Exact Diagonalization: Introduction

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Matrix

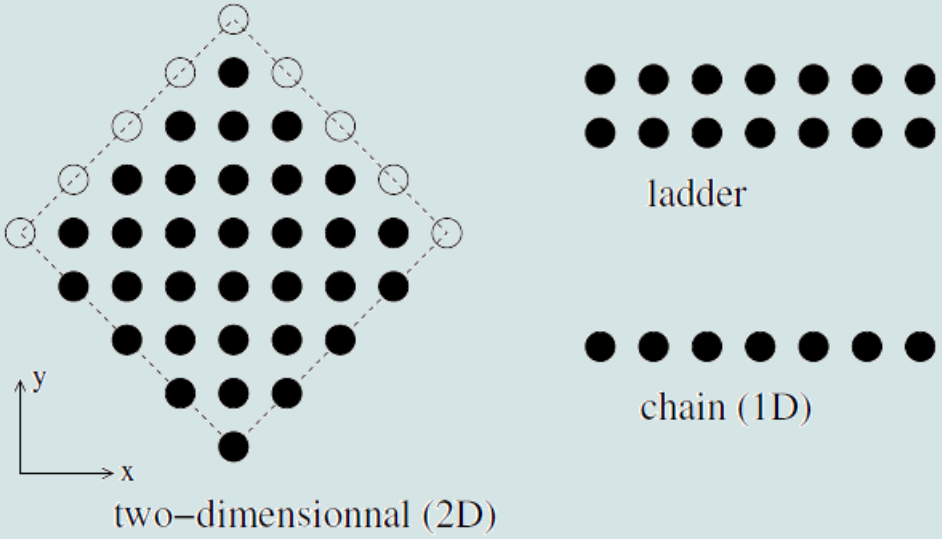
$$H = \begin{pmatrix}
0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\
0 & 0 & 0 & 0 & -t & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\
0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & -t & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\
0 & 0 & 0 & U & 0 & 0 & -t & 0 & 0 & -t & 0 & 0 & 0 & 0 & 0 & 0 \\
0 & -t & 0 & 0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

Ingredients

- Hilbert space
  - Basis representation, Lookup techniques
  - Symmetries
- Hamiltonian Matrix
  - Sparse Matrix representation (memory/disk)
  - Matrix recalculation on the fly (matrix–free)
- Linear Algebra : Eigensolver / Time propagation
  - LAPACK full diagonalization
  - Lanczos type diagonalization (needs only operations)
  - More exotic eigensolver techniques, imaginary-time propagation,
- Observables
  - Static quantities (multipoint correlation functions, correlation density matrices,...)
  - Dynamic observables (spectral functions, density of states,...)
  - Real-time evolution

Lattice model

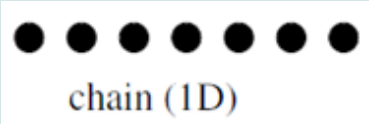
Direct diagonalization of Hamiltonian matrix on finite clusters



- Hilbert space, Symmetries
- Hamiltonian matrix
- Linear Algebra
- Observables

Representation of Many-Body States

- Mapping to (binary) integers:
  - Spin–1/2 Heisenberg:



$$|j,m\rangle = |\uparrow\rangle \otimes \cdots\cdots \otimes |\downarrow\rangle$$

    - For example

$$|\uparrow\downarrow\uparrow\rangle = |101\rangle = |5\rangle$$

  - Hubbard:
    - For example

$$|01\rangle_{\downarrow}|10\rangle_{\uparrow} = 6$$

Symmetries in ED I

- The inclusion of symmetries in an ED code has two major advantages:
  - Quantum number resolved energies and states.
  - Reduction of the Hilbert space to be diagonalized.
- Given group G with generators $\{g_p\}$
  - $[H, g_p] = 0$ → H block diagonal (Hilbert space can be divided)

Symmetries in ED II

- Consider the simplest parent Hamiltonian, *the Heisenberg model* on a chain.

$$H = J\sum_i \mathbf{S}_i \mathbf{S}_{i+1}$$

- The dimension of Hilber space is 2^N
  - For exmaple $N = 20 \rightarrow 2^{20} = 1048576 \cong 10^6$
    - To store a *real number* (*double precision*) in computer we need 8 Bytes.
    - To store the matrix element of the above Hamiltonian we need:
    - Number of bytes $= 8 \cdot (10^6)^2 \cong 8000\text{GB}$
- Considering the S_z symmetry
  - For example, the most amount of basis is total $S_z = 0$
    - 10 up–spin, 10 down–spin

$$C_{10}^{20} = \frac{20!}{10!10!} = 184756 \cong 10^5$$

    - Number of bytes $= 8\ (10^5)^2 \cong 80\text{GB}$

Symmetries in ED III

- Continuous:
- $U(1)$ related symmetries
  - Conservation of particle number(s)
  - Conservation of total S_z
- $SU(2)$ symmetry
  - Difficult to implement together with spatial symmetries
  - For $S_z = 0$ an operation called "spin inversion (Z_2)" splits the Hilbert space in even and odd spin sectors.
- Spatial symmetry groups:
  - Translation symmetry (abelian symmetry, therefore 1D irreps)
  - Pointgroup symmetries (in general non–abelian)

Sparse Matrix

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

Hamiltonian Matrix Storage

- Different possibilities exist:
  - Store Hamiltonian matrix elements in memory in a sparse matrix format
    - Fast matrix vector multiplies, but obviously limited by available memory.
  - Store Hamiltonian matrix elements on disk in a sparse matrix format.
    - In principle possible due to the vast disk space available, but I/O speed is much slower than main memory access times. Difficult to parallelize.
  - Recalculate the Hamiltonian matrix elements in each iterations “on the fly”.
    - Needed for the cutting edge simulations, where the whole memory is used by the Lanczos vectors. Can be parallelized on most architectures.

Diagonalization routine

- If *H* is dense or system small enough
  - Use
    - Jacobi
    - Householder
    - LAPACK
    - ...
  - (all these apply orthogonal transformations to *H* until tridiagonal form, then quickly diagonalize)
- If *H* is sparse
  - Use
    - ARPACK
    - IETL/ALPS
    - DiagHam
  - (these are iterative solvers based on variants of Lanczos algorithm which preserves the sparseness of *H*)

LAPACK

- Complete diagonalization routine written in F77 (Fortran)
- Support all kind of data structure
  - Real, Real (double precision), complex, complex (double precision)
- Support most of matrix formation
  - Symmetric, Hermitian, Tri–digonal, ...
- Useful for:
  - Simple problems, testing
  - Matrix *H* dense
  - Many eigenstates required
- But
  - *H* must be stored
  - Entire matrix must be diagonalized

Linear Algebra I

- Lanczos algorithm:
  - C. Lanczos, J. Res. Natl. Bur. Stand. 45, 255 (1950).
  - Iterative "Krylov" space method which brings matrices into tridiagonal form.
  - Method of choice in many large–scale ED programs.
    - Works well for sparse, short–range H
    - Very rapid convergence but numerically unstable (can be controlled by a suitable techniques).
    - Easy to implement and memory efficient – only 3 vectors needed at once
  - If the ground state (energy) or some low energy spectrum is interesting, the Lanczos method may help us. Using Lanczos and considering the $S_z = 0$ symmetry of the model above, the required memory to get the ground state (energy) and few low lying states is:
    - Number of bytes $\cong 30 \times 184756 = 5542680$Bytes $\cong$ 55MB
    - The required memory is available as RAM in any personal computer.

Linear Algebra II

- "modified Lanczos" algorithm:
  - E. Gagliano, et al. Phys. Rev. B 34, 1677 (1986).
  - actually more like a Power–method, therefore rather slow convergence.
  - needs only two vectors in memory
  - At each step the approximate groundstate wavefunction is available
  - Difficult to get excited states
- Jacobi-Davidson Algorithm:
  - E. R. Davidson, Comput. Phys. 7, 519 (1993).
  - subspace expanded by diagonal approximation to inverse iteration
  - varying number of vectors in memory
  - higher-order convergence than Lanczos (usually)
    - Rapid convergence, especially for diagonally dominant matrices (Hubbard model)
    - Often used in DMRG programs as well.

