Bootstrapping Nature: Non-perturbative Approaches to Critical Phenomena, Training Week
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Part II. Principles of key numerical methods

Exact diagonalization, use of symmetries
- 1D, 2D examples

Matrix- and tensor-product states
- very brief intro, some examples of recent use

Quantum Monte Carlo methods
- brief review of classical MC
- path integrals, stochastic series expansion
- fermion determinant QMC

Exact Diagonalization

Using basis states incorporating conservation laws (symmetries)

- magnetization conservation, momentum states, parity, spin inversion
- 1D systems, discussion without group theory
  - only basic quantum mechanics and common sense needed

Lanczos diagonalization

- ground state, low excitations

Characterization of different ground states

- critical ground state of the Heisenberg chain
- quantum phase transition to a valence-bond solid in a J_1-J_2 chain
- 2D Néel order, Anderson tower of rotor states

Computational basis states

Using example: the Heisenberg S=1/2 chain

$$H = J\sum_{i=1}^{N} \mathbf{S}_i \cdot \mathbf{S}_{i+1} = J\sum_{i=1}^{N} [S_i^x S_{i+1}^x + S_i^y S_{i+1}^y + S_i^z S_{i+1}^z],$$

$$= J\sum_{i=1}^{N} [S_i^z S_{i+1}^z + \tfrac{1}{2}(S_i^+ S_{i+1}^- + S_i^- S_{i+1}^+)]$$

Most efficient way computationally; enumerate the states

- construct the hamiltonian matrix using **bit-representation** of integers

$$|0\rangle = |\downarrow,\downarrow,\downarrow,\ldots,\downarrow\rangle \quad (=0\ldots000)$$
$$|1\rangle = |\uparrow,\downarrow,\downarrow,\ldots,\downarrow\rangle \quad (=0\ldots001)$$
$$|2\rangle = |\downarrow,\uparrow,\downarrow,\ldots,\downarrow\rangle \quad (=0\ldots010)$$
$$|3\rangle = |\uparrow,\uparrow,\downarrow,\ldots,\downarrow\rangle \quad (=0\ldots011)$$

$$H_{ij} = \langle i|H|j\rangle$$
$$i,j = 0,\ldots,2^N-1$$

bit representation perfect for S=1/2 systems, integer i represents a state

- use >1 bit/spin for S>1/2, or integer vector
- construct H by examining/flipping bits

Alternative: use array state(1:N) with values 0,1, along with

- function statelabel(state) to produce the index i
- function makestate(i), to create array state for given state label i

Diagonalizing the hamiltonian matrix

- on the computer
- gives the eigenvalues and eigenvectors

If U is the matrix whose columns are the eigenvectors of H, then

$$\langle n|A|n\rangle = [U^{T*}AU]_{nn}$$

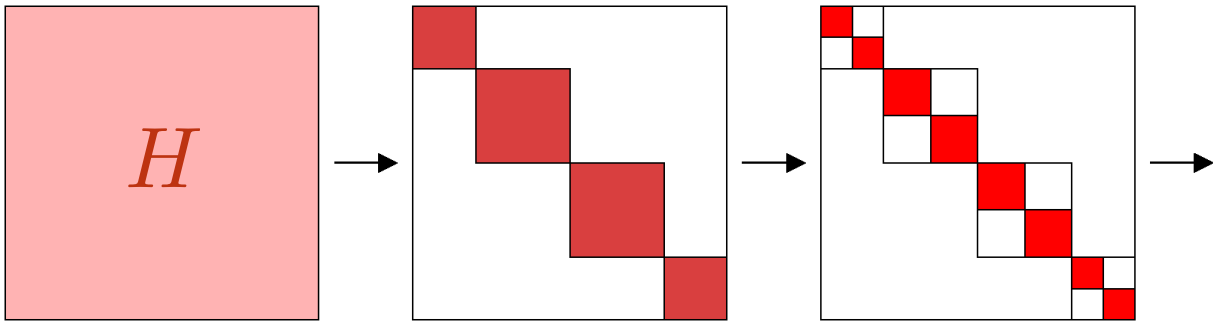
is the expectation value of some operator A in the n:th eigenstate

