Quantum Cluster Methods

An introduction

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Outline

- Exact Diagonalizations
- Clusters and Cluster Perturbation Theory (CPT)
- The Self-Energy Functional Approach
- The Variational Cluster Approximation (VCA)
- Cluster Dynamical Mean Field Theory (CDMFT)

Part I

Exact Diagonalizations

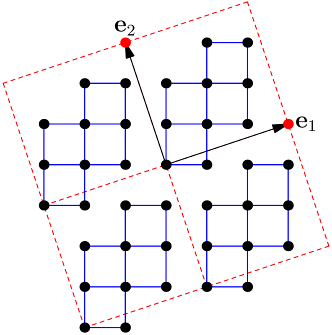
An old Persian Legend, revisited

The Hubbard Model on finite cluster

- Simple Hubbard model (conserves $N_\uparrow$ and $N_\downarrow$ separately):

$$H = \sum_{a,b,\sigma} t_{ab} c^\dagger_{a\sigma} c_{b\sigma} + U \sum_a n_{a\uparrow} n_{a\downarrow} - \mu \sum_a n_a$$

- Typical cluster (L sites):



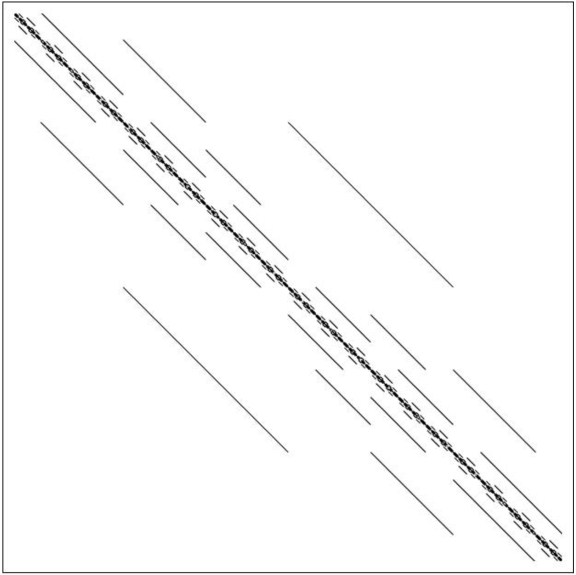
Hamiltonian matrix : 2 sites

- Half-filled Hubbard model $L = 2$

$$\begin{pmatrix} U-2\mu & -t & -t & 0 \\ -t & -2\mu & 0 & -t \\ -t & 0 & -2\mu & -t \\ 0 & -t & -t & U-2\mu \end{pmatrix}$$

Hamiltonian matrix : 6 sites

Sparse matrix structure
400×400



Hamiltonian matrix : example

- Dimension of the Hilbert space (half-filled Hubbard model):

$$d = \left(\frac{L!}{[(L/2)!]^2} \right)^2 \sim 2\frac{4^L}{\pi L}$$

- One double-precision vector means 1.23 GB of memory

L	dimension
2	4
4	36
6	400
8	4 900
10	63 504
12	853 776
14	11 778 624
16	165 636 900

Steps

1. Building a basis
2. Constructing the Hamiltonian matrix
3. Finding the ground state (e.g. by the Lanczos method)
4. Calculating the one-body Green function

Coding of the states

- Basis of occupation number eigenstates:

$$(c^\dagger_{1\uparrow})^{n_{1\uparrow}} \cdots (c^\dagger_{L\uparrow})^{n_{L\uparrow}} (c^\dagger_{1\downarrow})^{n_{1\downarrow}} \cdots (c^\dagger_{L\downarrow})^{n_{L\downarrow}} |0\rangle$$

- Binary representation of basis states:

$$|b\rangle \;\; \text{where} \;\; b = b_\uparrow + 2^L b_\downarrow$$

  Example :
  $b = (0101010101|1010101010) = 341 \cdot 2^{10} + 682 = 349,866$

- Need a direct table:

$$b_\uparrow = B_\uparrow(i_\uparrow) \qquad b_\downarrow = B_\downarrow(i_\downarrow)$$

- …and a reverse table:

consecutive label   mod   int. division

$$i = I_\uparrow(b_\uparrow) + d_{N\uparrow} I_\downarrow(b_\downarrow) \qquad i_\uparrow = i \% d_{N\uparrow} \quad i_\downarrow = i / d_{N\uparrow}$$

Coding of the states (2)

- Tensor product structure of the Hilbert space: $V = V_{N_\uparrow} \otimes V_{N_\downarrow}$
- dimension:

$$d = d(N_\uparrow)d(N_\downarrow) \qquad\qquad d(N_\sigma) = \frac{L!}{N_\sigma!(L - N_\sigma)!}$$

- Example (6 sites):

	0	1	2	3	4	5	6
0	1	6	15	20	15	6	1
1	6	36	90	120	90	36	6
2	15	90	225	300	225	90	15
3	20	120	300	400	300	120	20
4	15	90	225	300	225	90	15
5	6	36	90	120	90	36	6
6	1	6	15	20	15	6	1

Constructing the Hamiltonian matrix

- Form of Hamiltonian:

$$H = K_\uparrow \otimes 1 + 1 \otimes K_\downarrow + V_{\text{int.}} \qquad K = \sum_{a,b} t_{ab} c_a^\dagger c_b$$

- K is stored in sparse form.
- $V_{\text{int.}}$ is diagonal and is stored.
- Matrix elements of $V_{\text{int.}}$: 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.

$$\langle b'|K|b\rangle = (-1)^{M_{ab}} t_{ab} \qquad M_{ab} = \sum_{c=a+1}^{b-1} n_c$$

The Lanczos algorithm

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

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

- Lanczos three-way recursion:

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

$$a_n = \frac{\langle\phi_n|H|\phi_n\rangle}{\langle\phi_n|\phi_n\rangle} \qquad b_n^2 = \frac{\langle\phi_n|\phi_n\rangle}{\langle\phi_{n-1}|\phi_{n-1}\rangle} \qquad b_0 = 0$$

The Lanczos algorithm (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

$$H = \begin{pmatrix} a_0 & b_1 & 0 & 0 & \cdots & 0 \\ b_1 & a_1 & b_2 & 0 & \cdots & 0 \\ 0 & b_2 & a_2 & b_3 & \cdots & 0 \\ \vdots & \vdots & \vdots & \vdots & \ddots & \vdots \\ 0 & 0 & 0 & 0 & \cdots & a_N \end{pmatrix}$$

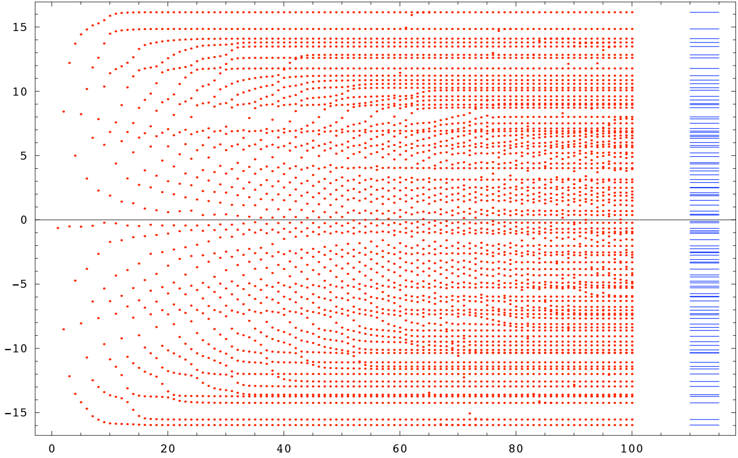
- At each step n, find the lowest eigenvalue of that matrix
- Stop when the lowest eigenvalue E_0 has converged ($\Delta E_0 / E_0 < 10^{-12}$)
- Then re-run to find eigenvector $|\psi\rangle = \sum_n \psi_n |n\rangle$ as the $|\phi_n\rangle$'s are not kept in memory.