Lanczos

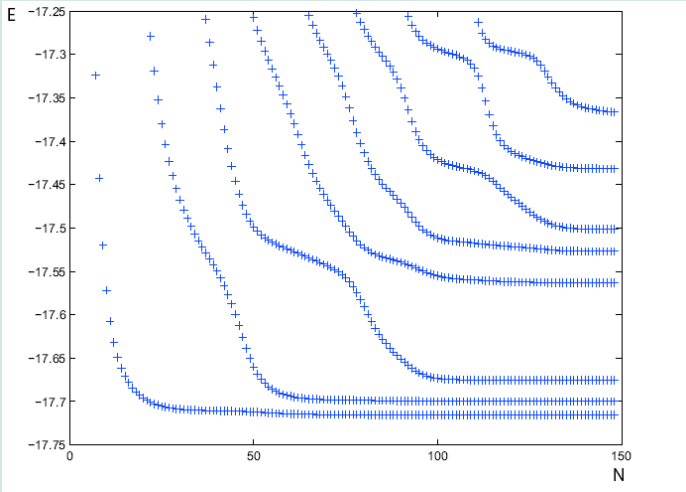
$$b_0 = 0$$

$$|\phi'\rangle = H|\phi_n\rangle - b_n|\phi_{n-1}\rangle$$
$$a_n = \langle\phi_n|\phi'\rangle$$
$$|\phi''\rangle = |\phi'\rangle - a_n|\phi_n\rangle$$
$$b_{n+1} = \|\phi''\| = \sqrt{\langle\phi''|\phi''\rangle}$$
$$|\phi_{n+1}\rangle = |\phi''\rangle / b_{n+1}$$

- At each step n, find the lowest eigenvalue of that matrix
- Stop when the lowest eigenvalue E_0 has converged ($\Delta E_0/E_0 < 10^{-12}$)

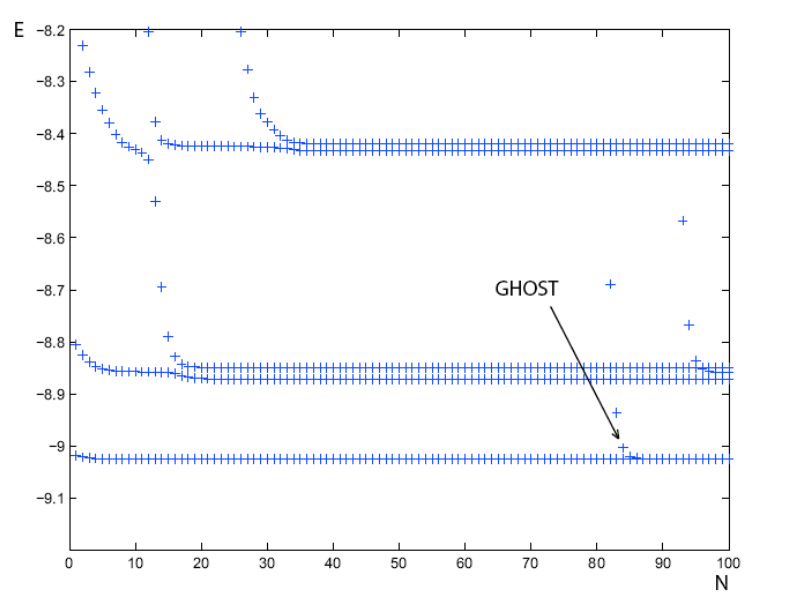
$$H^N|\phi_0\rangle = a_N|\phi_N\rangle \ , \ |N\rangle = \frac{|\phi_N\rangle}{\sqrt{\langle\phi_N|\phi_N\rangle}} \ , \ \text{Krylov space}$$

$$T = \begin{matrix} \langle 1| \\ \langle 2| \\ \langle 3| \\ \langle \cdots| \\ \langle N-1| \\ \langle N| \end{matrix} \begin{pmatrix} a_1 & b_2 & & & & \\ b_2 & a_2 & b_3 & & & \\ & b_3 & a_3 & b_4 & & \\ & & \ddots & \ddots & \ddots & \\ & & & b_{N-1} & a_{N-1} & b_N \\ & & & & b_N & a_N \end{pmatrix}$$



Roundoff errors and ghosts

- In exact arithmetic the vectors $\{\phi_i\}$ are orthogonal and the Lanczos iterations stop after at most N – 1 steps. The eigenvalues of T are then the exact eigenvalues of H.
- Roundoff errors in finite precision cause a loss of orthogonality so that the matrix T contains extra spurious eigenvalues, called “ghosts”.



Roundoff errors and ghosts

- There are two ways to deal with that:
  - Reorthogonalization of the vectors after every step. This requires storing all of the vectors $\{\phi_i\}$ and is memory intensive. (you don't want to do it)
  - Control of the effects of roundoff.
- We will discuss the second solution as it is faster and needs less memory.
- The main effect of roundoff errors is that the matrix T contains extra spurious eigenvalues, called "ghosts". These ghosts are not real eigenvalues of H.
- However they converge towards real eigenvalues of H over time and increase their multiplicities.

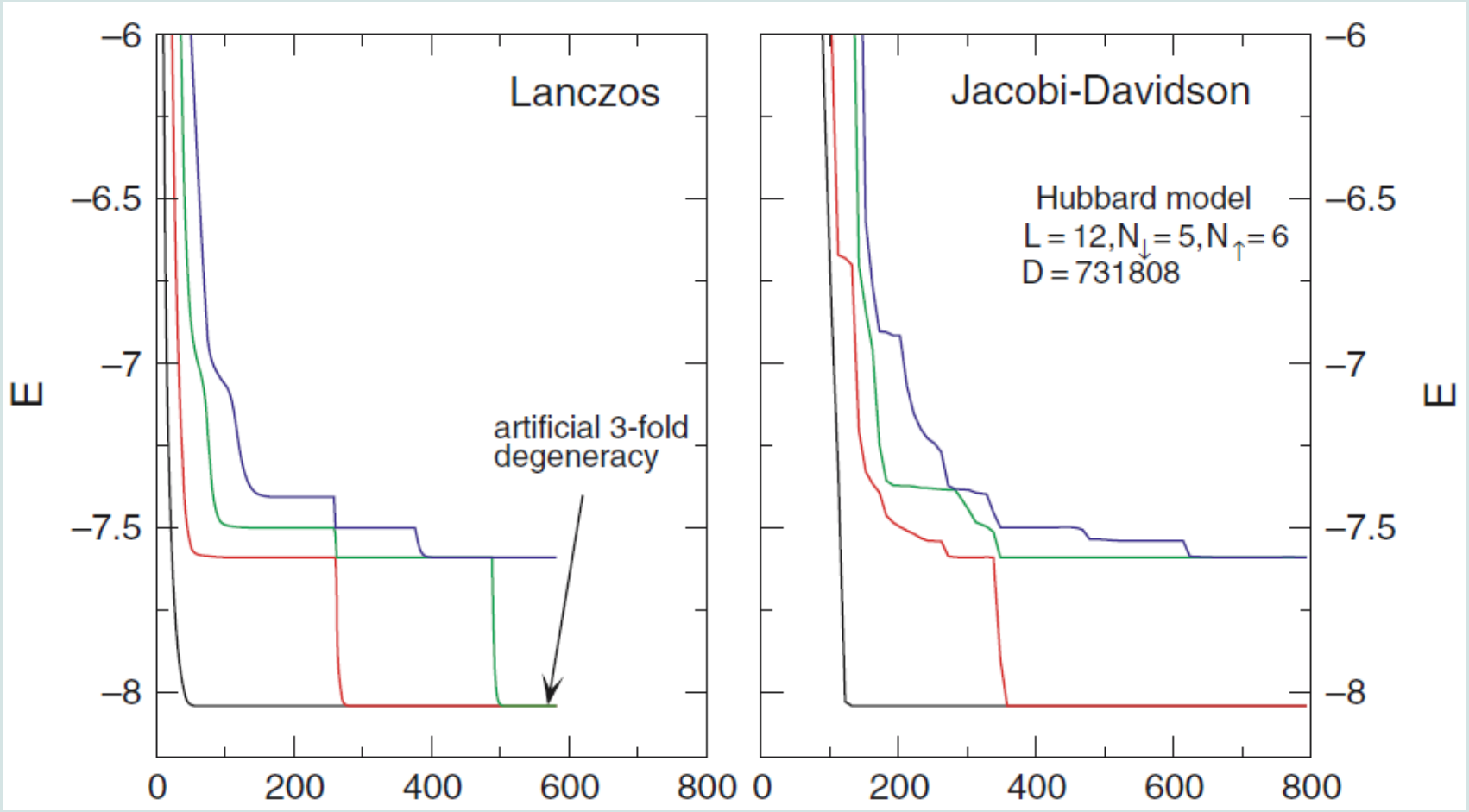
Roundoff errors and ghosts

- A simple criterion distinguishes ghosts from real eigenvalues. Ghosts are caused by roundoff errors. Thus they do not depend on the starting vector ϕ_l. As a consequence these ghosts are also eigenvalues of the matrix T', which can be obtained from T' by deleting the first row and column:

$$T' = \begin{pmatrix} \cancel{a_1} & \cancel{b_2} & & & & & \\ \cancel{b_2} & a_2 & b_3 & & & & \\ & b_3 & a_3 & b_4 & & & \\ & & \ddots & \ddots & \ddots & & \\ & & & b_{N-1} & a_{N-1} & b_N & \\ & & & & b_N & a_N & \end{pmatrix}$$

- Criterion to distinguish ghosts from real eigenvalues:
  - All multiple eigenvalues are real, but their multiplicities might be too large.
  - All single eigenvalues of T which are not eigenvalues of T' are also real.