Problem: Matrix size $M=2^N$ becomes too large quickly

- maximum number of spins in practice; N≈20
- M^2 matrix elements to store, time to diagonalize $\propto M^3$

Using conservation laws (symmetries) for block-diagonalization

We can choose the basis in such a way that the H becomes block-diagonal



- the blocks can be diagonalized individually
- we can reach larger N (but not much larger, N≈40 is max)

Simplest example; magnetization conservation

$$m_z = \sum_{i=1}^{N} S_i^z$$

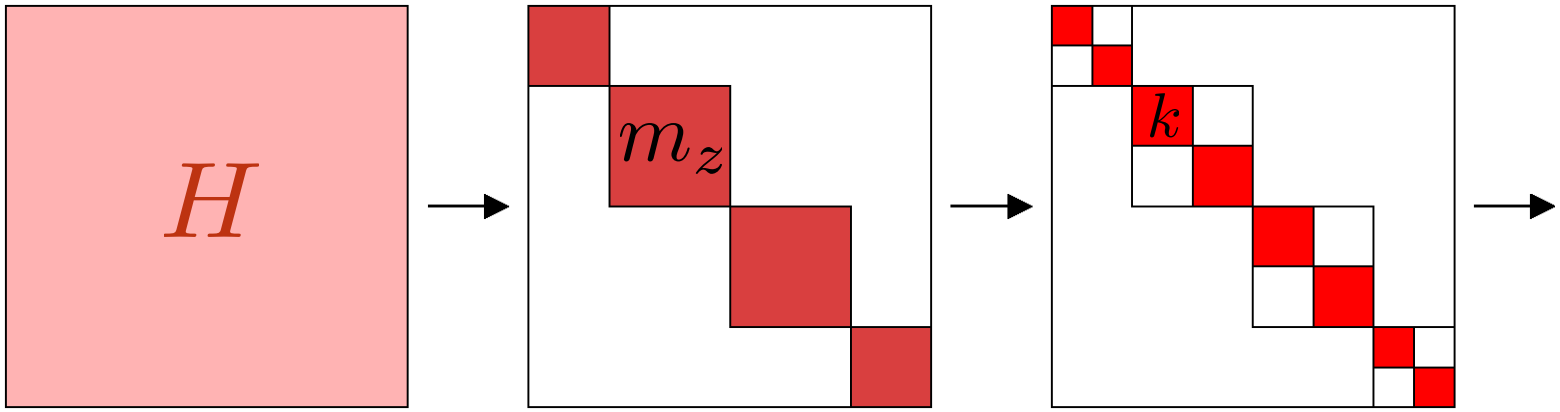
- blocks correspond to fixed values of m_z
- no H matrix elements between states of different m_z
- A block contains states with a given m_z
  - corresponds to ordering the states in a particular way

Number of states in the largest block (m_z =0): $N!/[(N/2)!]^2$

Example

N=4, m=0

s_1=3	(0011)
s_2=5	(0101)
s_3=6	(0110)
s_4=9	(1001)
s_5=10	(1010)
s_6=12	(1100)

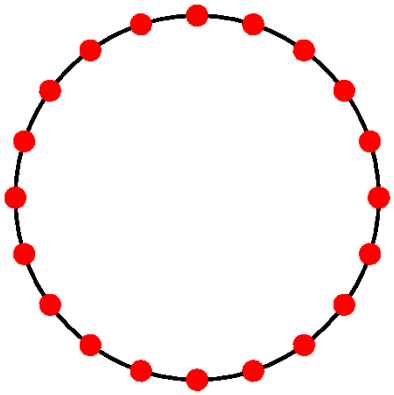


Other symmetries (conserved quantum numbers)

- can be used to further split the blocks
- but more complicated
  - basis states have to be constructed to obey symmetries
  - e.g., momentum states (using translational invariance)

Momentum states (translationally invariant systems)

A periodic chain (ring), translationally invariant



- the eigenstates have a momentum (crystal momentum) k

$$T|n\rangle = \mathrm{e}^{ik}|n\rangle \qquad k = m\frac{2\pi}{N}, \quad m = 0, \ldots, N-1,$$

