Quantum Cluster Methods for Strongly Correlated Electron Systems: Variational Approach

Peyman Sahebsara

Advanced School of Recent Progress in
Condensed Matter Physics and Strongly Correlated Systems

IPM

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UNIVERSITÉ DE SHERBROOKE

Réseau québécois de calcul de haute performance

NSERC CRSNG

Menu

Part I :

Correlated Electron Systems

Part II :

Quantum Cluster Methods

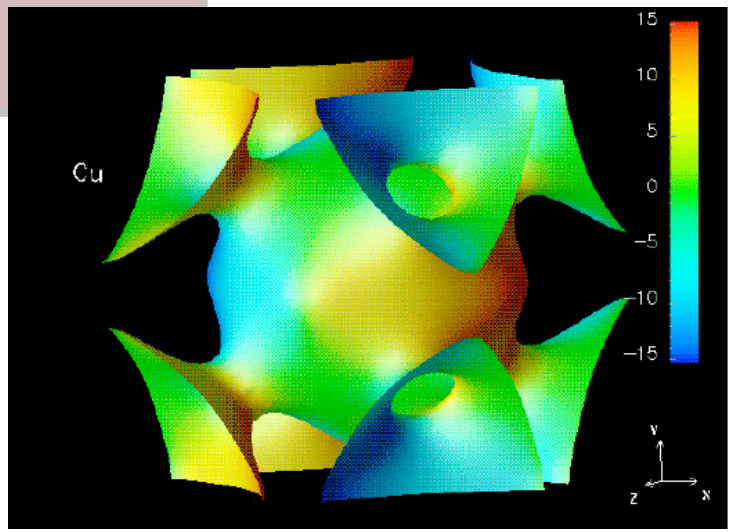
Part III:

Variational Approach

Part I

Uncorrelated Electron Systems (Standard Solid State Physics)

Uncorrelated Electron Systems



- Each electron moves in a periodic potential
- Electron states form bands with dispersion $\varepsilon_n(\mathrm{k})$
- The ground state is a filled Fermi surface: (e.g. copper)
- Interactions produce scattering of electrons, which are otherwise well-defined (quasi-)particles
- If the Fermi level crosses a band, the system is a conductor; otherwise it is an insulator (or a semiconductor).

Uncorrelated Electron Systems

The "theory of everything" in solids :

$$H = \underbrace{\sum_i \frac{\mathbf{p}_i^2}{2m}}_{\text{electrons}} + \underbrace{\sum_i \frac{\mathbf{P}_i^2}{2M_i}}_{\text{nuclei}} + \sum_{i<j} \frac{e^2}{|\mathbf{r}_i - \mathbf{r}_j|} - \sum_{i,j} \frac{Z_j e^2}{|\mathbf{r}_i - \mathbf{R}_j|} + \sum_{i<j} \frac{Z_i Z_j e^2}{|\mathbf{R}_i - \mathbf{R}_j|} + \text{spin orbit} + \text{Pauli spin}$$

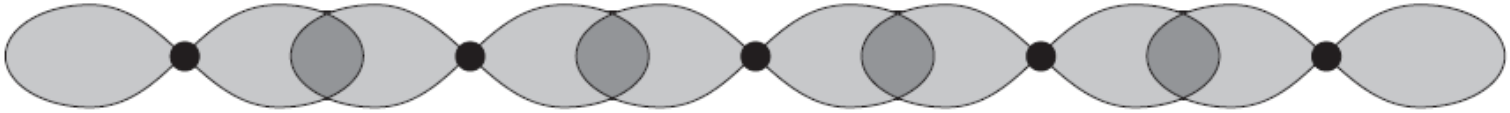
. . . is reduced to something manageable :

