.}(i\omega_n) \]

- \( G_{i,j}^\text{env.}(i\omega_n) \) unknown.
  Rather, treat \( G_0^{-1} \) 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

- $G_0$ has the analytic properties of a Green function: poles on the real axis and positive residues.
- Could be represented by a (quasi-infinite) set of poles:
  \[ G_0^{-1}(i\omega_n) = i\omega_n + \mu - \Gamma(i\omega_n) \]
  \[ \Gamma(i\omega_n) = \sum_r \frac{\theta_r^2}{i\omega_n - \epsilon_r} \quad \text{(hybridization function)} \]
- Interacting Green function of the effective theory for the “impurity” site:
  \[ G_{\text{imp.}}(i\omega_n) = \frac{1}{i\omega_n + \mu - \Gamma(i\omega_n) - \Sigma(i\omega_n)} \]
Hamiltonian representation

$G_{\text{imp.}}$ can be obtained from the following Hamiltonian:

$$H_{\text{imp.}} = \sum_{r=1}^{N_b} \theta_r \left( c_0^\dagger a_r + \text{H.c.} \right) + \sum_{r=1}^{N_b} \epsilon_r a_r^\dagger a_r - \mu c_0^\dagger c_0 + U n_0^\uparrow n_0^\downarrow$$

\[\text{hyb. amplitude} \quad \rightarrow \quad \text{bath orbital} \quad \rightarrow \quad \text{bath energy}\]

One-body matrix:

$$T = \begin{pmatrix} -\mu & \theta^{\dagger} [1 \times N_b] \\ \theta [N_b \times 1] & \epsilon [N_b \times N_b] \end{pmatrix}$$
Proof ($U = 0$)

\[ G_{\text{full}}^{-1}(\omega) = i\omega_n - T = \begin{pmatrix} A_{11} & A_{12} \\ A_{21} & A_{22} \end{pmatrix} \]

Need to compute \( G = B_{11} \), where

\[
\begin{pmatrix} A_{11} & A_{12} \\ A_{21} & A_{22} \end{pmatrix} \begin{pmatrix} B_{11} & B_{12} \\ B_{21} & B_{22} \end{pmatrix} = 1
\]

or

\[
A_{11}B_{11} + A_{12}B_{21} = 1 \quad A_{21}B_{11} + A_{22}B_{21} = 0
\]

\[
B_{21} = -A_{22}^{-1}A_{21}B_{11} \implies \left[A_{11} - A_{12}A_{22}^{-1}A_{21}\right] B_{11} = 1
\]
therefore

\[ B_{11}^{-1} = G^{-1} = i \omega_n - \mu - \theta \frac{1}{i \omega_n - \epsilon} \theta^\dagger \]

\[ = i \omega_n - \mu - \Gamma(i \omega_n) \]

where

\[ \Gamma(i \omega_n) = \theta \frac{1}{i \omega_n - \epsilon} \theta^\dagger = \sum_{r=1}^{N_b} \frac{\theta_r^2}{i \omega_n - \epsilon_r} \]

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

\[ G_{\text{imp.}}(i \omega_n) = \frac{1}{i \omega_n + \mu - \Gamma(i \omega_n) - \Sigma(i \omega_n)} \]
The self-consistency condition

- Full Green function in the DMFT approximation:

\[ G(i\omega_n, k) = \frac{1}{i\omega_n - \varepsilon(k) + \mu - \Sigma(i\omega_n)} \]

- The local Green function

\[ \bar{G}(i\omega_n) = \frac{1}{N} \sum_k G(i\omega_n, k) \]

must coincide with \( G_{\text{imp.}}(i\omega_n) \):

\[ \bar{G}(i\omega_n)^{-1} = i\omega_n + \mu - \Gamma(i\omega_n) - \Sigma(i\omega_n) \]

\[ = G_0^{-1}(i\omega_n) - \Sigma(i\omega_n) \]
The DMFT self-consistency loop

Initial guess for $\Gamma(i\omega_n)$

Impurity solver: Compute $G_{\text{imp.}}(i\omega_n)$

\[
\tilde{G}(i\omega_n) = \frac{1}{N} \sum_k \left[ G_0^{-1}(i\omega_n, k) - \Sigma(i\omega_n) \right]^{-1}
\]

$\Gamma(i\omega_n) \rightarrow i\omega_n + \mu - \tilde{G}(i\omega_n) - \Sigma(i\omega_n)$

$\Gamma$ converged? Yes exit

No
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 $H_{\text{imp.}}$)
    Hence self-consistency relation only approximately satisfied
  - real-frequency information
  - zero temperature
- Other real frequency methods: CI and natural basis, etc.
The DMFT self-consistency loop (discrete bath version)

1. Start with a guess value of \((\theta_r, \epsilon_r)\).
2. Calculate the impurity Green function \(G_{\text{imp}}(i\omega_n)\) (ED).
3. Calculate the superlattice-averaged Green function

\[
\bar{G}(i\omega_n) = \sum_k \frac{1}{G_0^{-1}(k) - \Sigma(i\omega_n)} \quad \text{and} \quad \mathcal{G}_0^{-1}(i\omega_n) = \bar{G}^{-1} + \Sigma(i\omega_n)
\]

4. Minimize the following \textbf{distance function}:

\[
d(\theta, \epsilon) = \sum_{\omega_n} W(i\omega_n) \text{tr} \left| G_{\text{imp}}^{-1}(i\omega_n) - \bar{G}^{-1}(i\omega_n) \right|^2
\]

over the set of bath parameters. Thus obtain a new set \((\theta_r, \epsilon_r)\).
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.


$N(\omega)$ for the half-filled 3D Hubbard model.

Exact diagonalization solver.

The Mott transition (cont.)

$N(\omega)$ in the 2D, half-filled Hubbard model.