Degenracy


Lanczos
Jacobi-Davidson
Hubbard model
L = 12, N↓ = 5, N↑ = 6
D = 731808
artificial 3-fold
degeneracy
E
E
–6
–6.5
–7
–7.5
–8
0
200
400
600
800

Green's function–Continued fraction

- Zero temperature Green's function

$$G_{ij}(t) = -i\left\langle \Omega \middle| c_i(t) c_j^+(0) \middle| \Omega \right\rangle$$

$$G_{ij}(\omega) = \left\langle \Omega \middle| c_i \frac{1}{\omega - H + E_0} c_j^+ \middle| \Omega \right\rangle$$

- Consider the diagonal element

$$\left|\phi_i\right\rangle = c_i^+ \left|\Omega\right\rangle \Rightarrow G_{ii} = \left\langle \phi_i \middle| \frac{1}{\omega - H + E_0} \middle| \phi_i \right\rangle$$

- Use the expansion

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

Green's function–Continued fraction

- Truncated expansion evaluated exactly in Krylov subspace generated by $|\phi_i\rangle$
- We perform a Lanczos procedure on $|\phi_i\rangle$, then G_{ii} is given by Jacobi continued fraction

$$G_{ii} = \cfrac{\langle \phi_i | \phi_i \rangle}{\omega - a_0 - \cfrac{b_1^2}{\omega - a_1 - \cfrac{b_2^2}{\omega - a_2 - \cdots}}}$$

Green's function–Continued fraction

- Non-diagonal element

$$G_{ij}^{+}(\omega) = \left\langle \Omega \middle| (c_i + c_j) \frac{1}{\omega - H + E_0} (c_i + c_j)^{+} \middle| \Omega \right\rangle$$

- Define $|\phi_k\rangle = (c_i + c_j)^{+} |\Omega\rangle$, we obtain

$$G_{ij}^{+} = \cfrac{\langle \phi_k | \phi_k \rangle}{\omega - a_0 - \cfrac{b_1^2}{\omega - a_1 - \cfrac{b_2^2}{\omega - a_2 - \cdots}}}$$

- Since $G_{ij} = G_{ji}$, then

$$G_{ij} = \frac{1}{2}[G_{ij}^{+} - G_{ii} - G_{jj}]$$

Green's function–Lehmann representation

- Lehmann representation

$$G_{ij}(\omega) = \sum_m \left\langle \Omega \middle| c_i \middle| m \right\rangle \frac{1}{\omega - E_m + E_0} \left\langle m \middle| c_j^+ \middle| \Omega \right\rangle + \sum_n \left\langle \Omega \middle| c_j \middle| n \right\rangle \frac{1}{\omega + E_n - E_0} \left\langle n \middle| c_i^+ \middle| \Omega \right\rangle$$

$$= \sum_m \frac{\left| \left\langle \Omega \middle| c_i \middle| m \right\rangle \right|^2}{\omega - E_m + E_0} + \sum_n \frac{\left| \left\langle n \middle| c_i^+ \middle| \Omega \right\rangle \right|^2}{\omega + E_n - E_0}$$

$$\left| \phi_i \right\rangle = c_i^+ \left| \Omega \right\rangle \quad , \quad i = 1 \ldots L$$

- Extended Krylov space form a band Hamiltonian ($2L+1$ diagonals)

$$H^N \left| \phi_i \right\rangle = a_i^{(N)} \left| \phi_i^N \right\rangle \quad , \quad i = 1 \ldots L$$

Green's function–Recursion

- Green's function

$$G_{ij}(\omega) = \left\langle \Omega \middle| c_i \frac{1}{\omega - H + E_0} c_j^{+} \middle| \Omega \right\rangle = \left\langle \phi_1 \middle| \frac{1}{\omega - H + E_0} \middle| \phi_1 \right\rangle$$

$$\left|\phi_i\right\rangle = c_i^{+}\left|\Omega\right\rangle \ , \ \ i = 1 \ldots L$$

- $\boldsymbol{HQ} = \boldsymbol{QT}$

$$\mathbf{T} = \begin{pmatrix} a_1 & b_{21} & b_{32} & \cdots & & \\ b_{21} & a_2 & b_{31} & b_{42} & & \\ b_{32} & b_{31} & a_3 & b_{41} & & \\ \vdots & b_{42} & \ddots & \ddots & \ddots & \\ & & & b_{N-1,1} & a_{N-1} & b_{N,1} \\ & & & & b_{N,1} & a_N \end{pmatrix} \qquad \mathbf{Q} = \begin{bmatrix} \boldsymbol{\varphi}_1 & \boldsymbol{\varphi}_2 & \boldsymbol{\varphi}_3 & \cdots \end{bmatrix}$$

- where $\boldsymbol{\varphi}_i$ is calcuated by band Lanczos method

Green's function–Recursion

- Recursion

$$G_{ij}(\omega) = \boldsymbol{\varphi}_1 \frac{1}{\omega - \mathbf{H} + E_0} \boldsymbol{\varphi}_1$$

$$= \boldsymbol{\varphi}_1 \mathbf{Q}\mathbf{Q}^{+} \frac{1}{\omega - \mathbf{H} + E_0} \mathbf{Q}\mathbf{Q}^{+} \boldsymbol{\varphi}_1$$

$$= \boldsymbol{\varphi}_1 \mathbf{Q} \frac{1}{\omega - \mathbf{T} + E_0} \mathbf{Q}^{+} \boldsymbol{\varphi}_1$$

$$= \left[\frac{1}{\omega - \mathbf{T} + E_0} \right]_{11}$$

- where

$$\mathbf{Q}^{+}\boldsymbol{\varphi}_1 = \begin{bmatrix} \boldsymbol{\varphi}_1 \\ \boldsymbol{\varphi}_2 \\ \boldsymbol{\varphi}_3 \\ \vdots \end{bmatrix} \boldsymbol{\varphi}_1 = \begin{bmatrix} 1 \\ 0 \\ 0 \\ 0 \end{bmatrix}$$

Finite Temperature Lanczos Methods

- These methods (FTLM, LTLM) combine the Lanczos method and random sampling to go to larger systems.
- For high to moderate temperatures these methods can obtain results basically in the thermodynamic limit.
- The Low Temperature Lanczos Method can also go to low temperatures to get correct results on a given sample. Finite size effects however persist.
- Like the $T = 0$ ED method it is most useful, where QMC or T–DMRG etc fail, such as frustrated and fermionic models.

FTLM

- In the canonical ensemble, the thermal average of a physical quantity A at finite–T in orthonormal basis $|n\rangle$ is defined as

$$\langle A \rangle = \frac{1}{Z} \sum_{n}^{N} \langle n | A e^{-\beta H} | n \rangle$$

$$Z = \sum_{n}^{N} \langle n | e^{-\beta H} | n \rangle$$

- High temperature expansion gives

$$\langle A \rangle = \frac{1}{Z} \sum_{n}^{N} \sum_{k=0}^{\infty} \frac{(-\beta)^k}{k!} \langle n | H^k A | n \rangle$$

$$Z = \sum_{n}^{N} \sum_{k=0}^{\infty} \frac{(-\beta)^k}{k!} \langle n | H^k | n \rangle$$

  - From two successive Lanczos procedures for two operators

$$\langle n | H^k B H^l A | n \rangle = \sum_{i=0}^{M} \sum_{j=0}^{M} \langle n | \psi_i \rangle \langle \psi_i | B | \tilde{\psi}_j \rangle \langle \tilde{\psi}_j | A | n \rangle (\varepsilon_i)^k (\tilde{\varepsilon}_j)^l$$

FTLM

- We obtain ($k < M$)

$$\langle n|H^k A|n\rangle = \sum_{i=0}^{M} \langle n|\psi_i^{(n)}\rangle\langle\psi_i^{(n)}|A|n\rangle(\varepsilon_i^{(n)})^k$$

  - The superscript (n) means that $|\psi_i^{(n)}\rangle$ and $\varepsilon_i^{(n)}$ are obtained in Lanczos algorithm with the initial state $|\psi_i^{(n)}\rangle$
  - Extend the results to $k > M$, the approximate expressions are

$$\langle A\rangle \approx \frac{1}{Z}\sum_{n}^{N}\sum_{k=0}^{\infty}\frac{(-\beta)^k}{k!}\sum_{i=0}^{M}\langle n|\psi_i^{(n)}\rangle\langle\psi_i^{(n)}|A|n\rangle(\varepsilon_i^{(n)})^k = \frac{1}{Z}\sum_{n}^{N}\sum_{i=0}^{M} e^{-\beta\varepsilon_i^{(n)}}\langle n|\psi_i^{(n)}\rangle\langle\psi_i^{(n)}|A|n\rangle$$

$$Z \approx \sum_{n}^{N}\sum_{k=0}^{\infty}\frac{(-\beta)^k}{k!}\sum_{i=0}^{M}\langle n|\psi_i^{(n)}\rangle\langle\psi_i^{(n)}|n\rangle(\varepsilon_i^{(n)})^k = \frac{1}{Z}\sum_{n}^{N}\sum_{i=0}^{M} e^{-\beta\varepsilon_i^{(n)}}\langle n|\psi_i^{(n)}\rangle\langle\psi_i^{(n)}|n\rangle$$