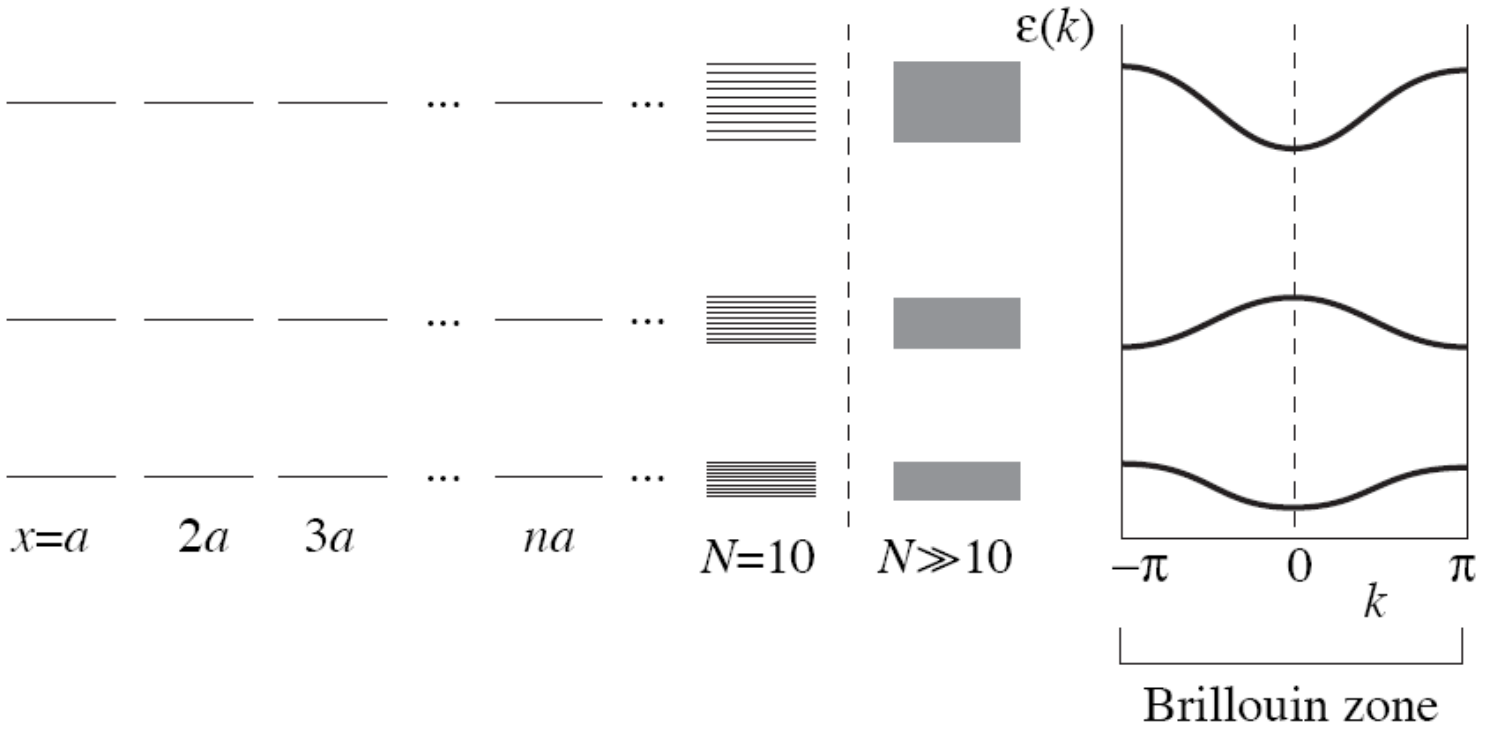
$$H = \sum_i \frac{\mathbf{p}_i^2}{2m} + \sum_i V_{sc}(\mathbf{r}_i, \{\mathbf{R}_j\})$$