Exact diagonalization solver with $N_b = 5$. 
Antiferromagnetic order in cold atom systems with harmonic trap

\[ H = \sum_{\mathbf{r}, \mathbf{r}', \sigma} t_{\mathbf{r}, \mathbf{r}'} c_{\mathbf{r}\sigma}^{\dagger} c_{\mathbf{r}'\sigma} + U \sum_{\mathbf{r}} n_{\mathbf{r}\uparrow} n_{\mathbf{r}\downarrow} - \sum_{\mathbf{r}, \sigma} \left( V_r - \mu \right) n_{\mathbf{r}, \sigma} \]

Outline

Introduction

Dynamical Mean Field Theory

Cluster Perturbation Theory
  kinematics
  periodization
  Applications

Cluster Dynamical Mean Field Theory

The self-energy functional approach

Exact Diagonalizations
Clusters and superlattices

10-site cluster

Reduced Brillouin zone
CPT Green function

\[ H = H' + V \]

\[ t = t' + V \]

- Treat \( V \) at lowest order in Perturbation theory
- At this order, the Green function is

\[ G^{-1}(\omega) = G'^{-1}(\omega) - V \]


Interlude: Fourier transforms

Unitary matrices performing Fourier transforms:

\[
U_{k,r} = \frac{1}{\sqrt{N}} e^{-i k \cdot r} \quad V_{\tilde{k}\tilde{r}} = \sqrt{\frac{L}{N}} e^{-i \tilde{k} \cdot \tilde{r}} \quad W_{K,R} = \frac{1}{\sqrt{L}} e^{-i K \cdot R}
\]

complete \quad superlattice \quad cluster

Various representations of the annihilation operator

\[
c(k) = \sum_r U_{kr} c_r \quad c_K(\tilde{k}) = \sum_{\tilde{r}, R} V_{\tilde{k}\tilde{r}} W_{KR} c_{\tilde{r}+R}
\]

\[
c_R(\tilde{k}) = \sum_{\tilde{r}} V_{\tilde{k}\tilde{r}} c_{\tilde{r}+R} \quad c_{\tilde{r}, K} = \sum_R W_{KR} c_{\tilde{r}+R}
\]

Caveat: \( U \neq V \otimes W \)

The matrix \( \Lambda = U(V \otimes W)^{-1} \) relates \((K, \tilde{k})\) to \(k\):

\[
c(\tilde{k} + K) = \Lambda_{K,K'}(\tilde{k}) c_{K'}(\tilde{k})
\]
More accurate notation:

\[ G^{-1}(\tilde{k}, \omega) = G'^{-1}(\omega) - V(\tilde{k}) \]

But

\[ G'^{-1} = \omega - t' - \Sigma \]
\[ G_0^{-1} = \omega - t' - V \]

Thus: The lattice self-energy is approximated as the cluster self-energy

\[ G^{-1}(\tilde{k}, \omega) = G_0^{-1}(\tilde{k}, \omega) - \Sigma(\omega) \]

Example: 2-site cluster (1D):

\[ t' = -t \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix} \quad V(\tilde{k}) = -t \begin{pmatrix} 0 & e^{-2i\tilde{k}} \\ e^{2i\tilde{k}} & 0 \end{pmatrix} \]
Periodization

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

\[ G_{\text{cpt}}(k, \omega) = \frac{1}{L} \sum_{R,R'} e^{-i k \cdot (R-R')} G_{RR'}(\tilde{k}, \omega). \]

- Periodizing (1D case, 12-site cluster):

Green function periodization

Self-energy periodization
Periodization (2)

\[ G_{KK'}(\tilde{k}, \omega) = W_{KR} W_{K'R'}^* G_{RR'}(\tilde{k}, \omega) \quad \text{or} \quad G \rightarrow WGW^\dagger \]

Converted to the full wavevector basis \((k = K + \tilde{k})\) with \(\Lambda:\)

\[ G(\tilde{k} + K, \tilde{k} + K') = \left( \Lambda(\tilde{k}) G \Lambda^\dagger(\tilde{k}) \right)_{KK'} \]

\[ = \frac{1}{L^2} \sum_{R,R',K_1,K_1'} e^{-i(\tilde{k}+K-K_1) \cdot R} e^{i(\tilde{k}+K'-K_1') \cdot R'} G_{K_1K_1'} \]

\[ = \frac{1}{L} \sum_{R,R'} e^{-i(\tilde{k}+K) \cdot R} e^{i(\tilde{k}+K') \cdot R'} G_{RR'}(\tilde{k}, \omega). \]

Then set \(K = K'.\)

Replace \(\tilde{k}\) by \(k = \tilde{k} + K\) in \(G_{RR'}(\tilde{k}, \omega)\), since \(V(\tilde{k})\) is unchanged when \(\tilde{k}\) is shifted by a reciprocal superlattice vector.

\[ G_{\text{per.}}(k, \omega) = \frac{1}{L} \sum_{RR'} e^{-ik \cdot (R-R')} G_{RR'}(k, \omega) \]
One-dimensional example

Evolution of spectral function with increasing $U/t$: 
Averages of one-body operators

General one-body operator:

\[ O = s_{\alpha\beta} c_\alpha^\dagger c_\beta \quad s^\dagger = s \]

Average:

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

\[ = \frac{L}{N} \sum_{\tilde{k}} \int_0^\infty \frac{d\omega}{\pi} \text{Re} \left\{ \text{tr} \left[ s(\tilde{k}) G(\tilde{k}, i\omega) \right] - \frac{\text{tr} s(\tilde{k})}{i\omega - p} \right\} \]
Application: Pseudogap in h-doped cuprates

Application: Pseudogap in e-doped cuprates

Application: Fermi surface maps

\[ U = 2, \, n = \frac{5}{6} \]
\[ U = 8, \, n = \frac{5}{6} \]
\[ U = 4, \, n = \frac{7}{6} \]
\[ U = 8, \, n = \frac{7}{6} \]


Kitaev-Hubbard model on a honeycomb lattice:

\[
H = \sum_{\langle i,j \rangle} \left\{ c_i^{\dagger} \left( \frac{t + t' \sigma^\alpha}{2} \right) c_j + \text{H.c.} \right\} + U \sum_i n_{i\uparrow} n_{i\downarrow}
\]
Interacting topological insulators (cont.)
CPT : features

- 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.