Lanczos method: characteristics

- Typical required number of iterations: from 20 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, periodic re-orthogonalization may be required, as orthogonality leaks will occur
- For degenerate ground states and low lying states (e.g. in DMRG), the Davidson method is generally preferable

Lanczos method: illustration of the convergence

100 iterations on a matrix of dimension 600: eigenvalues of the tridiagonal projection as a function of iteration step



Lanczos method for the Green function

- Zero temperature Green function:

$$
\begin{aligned}
G_{\mu\nu}(\omega) &= G_{\mu\nu,e}(\omega) + G_{\mu\nu,h}(\omega) \\
G_{\mu\nu,e}(\omega) &= \langle\Omega|c_\mu \frac{1}{\omega - H + E_0} c_\nu^\dagger|\Omega\rangle \\
G_{\mu\nu,h}(\omega) &= \langle\Omega|c_\nu^\dagger \frac{1}{\omega + H - E_0} c_\mu|\Omega\rangle
\end{aligned}
$$

- Consider the diagonal element

$$
|\phi_\mu\rangle = c_\mu^\dagger|\Omega\rangle \implies G_{\mu\mu,e} = \langle\phi_\mu|\frac{1}{\omega - H + E_0}|\phi_\mu\rangle
$$

- Use the expansion

$$
\frac{1}{z - H} = \frac{1}{z} + \frac{1}{z^2}H + \frac{1}{z^3}H^2 + \cdots
$$

Lanczos method for the Green function (2)

- Truncated expansion evaluated exactly in Krylov subspace generated by $|\phi_\mu\rangle$ if we perform a Lanczos procedure on $|\phi_\mu\rangle$.
- Then $G_{\mu\mu,e}$ is given by a Jacobi continued fraction:

$$G_{\mu\mu,e}(\omega) = \cfrac{\langle\phi_\mu|\phi_\mu\rangle}{\omega - a_0 - \cfrac{b_1^2}{\omega - a_1 - \cfrac{b_2^2}{\omega - a_2 - \cdots}}}$$

- The coefficients a_n and b_n are stored in memory
- What about non diagonal elements $G_{\mu\nu,e}$?

See, e.g., E. Dagotto, Rev. Mod. Phys. 66:763 (1994)

Lanczos method for the Green function (3)

- Trick: Define the combination

$$G^{+}_{\mu\nu,e}(\omega) = \langle\Omega|(c_\mu + c_\nu)\frac{1}{\omega - H + E_0}(c_\mu + c_\nu)^\dagger|\Omega\rangle$$

- $G^{+}_{\mu\nu,e}(\omega)$ can be calculated like $G_{\mu\mu,e}(\omega)$
- Since $G_{\mu\nu,e}(\omega) = G_{\nu\mu,e}(\omega)$, then

$$G_{\mu\nu,e}(\omega) = \frac{1}{2}\left[G^{+}_{\mu\nu,e}(\omega) - G_{\mu\mu,e}(\omega) - G_{\nu\nu,e}(\omega)\right]$$

- Likewise for $G_{\mu\nu,h}(\omega)$

Lehman representation

- Lehmann representation of the Green function

$$G_{\mu\nu}(\omega) = \sum_m \langle\Omega|c_\mu|m\rangle \frac{1}{\omega - E_m + E_0} \langle m|c_\nu^\dagger|\Omega\rangle + \sum_n \langle\Omega|c_\nu^\dagger|n\rangle \frac{1}{\omega + E_n - E_0} \langle n|c_\mu|\Omega\rangle$$

- Define the matices

$$Q^{(e)}_{\mu m} = \langle\Omega|c_\mu|m\rangle \qquad Q^{(h)}_{\mu n} = \langle\Omega|c_\mu^\dagger|n\rangle$$

- Then

$$\begin{aligned} G_{\mu\nu}(\omega) &= \sum_m \frac{Q^{(e)}_{\mu m} Q^{(e)*}_{\nu m}}{\omega - \omega^{(e)}_m} + \sum_n \frac{Q^{(h)}_{\mu n} Q^{(h)*}_{\nu n}}{\omega - \omega^{(h)}_n} \\ &= \sum_r \frac{Q_{\mu r} Q^*_{\nu r}}{\omega - \omega_r} \end{aligned}$$

Alternate way : The Band Lanczos method

- Define $|\phi_\mu\rangle = c_\mu^\dagger|\Omega\rangle$, $\mu = 1, \ldots, L$.
- Extended Krylov space :

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

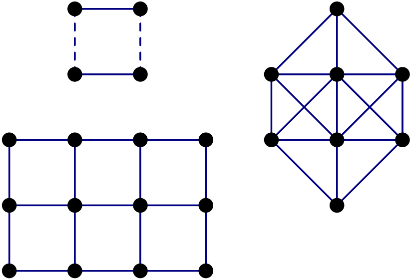
- States are built iteratively and orthogonalized
- Possible linearly dependent states are eliminated ('deflation')
- A band representation of the Hamiltonian ($2L + 1$ diagonals) is formed in the Krylov subspace.
- It is diagonalized and the eigenpairs are used to build an approximate Lehmann representation

http://www.cs.utk.edu/ dongarra/etemplates/node131.html

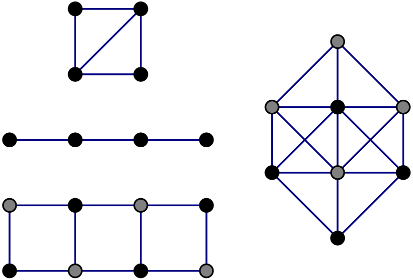
Lanczos vs Band Lanczos

- The usual Lanczos method for the Green function needs 3 vectors in memory, and $L(L+1)$ 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 $\mathfrak{G}$
- The most common occurences are :
  - C_1 : The trivial group (no symmetry)
  - C_2 : The 2-element group (e.g. left-right symmetry)
  - C_{2v} : 2 reflections, 1 π-rotation
  - C_{4v} : 4 reflections, 1 π-rotation, 2 $\pi/2$-rotations
  - C_{3v} : 3 reflections, 3 $2\pi/3$-rotations
  - C_{6v} : 6 reflections, 1 π, 2 $\pi/3$, 2 $\pi/6$ rotations
- States in the Hilbert space fall into a finite number of irreducible representations (irreps) of $\mathfrak{G}$
- The Hamiltonian H' is block diagonal w.r.t. to irreps.

Group characters

C_2	E	C_2
A	1	1
B	1	-1

C_{2v}	e	c_2	σ_1	σ_2
A_1	1	1	1	1
A_2	1	1	-1	-1
B_1	1	-1	1	-1
B_2	1	-1	-1	1

C_{4v}	e	c_2	$2c_4$	$2\sigma_1$	$2\sigma_2$
A_1	1	1	1	1	1
A_2	1	1	1	-1	-1
B_1	1	1	-1	1	-1
B_2	1	1	-1	-1	1
E	2	-2	0	0	0

Taking advantage of cluster symmetries...

order of the group

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

dimension of irrep.