The operator T translates the state by one lattice spacing

- for a spin basis state

$$T|S_1^z, S_2^z, \ldots, S_N^z\rangle = |S_N^z, S_1^z, \ldots, S_{N-1}^z\rangle$$

[T,H]=0 → momentum blocks of H

- can use eigenstates of T with given k as basis (H blocks labeled by k)

A momentum state can be constructed from any **representative** state

$$|a(k)\rangle = \frac{1}{\sqrt{N_a}} \sum_{r=0}^{N-1} \mathrm{e}^{-ikr} T^r |a\rangle, \qquad |a\rangle = |S_1^z, \ldots, S_N^z\rangle$$

Construct ordered list of representatives

If |a> and |b> are representatives, then

$$T^r|a\rangle \neq |b\rangle \quad r \in \{1, \ldots, N-1\}$$

4-site examples

(**0011**)→(0110),(1100),(1001)

(**0101**)→(1010)

Convention: the representative is the one corresponding to the smallest integer

$$|a(k)\rangle = \frac{1}{\sqrt{N_a}} \sum_{r=0}^{N-1} \mathrm{e}^{-ikr} T^r |a\rangle, \qquad |a\rangle = |S_1^z, \ldots, S_N^z\rangle \qquad k = m\frac{2\pi}{N}$$

The sum can contain several copies of the same state

- if $T^R|a\rangle = |a\rangle \quad \text{for some } R < N$
- the total weight for this component is

$$1 + \mathrm{e}^{-ikR} + \mathrm{e}^{-i2kR} + \ldots + \mathrm{e}^{-ik(N-R)}$$

- vanishes (state incompatible with k and not in k block) unless kR=n2π
- the total weight of the representative is then N/R

$$kR = n2\pi \rightarrow \frac{mR}{N} = n \rightarrow m = n\frac{N}{R} \rightarrow \mathrm{mod}(m, N/R) = 0$$

Normalization of a state |*a*(k)> with periodicity R_a

$$\langle a(k)|a(k)\rangle = \frac{1}{N_a} \times R_a \times \left(\frac{N}{R_a}\right)^2 = 1 \rightarrow N_a = \frac{N^2}{R_a}$$

Basis construction: find all allowed representatives and their periodicities

(a_1, a_2, a_3, ..., a_M)
(R_1, R_2, R_3, ..., R_M)

The block size **M** is initially not known

- approximately 1/N of total size of fixed m_z block
- depends on the periodicity constraint for given k

The Hamiltonian matrix. Write $S = 1/2$ chain hamiltonian as

$$H_0 = \sum_{j=1}^{N} S_j^z S_{j+1}^z, \quad H_j = \tfrac{1}{2}(S_j^+ S_{j+1}^- + S_j^+ S_{j+1}^-), \quad j = 1, \ldots, N$$

Act with H on a momentum state

$$H|a(k)\rangle = \frac{1}{\sqrt{N_a}} \sum_{r=0}^{N-1} \mathrm{e}^{-ikr} T^r H|a\rangle = \frac{1}{\sqrt{N_a}} \sum_{j=0}^{N} \sum_{r=0}^{N-1} \mathrm{e}^{-ikr} T^r H_j|a\rangle,$$

$H_j|a\rangle$ is related to some representative: $H_j|a\rangle = h_a^j T^{-l_j}|b_j\rangle$

$$H|a(k)\rangle = \sum_{j=0}^{N} \frac{h_a^j}{\sqrt{N_a}} \sum_{r=0}^{N-1} \mathrm{e}^{-ikr} T^{(r-l_j)}|b_j\rangle$$

Shift summation index r and use definition of momentum state

$$H|a(k)\rangle = \sum_{j=0}^{N} h_a^j \mathrm{e}^{-ikl_j} \sqrt{\frac{N_{b_j}}{N_a}}|b_j(k)\rangle \qquad \rightarrow \text{matrix elements}$$

$$\langle a(k)|H_0|a(k)\rangle = \sum_{j=1}^{N} S_j^z S_j^z,$$

$$\langle b_j(k)|H_{j>0}|a(k)\rangle = \mathrm{e}^{-ikl_j} \frac{1}{2} \sqrt{\frac{R_a}{R_{b_j}}}, \qquad |b_j\rangle \propto T^{-l_j} H_j|a\rangle,$$