$\Rightarrow$ A first step towards CDMFT or VCA
Outline

Introduction

Dynamical Mean Field Theory

Cluster Perturbation Theory

Cluster Dynamical Mean Field Theory
  The hybridization function
  The CDMFT self-consistency condition

Applications
  The Dynamical Cluster Approximation (DCA)

The self-energy functional approach

Exact Diagonalizations
Generalization of DMFT to small clusters

- $H_{\text{imp.}} \rightarrow H'$
- Simple adaptation of DMFT
- Scalar equations → matrix equations

Dynamical mean field $G_0$:

$$S_{\text{eff}}[c, c^*] = \int_0^\beta d\tau \, d\tau' \sum_{\alpha, \beta} c_\alpha^*(\tau) G_{0,\alpha\beta}^{-1}(\tau - \tau') c_\beta(\tau') + \int_0^\beta d\tau \, H_1(c, c^*)$$
The hybridization function

In the frequency domain:

\[ G_0^{-1}(i\omega_n) = i\omega_n - t' - \Gamma(i\omega_n) \quad \text{where} \quad G_0(i\omega_n) = \int_0^\beta e^{i\omega_n\tau} G_0(\tau) \]

Spectral representation of \( \Gamma \):

\[ \Gamma_{\alpha\beta}(i\omega_n) = \sum_r \frac{\theta_{ar} \theta_{\beta r}^*}{i\omega_n - \epsilon_r} = \theta \frac{1}{i\omega_n - \epsilon} \theta^\dagger \]

Corresponding Hamiltonian: Anderson impurity model

\[ H' = \sum_{\alpha,\beta} t'_{\alpha\beta} c_{\alpha}^\dagger c_{\beta} + U \sum_i n_{i\uparrow} n_{i\downarrow} + \sum_{r,\alpha} \theta_{r\alpha}(c_{\alpha}^\dagger a_r + \text{H.c.}) + \sum_r \epsilon_r a_r^\dagger a_r \]
Discrete bath systems

The CDMFT Procedure (discrete bath)

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

\[
\tilde{G}(\omega) = \sum_{\tilde{k}} \frac{1}{G^{-1}_{0}(\tilde{k}) - \Sigma(\omega)} \quad \text{and} \quad G^{-1}_{0}(\omega) = \tilde{G}^{-1} + \Sigma(\omega)
\]

4. Minimize the following distance function:

\[
d(\theta, \epsilon) = \sum_{\omega_n} W(i\omega_n) \text{tr} \left| G'^{-1}(i\omega_n) - \tilde{G}^{-1}(i\omega_n) \right|^2
\]

over the set of bath parameters. Thus obtain a new set \((\theta_{\alpha r}, \epsilon_r)\).
5. Go back to step (2) until convergence.
The CDMFT self-consistency loop

Initial guess for $\Gamma(i\omega_n)$

Impurity solver: Compute $G'(i\omega_n)$

\[
\tilde{G}(i\omega_n) = \frac{L}{N} \sum_k \left[ G_0^{-1}(i\omega_n, k) - \Sigma(i\omega_n) \right]^{-1}
\]

$\Gamma(i\omega_n) \rightarrow i\omega_n - t' + \mu - \tilde{G}(i\omega_n) - \Sigma(i\omega_n)$ (QMC)

minimize $\sum_{\omega_n} W(i\omega_n) \text{tr} \left| G'^{-1}(i\omega_n) - \tilde{G}^{-1}(i\omega_n) \right|^2$ (ED)

$\Gamma$ converged?

No

Yes → exit
Digression: Superconductivity

- Superconductivity is described by pairing fields:
  \[
  \Delta = \sum_{r,r'} \Delta_{rr'} c_r^\uparrow c_{r'}^\downarrow + \text{H.c}
  \]

- \textit{s-wave pairing: } \Delta_{rr'} = \delta_{rr'}

- \textit{d}_{x^2-y^2} pairing:
  \[
  \Delta_{rr'} = \begin{cases} 
  1 & \text{if } r - r' = \pm x \\
  -1 & \text{if } r - r' = \pm y 
  \end{cases}
  \]

- \textit{d}_{xy} pairing:
  \[
  \Delta_{rr'} = \begin{cases} 
  1 & \text{if } r - r' = \pm (x+y) \\
  -1 & \text{if } r - r' = \pm (x-y) 
  \end{cases}
  \]

- Pairing fields are introduced in the bath, and measured on the cluster
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: $c_{\alpha \downarrow} \rightarrow c_{\alpha \downarrow}^\dagger$ and $a_{r \downarrow} \rightarrow a_{r \downarrow}^\dagger$

Structure of the one-body matrix:

$$\begin{pmatrix}
c_{\uparrow} & \theta_{\uparrow} & 0 & 0 \\
\theta_{\uparrow}^\dagger & \epsilon_{\uparrow} & 0 & \Delta_b \\
c_{\downarrow}^\dagger & 0 & -t_{\downarrow} & -\theta_{\downarrow} \\
a_{\downarrow}^\dagger & \Delta_b^\dagger & -\theta_{\downarrow}^\dagger & -\epsilon_{\downarrow}
\end{pmatrix}$$
Application: dSC and AF in the 2D Hubbard model

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

![Graphs showing the coexistence of different parameters](image)

Effect of the distance function

▶ What weights $W(i\omega_n)$ to use?
▶ $W \sim 1/\omega$ better in the underdoped region
▶ Sharp cutoff better in the overdoped region

Application: The Mott transition

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

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

\[ U/t \]

\[ D \]

\[ t = t' \]

\[ t = 0.7t' \]

Mott transition and superconductivity


P. Sémon et al., ArXiv:1402.7087
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

\[ H = \sum_{r,r',\sigma} t_{r,r'} c_{r\sigma}^\dagger c_{r'\sigma} + U \sum_r n_{r\uparrow} n_{r\downarrow} + \sum_{r\neq r'} V_{rr'} n_{r\uparrow} n_{r'\downarrow} - \mu \sum_r n_{r,\sigma} \]

▶ 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.)