Uncorrelated Electron Systems

1 Dimension

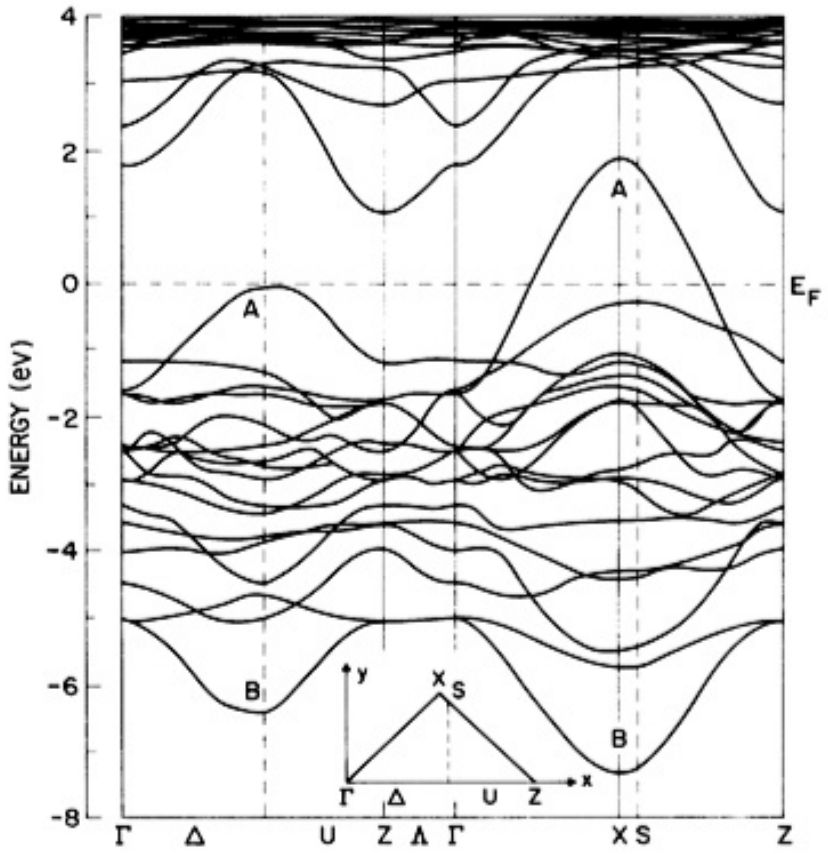
$$\psi_{\mathbf{k},n}(\mathbf{k}) = \sum_{\mathbf{n}} \mathrm{e}^{-i\mathbf{k}\cdot\mathbf{n}} w_n(\mathbf{r}-\mathbf{n})$$





Band structure of La_2CuO_4

- According to this, the material is a metal.
- In reality, it is an antiferromagnetic insulator!



Mattheiss, *Phys. Rev. Lett.* 58, 1028 (1987)

Electron Correlations

- They are strong deviations from the independent-electron picture
- Many families of materials are not adequately described by band theory, or by Fermi liquid theory :
  - High-T_c cuprate superconductors
  - Organic superconductors (quasi-1D or quasi-2D)
  - Most magnetic systems,
  - etc.
- Correlations make life difficult (and interesting...)

The Hubbard Model

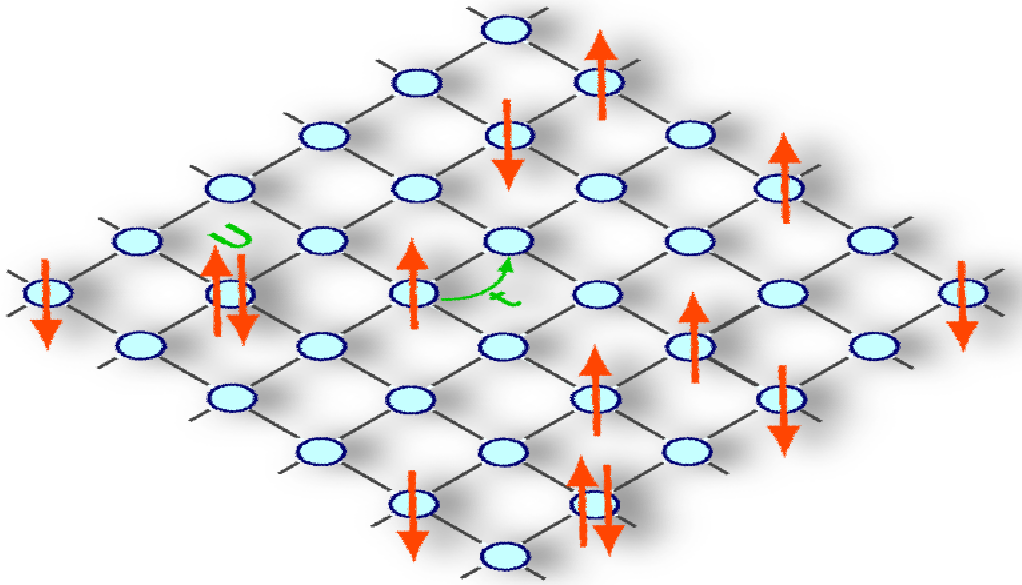
The Hubbard Model

- Used independently by Gutzwiller, Hubbard, Kanamori
- Basic assumption :

  Keep only local Coulomb repulsion (in the Wannier sense)
- One-band Hamiltonian:

$$H = \sum_{i,j,\sigma} t_{ij} c_{i\sigma}^{\dagger} c_{j\sigma} + U \sum_{i} n_{i\uparrow} n_{i\downarrow} + \mu \sum_{i} n_{i}$$

