Summer School on Computational Statistical Physics
August 4-11, 2010, NCCU, Taipei, Taiwan

BOSTON UNIVERSITY

Exact diagonalization methods

Anders W. Sandvik, Boston University

Representation of states in the computer

- bit representation and operations for S=1/2 spins

Using basis states incorporating conservation laws (symmetries)

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

Lanczos diagonalization (ground state, low excitations)

Numerical diagonalization of the hamiltonian

To find the ground state (maybe excitations, T>0 properties)
of the Heisenberg S=1/2 chain

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

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

Simplest 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

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

spin-state manipulations with bit operations

Let **a[i]** refer to the **i:th** bit of an **integer a**

- In Fortran 90 the bit-level function **ieor(a,2**i)** can be used to flip bit i of a
- bits i and j can be flipped using **ieor(a,2**i+2**j)**

				j			i	
a	0	1	0	1	0	0	1	1
$2^i + 2^j$	0	0	0	1	1	0	0	0
$\mathrm{ieor}(a, 2^i + 2^j)$	0	1	0	0	1	0	1	1

Other Fortran 90 functions

ishftc(a,-1,N)
- shifts N bits to the "left"

btest(a,b)
- checks (T or F) bit b of a

ibset(a,b), ibclr(a,b)
- sets to 1 or 1 bit b of a

Translations and reflections of states

r	T^r	T^rP
0	27 0 0 0 1 1 0 1 1	216 1 1 0 1 1 0 0 0
1	54 0 0 1 1 0 1 1 0	177 1 0 1 1 0 0 0 1
2	108 0 1 1 0 1 1 0 0	99 0 1 1 0 0 0 1 1
3	216 1 1 0 1 1 0 0 0	198 1 1 0 0 0 1 1 0
4	177 1 0 1 1 0 0 0 1	141 1 0 0 0 1 1 0 1
5	99 0 1 1 0 0 0 1 1	27 0 0 0 1 1 0 1 1
6	198 1 1 0 0 0 1 1 0	54 0 0 1 1 0 1 1 0
7	141 1 0 0 0 1 1 0 1	108 0 1 1 0 1 1 0 0

The S=1/2 Heisenberg chain hamiltonian can be constructed according to:

```
do a = 0, 2^N − 1
    do i = 0, N − 1
        j = mod(i + 1, N)
        if (a[i] = a[j]) then
            H(a, a) = H(a, a) + 1/4
        else
            H(a, a) = H(a, a) − 1/4
            b = flip(a, i, j); H(a, b) = 1/2
        endif
    enddo
enddo
```

j is the “right” nearest-neighbor of i

- periodic boundary conditions

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

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

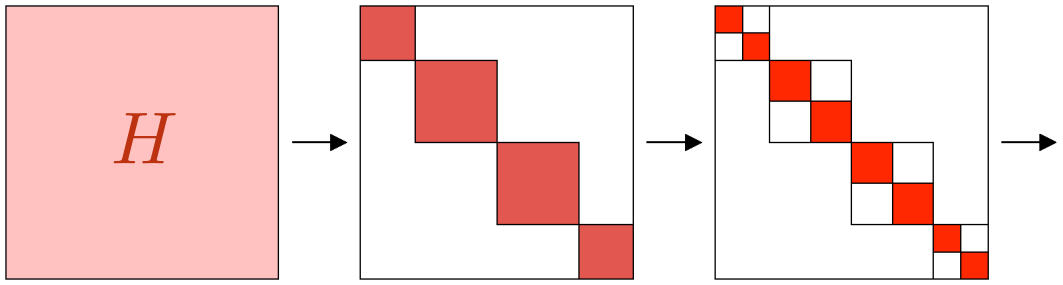
is the expectation value of some operator A in the n:th eigenstate