The Dynamical Cluster Approximation

- Based on periodic clusters
- Self-consistency condition:

\[
\frac{1}{i\omega_n - \tilde{t}_K - \Gamma_K(\omega) - \Sigma_K(\omega)} = \frac{L}{N} \sum_{\tilde{k}} \frac{1}{i\omega_n - \epsilon(\tilde{k} + K) - \Sigma_K(\omega)}
\]

where

\[
\tilde{t}_K = \frac{L}{N} \sum_{\tilde{k}} \epsilon(\tilde{k} + K)
\]

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

DCA on superconductivity

Outline

Introduction

Dynamical Mean Field Theory

Cluster Perturbation Theory

Cluster Dynamical Mean Field Theory

The self-energy functional approach
  The variational principle
  Calculating the Potthoff functional
  The Variational Cluster Approximation

Optimization
  Thermodynamic consistency

Applications
  The (Cluster) Dynamical Impurity Approximation

Exact Diagonalizations
Motivation

- CPT cannot describe broken symmetry states, because of the finite cluster size
- Idea: add a Weiss field term to the cluster Hamiltonian \( H' \), e.g., for antiferromagnetism:

\[
H'_M = M \sum_a e^{iQ \cdot r_a} (n_{a\uparrow} - n_{a\downarrow})
\]

- This term favors AF order, but does not appear in \( H \), and must be subtracted from \( V \) (\( H = H' + V \))
- Need a principle to set the value of \( M \): energy minimization?
- Better: Potthoff’s self-energy functional approach
The Luttinger-Ward functional

- Luttinger-Ward (or Baym-Kadanoff) functional:

\[ \Phi[G] = \cdots + \frac{\delta\Phi[G]}{\delta G} \delta G + \cdots \]

- Relation with self-energy:

\[ \frac{\delta\Phi[G]}{\delta G} = \Sigma \]

- Legendre transform:

\[ F[\Sigma] = \Phi[G] - \text{Tr} (\Sigma G) \]

\[ \frac{\delta F[\Sigma]}{\delta \Sigma} = \frac{\delta\Phi[G]}{\delta G} \frac{\delta G[\Sigma]}{\delta \Sigma} - \Sigma \frac{\delta G[\Sigma]}{\delta \Sigma} - G = -G \]

The variational principle

- Free energy functional:

\[ \Omega_t[\Sigma] = F[\Sigma] - \text{Tr} \ln(-G_{0t}^{-1} + \Sigma) \]

- Stationary at the physical self-energy (Euler equation):

\[ \frac{\delta \Omega_t[\Sigma]}{\delta \Sigma} = -G + (G_{0t}^{-1} - \Sigma)^{-1} = 0 \]

- At the physical self-energy \( \Sigma^* \), \( \Omega_t[\Sigma^*] = \text{grand potential} \)

- Approximation strategies with variational principles:
  - Type I: Simplify the Euler equation
  - Type II: Approximate the functional (Hartree-Fock, FLEX)
  - Type III: Restrict the variational space, but keep the functional exact
To evaluate $F$, use its universal character: its functional form depends only on the interaction.

Introduce a reference system $H'$, which differs from $H$ by one-body terms only (example: the cluster Hamiltonian).

Suppose $H'$ can be solved exactly. Then, at the physical self-energy $\Sigma$ of $H'$,

$$\Omega' = F[\Sigma] + \text{Tr} \ln(-G')$$

by eliminating $F$:

$$\Omega_t[\Sigma] = \Omega' - \text{Tr} \ln(-G') - \text{Tr} \ln(-G_{0t}^{-1} + \Sigma)$$

$$= \Omega' - \text{Tr} \ln(-G') + \text{Tr} \ln(-G)$$

$$= \Omega' - \text{Tr} \ln(-G') - \text{Tr} \ln(-G'^{-1} + V)$$

$$= \Omega' - \text{Tr} \ln(1 - VG')$$
The Potthoff functional

- Making the trace explicit, one finds
  \[ \Omega_t[\Sigma] = \Omega' - T \sum_{\omega} \sum_{\tilde{k}} \text{tr} \ln \left[ 1 - V(\tilde{k})G'(\tilde{k}, \omega) \right] \]
  \[ = \Omega' - T \sum_{\omega} \sum_{\tilde{k}} \ln \det \left[ 1 - V(\tilde{k})G'(\tilde{k}, \omega) \right] \]

- The sum over frequencies is to be performed over Matsubara frequencies (or an integral along the imaginary axis at \( T = 0 \)).
- The variation is done over one-body parameters of the cluster Hamiltonian \( H' \)
- In the above example, the solution is found when \( \partial \Omega / \partial M = 0 \).
Calculating the functional I : exact form

▶ It can be shown that

\[ \text{Tr } \ln(-G) = -T \sum_m \ln(1 + e^{-\beta \omega_m}) + T \sum_m \ln(1 + e^{-\beta \zeta_m}) \]

▶ Use the Lehmann representation of the GF:

\[ G'_{\alpha\beta}(\omega) = \sum_r Q_{\alpha r} Q^*_{\beta r} \sqrt{\frac{1}{\omega - \omega_r}} \]

\[ G'(\omega) = Q \frac{1}{\omega - \Lambda} Q^\dagger \]

Calculating the functional $I$ : exact form (2)

- A similar representation holds for the CPT Green function

$$G(\tilde{k}, \omega) = \frac{1}{G^{-1} - V(\tilde{k})} = \frac{1}{[Q \frac{1}{\omega - \Lambda} Q^\dagger]^{-1} - V(\tilde{k})}$$

$$= Q \frac{1}{\omega - L(\tilde{k})} Q^\dagger \quad L(\tilde{k}) = \Lambda + Q^\dagger V(\tilde{k}) Q$$

- Let $\omega_r(\tilde{k})$ be the eigenvalues of $L(\tilde{k})$, i.e., the poles of $G(\tilde{k}, \omega)$. Then

$$\Omega(x) = \Omega'(x) - \sum_{\omega'_r < 0} \omega'_r + \frac{L}{N} \sum \sum \omega_r(\tilde{k})$$

Note: the zeros of $G'$ and $G$ are the same, since they have the same self-energy.