- It is very expensive to calculate all n

FTLM

- Stochastic sampling of Krylov space: Replace the summation of the full Hilbert space by a sum over random number of states

$$\langle A \rangle \approx \frac{1}{Z} \sum_s \sum_r^R \sum_i^M e^{-\beta \varepsilon_i^{(r)}} \left\langle r \middle| \psi_i^{(r)} \right\rangle \left\langle \psi_i^{(r)} \middle| A | r \right\rangle$$

$$Z = \sum_s \sum_r^R \sum_i^M e^{-\beta \varepsilon_i^{(r)}} \left| \left\langle r \middle| \psi_i^{(r)} \right\rangle \right|^2$$

- Σ_s over symmetry sector of dimension N_s
- Σ_r over R random starting vectors $|r\rangle$

LTLM

- Since FTLM is related to high–T expansion, i.e., $T \rightarrow \infty$ limit correct, the limit of $T \rightarrow 0$ does not lead to the ground state expectation value.

$$\langle A \rangle \approx \frac{1}{Z} \sum_{s}^{R} \sum_{r}^{M} \sum_{i}^{M} \sum_{j}^{M} e^{-\beta \varepsilon_i^{(r)}/2} e^{-\beta \varepsilon_j^{(r)}/2} \langle r | \psi_j^{(r)} \rangle \langle \psi_j^{(r)} | A | \psi_i^{(r)} \rangle \langle \psi_i^{(r)} | r \rangle$$

$$Z = \sum_{s}^{R} \sum_{r}^{M} \sum_{i}^{M} e^{-\beta \varepsilon_i^{(r)}} \left| \langle r | \psi_i^{(r)} \rangle \right|^2$$

  - One more Lanczos procedure for each sampling
  - In the limit of $T \rightarrow 0$

$$\langle A \rangle \approx \langle \psi_0 | A | \psi_0 \rangle$$

Strongly Correlated Systems

- Hubbard model
- Heisenberg model
- High-T_c superconductor
- Quantum Phase Transitions

Applications

- Quantum Magnets: nature of novel phases, critical points in 1D, dynamical correlation functions in 1D & 2D
- Fermionic models (Hubbard/t–J): gaps, pairing properties, correlation exponents, etc
- Fractional Quantum Hall states: energy gaps, overlap with model states, entanglement spectra
- Quantum dimer models or other constrained models (anyon chain..)
- Full Configuration Interaction in Quantum Chemistry

Largest system reached

- $S = 1/2$ spin models
  - square lattice: $N = 40$
  - triangular lattice: $N = 39$
    - maximum dimension of basis: 1.5 billion
- t–J models
  - checkerboard lattice with 2 holes: $N = 32$
  - square lattice with 2 holes: $N = 32$
    - maximum dimension of basis: 2.8 billion
- Hubbard models
  - square lattice at half filling: $N = 20$
  - quantum dot structure: $N = 20$
    - maximum dimension of basis: 3 billion
- Holstein models
  - chain with $N = 14$ + phonon pseudo-sites
    - maximum dimension of basis: 30 billion

Exact diagonalization is expensive!

- Why use ED then?
  - Robust, unbiased and completely versatile–almost anything can be calculated!
  - There are models which are not easy to access via other models (e.g. frustrated magnets)
  - Error is at least as low as 10^{-14} – numerical precision
  - Exploiting symmetries reduces computational effort and gives physical information about eigenstates (good quantum numbers)

The best we can do: Low-lying states

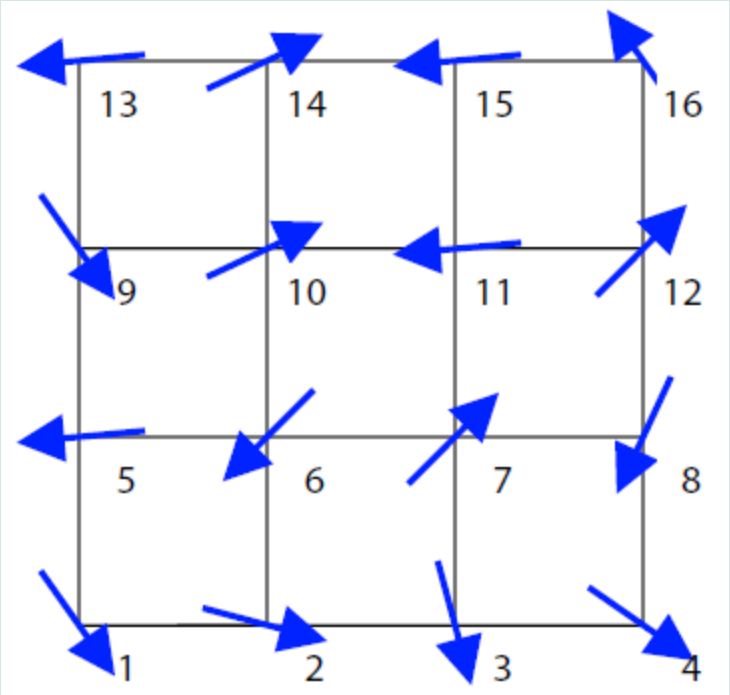
- Low-lying states sufficient for low–temperature physics;
- Low-lying states important for quantum phase transitions, e.g. magnetization jumps.
- Several methods available to obtain extreme eigenvalues: projection, Lanczos, DMRG.

Exact Diagonalization: Application

Spin–1/2

Heisenberg model

$$\mathcal{H} = -J \sum_{\langle ij \rangle \sigma} \mathbf{S}_i \mathbf{S}_j + h \sum_i \mathbf{B}\mathbf{S}_i$$



Spin–1/2 system

- Define ladder operators:

$$S_i^+ = S_i^x + iS_i^y$$

$$S_i^- = S_i^x - iS_i^y$$

- The basis of Hilbert space

$$|j,m\rangle = \left|\uparrow\right\rangle \otimes \cdots \otimes \left|\downarrow\right\rangle$$

- The Hamiltonian becomes

$$H = J\sum_{ij} S_i^z S_j^z + [S_i^x S_j^x + S_i^y S_j^y] = J\sum_{ij} S_i^z S_j^z + \frac{1}{2}[S_i^+ S_j^- + S_i^- S_j^+]$$

Three spin–1/2 Heisenberg model

- Non-periodic boundary condition

$$H = JS_1^z S_2^z + J\frac{1}{2}[S_1^+ S_2^- + S_1^- S_2^+] + JS_2^z S_3^z + J\frac{1}{2}[S_2^+ S_3^- + S_2^- S_3^+]$$

- The size of the system is $2^3 = 8$
- The trial basis states are

$$|\downarrow\downarrow\downarrow\rangle = |000\rangle = |0\rangle$$
$$|\downarrow\downarrow\uparrow\rangle = |001\rangle = |1\rangle$$
$$|\downarrow\uparrow\downarrow\rangle = |010\rangle = |2\rangle$$
$$|\downarrow\uparrow\uparrow\rangle = |011\rangle = |3\rangle$$
$$|\uparrow\downarrow\downarrow\rangle = |100\rangle = |4\rangle$$
$$|\uparrow\downarrow\uparrow\rangle = |101\rangle = |5\rangle$$
$$|\uparrow\uparrow\downarrow\rangle = |110\rangle = |6\rangle$$
$$|\uparrow\uparrow\uparrow\rangle = |111\rangle = |7\rangle$$

The Hamiltonian matrix

- The Hamiltonian in the given basis is

$$H = \begin{array}{c} \\ \langle\downarrow\downarrow\downarrow| \\ \langle\downarrow\downarrow\uparrow| \\ \langle\downarrow\uparrow\downarrow| \\ \langle\downarrow\uparrow\uparrow| \\ \langle\uparrow\downarrow\downarrow| \\ \langle\uparrow\downarrow\uparrow| \\ \langle\uparrow\uparrow\downarrow| \\ \langle\uparrow\uparrow\uparrow| \end{array} \begin{array}{c} \begin{array}{cccccccc} |\downarrow\downarrow\downarrow\rangle & |\downarrow\downarrow\uparrow\rangle & |\downarrow\uparrow\downarrow\rangle & |\downarrow\uparrow\uparrow\rangle & |\uparrow\downarrow\downarrow\rangle & |\uparrow\downarrow\uparrow\rangle & |\uparrow\uparrow\downarrow\rangle & |\uparrow\uparrow\uparrow\rangle \end{array} \\ \begin{pmatrix} \frac{J}{2} & & & & & & & \\ & 0 & \frac{J}{2} & & & & & \\ & \frac{J}{2} & -\frac{J}{2} & 0 & 0 & \frac{J}{2} & & \\ & & 0 & 0 & 0 & \frac{J}{2} & & \\ & & 0 & 0 & 0 & 0 & & \\ & & \frac{J}{2} & \frac{J}{2} & 0 & -\frac{J}{2} & \frac{J}{2} & \\ & & & & & \frac{J}{2} & 0 & \\ & & & & & & & \frac{J}{2} \end{pmatrix} \end{array}$$