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

group character

See, e.g. Poilblanc & Laflorencie cond-mat/0408363

Taking advantage of cluster symmetries (2)

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

fermionic phase

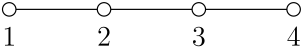
$$|\psi\rangle = \frac{d_\alpha}{|\mathfrak{G}|}\sum_g \chi_g^{(\alpha)*} g|b\rangle \qquad g|b\rangle = \phi_g(b)|gb\rangle$$

- Then matrix elements take the form

$$\langle\psi_2|\,H|\,\psi_1\rangle = \frac{d_\alpha}{|\mathfrak{G}|}\sum_g \chi_h^{(\alpha)*}\phi_g(b)\langle gb_2|H|b_1\rangle$$

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

$$c_1^{(A)} = c_1 + c_4 \qquad c_1^{(B)} = c_1 - c_4$$
$$c_2^{(A)} = c_2 + c_3 \qquad c_2^{(B)} = c_2 - c_3$$



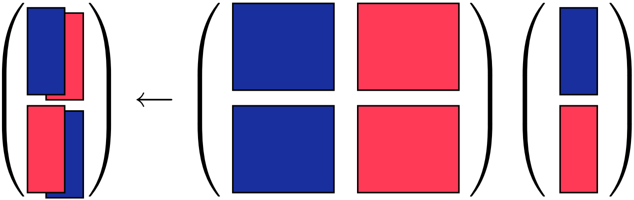
Taking advantage of cluster symmetries (3)

Example : number of matrix elements of the kinetic energy operator (Nearest neighbor) on a 3×4 cluster with C_{2v} symmetry:

	A_1	A_2	B_1	B_2
dim.	$213,840$	$213,248$	$213,440$	$213,248$
value				
-2	96	736	704	0
$-\sqrt{2}$	$12,640$	$6,208$	$7,584$	$5,072$
-1	$2,983,264$	$2,936,144$	$2,884,832$	$2,911,920$
1	$952,000$	$997,168$	$1,050,432$	$1,021,392$
$\sqrt{2}$	$5,088$	$2,304$	$3,232$	$2,992$
2	32	0	0	0

Large dimensions : need for parallelization

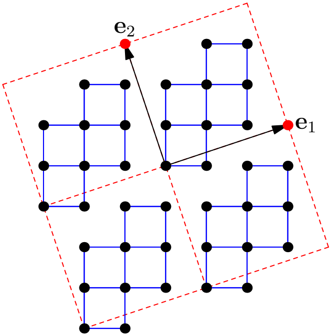
- Memory needs exceed single cpu capacity beyond $L \sim 14$
- A half-filled 16-site system has dimension 165,636,900
  $\rightarrow$ 1.23 GB for a state vector.
- Need to distribute the problem over many processors
- The main task is matrix-vector multiplication:



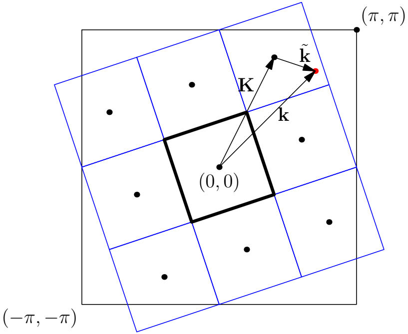
Part II

Cluster Perturbation Theory

Clusters and superlattices



10-site cluster



Reduced Brillouin zone

Basic Idea

lattice Hamiltonian ↵ ↳ cluster Hamiltonian

$$H = H' + V$$

↳ inter-cluster hopping terms

hopping matrix ↵ ↳ cluster hopping matrix

$$\mathsf{t} = \mathsf{t}' + \mathsf{V}$$

↳ inter-cluster hopping

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

$$\mathsf{G}^{-1}(\omega) = \mathsf{G}'^{-1}(\omega) - \mathsf{V}$$

↳ cluster Green function

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)

Interlude : Fourier transforms

i, j : lattice site index

m, n : lattice site index

a, b : cluster site index

$\mathbf{k}$: full wavevector

$\tilde{\mathbf{k}}$: redcued wavevector

$\mathbf{K}$: cluster wavevector

$$f_j = \sum_{\mathbf{k}} \mathrm{e}^{i\mathbf{k}\cdot\mathbf{r}_j} f(\mathbf{k}) \qquad f(\mathbf{k}) = \frac{1}{N} \sum_{j} \mathrm{e}^{-i\mathbf{k}\cdot\mathbf{r}_j} f_j$$

$$f_m = \sum_{\tilde{\mathbf{k}}} \mathrm{e}^{i\tilde{\mathbf{k}}\cdot\mathbf{r}_m} f(\tilde{\mathbf{k}}) \qquad f(\tilde{\mathbf{k}}) = \frac{L}{N} \sum_{m} \mathrm{e}^{-i\tilde{\mathbf{k}}\cdot\mathbf{r}_m} f_m$$

$$f_a = \frac{1}{\sqrt{L}} \sum_{\mathbf{K}} \mathrm{e}^{i\mathbf{K}\cdot\mathbf{r}_a} f_{\mathbf{K}} \qquad f_{\mathbf{K}} = \frac{1}{\sqrt{L}} \sum_{a} \mathrm{e}^{-i\mathbf{K}\cdot\mathbf{r}_a} f_a$$

Basic Idea (cont.)

- More accurate formulation

$$\mathsf{G}^{-1}(\tilde{\mathbf{k}},\omega) = \mathsf{G}'^{-1}(\omega) - \mathsf{V}(\tilde{\mathbf{k}}) \ .$$

- But

$$\begin{aligned} \mathsf{G}'^{-1} &= \omega - \mathsf{t}' - \Sigma \\ \mathsf{G_0}^{-1} &= \omega - \mathsf{t}' - \mathsf{V} \ , \end{aligned}$$

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

$$\mathsf{G}^{-1}(\tilde{\mathbf{k}},\omega) = \mathsf{G_0}^{-1}(\tilde{\mathbf{k}},\omega) - \Sigma(\omega) \ ,$$

- Example : 2-site cluster (1D):

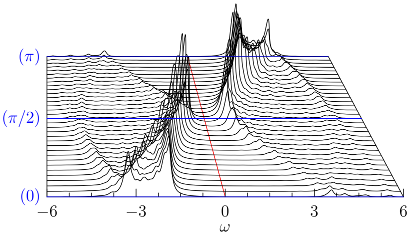
$$\mathsf{t}' = -t \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix} \qquad \mathsf{V}(\tilde{k}) = -t \begin{pmatrix} 0 & e^{-2i\tilde{k}} \\ e^{2i\tilde{k}} & 0 \end{pmatrix}$$

Periodization

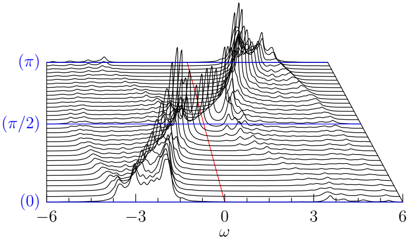
- CPT breaks translation invariance, which needs to be restored:

$$G_{\text{cpt}}(\mathbf{k},\omega) = \frac{1}{L}\sum_{a,b} \mathrm{e}^{-i\mathbf{k}\cdot(\mathbf{r}_a - \mathbf{r}_b)} G_{ab}(\tilde{\mathbf{k}},\omega) \ .$$