The Hubbard Model



$$H = \sum_{i,j,\sigma} t_{ij} c^{\dagger}_{i\sigma} c_{j\sigma} + U \sum_{i} n_{i\uparrow} n_{i\downarrow} + \mu \sum_{i} n_{i}$$

Hubbard Model

c_α : Destroys electron in state α (=$i\sigma$) of wavefunctions $\varphi_\alpha(\mathrm{r})$

$c_\alpha^\dagger$: Creates electron in state α

$n_\alpha = c_\alpha^\dagger c_\alpha$: number of electrons (0 or 1) in state α

$$\{c_\alpha^\dagger, c_\beta\} = \delta_{\alpha\beta} \quad , \quad \{c_\alpha, c_\beta\} = \{c_\alpha^\dagger, c_\beta^\dagger\} = 0$$

$$H = \sum_{i,j,\sigma} t_{ij} c_{i\sigma}^\dagger c_{j\sigma} + U \sum_i n_{i\uparrow} n_{i\downarrow} + \mu \sum_i n_i$$

Real Space :

$$\alpha \rightarrow (\mathbf{r}, \sigma)$$

k Space :

$$\alpha \rightarrow (\mathbf{k}, b, \sigma)$$

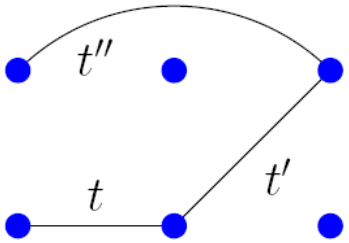
Hubbard model : noninteracting limit

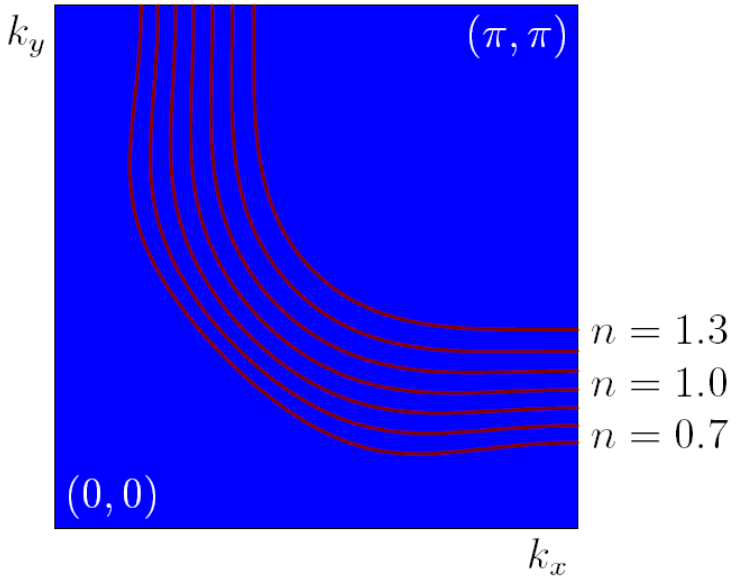
U = 0 : reduces to band theory

$$\varepsilon(k) = \frac{1}{N}\sum_{i,j} t_{ij} e^{-i(n_i - n_j)\cdot k}$$

Ex : square lattice with NN hopping *t*, NNN hopping *t'* and 3rd neighbor *t"*

$$\varepsilon(k) = -2t(\cos k_x + \cos k_y)$$
$$-2t'\left(\cos(k_x + k_y) + \cos(k_x - k_y)\right)$$
$$-2t''\left(\cos 2k_x + \cos 2k_y\right)$$





Hubbard model : large-U limit

- Electrons localized so as to minimize the double-occupancy
- Ground state may be highly degenerate as $U \to \infty$
- half-filled case $\to$ Heisenberg model :

$$H \to J \sum_{i,j} S_i \cdot S_j \quad , \quad \left(J = \frac{4t^2}{U} \quad , \quad S = \frac{1}{2} c_\alpha^\dagger \sigma_{\alpha\beta} c_\beta \right)$$

- Tendency towards antiferromagnetism!
- Hence the HM describes undoped cuprates well.

Hubbard model : large-U limit (cont.)