Magnetization

- The magnetization is

$$M_z = \sum_i S_i^z$$

- The size of the largest block is

$M_z = 1/2 \text{ or } -1/2$

$C_1^3 = 3$

- The new basis states become

$$\left|\downarrow\downarrow\downarrow\right\rangle = \left|M_z = -\tfrac{3}{2}\right\rangle = \left|0\right\rangle \qquad \left|\downarrow\uparrow\uparrow\right\rangle = \left|M_z = \tfrac{1}{2}\right\rangle = \left|3\right\rangle$$
$$\left|\downarrow\downarrow\uparrow\right\rangle = \left|M_z = -\tfrac{1}{2}\right\rangle = \left|1\right\rangle \qquad \left|\uparrow\downarrow\uparrow\right\rangle = \left|M_z = \tfrac{1}{2}\right\rangle = \left|5\right\rangle$$
$$\left|\downarrow\uparrow\downarrow\right\rangle = \left|M_z = -\tfrac{1}{2}\right\rangle = \left|2\right\rangle \qquad \left|\uparrow\uparrow\downarrow\right\rangle = \left|M_z = \tfrac{1}{2}\right\rangle = \left|6\right\rangle$$
$$\left|\uparrow\downarrow\downarrow\right\rangle = \left|M_z = -\tfrac{1}{2}\right\rangle = \left|4\right\rangle \qquad \left|\uparrow\uparrow\uparrow\right\rangle = \left|M_z = \tfrac{3}{2}\right\rangle = \left|7\right\rangle$$

Magnetization

- The Hamiltonian becomes

$$H = \begin{array}{c} \left\langle -\frac{3}{2}\right| \\ \left\langle -\frac{1}{2}\right| \\ \left\langle -\frac{1}{2}\right| \\ \left\langle -\frac{1}{2}\right| \\ \left\langle \frac{1}{2}\right| \\ \left\langle \frac{1}{2}\right| \\ \left\langle \frac{1}{2}\right| \\ \left\langle \frac{3}{2}\right| \end{array} \begin{pmatrix} \frac{J}{2} & & & & & & & \\ & 0 & \frac{J}{2} & & & & & \\ & \frac{J}{2} & -\frac{J}{2} & \frac{J}{2} & & & & \\ & & \frac{J}{2} & 0 & & & & \\ & & & & 0 & \frac{J}{2} & & \\ & & & & \frac{J}{2} & -\frac{J}{2} & \frac{J}{2} & \\ & & & & & \frac{J}{2} & 0 & \\ & & & & & & & \frac{J}{2} \end{pmatrix}$$

How does the computer work

- Declare a vector $A[m]$ to store basis states
- For example:

  $A[1]=0 \quad A[2]=1 \quad A[3]=2 \quad A[4]=3$

  $A[5]=4 \quad A[6]=5 \quad A[7]=6 \quad A[8]=7$
- Next, act H on the basis states
- For example:

$$H|A[3]\rangle = H|2\rangle = H|\downarrow\uparrow\downarrow\rangle = \frac{J}{2}|\downarrow\downarrow\uparrow\rangle + \frac{J}{2}|\uparrow\downarrow\downarrow\rangle = \frac{J}{2}|1\rangle + \frac{J}{2}|4\rangle$$

- Then, we need to find out the corresponding index with respect to the basis

  $|1\rangle = |A[2]\rangle \ , \ j_1 = 2$

  $|4\rangle = |A[5]\rangle \ , \ j_2 = 5$

How does the computer work

- The most efficient way: declare a vector $B[m]$, $m = 0$ to 7
- Therefore we have

$$B[0]=1 \quad B[1]=2 \quad B[2]=3 \quad B[3]=4$$
$$B[4]=5 \quad B[5]=6 \quad B[6]=7 \quad B[7]=8$$

- and

$$B[A[2]] = 2 = j_1$$
$$B[A[4]] = 4 = j_2$$

- The matrix elements are

$$H(i, j_1) = H(3,2) = \frac{J}{2}$$
$$H(i, j_2) = H(3,4) = \frac{J}{2}$$

Two-Table method

- Divide lattice to two sublattice
- For example: site–1,2 and site–3

$$i = 2^2 i_3 + i_{1,2}$$

$$j = j_3 + j_{1,2}$$

$\lvert\downarrow\rangle$	0	1	$\lvert\downarrow\downarrow\rangle$	0	0	1
$\lvert\downarrow\rangle$	0	1	$\lvert\downarrow\uparrow\rangle$	1	1	2
$\lvert\downarrow\rangle$	0	1	$\lvert\uparrow\downarrow\rangle$	2	2	3
$\lvert\downarrow\rangle$	0	1	$\lvert\uparrow\uparrow\rangle$	3	3	4
$\lvert\uparrow\rangle$	1	5	$\lvert\downarrow\downarrow\rangle$	0	0	5
$\lvert\uparrow\rangle$	1	5	$\lvert\downarrow\uparrow\rangle$	1	1	6
$\lvert\uparrow\rangle$	1	5	$\lvert\uparrow\downarrow\rangle$	2	2	7
$\lvert\uparrow\rangle$	1	5	$\lvert\uparrow\uparrow\rangle$	3	3	8

Two spin–3/2 Heisenberg model

$$H = JS_1^z S_2^z + J\frac{1}{2}[S_1^+ S_2^- + S_1^- S_2^+]$$

- The size of the system is $4^2 = 16$

$$\left|-\tfrac{3}{2}\,-\tfrac{3}{2}\right\rangle \quad \left|\tfrac{1}{2}\,-\tfrac{3}{2}\right\rangle$$
$$\left|-\tfrac{3}{2}\,-\tfrac{1}{2}\right\rangle \quad \left|\tfrac{1}{2}\,-\tfrac{1}{2}\right\rangle$$
$$\left|-\tfrac{3}{2}\,\tfrac{1}{2}\right\rangle \quad \left|\tfrac{1}{2}\,\tfrac{1}{2}\right\rangle$$
$$\left|-\tfrac{3}{2}\,\tfrac{3}{2}\right\rangle \quad \left|\tfrac{1}{2}\,\tfrac{3}{2}\right\rangle$$
$$\left|-\tfrac{1}{2}\,-\tfrac{3}{2}\right\rangle \quad \left|\tfrac{3}{2}\,-\tfrac{3}{2}\right\rangle$$
$$\left|-\tfrac{1}{2}\,-\tfrac{1}{2}\right\rangle \quad \left|\tfrac{3}{2}\,-\tfrac{1}{2}\right\rangle$$
$$\left|-\tfrac{1}{2}\,\tfrac{1}{2}\right\rangle \quad \left|\tfrac{3}{2}\,\tfrac{1}{2}\right\rangle$$
$$\left|-\tfrac{1}{2}\,\tfrac{3}{2}\right\rangle \quad \left|\tfrac{3}{2}\,\tfrac{3}{2}\right\rangle$$

Two-bit per-site

$$|00\rangle = \left|-\tfrac{3}{2}\right\rangle$$

$$|01\rangle = \left|-\tfrac{3}{2}\right\rangle$$

$$|10\rangle = \left|\tfrac{1}{2}\right\rangle$$

$$|11\rangle = \left|\tfrac{3}{2}\right\rangle$$

$$\left|-\tfrac{3}{2}-\tfrac{3}{2}\right\rangle = |00\ \ 00\rangle \qquad \left|\tfrac{1}{2}-\tfrac{3}{2}\right\rangle = |10\ \ 00\rangle$$

$$\left|-\tfrac{3}{2}-\tfrac{1}{2}\right\rangle = |00\ \ 01\rangle \qquad \left|\tfrac{1}{2}-\tfrac{1}{2}\right\rangle = |10\ \ 01\rangle$$

$$\left|-\tfrac{3}{2}\ \tfrac{1}{2}\right\rangle = |00\ \ 10\rangle \qquad \left|\tfrac{1}{2}\ \tfrac{1}{2}\right\rangle = |10\ \ 10\rangle$$

$$\left|-\tfrac{3}{2}\ \tfrac{3}{2}\right\rangle = |00\ \ 11\rangle \qquad \left|\tfrac{1}{2}\ \tfrac{3}{2}\right\rangle = |10\ \ 11\rangle$$

$$\left|-\tfrac{1}{2}-\tfrac{3}{2}\right\rangle = |01\ \ 00\rangle \qquad \left|\tfrac{3}{2}-\tfrac{3}{2}\right\rangle = |11\ \ 00\rangle$$

$$\left|-\tfrac{1}{2}-\tfrac{1}{2}\right\rangle = |01\ \ 01\rangle \qquad \left|\tfrac{3}{2}-\tfrac{1}{2}\right\rangle = |11\ \ 01\rangle$$

$$\left|-\tfrac{1}{2}\ \tfrac{1}{2}\right\rangle = |01\ \ 10\rangle \qquad \left|\tfrac{3}{2}\ \tfrac{1}{2}\right\rangle = |11\ \ 10\rangle$$

$$\left|-\tfrac{1}{2}\ \tfrac{3}{2}\right\rangle = |01\ \ 11\rangle \qquad \left|\tfrac{3}{2}\ \tfrac{3}{2}\right\rangle = |11\ \ 11\rangle$$