- Periodizing the Green function vs the self-energy (1D case):



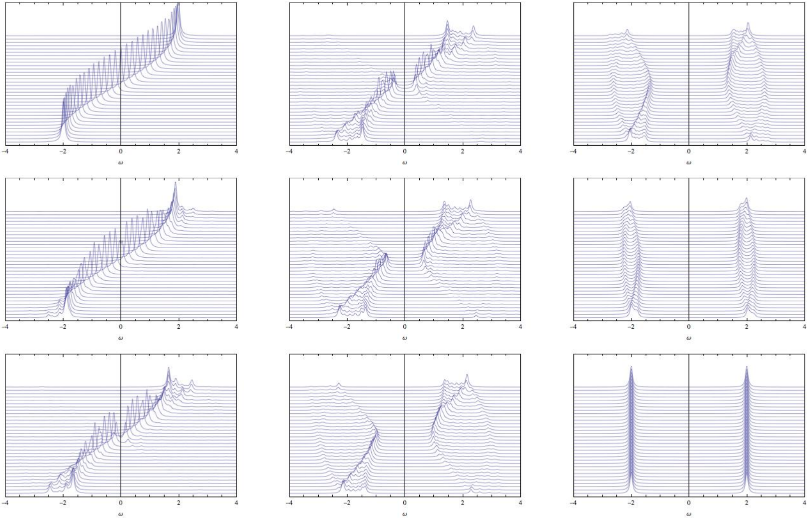
Green function periodization



Self-energy periodization

One-dimensional example

Evolution of spectral function with increasing U/t:



Interlude : Relation with spectral function

$$\boxed{A(\mathbf{k},\omega) = -2 \lim_{\eta\to 0^+} \mathrm{Im}\, G(\mathbf{k},\omega+i\eta)}$$

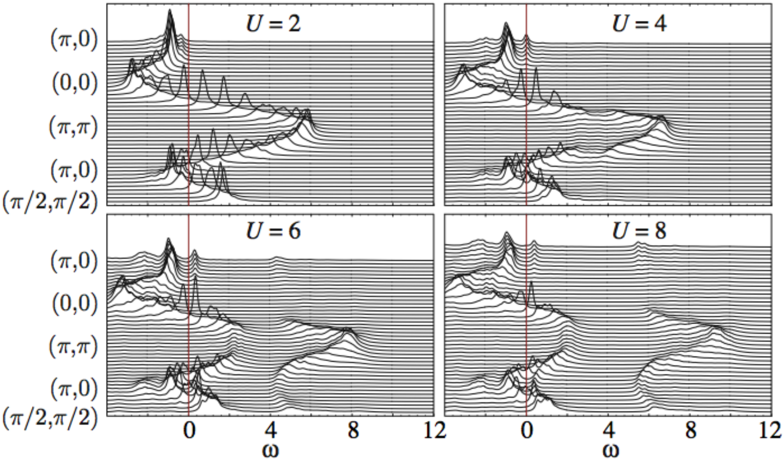
- Lehmann representation:

$$\begin{aligned} G_{\alpha\beta}(\omega) &= \sum_m \langle\Omega|c_\alpha|m\rangle \frac{1}{\omega - E_m + E_0} \langle m|c^\dagger_\beta|\Omega\rangle \\ &+ \sum_n \langle\Omega|c^\dagger_\beta|n\rangle \frac{1}{\omega + E_n - E_0} \langle n|c_\alpha|\Omega\rangle \end{aligned}$$

- But : $-\lim_{\eta\to 0^+} \mathrm{Im}\, \dfrac{1}{\omega+i\eta} = \lim_{\eta\to 0^+} \dfrac{\eta}{\omega^2+\eta^2} = \pi\delta(\omega)$
- Therefore :

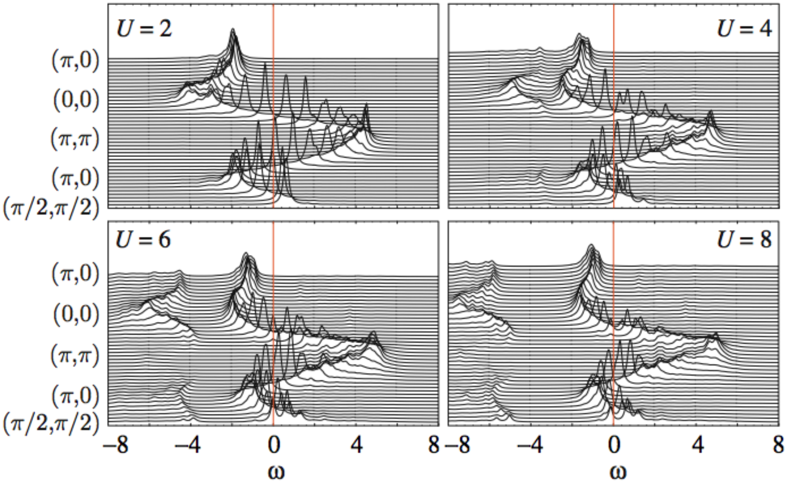
$$\begin{aligned} A(\mathbf{k},\omega) &= \sum_m |\langle m|c^\dagger_{\mathbf{k}}|\Omega\rangle|^2 2\pi\delta(\omega - E_m + E_0) \\ &+ \sum_n |\langle n|c_{\mathbf{k}}|\Omega\rangle|^2 2\pi\delta(\omega + E_n - E_0) \end{aligned}$$

h-doped cuprates : Pseudogap from CPT



Sénéchal and Tremblay., Phys. Rev. Lett. **92**, 126401 (2004)

e-doped cuprates : Pseudogap from CPT



Sénéchal and Tremblay., Phys. Rev. Lett. **92**, 126401 (2004)

CPT : characteristics

- Exact at $U = 0$
- Exact at $t_{ij} = 0$
- Exact short-range correlations
- Allows all values of the wavevector
- But : No long-range order
- Controlled by the size of the cluster

Part III

The self-energy functional approach

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:

$$H'_M = M \sum_a \mathrm{e}^{i\overbrace{\mathbf{Q}}^{(\pi,\pi)}\cdot\mathbf{r}_a} (n_{a\uparrow} - n_{a\downarrow})$$

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

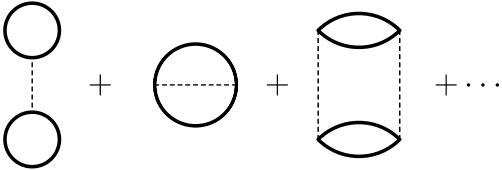
The Potthoff variational principle

- Variational principle for the Green function:

$$\Omega_{\mathsf{t}}[\mathsf{G}] = \Phi[\mathsf{G}] - \operatorname{Tr}\left((\mathsf{G}_{0\mathsf{t}}^{-1} - \mathsf{G}^{-1})\mathsf{G}\right) + \underbrace{\operatorname{Tr}}_{\operatorname{Tr}(A) = \sum_{\omega,\alpha} A_{\alpha\alpha}(\omega)} \ln(-\mathsf{G}).$$