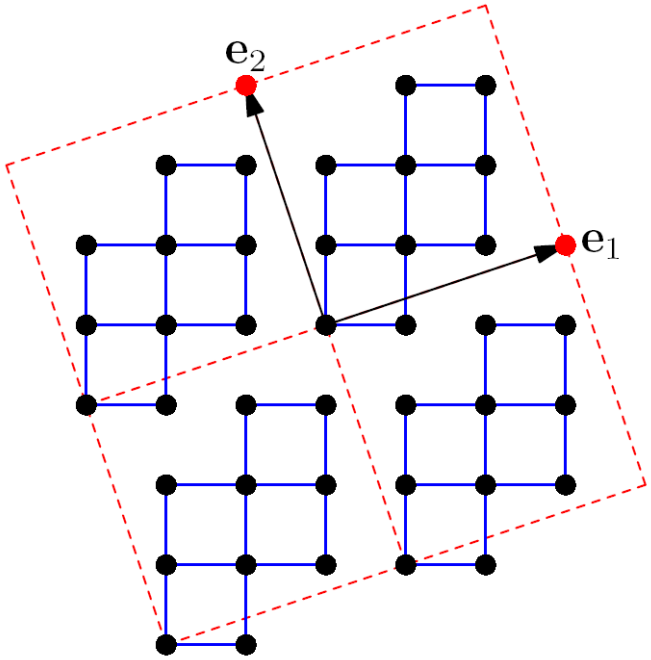
Away from half-filling, the HM goes to the *t*-*J* model when $U >> t$. (Anderson 1987)

$$H = \sum_{i,j,\sigma} t_{ij} c_{i\sigma}^{\dagger} c_{j\sigma} + \sum_{i,j} J_{ij} S_i \cdot S_j \quad , \quad \left(J_{ij} = \frac{4t_{ij}^2}{U} \right)$$

- The *t*-*J* model makes sense only when $J << t$.
- Single-occupancy constraint : no site is allowed to have two electrons

The Hubbard Model on finite cluster

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



Typical cluster (L=10 sites):

The Hubbard Model on finite cluster

A band structure calculation involves the self-consistent of the Schrödinger equation for a single electron :

an eigenproblem of dimension N ~10^3

But the HM is a full many-body problem, not an effective one-body problem.

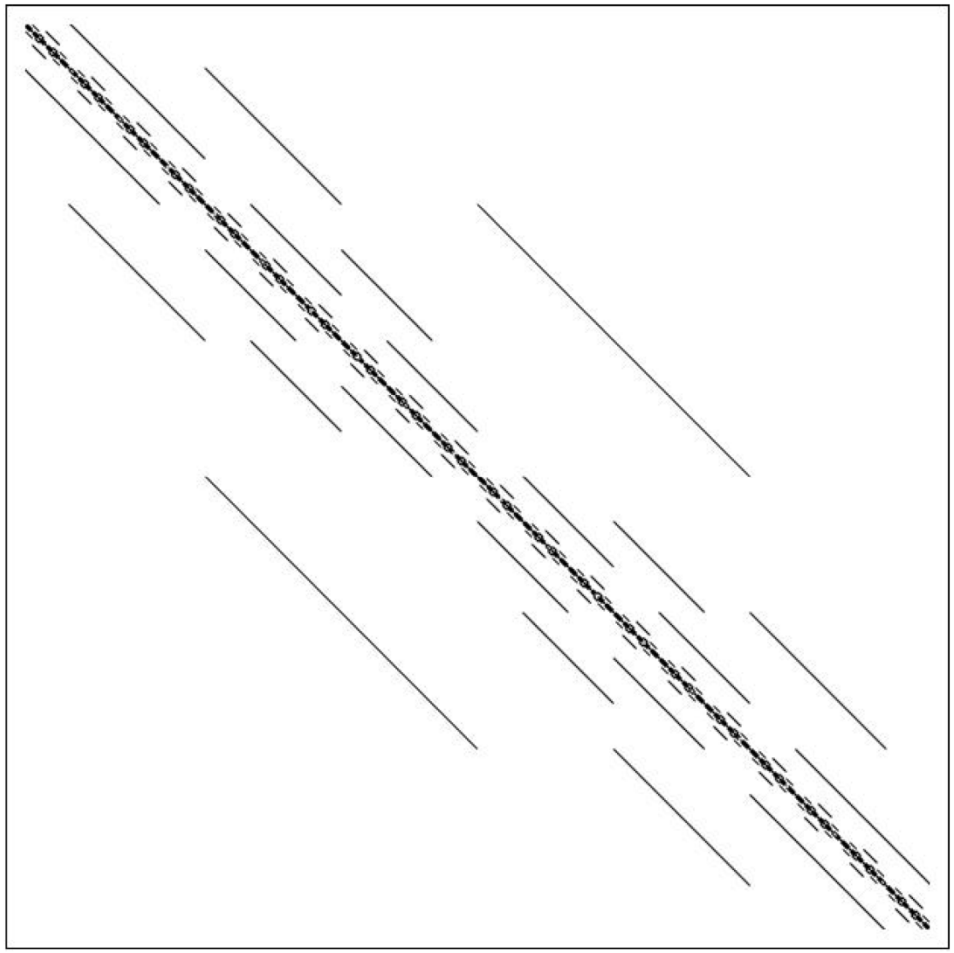
Finding just the ground state of the Hubbard model with $N_\uparrow + N_\downarrow$ electrons on L sites requires solving an eigensystem of dimension