Calculating the functional II: numerical integral

Except for very small clusters ($L \sim 4$), it is much faster to perform a numerical integration over frequencies:

$$\Omega(\mathbf{x}) = \Omega'(\mathbf{x}) - \int_{0}^{\infty} \frac{d\omega}{\pi} \frac{L}{N} \sum_{\tilde{k}} \ln \left| \det (1 - V(\tilde{k}) G'(i\omega)) \right| - L(\mu - \mu')$$

The integral must be done using an adaptive method that refines a mesh where necessary.

For instance: The CUBA library [http://www.feynarts.de/cuba/](http://www.feynarts.de/cuba/)

Grid of 17,095 points used in an adaptive integration over wavevectors
The variational Cluster Approximation: procedure

1. Set up a superlattice of clusters
2. Choose a set of variational parameters, e.g. Weiss fields for broken symmetries
3. Set up the calculation of the Potthoff functional:
4. Use an optimization method to find the stationary points
   ▶ E.g. the Newton-Raphson method, or a quasi-Newton method
5. Adopt the cluster self-energy associated with the stationary point with the lowest $\Omega$ and use it as in CPT or CDMFT.
6. Adopt the value of $\Omega$ as the best estimate of the grand potential
Need to find the stationary points of $\Omega(x)$ with as few evaluations as possible

Example: the *Newton-Raphson* method:
- Evaluate $\Omega$ at a number of points at and around $x_0$ that just fits a quadratic form
- Move to the stationary point $x_1$ of that quadratic form and repeat
- Stop when $|x_i - x_{i-1}|$, or the numerical gradient $|\nabla \Omega|$, converges
- Not robust: it converges fast when started close enough to the solution, but it can err. . .

Proceed adiabatically through external parameter space (e.g. as function of $U$ or $\mu$)
Example clusters

B10

3 × 4

T9

T15
Thermodynamic consistency

The electron density \( n \) may be calculated either as

\[
    n = \text{Tr} \, G \quad \text{or} \quad n = -\frac{\partial \Omega}{\partial \mu}
\]

The two methods give different results, except if the cluster chemical potential \( \mu' \) is a variational parameter.

2 × 2 cluster

\( U = 8 \)

normal state
VCA vs Mean-Field Theory

- **Differ from Mean-Field Theory:**
  - Interaction is left intact, it is not factorized
  - Retains exact short-range correlations
  - Weiss field $\neq$ order parameter
  - More stringent that MFT
  - Controlled by the cluster size

- **Similarities with MFT:**
  - No long-range fluctuations (no disorder from Goldstone modes)
  - Yet: no LRO for Néel AF in one dimension
  - Need to compare different orders
  - Yet: they may be placed in competition / coexistence
Application: Néel Antiferromagnetism

- Used the Weiss field

\[ H'_M = M \sum_r e^{iQ \cdot r} (n_{r\uparrow} - n_{r\downarrow}) \]

- Profile of \( \Omega \) for the half-filled, square lattice Hubbard model:
Néel Antiferromagnetism (cont.)

Best scaling factor:

\[ q = \frac{\text{number of links}}{2 \times \text{number of sites}} \]
Need to add a pairing field

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

- **s-wave pairing**: \( \Delta_{rr'} = \delta_{rr'} \)

- **\( d_{x^2-y^2} \) pairing**:

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

- **\( d_{xy} \) pairing**:

\[
\Delta_{rr'} = \begin{cases} 
1 & \text{if } r - r' = \pm (x + y) \\
-1 & \text{if } r - r' = \pm (x - y)
\end{cases}
\]
Competing SC and AF orders

One-band Hubbard model for the cuprates: $t' = -0.3, t'' = 0.2, U = 8$:

M. Guillot, MSc thesis, Univ. de Sherbrooke (2007)
Example: Homogeneous coexistence of dSC and AF orders
The (Cluster) Dynamical Impurity Approximation (CDIA)

- The bath parameters ($\epsilon_\mu$, $\theta_{\alpha \mu}$, etc) are variational parameters.
- The bath makes a contribution to the Potthoff functional:

$$\Omega_{\text{bath}} = \sum_{\epsilon_\alpha < 0} \epsilon_\alpha$$

- One can in principle use the same procedure as in VCA.
- ... but in practice it is more difficult.
- The presence of the bath increases the resolution of the approach in the time domain, at the cost of spatial resolution, for a fixed total number of orbitals (cluster + bath).
- Euler equations for the stationary point:

$$\sum_{\omega_n} \text{tr} \left\{ \left[ G'(i\omega_n) - \bar{G}(i\omega_n) \right] \cdot \frac{\partial \Sigma'(i\omega_n)}{\partial \theta} \right\} = 0.$$
The 1D Hubbard model

(A)

(B)

(C)

(D)

(E)

(F)
Ground state energy as a function of doping ($U = 4t$)

\[ E_0 \text{ sharp, } \langle K + V \rangle, \hspace{1cm} \text{exact} \]

\[ E_0 \text{ sharp, } \Omega + \mu n, \hspace{1cm} \text{SFA} \]
First-order character of the Mott transition (CDIA)

M. Balzer et al., Europhys. Lett. 85, 17002 (2009)
The Mott transition may not show up as first-order in CDMFT, even though it is in the CDIA.

The choice of distance function matters.

Outline

Introduction
Dynamical Mean Field Theory
Cluster Perturbation Theory
Cluster Dynamical Mean Field Theory
The self-energy functional approach

Exact Diagonalizations
  The Hilbert space
  Coding the states
  The Lanczos method
  Calculating the Green function
  Cluster symmetries
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The exact diagonalization procedure

1. Build a basis
2. Construct the Hamiltonian matrix (stored or not)
3. Find the ground state (e.g. by the Lanczos method)
   - Calculate ground state properties (expectation values, etc.)
4. Calculate a representation of the one-body Green function:
   - Continuous-fraction representation
   - Lehmann representation
5. Calculate dynamical properties from the Green function
The Hubbard model on a cluster of size $L$

- $N_{↑}$ and $N_{↓}$ separately conserved in the simple Hubbard model
- Dimension of the Hilbert space (half-filling):
  \[
  d = \left( \frac{L!}{[(L/2)!]^2} \right)^2 \sim 2 \frac{4^L}{\pi L}
  \]
- $L = 16$ : One double-precision vector requires 1.23 GB of memory