- Where $\Phi[\mathsf{G}]$ is the Luttinger-Ward functional:

$\Phi =$



- ... with the property

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

M. Potthoff, Eur. Phys. J. B **32**, 429?436 (2003)

The Potthoff variational principle (2)

- Here, Tr means a sum over frequencies, site indices (or wavevectors) and spin/band indices.
- The functional is stationary at the physical Green function (Euler eq.):

$$\frac{\delta \Omega_{\mathsf{t}}[\mathsf{G}]}{\delta \mathsf{G}} = \Sigma - \mathsf{G}_{0\mathsf{t}}^{-1} + \mathsf{G}^{-1} = 0.$$

- Approximation schemes:
  - 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

The Potthoff variational principle (3)

- Potthoff : Use the self-energy rather than the Green function

$$\begin{aligned} \Omega_{\mathsf{t}}[\Sigma] &= F[\Sigma] - \mathrm{Tr}\,\ln(-\mathsf{G}_{0\mathsf{t}}^{-1} + \Sigma) \\ F[\Sigma] &= \Phi[\mathsf{G}] - \mathrm{Tr}\,(\Sigma \mathsf{G}) \end{aligned}$$

- F is the Legendre transform of Φ:

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

- New Euler equation:

$$\frac{\delta \Omega_{\mathsf{t}}[\Sigma]}{\delta \Sigma} = -\mathsf{G} + (\mathsf{G}_{0\mathsf{t}}^{-1} - \Sigma)^{-1} = 0$$

- At the physical self-energy, $\Omega_{\mathsf{t}}[\Sigma]$ is the thermodynamic grand potential

The Reference System

- To evaluate F, use its universal character : its functional form depends only on the interaction.
- Introduce a reference rystem 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 Σ of H',

$$\Omega' = F[\Sigma] - \mathrm{Tr}\,\ln(-\mathsf{G}')$$

- by eliminating F:

$$\begin{aligned}\Omega_{\mathsf{t}}[\Sigma] &= \Omega' + \mathrm{Tr}\,\ln(-\mathsf{G}') - \mathrm{Tr}\,\ln(-\mathsf{G}_{0\mathsf{t}}^{-1} + \Sigma) \\ &= \Omega' + \mathrm{Tr}\,\ln(-\mathsf{G}') - \mathrm{Tr}\,\ln(-\mathsf{G}) \\ &= \Omega' - \mathrm{Tr}\,\ln(1 - \mathsf{V}\mathsf{G}')\end{aligned}$$

The Potthoff functional

- Making the trace explicit, one finds

$$\begin{aligned}\Omega_{\mathsf{t}}[\Sigma] &= \Omega' - T\sum_{\omega}\sum_{\tilde{\mathbf{k}}} \mathrm{tr}\,\ln\left[1 - \mathsf{V}(\tilde{\mathbf{k}})\mathsf{G}'(\tilde{\mathbf{k}},\omega)\right] \\ &= \Omega' - T\sum_{\omega}\sum_{\tilde{\mathbf{k}}} \ln\det\left[1 - \mathsf{V}(\tilde{\mathbf{k}})\mathsf{G}'(\tilde{\mathbf{k}},\omega)\right]\end{aligned}$$

- 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 particular, the Weiss field M is to be varied until Ω is stationary

Calculating the functional I : exact form

- It can be shown that

$$\mathrm{Tr}\ \ln(-\mathsf{G}) = -T\sum_m \ln(1+\mathrm{e}^{-\beta\omega_m}) + T\sum_m \ln(1+\mathrm{e}^{-\beta\zeta_m})$$

poles of G

zeros of G

- Use the Lehmann representation of the GF:

$$G'_{\mu\nu}(\omega) = \sum_r \frac{Q_{\mu r}Q^*_{\nu r}}{\omega-\omega_r} \qquad \mathsf{G}(\omega) = \mathsf{Q}\frac{1}{\omega-\Lambda}\mathsf{Q}^\dagger$$

diagonal(ω_r)

M. Potthoff, Eur. Phys. J. B, 36:335 (2003)

Calculating the functional I : exact form (2)

- A similar representation holds for the CPT Green function

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

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

- Let $\omega_r(\tilde{\mathbf{k}})$ be the eigenvalues of $\mathsf{L}(\tilde{\mathbf{k}})$. Then

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

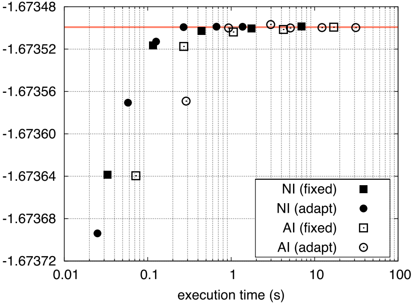
variational parameters

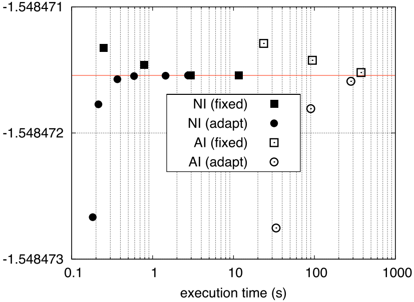
M. Aichhorn et al., Phys. Rev. B 74 : 235117 (2006)

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:

$$\Omega(\mathsf{x}) = \Omega'(\mathsf{x}) - \int_0^\infty \frac{dx}{\pi} \frac{L}{N} \sum_{\tilde{\mathbf{k}}} \ln \left| \det(1 - \mathsf{V}(\tilde{\mathbf{k}})\mathsf{G}'(ix)) \right| - L(\mu - \mu')$$

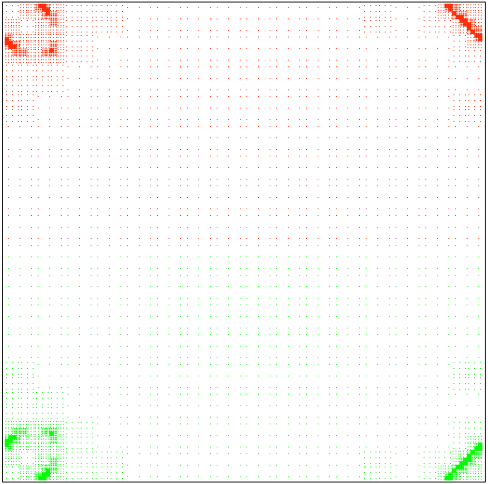




D. Sénéchal, proceedings of HPCS 2008, IEEE (2008)

Evaluation of integrals

- For frequency integrals: Gaussian integration on three segments
- For wavevector integrals, adaptive mesh of points:
  - Start with a coarse, regular grid
  - On each plaquette, compare 4 and 9 point Gaussian integrals. Subdivide into 4 sub-plaquettes if necessary.
  - Easy with recursive calls



Part IV

The Variational Cluster Approximation

Basic Idea

- Set up a superlattice of clusters
- Choose a set of variational parameters, e.g. Weiss fields for broken symmetries
- Set up the calculation of the Potthoff functional:

$$\Omega_{\mathsf{t}}[\Sigma] = \Omega' - \frac{TL}{N} \sum_{\omega} \sum_{\tilde{\mathbf{k}}} \ln \det \left[\mathsf{1} - \mathsf{V}(\tilde{\mathbf{k}}) \mathsf{G}'(\tilde{\mathbf{k}}, \omega) \right]$$