Reflection symmetry (parity)

Define a reflection (parity) operator

$$P|S_1^z, S_2^z, \ldots, S_N^z\rangle = |S_N^z, \ldots, S_2^z, S_1^z\rangle$$

Consider a hamiltonian for which [H,P]=0 and [H,T]=0; but note that [P,T]≠0

Can we still exploit both P and T at the same time? Consider the state

$$|a(k,p)\rangle = \frac{1}{\sqrt{N_a}} \sum_{r=0}^{N-1} \mathrm{e}^{-ikr} T^r (1+pP)|a\rangle, \quad p = \pm 1$$

This state has momentum k, but does it have parity p? Act with P

$$P|a(k,p)\rangle = \frac{1}{\sqrt{N_a}} \sum_{r=0}^{N-1} \mathrm{e}^{-ikr} T^{-r} (P+p)|a\rangle \qquad PT^r = T^{-r}P$$

$$= p\frac{1}{\sqrt{N_a}} \sum_{r=0}^{N-1} \mathrm{e}^{ikr} T^r (1+pP)|a\rangle \;\; = p|a(k,p)\rangle \text{ if } k = 0 \text{ or } k = \pi$$

k=0,π momentum blocks are split into p=+1 and p=–1 sub-blocks

- [T,P]=0 in the k=0,π blocks
- physically clear because -k=k on the lattice for k=0,π
- we can exploit parity in a different way for other k → real basis (semi-momentum states, will not discuss here)

Spin-inversion symmetry

Spin inversion operator: $Z|S_1^z, S_2^z, \ldots, S_N^z\rangle = |-S_1^z, -S_2^z, \ldots, -S_N^z\rangle$

In the magnetization block $m^z=0$ we can use eigenstates of Z

$$|\alpha(k,p,z)\rangle = \frac{1}{\sqrt{N_a}} \sum_{r=0}^{N-1} \mathrm{e}^{-ikr} T^r (1+pP)(1+zZ)|a\rangle$$

$$Z|\alpha(k,p,z)\rangle = z|\alpha(k,p,z)\rangle, \quad z = \pm 1$$

Example: block sizes

$m_z=0$, k=0 (largest momentum block)

	$(p=\pm1, z=\pm1)$			
N	$(+1,+1)$	$(+1,-1)$	$(-1,+1)$	$(-1,-1)$
8	7	1	0	2
12	35	15	9	21
16	257	183	158	212
20	2518	2234	2136	2364
24	28968	27854	27482	28416
28	361270	356876	355458	359256
32	4707969	4690551	4685150	4700500

Total spin S conservation

- difficult to exploit
- complicated basis states
- calculate S using **$S^2=S(S+1)$**

$$\mathbf{S}^2 = \sum_{i=1}^{N}\sum_{j=1}^{N} \mathbf{S}_i \cdot \mathbf{S}_j$$

$$= 2\sum_{i<j} \mathbf{S}_i \cdot \mathbf{S}_j + \frac{3}{4}N$$

The Lanczos method

If we need only the ground state and a small number of excitations
- can use "Krylov space" methods, which work for much larger matrices
- basis states with 10^7 states or more can be easily handled (30-40 spins)

The Krylov space and "projecting out" the ground state

Start with an arbitrary state $|\psi\rangle$
- it has an expansion in eigenstates of H; act with a high power Λ of H

$$H^\Lambda|\Psi\rangle = \sum_n c_n E_n^\Lambda |n\rangle = E_0^\Lambda \left(c_0|0\rangle + c_1 \left(\frac{E_1}{E_0}\right)^\Lambda |1\rangle + \dots \right)$$

For large Λ, if the state with largest $|E_n|$ dominates the sum
- one may have to subtract a constant, using *H–C*, to ensure ground state
- even better to use linear combination of states generated for different Λ

$$|\psi_a\rangle = \sum_{m=0}^{\Lambda} \psi_a(m) H^m |\Psi\rangle, \quad a = 0, \dots, \Lambda$$

- diagonalize H in this basis

In the **Lanczos basis**, H is tridiagonal, convenient to generate and use
- Normally M=50-200 basis states is enough; easy to diagonalize H