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<td>11 778 624</td>
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<tr>
<td>16</td>
<td>165 636 900</td>
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Two-site cluster: Hamiltonian matrix

- Half-filled, two-site Hubbard model: 4 states
- States and Hamiltonian matrix:

\[
\begin{pmatrix}
|01, 01\rangle & \begin{pmatrix} U - 2\mu & -t & -t & 0 \\
-t & -2\mu & 0 & -t \\
-t & 0 & -2\mu & -t \\
0 & -t & -t & U - 2\mu
\end{pmatrix} \\
|01, 10\rangle & \begin{pmatrix} U - 2\mu & -t & -t & 0 \\
-t & -2\mu & 0 & -t \\
-t & 0 & -2\mu & -t \\
0 & -t & -t & U - 2\mu
\end{pmatrix} \\
|10, 01\rangle & \begin{pmatrix} U - 2\mu & -t & -t & 0 \\
-t & -2\mu & 0 & -t \\
-t & 0 & -2\mu & -t \\
0 & -t & -t & U - 2\mu
\end{pmatrix} \\
|10, 10\rangle & \begin{pmatrix} U - 2\mu & -t & -t & 0 \\
-t & -2\mu & 0 & -t \\
-t & 0 & -2\mu & -t \\
0 & -t & -t & U - 2\mu
\end{pmatrix}
\]

spin $\uparrow$ occupation $\leftrightarrow$ spin $\downarrow$ occupation
Six-site cluster: Hamiltonian matrix

Sparse matrix structure
400 × 400
Coding the states

- Tensor product structure of the Hilbert space: \( V = V_{N_{\uparrow}} \otimes V_{N_{\downarrow}} \)
- Dimension:
  
  \[
  d = d(N_{\uparrow})d(N_{\downarrow}) \\
  d(N_{\sigma}) = \frac{L!}{N_{\sigma}!(L - N_{\sigma})!}
  \]

- Example (6 sites):

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<td>15</td>
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<td>1</td>
</tr>
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</table>
Coding the states (2)

- Basis of occupation number eigenstates:

\[ (c_{1\uparrow}^\dagger)^{n_{1\uparrow}} \cdots (c_{L\uparrow}^\dagger)^{n_{L\uparrow}} (c_{1\downarrow}^\dagger)^{n_{1\downarrow}} \cdots (c_{L\downarrow}^\dagger)^{n_{L\downarrow}} |0 \rangle \quad n_{i\sigma} = 0 \text{ or } 1 \]

- Correspondence with binary representation of integers:

\[ b_\sigma = (n_{1\sigma} n_{2\sigma} \cdots n_{L\sigma})_2 \]

- For a given \((N_{\uparrow}, N_{\downarrow})\), we need a direct table:

\[ b_{\uparrow} = B_{\uparrow}(i_{\uparrow}) \quad b_{\downarrow} = B_{\downarrow}(i_{\downarrow}) \]

- …and a reverse table:

\[ i = I_{\uparrow}(b_{\uparrow}) + d_{N_{\uparrow}} I_{\downarrow}(b_{\downarrow}) \quad i_{\uparrow} = i \% d_{N_{\uparrow}} \quad i_{\downarrow} = i / d_{N_{\uparrow}} \]
Constructing the Hamiltonian matrix

- Form of Hamiltonian:

\[ H = K_{\uparrow} \otimes 1 + 1 \otimes K_{\downarrow} + V_{\text{int.}} \]

\[ K = \sum_{a,b} t_{ab} c_a^\dagger c_b \]

- \( K \) is stored in sparse form.
- \( V_{\text{int.}} \) is diagonal and is stored.
- Matrix elements of \( V_{\text{int.}} \): \( \text{bit\_count}(b_{\uparrow} \& b_{\downarrow}) \)
- Two basis states \(|b_{\sigma}\rangle\) and \(|b'_{\sigma}\rangle\) are connected with the matrix \( K \) if their binary representations differ at two positions \( a \) and \( b \).

\[ \langle b'\mid K \mid b \rangle = (-1)^{M_{ab}} t_{ab} \]

\[ M_{ab} = \sum_{c=a+1}^{b-1} n_c \]

- We find it practical to construct and store all terms of the Hamiltonian separately.
The Lanczos method

- Finds the lowest eigenpair by an iterative application of $H$
- Start with random vector $|\phi_0\rangle$
- An iterative procedure builds the Krylov subspace:

$$\mathcal{K} = \text{span}\left\{|\phi_0\rangle, H|\phi_0\rangle, H^2|\phi_0\rangle, \cdots, H^M|\phi_0\rangle\right\}$$

- Lanczos three-way recursion for an orthogonal basis $\{|\phi_n\rangle\}$:

$$|\phi_{n+1}\rangle = H|\phi_n\rangle - a_n|\phi_n\rangle - b_n^2|\phi_{n-1}\rangle$$

$$a_n = \frac{\langle \phi_n | H | \phi_n \rangle}{\langle \phi_n | \phi_n \rangle}, \quad b_n^2 = \frac{\langle \phi_n | \phi_n \rangle}{\langle \phi_{n-1} | \phi_{n-1} \rangle}, \quad b_0 = 0$$
The Lanczos method (2)

- In the basis of normalized states \( |n\rangle = |\phi_n\rangle / \sqrt{\langle \phi_n | \phi_n \rangle} \), the projected Hamiltonian has the tridiagonal form

\[
\begin{pmatrix}
 a_0 & b_1 & 0 & 0 & \cdots & 0 \\
 b_1 & a_1 & b_2 & 0 & \cdots & 0 \\
 0 & b_2 & a_2 & b_3 & \cdots & 0 \\
 \vdots & \vdots & \vdots & \vdots & \ddots & \vdots \\
 0 & 0 & 0 & 0 & \cdots & a_N
\end{pmatrix}
\]

- At each step \( n \), find the lowest eigenvalue of that matrix
- Stop when the estimated Ritz residual \( \| T |\psi\rangle - E_0 |\psi\rangle \| \) is small enough
- Run again to find eigenvector \( |\psi\rangle = \sum_n \psi_n |n\rangle \) as the \( |\phi_n\rangle \)'s are not kept in memory.
The Lanczos method: features