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



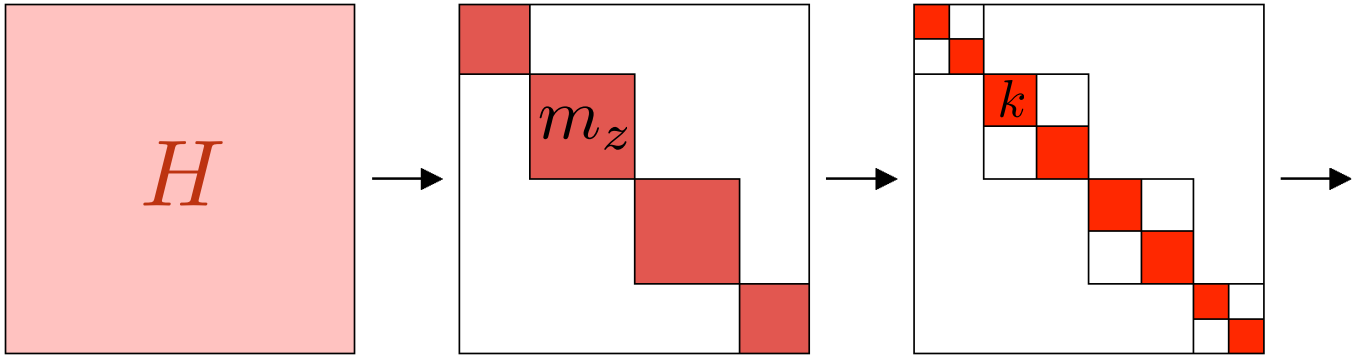
- the blocks can be diagonalized individually
- we can reach larger N (but not much larger, N≈40 is max)

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 is constructed by only including 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): $N!/[(N/2)!]^2$



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)

Pseudocode: using magnetization conservation

Constructing the basis in the block of $n_\uparrow$ spins ↑

Store state-integers in ordered list **s_a, a=1,....,M**

```
do s = 0, 2^N − 1
    if (Σ_i s[i] = n_↑) then a = a + 1; s_a = s endif
enddo
M = a
```

Example; N=4, $n_\uparrow$=2

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

How to locate a state (given integer s) in the list?

- stored map s→a may be too big for s=0,...,2^N-1
- instead, we search the list s_a (here simplest way)

```
subroutine findstate(s, b)
b_min = 1; b_max = M
do
    b = b_min + (b_max − b_min)/2
    if (s < s_b) then
        b_max = b − 1
    elseif (s > s_b) then
        b_min = b + 1
    else
        exit
    endif
enddo
```

Finding the location ***b***
of a state-integer ***s*** in the list

- using bisection in the ordered list

Pseudocode; hamiltonian construction

- recall: states labeled a=1,...,M
- corresponding state-integers (bit representation) stored as s_a
- bit i, $s_a[i]$, corresponds to S^z_i

```
do a = 1, M
    do i = 0, N − 1
        j = mod(i + 1, N)
        if (s_a[i] = s_a[j]) then
            H(a, a) = H(a, a) + 1/4
        else
            H(a, a) = H(a, a) − 1/4
            s = flip(s_a, i, j)
            call findstate(s, b)
            H(a, b) = H(a, b) + 1/2
        endif
    enddo
enddo
```

loop over states

loop over sites

check bits of state-integers

state with bits i and j flipped

Magnetization expectation value

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

when we have diagonalized H, we have its eigenvectors

- stored as the columns of the diagonalizing matrix U(i,n)=vec(i,n)
- vec(i,n) is the i:th component of eigenvector n

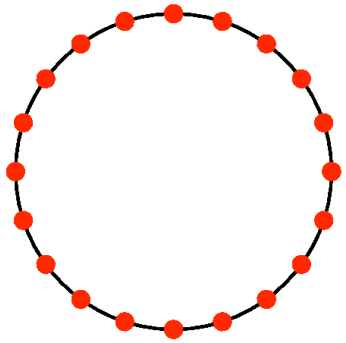
$$|n\rangle_{\text{eigen}} = \sum_{i=1}^{M} \phi_i |i\rangle \qquad (M = 2^N)$$

To calculate <n|m_z|n> (or any observable diagonal in the spin-z basis):

$$\begin{aligned} \langle n|m_z|n\rangle &= \sum_{i,j} \phi_i \phi_j \langle j|m_z|i\rangle \\ &= \sum_{i} \phi_i^2 \langle i|m_z|i\rangle \\ &= \sum_{i} \phi_i^2 m_z(i) \end{aligned}$$