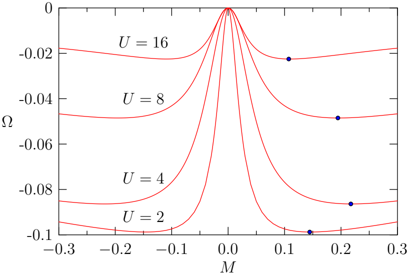
- Use an optimization method to find the stationary points
- Adopt the cluster self-energy associated with the stationary point with the lowest Ω and use it as in CPT

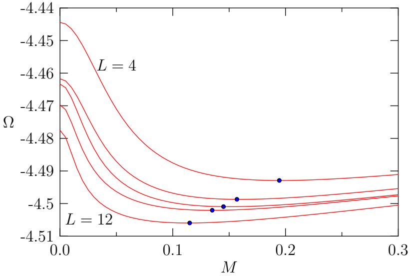
Example : Néel Antiferromagnetism

- Used the Weiss field

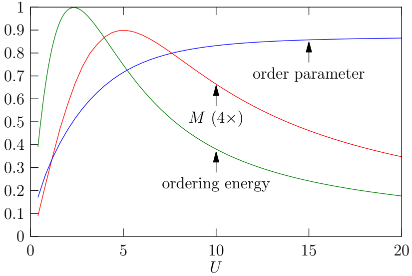
$$H'_M = M \sum_a \mathrm{e}^{i\overset{(\pi,\pi)}{\mathbf{Q}}\cdot\mathbf{r}_a}(n_{a\uparrow} - n_{a\downarrow})$$

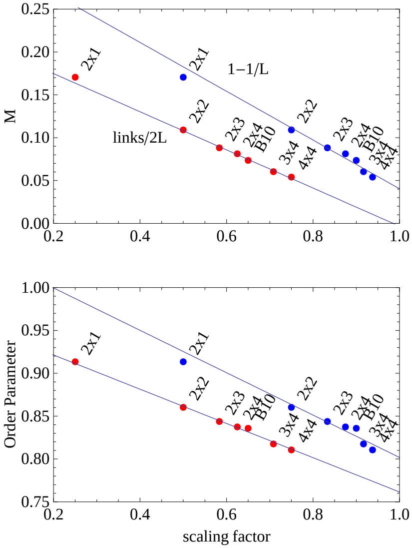
- Profile of Ω for the half-filled, square lattice Hubbard model:





Example : Néel Antiferromagnetism (2)

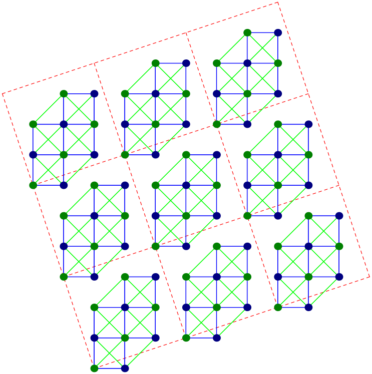




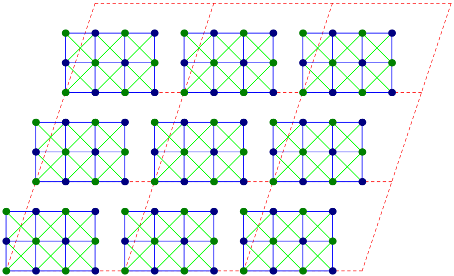
Best scaling factor :

$$q = \frac{\text{number of links}}{2 \times \text{number of sites}}$$

Example clusters



B10



3×4

Superconductivity

- Need to add a pairing field

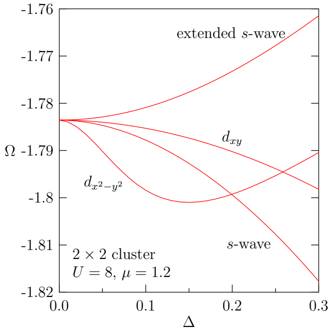
$$\mathcal{O}_{\mathrm{sc}} = \sum_{ij} \Delta_{ij} c_{i\uparrow} c_{j\downarrow} + \mathrm{H.c}$$

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

$$\Delta_{ij} = \begin{cases} 1 & \text{if} \quad \mathbf{r}_i - \mathbf{r}_j = \pm\hat{\mathbf{x}} \\ -1 & \text{if} \quad \mathbf{r}_i - \mathbf{r}_j = \pm\hat{\mathbf{y}} \end{cases}$$

- d_{xy} pairing:

$$\Delta_{ij} = \begin{cases} 1 & \text{if} \quad \mathbf{r}_i - \mathbf{r}_j = \pm(\hat{\mathbf{x}} + \hat{\mathbf{y}}) \\ -1 & \text{if} \quad \mathbf{r}_i - \mathbf{r}_j = \pm(\hat{\mathbf{x}} - \hat{\mathbf{y}}) \end{cases}$$



Superconductivity (2)

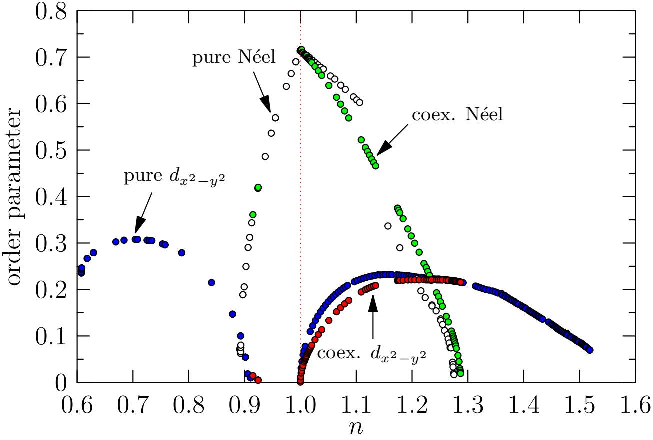
- Pairing fields violate particle number conservation
- The Hilbert space is enlarged to encompass all particle numbers with a given spin
- In practice, on uses the Nambu formalism, i.e., particle-hole transformation on the spin-down sector :

$$c_a = c_{a\uparrow} \quad \text{and} \quad d_a = c^\dagger_{a\downarrow}$$

Then the Hamiltonian looks like it conserves particle number, but not spin.