- Required number of iterations: typically from 50 to 200
- Extreme eigenvalues converge first
- Rate of convergence increases with separation between ground state and first excited state
- Cannot resolve degenerate ground states: only one state per ground state manifold is picked up
- If one is interested in low lying states, re-orthogonalization may be required, as orthogonality leaks will occur. But then Lanczos intermediate states need to be stored.
- For degenerate ground states and low lying states (e.g. in DMRG), the Davidson method is generally preferable
The Lanczos method: illustration of the convergence

149 iterations on a matrix of dimension 213,840: eigenvalues of the tridiagonal projection as a function of iteration step
Lanczos method for the Green function

- Zero temperature Green function:

\[ G_{\alpha \beta}(\omega) = G_{\alpha \beta}^{(e)}(\omega) + G_{\alpha \beta}^{(h)}(\omega) \]

\[ G_{\alpha \beta}^{(e)}(\omega) = \langle \Omega | c_{\alpha} \frac{1}{\omega - H + E_0} c_{\beta}^\dagger | \Omega \rangle \]

\[ G_{\alpha \beta}^{(h)}(\omega) = \langle \Omega | c_{\beta}^\dagger \frac{1}{\omega + H - E_0} c_{\alpha} | \Omega \rangle \]

- Consider the diagonal element

\[ |\phi_\alpha\rangle = c_{\alpha}^\dagger |\Omega\rangle \implies G_{\alpha \alpha}^{(e)} = \langle \phi_\alpha | \frac{1}{\omega - H + E_0} | \phi_\alpha \rangle \]

- Use the expansion

\[ \frac{1}{z - H} = \frac{1}{z} + \frac{1}{z^2} H + \frac{1}{z^3} H^2 + \cdots \]
Truncated expansion evaluated exactly in Krylov subspace generated by $|\phi_\alpha\rangle$ if we perform a Lanczos procedure on $|\phi_\alpha\rangle$.

Then $G^{(e)}_{\alpha\alpha}$ is given by a Jacobi continued fraction:

$$G^{(e)}_{\alpha\alpha}(\omega) = \frac{\langle \phi_\alpha | \phi_\alpha \rangle}{\omega - a_0 - \frac{b_1^2}{\omega - a_1 - \frac{b_2^2}{\omega - a_2 - \cdots}}}$$

The coefficients $a_n$ and $b_n$ are stored in memory.

What about non diagonal elements $G^{(e)}_{\alpha\beta}$?

Trick: Define the combination

\[
G_{\alpha\beta}^{(e)+}(\omega) = \langle \Omega | (c_{\alpha} + c_{\beta}) \frac{1}{\omega - H + E_0} (c_{\alpha} + c_{\beta})^\dagger | \Omega \rangle
\]

\[G_{\alpha\beta}^{(e)+}(\omega)\) can be calculated like \(G_{\alpha\alpha}^{(e)}(\omega)\)

Since \(G_{\alpha\beta}(\omega) = G_{\beta\alpha}^{(e)}(\omega)\), then

\[
G_{\alpha\beta}^{(e)}(\omega) = \frac{1}{2} \left[ G_{\alpha\beta}^{(e)+}(\omega) - G_{\alpha\alpha}^{(e)}(\omega) - G_{\beta\beta}^{(e)}(\omega) \right]
\]

Likewise for \(G_{\alpha\beta}^{(h)}(\omega)\)
The Lehmann representation

\[ G_{\alpha\beta}(\omega) = \sum_{m} \frac{\langle \Omega | c_\alpha | m \rangle \langle m | c_\beta^\dagger | \Omega \rangle}{\omega - E_m + E_0} + \sum_{n} \frac{\langle \Omega | c_\beta^\dagger | n \rangle \langle n | c_\alpha | \Omega \rangle}{\omega + E_n - E_0} \]

Define the matrices

\[ Q^{(e)}_{\alpha m} = \langle \Omega | c_\alpha | m \rangle \quad \quad Q^{(h)}_{\alpha n} = \langle \Omega | c_\alpha^\dagger | n \rangle \]

Then

\[ G_{\alpha\beta}(\omega) = \sum_{m} \frac{Q^{(e)}_{\alpha m} Q^{(e)\star}_{\beta m}}{\omega - \omega^{(e)}_m} + \sum_{n} \frac{Q^{(h)}_{\alpha n} Q^{(h)\star}_{\beta n}}{\omega - \omega^{(h)}_n} \]

\[ = \sum_{r} \frac{Q_{\alpha r} Q_{\beta r}^\star}{\omega - \omega_{r}} \quad \quad QQ^\dagger = 1 \]
The Band Lanczos method

- Define $|\phi_\alpha\rangle = c_\alpha^\dagger |\Omega\rangle$, $\alpha = 1, \ldots, L$.

- Extended Krylov space:

$$\left\{|\phi_1\rangle, \ldots, |\phi_L\rangle, H|\phi_1\rangle, \ldots, H|\phi_L\rangle, \ldots, (H)^M|\phi_1\rangle, \ldots, (H)^M|\phi_L\rangle\right\}$$

- States are built iteratively and orthogonalized.
- Possible linearly dependent states are eliminated (‘deflation’).
- A band representation of the Hamiltonian ($2L + 1$ diagonals) is formed in the Krylov subspace.
- It is diagonalized and the eigenpairs are used to build an approximate Lehmann representation.

http://www.cs.utk.edu/dongarra/etemplates/node131.html
The usual Lanczos method for the Green function needs 3 vectors in memory, and $L(L + 1)$ distinct Lanczos procedures.

The band Lanczos method requires $3L + 1$ vectors in memory, but requires only 2 iterative procedures ((e) et (h)).