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

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 Ia> and Ib> 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 $T^R|a\rangle = |a\rangle \;\; \text{for some } R < N$
- 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) 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

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

```
do s = 0, 2^N − 1
    call checkstate(s, R)
    if R ≥ 0 then a = a + 1; s_a = s; R_a = R endif
enddo
M = a
```

M = size of the H-block

Uses a subroutine **checkstate**(s,R)
- *R* = periodicity if integer s is a new representative
- *R* = –1 if
  - the magnetization is not the one considered
  - some translation of |s> gives an integer < s
  - |s> is not compatible with the momentum

r	T^r	
0	27	0 0 0 1 1 0 1 1
1	54	0 0 1 1 0 1 1 0
2	108	0 1 1 0 1 1 0 0
3	216	1 1 0 1 1 0 0 0
4	177	1 0 1 1 0 0 0 1
5	99	0 1 1 0 0 0 1 1
6	198	1 1 0 0 0 1 1 0
7	141	1 0 0 0 1 1 0 1

Translations of the representative; cyclic permutation

Define function **cyclebits**(t,N)
- cyclic permutations of first N bits of integer t
- F90 function ishiftc(*t*,–1,*N*)

The representative has the lowest state-integer among all its translations

Pseudocode; checkstate() subroutine

```
subroutine checkstate(s, R)
R = -1
if (∑_i s[i] ≠ n_↑) return
t = s
do i = 1, N
    t = cyclebits(t, N)
    if (t < s) then
        return
    elseif (t = s) then
        if (mod(k, N/i) ≠ 0) return
        R = i; return
    endif
enddo
```

check the magnetization

check if translated state has lower integer representation

check momentum compatibility
- k is the integer corresponding to the momentum; k=0,...,N-1
- momentum = k2π/N

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

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

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

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

Pseudocode; hamiltonian construction

First, some elements needed; recall

$$H_j|a\rangle = h_a^j T^{-l_j}|b_j\rangle \qquad |b_j\rangle \propto T^{l_j} H_j|a\rangle$$

Finding the representative r of a state-integer s

- lowest integer among all translations

```
subroutine representative(s, r, l)
r = s; t = s; l = 0
do i = 1, N − 1
    t = cyclebits(t, N)
    if (t < r) then r = t; l = i endif
enddo
```

$$|r\rangle = T^l|s\rangle$$

```
subroutine findstate(s, b)
b_min = 1; b_max = M
do
    b = b_min + (b_max − b_min)/2
    if (s < s_b) then
        b_max = b − 1
    elseif (s > s_b) then
        b_min = b + 1
    else
        exit
    endif
    if (b_min > b_max then
        b = −1; exit
    endif
enddo
```

Finding the location of the representative in the state list

- may not be there, if the new state is incompatible with k
- **b=–1** for not found in list

Construct all the matrix elements

```
do a = 1, M
    do i = 0, N − 1
        j = mod(i + 1, N)
        if (s_a[i] = s_a[j]) then
            H(a, a) = H(a, a) + 1/4
        else
            H(a, a) = H(a, a) − 1/4
            s = flip(s_a, i, j)
            call representative(s, r, l)
            call findstate(r, b)
            if (b ≥ 0) then
                H(a, b) = H(a, b) + (1/2) √(R_a/R_b) e^{i2πkl/N}
            endif
        endif
    enddo
enddo
```

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

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

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

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 →
- **semi-momentum states**

Semi-momentum states

Mix momenta +k and –k for k≠0,π

$$|a^\sigma(k)\rangle = \frac{1}{\sqrt{N_a}} \sum_{r=0}^{N-1} C_k^\sigma(r) T^r |a\rangle \qquad C_k^\sigma(r) = \begin{cases} \cos(kr), & \sigma = +1 \\ \sin(kr), & \sigma = -1. \end{cases}$$

$$k = m\frac{2\pi}{N}, \quad m = 1, \ldots, N/2-1, \quad \sigma = \pm 1$$

States with same k, different σ are orthogonal

Semi-momentum states with parity

This state has definite parity with p=+1 or p=–1 for any k

$$|a^\sigma(k,p)\rangle = \frac{1}{\sqrt{N_a^\sigma}} \sum_{r=0}^{N-1} C_k^\sigma(r)(1+pP)T^r|a\rangle.$$