Magnetization $M_z = -3, -2, -1, 0, 1, 2, 3$

$$\left|-\tfrac{3}{2}-\tfrac{3}{2}\right\rangle = \left|00\ \ 00\right\rangle$$

$$\left|-\tfrac{3}{2}-\tfrac{1}{2}\right\rangle = \left|00\ \ 01\right\rangle \quad \left|-\tfrac{1}{2}-\tfrac{3}{2}\right\rangle = \left|01\ \ 00\right\rangle$$

$$\left|-\tfrac{3}{2}\,\tfrac{1}{2}\right\rangle = \left|00\ \ 10\right\rangle \quad \left|-\tfrac{1}{2}-\tfrac{1}{2}\right\rangle = \left|01\ \ 01\right\rangle \quad \left|\tfrac{1}{2}-\tfrac{3}{2}\right\rangle = \left|10\ \ 00\right\rangle$$

$$\left|-\tfrac{3}{2}\,\tfrac{3}{2}\right\rangle = \left|00\ \ 11\right\rangle \quad \left|-\tfrac{1}{2}\,\tfrac{1}{2}\right\rangle = \left|01\ \ 10\right\rangle \quad \left|\tfrac{1}{2}-\tfrac{1}{2}\right\rangle = \left|10\ \ 01\right\rangle \quad \left|\tfrac{3}{2}-\tfrac{3}{2}\right\rangle = \left|11\ \ 00\right\rangle$$

$$\left|-\tfrac{1}{2}\,\tfrac{3}{2}\right\rangle = \left|01\ \ 11\right\rangle \quad \left|\tfrac{1}{2}\,\tfrac{1}{2}\right\rangle = \left|10\ \ 10\right\rangle \quad \left|\tfrac{3}{2}-\tfrac{1}{2}\right\rangle = \left|11\ \ 01\right\rangle$$

$$\left|\tfrac{1}{2}\,\tfrac{3}{2}\right\rangle = \left|10\ \ 11\right\rangle \quad \left|\tfrac{3}{2}\,\tfrac{1}{2}\right\rangle = \left|11\ \ 10\right\rangle$$

$$\left|\tfrac{3}{2}\,\tfrac{3}{2}\right\rangle = \left|11\ \ 11\right\rangle$$

The Basis and lookup tables

$$A[1]=0 \quad A[2]=1 \quad A[3]=4 \quad A[4]=2 \quad A[5]=5 \quad A[6]=8 \quad A[7]=3 \quad A[8]=6$$
$$A[9]=9 \quad A[10]=12 \quad A[11]=7 \quad A[12]=10 \quad A[13]=13 \quad A[14]=11 \quad A[15]=14 \quad A[16]=15$$

$$B[0]=1 \quad B[1]=2 \quad B[2]=4 \quad B[3]=7 \quad B[4]=3 \quad B[5]=5 \quad B[6]=8 \quad B[7]=11$$
$$B[8]=6 \quad B[9]=9 \quad B[10]=12 \quad B[11]=14 \quad B[12]=10 \quad B[13]=13 \quad B[14]=15 \quad B[15]=16$$

Hamiltonian matrix elements

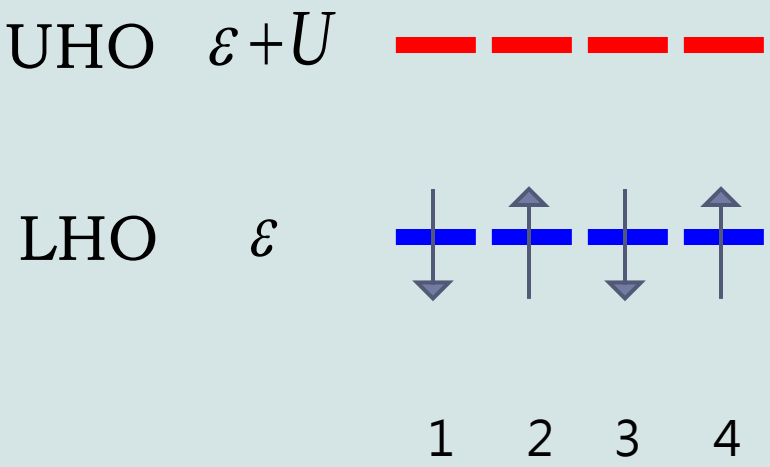
$$
H = \begin{array}{c}
\langle 0| \\ \langle 1| \\ \langle 4| \\ \langle 2| \\ \langle 5| \\ \langle 8| \\ \langle 3| \\ \langle 6| \\ \langle 9| \\ \langle 12| \\ \langle 7| \\ \langle 10| \\ \langle 13| \\ \langle 11| \\ \langle 14| \\ \langle 15|
\end{array}
\begin{pmatrix}
\frac{9}{4}J & & & & & & & & & & & & & & & \\
 & \frac{3}{4}J & \frac{3}{2}J & & & & & & & & & & & & & \\
 & \frac{3}{2}J & \frac{3}{4}J & & & & & & & & & & & & & \\
 & & & -\frac{3}{4}J & \sqrt{3}J & 0 & & & & & & & & & & \\
 & & & \sqrt{3}J & -\frac{3}{4}J & \sqrt{3}J & & & & & & & & & & \\
 & & & 0 & \sqrt{3}J & -\frac{3}{4}J & & & & & & & & & & \\
 & & & & & & -\frac{9}{4}J & \frac{3}{2}J & 0 & 0 & & & & & & \\
 & & & & & & \frac{3}{2}J & -\frac{1}{4}J & 2J & 0 & & & & & & \\
 & & & & & & 0 & 2J & -\frac{1}{4}J & \frac{3}{2}J & & & & & & \\
 & & & & & & 0 & 0 & \frac{3}{2}J & -\frac{9}{4}J & & & & & & \\
 & & & & & & & & & & -\frac{3}{4}J & \sqrt{3}J & 0 & & & \\
 & & & & & & & & & & \sqrt{3}J & \frac{1}{4}J & \sqrt{3}J & & & \\
 & & & & & & & & & & 0 & \sqrt{3}J & -\frac{3}{4}J & & & \\
 & & & & & & & & & & & & & \frac{3}{4}J & \frac{3}{2}J & \\
 & & & & & & & & & & & & & \frac{3}{2}J & \frac{3}{4}J & \\
 & & & & & & & & & & & & & & & \frac{9}{4}J
\end{pmatrix}
$$

Exact Diagonalization: Application

Hubbard Model

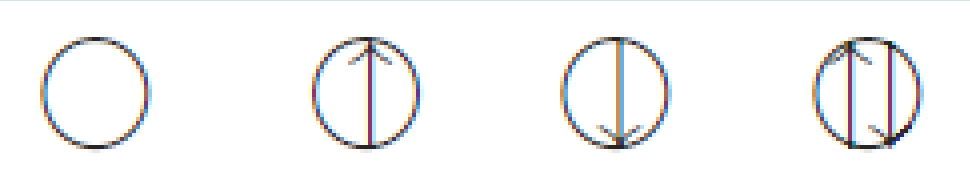
Hubbard Model

$$\mathcal{H} = -t\sum_{\langle ij\rangle\sigma} c_{i\sigma}^{+}c_{i\sigma} + \sum_{i} U\hat{n}_{i\uparrow}\hat{n}_{i\downarrow}$$



Atomic Ground State ($t = 0$)

- Four possible occupation of a single site



$$H = \begin{matrix} \langle 0| \\ \langle \uparrow| \\ \langle \downarrow| \\ \langle 2| \end{matrix} \begin{pmatrix} 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & U \end{pmatrix}$$

A. Non-interacting electrons

$$H_0 = \sum_{ij} t_{ij} c_i^+ c_j$$

- Assume ϕ_j to be Wannier wave functions (Fourier transform of Bloch orbitals)

$$t_{ij} = \left\langle \phi_i \left| -\frac{\hbar^2 \nabla^2}{2m} + \hat{v} \right| \phi_j \right\rangle$$