Constructing the Lanczos basis

First: construct **orthogonal but not normalized basis $\{f_m\}$.** Define

$$N_m = \langle f_m | f_m \rangle, \quad H_{mm} = \langle f_m | H | f_m \rangle$$

The first state $|f_0\rangle$ is arbitrary, e.g., random. The next one is

$$|f_1\rangle = H|f_0\rangle - a_0|f_0\rangle$$

Demand orthogonality

$$\langle f_1 | f_0 \rangle = \langle f_0 | H | f_0 \rangle - a_0 \langle f_0 | f_0 \rangle = H_{00} - a_0 N_0 \quad \rightarrow \quad a_0 = H_{00}/N_0$$

All subsequent states are constructed according to

$$|f_{m+1}\rangle = H|f_m\rangle - a_m|f_m\rangle - b_{m-1}|f_{m-1}\rangle$$

$$a_m = H_{mm}/N_m, \quad b_{m-1} = N_m/N_{m-1}$$

Easy to prove orthogonality of all these states ($\langle f_{m+1}|f_m\rangle = 0$ is enough)

The hamiltonian in the Lanczos basis

Rewrite the state generation formula

$$H|f_m\rangle = |f_{m+1}\rangle + a_m|f_m\rangle + b_{m-1}|f_{m-1}\rangle$$

Because of the orthogonality, the only non-0 matrix elements are

$$\begin{aligned}\langle f_{m-1}|H|f_m\rangle &= b_{m-1}N_{m-1} = N_m \\ \langle f_m|H|f_m\rangle &= a_m N_m \\ \langle f_{m+1}|H|f_m\rangle &= N_{m+1}\end{aligned}$$

But the f-states or not normalized. The normalized states are:

$$|\phi_m\rangle = \frac{1}{\sqrt{N_m}}|f_m\rangle$$

In this basis the Hamiltonian matrix is

$$\begin{aligned}\langle \phi_{m-1}|H|\phi_m\rangle &= \sqrt{b_{m-1}} \\ \langle \phi_m|H|\phi_m\rangle &= a_m \\ \langle \phi_{m+1}|H|\phi_m\rangle &= \sqrt{b_m}\end{aligned}$$

Operator expectation values

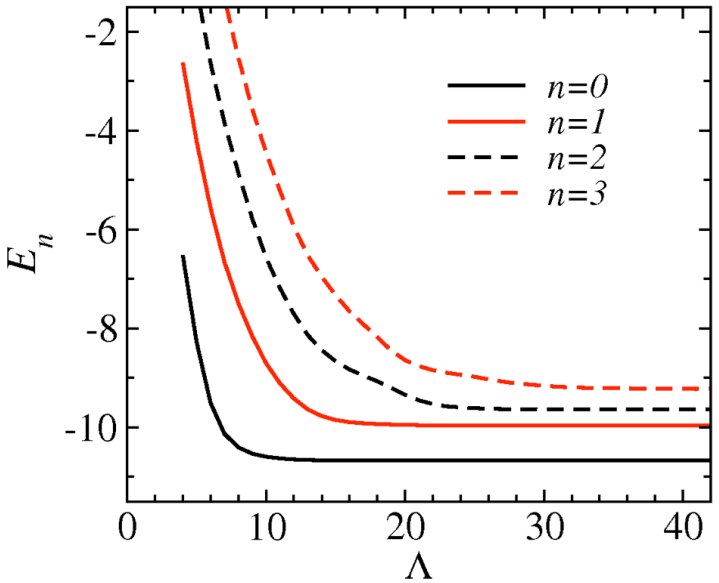
Diagonalizing the tri-diagonal matrix → eigenstates in the Lanczos basis