Superconductivity and Antiferromagnetism in the cuprates

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



M. Guillot, MSc thesis, Univ. de Sherbrooke (2007)

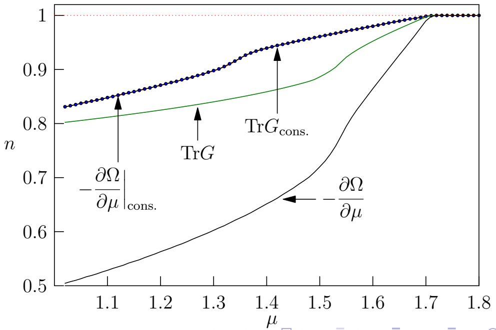
Thermodynamic consistency

- The electron density n may be calculated either as

$$n = \mathrm{Tr}\,\mathsf{G} \qquad \text{or} \qquad n = -\frac{\partial \Omega}{\partial \mu}$$

- The two methods give different results, except if the cluster chemical potential μ' is treated like a variational parameter:

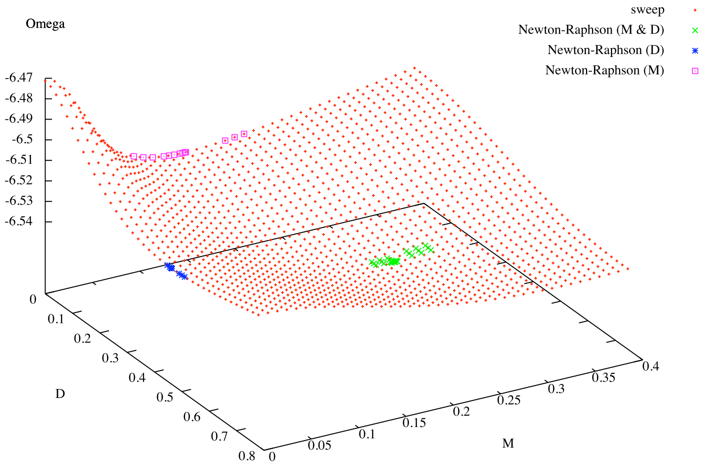
2×2 cluster
$U = 8$
normal state



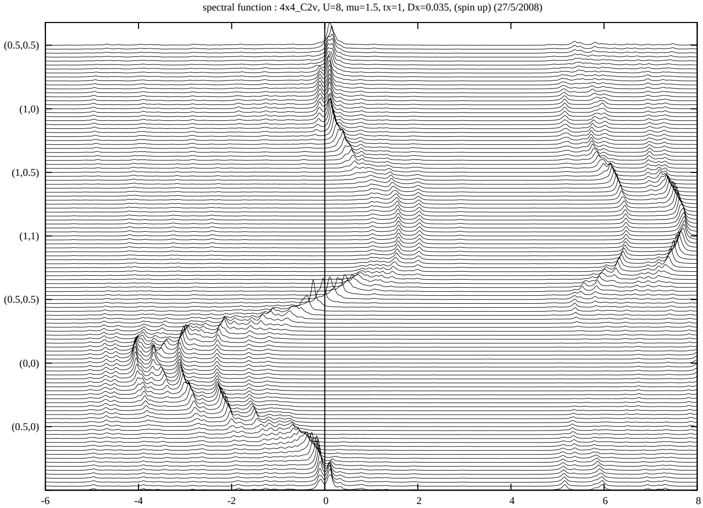
Optimization procedure

- Need to find the saddle points of $\Omega(\mathsf{x})$ with the least possible evaluations of $\Omega(\mathsf{x})$
- Use the Newton-Raphson algorithm:
  - Evaluate Ω 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 $|\mathsf{x}_i - \mathsf{x}_{i-1}|$, or the numerical gradient $|\nabla\Omega|$, converges
- The NR method is not robust : it converges fast when started close enough to the solution
- Proceed adiabatically through external parameter space (e.g. as function of U or μ)

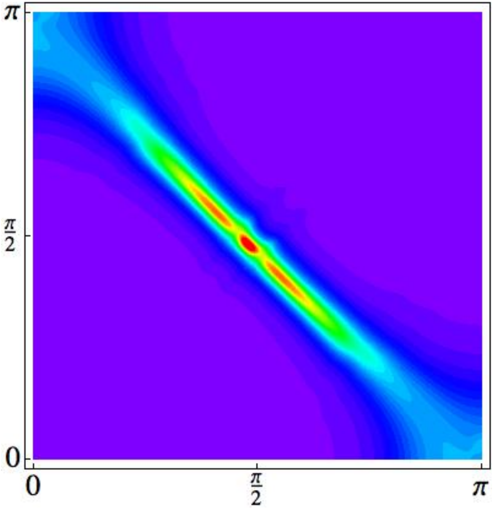
Example: Homogeneous coexistence of dSC and AF orders



Example: dSC on a 4×4 cluster, spectral function



Example: dSC on a 4×4 cluster, Fermi surface plot



VCA vs Mean-Field Theory

- Differs 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

Part V

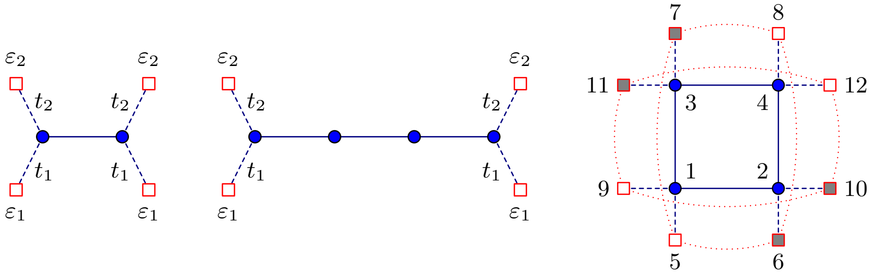
Cluster Dynamical Mean Field Theory

Basic Idea

- To add variational degrees of freedom in the form of a bath of uncorrelated 'sites'

$$H' = -\sum_{\mu,\nu} t_{\mu\nu} c^\dagger_\mu c_\nu + U \sum_a n_{a\uparrow} n_{a\downarrow} + \sum_{\mu,\alpha} \theta_{\mu\alpha} (c^\dagger_\mu a_\alpha + \mathrm{H.c.}) + \sum_\alpha \varepsilon_\alpha a^\dagger_\alpha a_a$$

$\hookrightarrow$ hybridization matrix $\hookrightarrow$ bath energies



The hybridization function

- If we trace over the bath degrees of freedom, the cluster Green function takes the form

$$\mathsf{G}'^{-1} = \omega - \mathsf{t} - \Gamma(\omega) - \Sigma(\omega)$$

- $\Gamma(\omega)$ is the hybridization function:

$$\Gamma_{\mu\nu}(\omega) = \sum_{\alpha} \frac{\theta_{\mu\alpha}\theta^*_{\nu\alpha}}{\omega - \varepsilon_\alpha}$$

The hybridization function (2)

- Proof: $(U = 0)$

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

- Given $A = \mathsf{G}_{\text{full}}^{-1}$, need to find B_{11}^{-1} :

$$\begin{pmatrix} A_{11} & A_{12} \\ A_{21} & A_{22} \end{pmatrix} = \begin{pmatrix} B_{11} & B_{12} \\ B_{21} & B_{22} \end{pmatrix}^{-1}$$

- Simple manipulations lead to

$$\left(A_{11} - A_{12}A_{22}^{-1}A_{21}\right) B_{11} = 1 \quad \to \quad \mathsf{G}^{-1} = \omega - \mathsf{t} - \boldsymbol{\theta}\frac{1}{\omega - \boldsymbol{\varepsilon}}\boldsymbol{\theta}^\dagger$$

- $U \neq 0$: simply add the free energy (by definition)

The hybridization function (3)

- $\Gamma(\omega)$ embodies the effect of the rest of the lattice on the cluster, in some effective dynamics. The action would take the form

$$S = -\int_0^\beta \mathrm{d}\tau \int_0^\beta \mathrm{d}\tau' \sum_{\mu\nu} c_\mu^*(\tau)\mathscr{G}_{\mu\nu}^{-1}(\tau-\tau')c_\nu(\tau') + U\int \mathrm{d}_0^\beta\tau \sum_a n_{a\uparrow}(\tau)n_{a\downarrow}(\tau)$$

where

$$\mathscr{G}(i\omega_n) = \int_0^\beta \mathrm{e}^{i\omega_n\tau}\mathscr{G}(\tau)$$

$$\mathscr{G}_{\mu\nu}^{-1}(i\omega_n) = i\omega_n\delta_{\mu\nu} - t_{\mu\nu} - \Gamma_{\mu\nu}(i\omega_n)$$

Baths and the SFA

- The Potthoff functional approach carries over unchanged in the presence of a bath
- The bath makes a contribution to the Potthoff functional:

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

- On can in principle use the same methods as in VCA
- 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 sites (cluster + bath).