- Assume t_{ij} is non–zero only when i,j are nearest neighbors

$$H_0 = -t \sum_{ij} \left(c_i^+ c_j + c_j^+ c_i \right)$$

- Diagonalize the Hamiltonian by a Fourier transformation

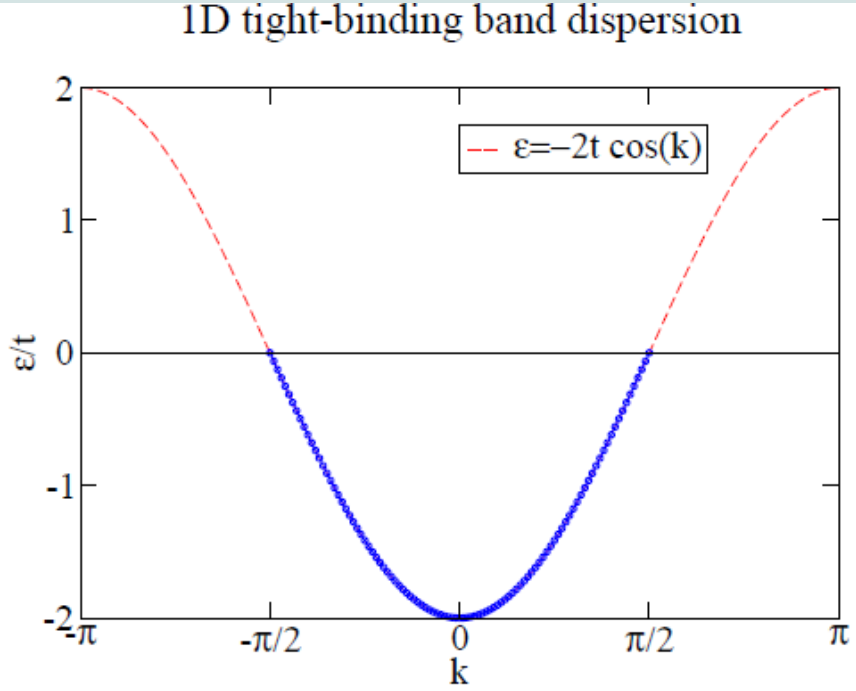
$$c_k^+ = \frac{1}{\sqrt{L}} \sum_j e^{ikj} c_j^+$$

A. Non-interacting electrons

- Then the Hamiltonian in ϕ_j basis becomes

$$H_0 = \sum_k \varepsilon_k c_k^+ c_k$$

where $\varepsilon_k = -2t\cos(k)$



$$|GS\rangle = \prod_{k<k_F} c_{k\uparrow}^+ c_{k\downarrow}^+ |0\rangle$$

A. Non-interacting electrons

- Particle-hole excitation

$$H_0|\psi_n\rangle = H_0 c^{+}_{k+q\uparrow} c_{k\uparrow}|GS\rangle = \varepsilon_{kq}|\psi_n\rangle$$

where $\varepsilon_k(q) = \varepsilon_{k+q} - \varepsilon_k$

- As the energy of the particle-hole excitation $\varepsilon_k(q)$ can be made arbitrarily small, $|GS\rangle$ characterizes a metal.

B. Electron-electron interaction

- Two-site case

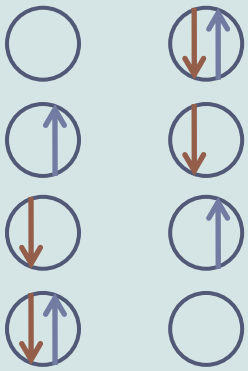
$$H = H_t + H_U = -t(c_{0\uparrow}^{+}c_{1\uparrow} + c_{1\uparrow}^{+}c_{0\uparrow} + c_{0\downarrow}^{+}c_{1\downarrow} + c_{1\downarrow}^{+}c_{0\downarrow}) + U(n_{0\uparrow}n_{0\downarrow} + n_{1\uparrow}n_{1\downarrow})$$

$$H = \begin{array}{c} \\ \langle 00| \\ \langle 0\uparrow| \\ \langle 0\downarrow| \\ \langle 02| \\ \langle \uparrow 0| \\ \langle \uparrow\uparrow| \\ \langle \uparrow\downarrow| \\ \langle \uparrow 2| \\ \langle \downarrow 0| \\ \langle \downarrow\uparrow| \\ \langle \downarrow\downarrow| \\ \langle \downarrow 2| \\ \langle 20| \\ \langle 2\uparrow| \\ \langle 2\downarrow| \\ \langle 22| \end{array} \begin{array}{c} \begin{array}{cccccccccccccc} |00\rangle & |0\uparrow\rangle & |0\downarrow\rangle & |02\rangle & |\uparrow 0\rangle & |\uparrow\uparrow\rangle & |\uparrow\downarrow\rangle & |\uparrow 2\rangle & |\downarrow 0\rangle & |\downarrow\uparrow\rangle & |\downarrow\downarrow\rangle & |\downarrow 2\rangle & |20\rangle & |2\uparrow\rangle \end{array} \\ \begin{pmatrix} & & & & & & & & & & & & & & & \\ & & -t & & & & & & & & & & & & & \\ & & & & & & & & -t & & & & & & & \\ & & & U & & -t & & & & -t & & & & & & \\ & -t & & & & & & & & & & & & & & \\ & & & & & & & & & & & & & & & \\ & & & -t & & & & & & & & & -t & & & \\ & & & & & & & U & & & & & & -t & & \\ & & -t & & & & & & & & & & & & & \\ & & & -t & & & & & & & & & -t & & & \\ & & & & & & & & & & & & & & & \\ & & & & & & & & & & & U & & & -t & \\ & & & & & -t & & & & -t & & & U & & & \\ & & & & & & & & -t & & & & & U & & \\ & & & & & & & & & & & -t & & & U & \\ & & & & & & & & & & & & & & & 2U \end{pmatrix} \end{array}$$

B. Electron-electron interaction

- Organizing the Hilbert space
  - Operators commute with Hamiltonian
    - Number operator $N = \sum n_{i\sigma}$
    - Total $S_z = \frac{1}{2} \sum (n_{i\uparrow} - n_{i\downarrow})$
- The structure of the Hamiltonian will be block diagonal where each block corresponds to a fixed value of N and S_z
- For example: $N = 2$, the size of this block is $C_2^4 = 6$, which is also the largest block of the Hamiltonian matrix
  - *Case1:* $S_z = 0$
    - The size is 4
  - *Case2:* $S_z = -1$
    - The size is 1
  - *Case3:* $S_z = 1$
    - The size is 1

$N = 2$ and $S_z = 0$



$\|01\rangle_\downarrow \|01\rangle_\uparrow$		5
$\|01\rangle_\downarrow \|10\rangle_\uparrow$		6
$\|10\rangle_\downarrow \|01\rangle_\uparrow$		9
$\|10\rangle_\downarrow \|10\rangle_\uparrow$		10
Site 1 Site 0	→ Binary	→ Decimal

- Declare a matrix A(1:4)

$$\left.\begin{array}{lcl} A(1) & \rightarrow & 5 \\ A(2) & \rightarrow & 6 \\ A(3) & \rightarrow & 9 \\ A(4) & \rightarrow & 10 \end{array}\right\} \text{Basis States}$$

$N = 2$ and $S_z = 0$: Diagonal elements

- Basis states

$$|\varphi_1\rangle = |A(1)\rangle = |5\rangle = |01\rangle_{\downarrow}|01\rangle_{\uparrow}$$

- Acting on-site Coulomb interaction H_U on the basis states

$$H_U = \begin{array}{c} {}_{\downarrow}\langle 01|_{\uparrow}\langle 01| \\ {}_{\downarrow}\langle 01|_{\uparrow}\langle 10| \\ {}_{\downarrow}\langle 10|_{\uparrow}\langle 01| \\ {}_{\downarrow}\langle 10|_{\uparrow}\langle 10| \end{array} \begin{pmatrix} U & & & \\ & 0 & & \\ & & 0 & \\ & & & U \end{pmatrix}$$

$N=2$ and $S_z=0$: Off-Diagonal elements

- Acting hopping terms H_t on the basis states

$$|\varphi_1\rangle = |A(1)\rangle = |5\rangle = |01\rangle_\downarrow |01\rangle_\uparrow = c^+_{0\downarrow} c^+_{0\uparrow} |0\rangle$$

$$\begin{aligned} H_t|\varphi_1\rangle &= -t(c^+_{0\uparrow}c_{1\uparrow} + c^+_{1\uparrow}c_{0\uparrow} + c^+_{0\downarrow}c_{1\downarrow} + c^+_{1\downarrow}c_{0\downarrow})c^+_{0\downarrow}c^+_{0\uparrow}|0\rangle \\ &= -tc^+_{1\uparrow}c_{0\uparrow}c^+_{0\downarrow}c^+_{0\uparrow}|0\rangle - tc^+_{1\downarrow}c_{0\downarrow}c^+_{0\downarrow}c^+_{0\uparrow}|0\rangle \\ &= +tc^+_{1\uparrow}c^+_{0\downarrow}c_{0\uparrow}c^+_{0\uparrow}|0\rangle - tc^+_{1\downarrow}c^+_{0\uparrow}c_{0\downarrow}c^+_{0\downarrow}|0\rangle \\ &= -tc^+_{0\downarrow}c^+_{1\uparrow}c_{0\uparrow}c^+_{0\uparrow}|0\rangle - tc^+_{1\downarrow}c^+_{0\uparrow}c_{0\downarrow}c^+_{0\downarrow}|0\rangle \\ &= -t|\varphi_2\rangle - t|\varphi_3\rangle \end{aligned}$$

- How does the computer work to come out the same results?