- (k,–1) and (k,+1) blocks
- the basis is of the same size as the original k-blocks
- but these states are real, not complex ⇒ computational advantage
- For k≠0,π, the p=-1 and p=+1 states are degenerate

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

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

$$Z|a^\sigma(k,p,z)\rangle = z|a^\sigma(k,p,z)\rangle, \quad z=\pm 1$$

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 **$S^2=S(S+1)$**

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

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

Example: Thermodynamics

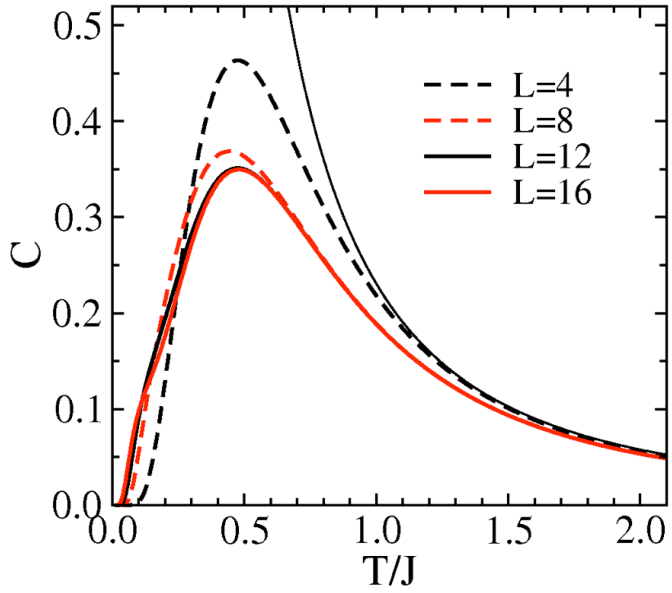
some quantities can be computed using only the magnetization m_z=0 sector

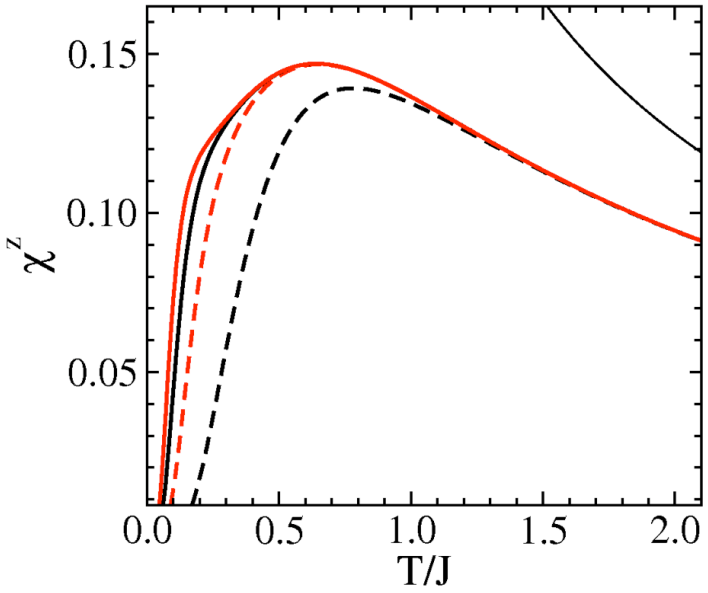
- spin-inversion symmetry can be used, smallest blocks
- spin-S state is **(2S+1)**-fold degenerate (no magnetix field) → weight factor
- possible spin dependence of expectation value → average over **m_z=–S,...,S**

$$C = \frac{d\langle H\rangle}{dt} = \frac{1}{T^2}\left(\langle H^2\rangle - \langle H\rangle^2\right)$$

$$\chi^z = \frac{d\langle m_z\rangle}{dh_z} = \frac{1}{T}\left(\langle m_z^2\rangle - \langle m_z\rangle^2\right)$$

$$\langle m_z\rangle = 0, \quad \langle m_z^2\rangle = \frac{\langle m_x^2 + m_y^2 + m_z^2\rangle}{3} = \frac{\langle S^2\rangle}{3} = \frac{S(S+1)}{3}$$