The CDMFT Procedure

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

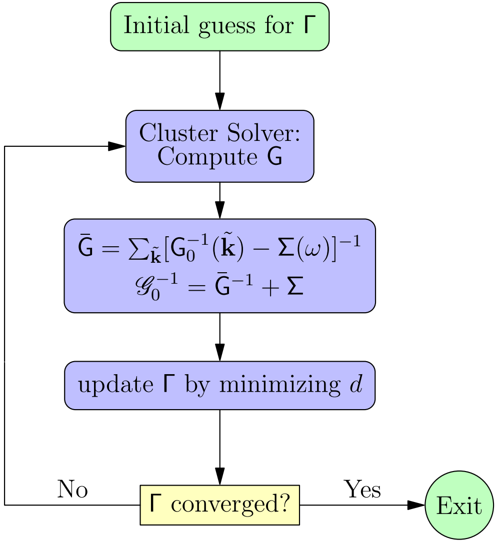
$$\bar{\mathsf{G}}(\omega) = \sum_{\tilde{\mathbf{k}}} \frac{1}{\mathsf{G}_0^{-1}(\tilde{\mathbf{k}}) - \Sigma(\omega)} \quad \text{and} \quad \mathscr{G}_0^{-1}(\omega) = \bar{\mathsf{G}}^{-1} + \Sigma(\omega)$$

4. Minimize the following distance function:

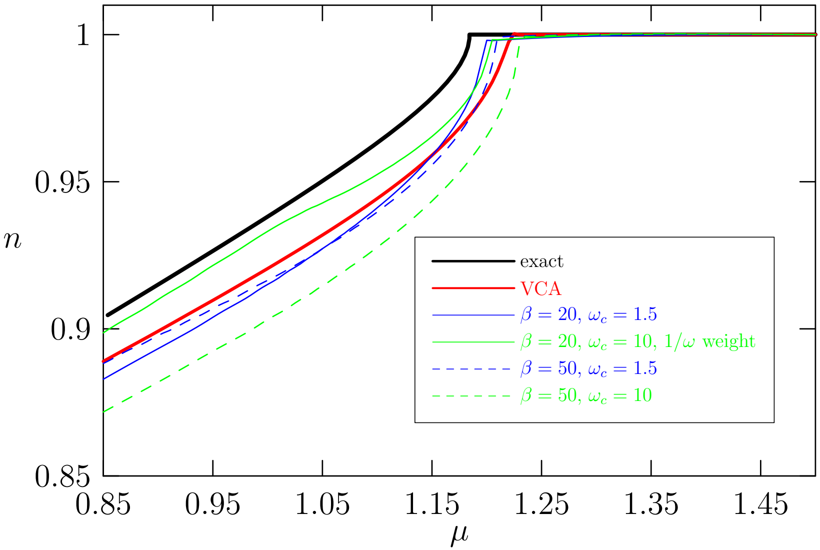
$$d = \sum_{\omega,\nu,\nu'} \left| \left(\omega + \mu - \mathsf{t}' - \Gamma(\omega) - \mathscr{G}_0^{-1}(\omega)\right)_{\nu\nu'} \right|^2$$

   over the set of bath parameters.
5. Go back to step (2) until convergence.

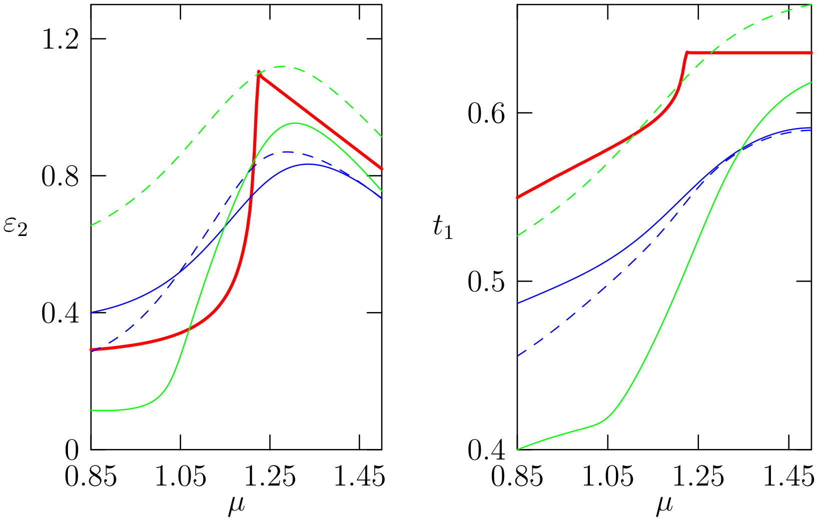
The CDMFT Procedure (2)



Example : the 1D Hubbard model

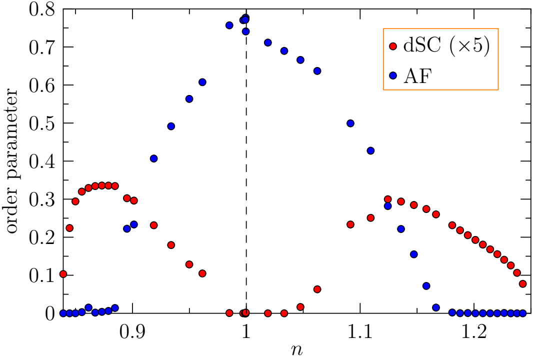


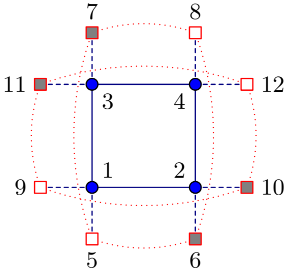
Example : the 1D Hubbard model (2)



Example : dSC and AF in the 2D Hubbard model

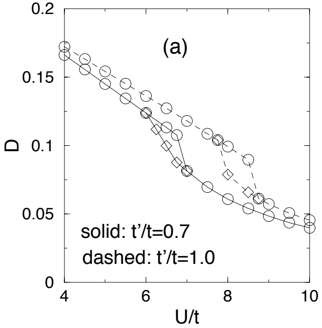
- Nine bath parameters
- Homogeneous coexistence of $d_{x^2-y^2}$ SC and Néel AF





Example : The Mott transition

- The CDMFT is well suited to detect the Mott transition
- This transition manifests itself as a jump in the double occupancy $\langle n_\uparrow n_\downarrow \rangle$
- In an exact SFA solution : discontinuity in the bath parameters (first order transition).
- in CDMFT : hysteresis is possible, because of the method's own dynamics for finding solutions



B. Kyung and A.-M. S. Tremblay. Physical Review Letters, 97 :046402 (2006)

QUESTIONS ?