$N=2$ and $S_z=0$: Off-Diagonal elements

- Acting hopping terms H_t on the basis states

$$|\phi\rangle = |\phi\rangle_\downarrow |\phi\rangle_\uparrow = [c^+_{r_1\downarrow}\cdots c^+_{r_N\downarrow}]|0\rangle_\downarrow [c^+_{r_1\uparrow}\cdots c^+_{r_N\uparrow}]|0\rangle_\uparrow$$

$$\begin{aligned} c^+_{r_i\uparrow}c_{r_j\uparrow}|\phi\rangle &= c^+_{r_i\uparrow}c_{r_j\uparrow}|\phi\rangle_\downarrow |\phi\rangle_\uparrow \\ &= c^+_{r_i\uparrow}c_{r_j\uparrow}[c^+_{r_1\downarrow}\cdots c^+_{r_N\downarrow}]|0\rangle_\downarrow [c^+_{r_1\uparrow}\cdots c^+_{r_N\uparrow}]|0\rangle_\uparrow \\ &= [c^+_{r_1\downarrow}\cdots c^+_{r_N\downarrow}]|0\rangle_\downarrow (-1)^N(-1)^N c^+_{r_i\uparrow}c_{r_j\uparrow}[c^+_{r_1\uparrow}\cdots c^+_{r_N\uparrow}]|0\rangle_\uparrow \\ &= |\phi\rangle_\downarrow c^+_{r_i\uparrow}c_{r_j\uparrow}|\phi\rangle_\uparrow \end{aligned}$$

- Count the number of electrons between site i and site j

$$c^+_{1\uparrow}c_{0\uparrow}|\phi_1\rangle = c^+_{1\uparrow}c_{0\uparrow}c^+_{0\downarrow}c^+_{0\uparrow}|0\rangle = (-1)^0|\phi_2\rangle$$

$$c^+_{1\uparrow}c_{0\uparrow}|\phi_1\rangle = c^+_{1\downarrow}c_{0\downarrow}c^+_{0\downarrow}c^+_{0\uparrow}|0\rangle = (-1)^0|\phi_3\rangle$$

$N = 2$ and $S_z = 0$: Off-Diagonal elements

- Similar to other basis states

$$H_t|\phi_1\rangle = -t|\phi_2\rangle - t|\phi_3\rangle$$
$$H_t|\phi_2\rangle = -t|\phi_1\rangle - t|\phi_4\rangle$$
$$H_t|\phi_3\rangle = -t|\phi_1\rangle - t|\phi_4\rangle$$
$$H_t|\phi_4\rangle = -t|\phi_2\rangle - t|\phi_3\rangle$$

- Therefore in these basis states, the Hamiltonian has the following matrix representation.

$$H_t = \begin{array}{c} {}_{\downarrow}\langle 01|_{\uparrow}\langle 01| \\ {}_{\downarrow}\langle 01|_{\uparrow}\langle 10| \\ {}_{\downarrow}\langle 10|_{\uparrow}\langle 01| \\ {}_{\downarrow}\langle 10|_{\uparrow}\langle 10| \end{array} \begin{pmatrix} & -t & -t & \\ -t & & & -t \\ -t & & & -t \\ & -t & -t & \end{pmatrix}$$

$N=2$ and $S_z=-1\ ,\ 1$

- For $S_z=1$, the basis state is

$$\rightarrow |00\rangle_{\downarrow}|11\rangle_{\uparrow}$$

$$|\phi\rangle = |00\rangle_{\downarrow}|\uparrow\uparrow\rangle_{\uparrow}$$

$$H_t|\phi\rangle = 0 \ \text{ and } \ H_U|\phi\rangle = 0$$

- For $S_z=-1$, the basis state is

$$\rightarrow |11\rangle_{\downarrow}|00\rangle_{\uparrow}$$

$$|\phi\rangle = |\downarrow\downarrow\rangle_{\downarrow}|00\rangle_{\uparrow}$$

$$H_t|\phi\rangle = 0 \ \text{ and } \ H_U|\phi\rangle = 0$$

$N = 0$ Block Diagonal Structure

$$H_t = \begin{array}{c} \\ {}_{\downarrow}\langle 00|_{\uparrow}\langle 11| \\ {}_{\downarrow}\langle 01|_{\uparrow}\langle 01| \\ {}_{\downarrow}\langle 01|_{\uparrow}\langle 10| \\ {}_{\downarrow}\langle 10|_{\uparrow}\langle 01| \\ {}_{\downarrow}\langle 10|_{\uparrow}\langle 10| \\ {}_{\downarrow}\langle 11|_{\uparrow}\langle 00| \end{array} \begin{array}{c} \begin{array}{cccc} |00\rangle_{\downarrow}|11\rangle_{\uparrow} & |01\rangle_{\downarrow}|01\rangle_{\uparrow} & |01\rangle_{\downarrow}|10\rangle_{\uparrow} & |10\rangle_{\downarrow}|01\rangle_{\uparrow} \end{array} \\ \left(\begin{array}{c|cccc|c} 0 & & & & & \\ \hline & U & -t & -t & & \\ & -t & & & -t & \\ & -t & & & -t & \\ & & -t & -t & U & \\ \hline & & & & & 0 \end{array}\right) \end{array} \begin{array}{c} \\ |11\rangle_{\downarrow}|00\rangle_{\uparrow} \end{array}$$

The Block Diagonal Structure

$$
H = \begin{array}{c}
\langle 00| \\ \langle 0\uparrow| \\ \langle \uparrow 0| \\ \langle 0\downarrow| \\ \langle \downarrow 0| \\ \langle \uparrow\uparrow| \\ \langle 02| \\ \langle \uparrow\downarrow| \\ \langle \downarrow\uparrow| \\ \langle 20| \\ \langle \downarrow\downarrow| \\ \langle \uparrow 2| \\ \langle 2\uparrow| \\ \langle \downarrow 2| \\ \langle 2\downarrow| \\ \langle 22|
\end{array}
\begin{pmatrix}
0 & & & & & & & & & & & & & & & \\
 & 0 & -t & & & & & & & & & & & & & \\
 & -t & 0 & & & & & & & & & & & & & \\
 & & & 0 & -t & & & & & & & & & & & \\
 & & & -t & 0 & & & & & & & & & & & \\
 & & & & & 0 & & & & & & & & & & \\
 & & & & & & U & -t & -t & & & & & & & \\
 & & & & & & -t & 0 & & -t & & & & & & \\
 & & & & & & -t & & 0 & -t & & & & & & \\
 & & & & & & & -t & -t & U & & & & & & \\
 & & & & & & & & & & 0 & & & & & \\
 & & & & & & & & & & & U & -t & & & \\
 & & & & & & & & & & & -t & U & & & \\
 & & & & & & & & & & & & & U & -t & \\
 & & & & & & & & & & & & & -t & U & \\
 & & & & & & & & & & & & & & & 2U
\end{pmatrix}
$$

Two-Table method

- For example: Up configuration and Down configuration

$$i = 2^2 i_1 + i_2$$

$$j = j_1 + j_2$$

$\|00\rangle$	0	0	$\|11\rangle$	3	1	1
$\|01\rangle$	1	1	$\|01\rangle$	1	1	2
$\|01\rangle$	1	1	$\|10\rangle$	2	2	3
$\|10\rangle$	2	3	$\|01\rangle$	1	1	4
$\|10\rangle$	2	3	$\|10\rangle$	2	2	5
$\|11\rangle$	3	5	$\|00\rangle$	0	1	6

How to implement

- Use subroutine (in Fortran 77 or c), module (in Fortran 90/95/2003), or object (in c++ or python) to structure your code
- Write an object (here it means subroutine, module, or object in different language) to store the symmetrized basis states and lookup table
- Write an object to calculate the matrix elements and assign it to a matrix
- Call the diagonalization routine using LAPACK/ARPACK/...
- Write an object to calculate the observable quantities

Main piece of wisdom

- DO NOT start writing your own code from the scratch (unless really forced to)