Compared with leading high-T forms

$\chi = (1/4)/T$

$C = (3/13)/T^2$

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

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

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

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

- 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 H-matrix is

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

Alternative way

generate the normalized basis directly

• start with $|\phi_0\rangle$ arbitrary, normalized, and then

$$|\phi_1\rangle = \frac{1}{N_1}\left(H|\phi_0\rangle - a_0|\phi_0\rangle\right)$$

$$|\phi_{m+1}\rangle = \frac{1}{N_{m+1}}\left(H|\phi_m\rangle - a_m|\phi_m\rangle - N_m|\phi_{m-1}\rangle\right) = \frac{|\gamma_{m+1}\rangle}{N_{m+1}}$$

The definition of N_m is different, and no b_m:

$$\begin{aligned} a_m &= \langle\phi_m|H|\phi_m\rangle \\ N_m &= \langle\gamma_m|\gamma_m\rangle^{-1/2} \end{aligned}$$

Generate $|\gamma_m\rangle$ first, normalize to get N_{m+1}

The H-matrix is

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

Operator expectation values

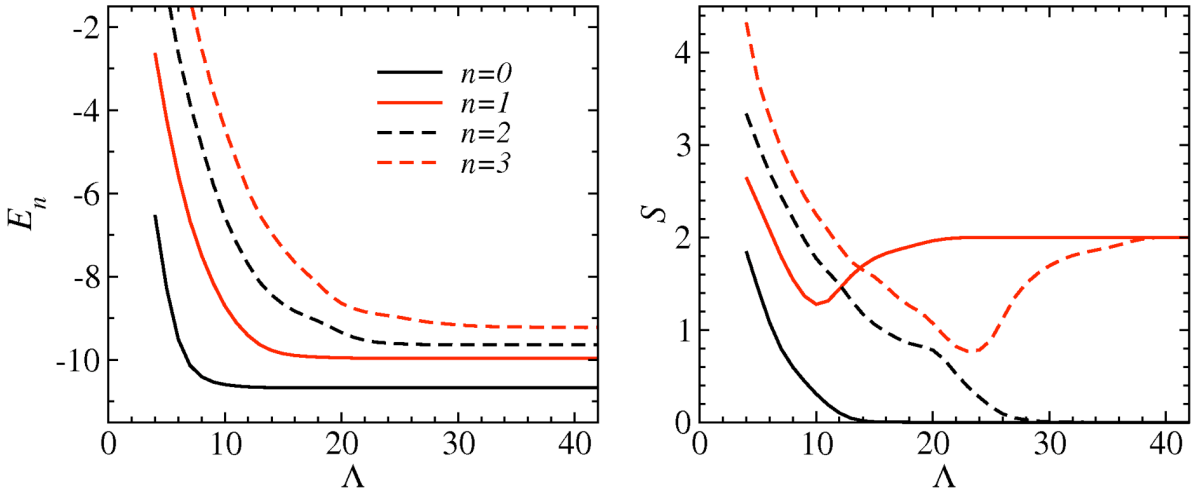
Diagonalizing the tri-diagonal matrix → eigenstates in the Lanczos basis

- 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

Spin correlations in the Heisenberg chain

Let's look at the (staggered) spin correlation function

$$C(r) = \langle \mathbf{S}_i \cdot \mathbf{S}_{i+r} \rangle (-1)^r$$

versus the distance r and at r=N/2 versus system size N

Theory (bosonization conformal field theory) predicts (for large r, N)

$$C(r) \propto \frac{\ln^{1/2}(r/r_0)}{r}$$

Plausible based on N up to 32
- other methods for larger N

Power-law correlations are a sign of a "critical" state; at the boundary between
- ordered (antiferromagnetic)
- disordered (spin liquid)