$$\frac{L!}{N_\uparrow!(L-N_\uparrow)!} \times \frac{L!}{N_\downarrow!(L-N_\downarrow)!}$$

The Hubbard Model on finite cluster

Half-filled Hubbard model $L = 6$

Sparse matrix structure
400×400



The Hubbard Model on finite cluster

Half-filled Hubbard model $L = 16$

For $N_\uparrow = N_\downarrow = 8$, this is 165 636 900.

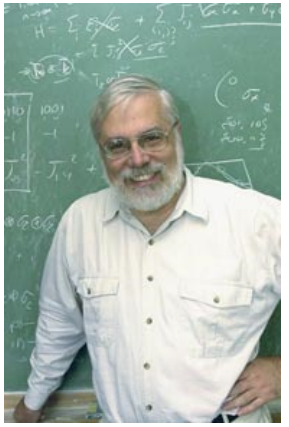
L	dimension
2	4
4	36
6	400
8	4 900
10	63 504
12	853 776
14	11 778 624
16	165 636 900

Solving the Hubbard Model

- Therefore, Hubbard model is difficult to solve
- The more difficult the model, the more there are methods to solve it!

Methods of Solving the Model

- Perturbation theory in U/t (a bad idea) or in t/U (more difficult)
- Self-consistent schemes based on perturbation theory (better)
- Two-particle self-consistent method (TPSC) [Tremblay et al.]
- Variational methods for the ground state (e.g. Gutzwiller)
- Various reductions to a 1-body Hamiltonian:
- Mean-field theory for the ordered state (Hartree-Fock)
- Slave-boson methods
- Monte Carlo simulations
- Exact diagonalizations on small periodic clusters
- Dynamical Mean-Field theory (DMFT)
- Quantum Cluster Approaches : CPT, DCA, CDMFT, VCA



The Lanczos Algorithm

Solving the Hubbard Model

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

Building a basis

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:

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

The Lanczos Algorithm

- Finds the lowest eigenpair by an iterative application of H
- Start with random vector $|\varphi_0\rangle$
- An iterative procedure builds the *Krylov subspace*:

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

The Lanczos Algorithm

- Lanczos three-way recursion:

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

with the coefficients:

$$a_n = \frac{\langle\phi_n|H|\phi_n\rangle}{\langle\phi_n|\phi_n\rangle}$$

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

The Lanczos Algorithm

The projected Hamiltonian has the tri-diagonal form

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

The basis contains normalized states

$$|n\rangle = |\phi_n\rangle / \sqrt{\langle \phi_n | \phi_n \rangle}$$

The Lanczos Algorithm

- 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 $|\varphi_n\rangle$'s are not kept in memory.

- 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

Lanczos Method and Green Function

$$G_{\mu\nu}(\omega) = G_{\mu\nu,e}(\omega) + G_{\mu\nu,h}(\omega)$$

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

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

Lanczos Method and Green Function

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 $G_{\mu\nu,e}$?

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

Lanczos Method and Green Function

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 $G_{\mu\nu,e}(\omega)$

We have

$$G_{\mu\nu,e}(\omega) = G_{\nu\mu,e}(\omega)$$

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

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

The Band Lanczos Algorithm

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

The Band Lanczos Algorithm

- 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

To be continued ...