If Memory allows it, the band Lanczos is much faster.
Cluster symmetries

Clusters with $C_{2v}$ symmetry

Clusters with $C_2$ symmetry
Cluster symmetries (2)

- Symmetry operations form a group $\mathbb{G}$
- The most common occurrences are:
  - $C_1$: The trivial group (no symmetry)
  - $C_2$: The 2-element group (e.g. left-right symmetry)
  - $C_{2v}$: 2 reflections, 1 $\pi$-rotation
  - $C_{4v}$: 4 reflections, 1 $\pi$-rotation, 2 $\pi/2$-rotations
  - $C_{3v}$: 3 reflections, 3 $2\pi/3$-rotations
  - $C_{6v}$: 6 reflections, 1 $\pi$, 2 $\pi/3$, 2 $\pi/6$ rotations
- States in the Hilbert space fall into a finite number of irreducible representations (irreps) of $\mathbb{G}$
- The Hamiltonian $H'$ is block diagonal w.r.t. to irreps.
- Easiest to implement with Abelian (i.e. commuting) groups
Taking advantage of cluster symmetries…

- Reduces the dimension of the Hilbert space by $\sim |G|$
- Accelerates the convergence of the Lanczos algorithm
- Reduces the number of Band Lanczos starting vectors by $|G|$,
- But: complicates coding of the basis states
- Make use of the projection operator:

$$P(\alpha) = \frac{d_\alpha}{|G|} \sum_{g \in G} \chi_g(\alpha)^* g$$

See, e.g. Poilblanc & Laflorence cond-mat/0408363
### Group characters

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<td>1</td>
</tr>
</tbody>
</table>

<table>
<thead>
<tr>
<th>$C_{4v}$</th>
<th>$e$</th>
<th>$c_2$</th>
<th>$2c_4$</th>
<th>$2\sigma_1$</th>
<th>$2\sigma_2$</th>
</tr>
</thead>
<tbody>
<tr>
<td>$A_1$</td>
<td>1</td>
<td>1</td>
<td>1</td>
<td>1</td>
<td>1</td>
</tr>
<tr>
<td>$A_2$</td>
<td>1</td>
<td>1</td>
<td>1</td>
<td>$-1$</td>
<td>$-1$</td>
</tr>
<tr>
<td>$B_1$</td>
<td>1</td>
<td>1</td>
<td>$-1$</td>
<td>1</td>
<td>$-1$</td>
</tr>
<tr>
<td>$B_2$</td>
<td>1</td>
<td>1</td>
<td>$-1$</td>
<td>$-1$</td>
<td>1</td>
</tr>
<tr>
<td>$E$</td>
<td>2</td>
<td>$-2$</td>
<td>0</td>
<td>0</td>
<td>0</td>
</tr>
</tbody>
</table>
Taking advantage of cluster symmetries (2)

- Need new basis states, made of sets of binary states related by the group action:

\[ |\psi\rangle = \frac{d^\alpha}{|G|} \sum_g \chi_g^{(\alpha)^*} g|b\rangle \quad g|b\rangle = \phi_g(b)|g\,b\rangle \]

- Then matrix elements take the form

\[ \langle \psi_2|H|\psi_1 \rangle = \frac{d^\alpha}{|G|} \sum_g \chi_h^{(\alpha)^*} \phi_g(b) \langle g\,b_2|H|b_1 \rangle \]

- When computing the Green function, one needs to use combinations of creation operators that fall into group representations. For instance (4 × 1):

\[ \begin{align*}
  c_1^{(A)} &= c_1 + c_4 \\
  c_2^{(A)} &= c_2 + c_3 \\
  c_1^{(B)} &= c_1 - c_4 \\
  c_2^{(B)} &= c_2 - c_3
\end{align*} \]

\[ \begin{array}{c|c|c|c|c}
  1 & 2 & 3 & 4 \\
\end{array} \]
Example: number of matrix elements of the kinetic energy operator (Nearest neighbor) on a $3 \times 4$ cluster with $C_{2v}$ symmetry:

<table>
<thead>
<tr>
<th>dim. value</th>
<th>$A_1$</th>
<th>$A_2$</th>
<th>$B_1$</th>
<th>$B_2$</th>
</tr>
</thead>
<tbody>
<tr>
<td>$-2$</td>
<td>96</td>
<td>736</td>
<td>704</td>
<td>0</td>
</tr>
<tr>
<td>$-\sqrt{2}$</td>
<td>12,640</td>
<td>6,208</td>
<td>7,584</td>
<td>5,072</td>
</tr>
<tr>
<td>$-1$</td>
<td>2,983,264</td>
<td>2,936,144</td>
<td>2,884,832</td>
<td>2,911,920</td>
</tr>
<tr>
<td>$1$</td>
<td>952,000</td>
<td>997,168</td>
<td>1,050,432</td>
<td>1,021,392</td>
</tr>
<tr>
<td>$\sqrt{2}$</td>
<td>5,088</td>
<td>2,304</td>
<td>3,232</td>
<td>2,992</td>
</tr>
<tr>
<td>$2$</td>
<td>32</td>
<td>0</td>
<td>0</td>
<td>0</td>
</tr>
</tbody>
</table>
Breaking the exponential barrier

Lu et al., arXiv:1402.0807v1
Breaking the exponential barrier (cont.)

Lu et al., arXiv:1402.0807v1
QUESTIONS ?
Interlude: The spectral function

\[ A(k, \omega) = -2 \lim_{\eta \to 0^+} \text{Im} \ G(k, \omega + i \eta) \]

▶ Lehmann representation:

\[ G_{\alpha\beta}(\omega) = \sum_m \frac{\langle \Omega | c_{\alpha} | m \rangle \langle m | c_{\beta}^\dagger | \Omega \rangle}{\omega - E_m + E_0} + \sum_n \frac{\langle \Omega | c_{\beta}^\dagger | n \rangle \langle n | c_{\alpha} | \Omega \rangle}{\omega + E_n - E_0} \]

▶ But: \( - \lim_{\eta \to 0^+} \text{Im} \ \frac{1}{\omega + i \eta} = \lim_{\eta \to 0^+} \frac{\eta}{\omega^2 + \eta^2} = \pi \delta(\omega) \)

▶ Therefore:

\[ A(k, \omega) = \sum_m |\langle m | c_{k}^\dagger | \Omega \rangle|^2 2\pi \delta(\omega - E_m + E_0) \]

prob. that energy is \( E_m \)

\[ + \sum_n |\langle n | c_{k} | \Omega \rangle|^2 2\pi \delta(\omega + E_n - E_0) \]