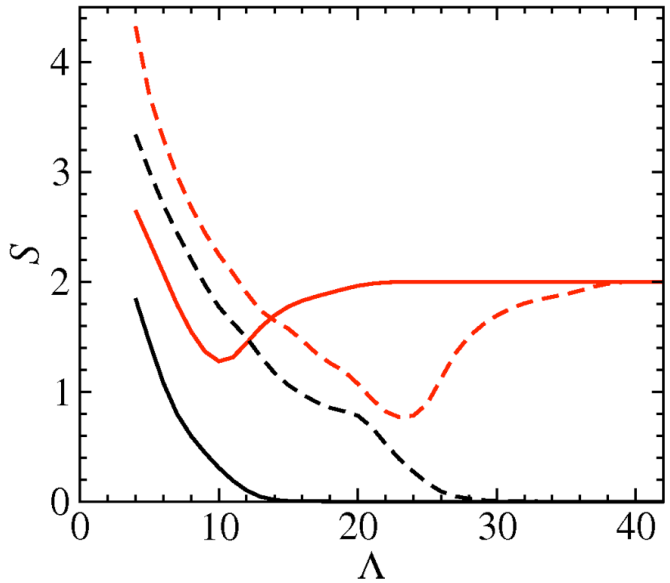
- eigenvectors v_n, energies E_n
- only some number of low-energy states (<< Λ) are correct eigenstates of H

To compute expectation values we go back to the original basis

$$\psi_n(a) = \sum_{m=0}^{\Lambda} v_n(m)\phi_m(a), \qquad a = 1, \ldots, M$$

Convergence properties of the Lanczos method





Example; 24-site chain
$m_z = 0$, $k = 0$, $p = 1$, $z = 1$
block size M=28416

Total spin S extracted assuming that
$\langle S^2 \rangle = S(S+1)$

Ground state converges first, then successively excited states

Break-down of orthogonality

- will eventually happen for large m
- causes artificial degeneracies
- cured by re-orthogonalization
- all states have to be stored

Explicit re-orthogonalization

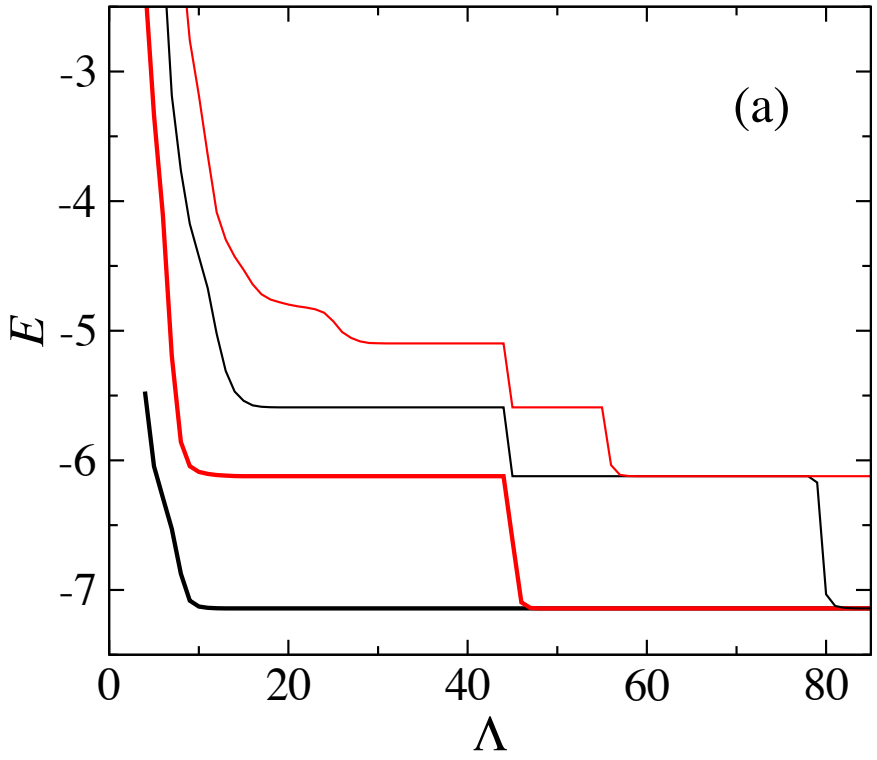
- at each Lanczos step

$$|\phi_{m+1}\rangle \rightarrow \frac{|\phi_{m+1}\rangle - q|\phi_i\rangle}{1-q^2}$$

$$q = \langle \phi_i | \phi_{m+1} \rangle$$

$$N = 16,\ k = 0,\ p = 1,\ z = 1$$

no orthogonalization



with orthogonalization