XIV Training Course on Strongly Correlated Systems
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Exact diagonalization studies

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Studies of small spin chains

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

Key elements of an actual program implementation
- pseudocode segments; actual program available for practice

How to characterize different kinds of ground states
- critical ground state of the Heisenberg chain
- quantum phase transition to a valence-bond solid in a J_1-J_2 chain

Complete 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; enumerate the states

- construct the hamiltonian matrix using bits

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

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

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

Diagonalizing the 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

Use some “canned” diagonalization subroutine

- Useful subroutines available at http://gams.nist.gov

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

- maximum $N\approx 20$
- M^2 matrix elements to store, time to diagonalize $\propto M^3$

Pseudocode; construction of the hamiltonian matrix

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

Define a function **flip**(a,i,j)

- "flips" (0↔1) bits i and j of the integer a
- In F90 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

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

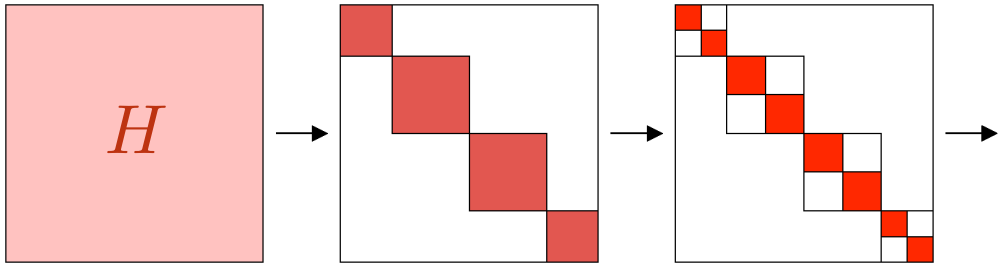
j is the “right” nearest-neighbor of i

- periodic boundary conditions

```
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
```

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
- block-diagonalization just amounts to including states with only given m_z

Number of states in the largest block (m_z =0):

$$\frac{N!}{(N/2)!(N/2)!}$$

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

Pseudocode: using magnetization conservation

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

Store state-integers in ordered list $\mathbf{s_a}$, **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)

```
subroutine findstate(s, b)
do
    b_min = 1; b_max = M
    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

Hamiltonian construction

```
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
```

Momentum states (translationally invariant systems)

A periodic chain (ring) is translationally invariant

- the eigenstates have a momentum (crystal momentum)
- quantum number 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)

The sum can contain several copies of the same state
If $T^R|a\rangle = |a\rangle \quad \text{for some } R$

- 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

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

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

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

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

Pseudocode; basis construction

```
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 state-integer s is a new representative
- store in list R_a, *a*=1,...,*M*
- *R* = –1 if some translation of |s⟩ gives a smaller integer

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*)

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
```

The representative is the lowest integer among all translations

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

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

Finding the representative r of a state-integer s

```
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
```

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

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

```
subroutine findstate(s, b)
do
    b_min = 1; b_max = M
    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
```

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. Introduce function

$$C_k^\sigma(r) = \begin{cases} \cos(kr), & \sigma = +1 \\ \sin(kr), & \sigma = -1. \end{cases}$$

Useful trigonometric relationships

$$\begin{aligned} C_k^\pm(-r) &= \pm C_k^\pm(r), \\ C_k^\pm(r+d) &= C_k^\pm(r)C_k^+(d) \mp C_k^\mp(r)C_k^-(d). \end{aligned}$$

Semi-momentum state

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

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

States with same k, different σ are orthogonal

$$\langle a^{-\sigma}(k)|a^\sigma(k)\rangle = \frac{1}{N_a} \sum_{r=1}^{R_a} \sin(kr)\cos(kr) = 0,$$

Normalization of semi-momentum states

$$N_a = \left(\frac{N}{R_a}\right)^2 \sum_{r=1}^{R_a} [C_k^\sigma(r)]^2 = \frac{N^2}{2R_a}$$

Hamiltonian: ac with H

$$H|a^\pm(k)\rangle = \sum_{j=0}^{N} h_a^j \sqrt{\frac{R_a}{R_{b_j}}} \left(C_k^+(l_j)|b_j^\pm(k)\rangle \mp C_k^-(l_j)|b_j^\mp(k)\rangle \right),$$

The matrix elements are

$$\langle b^\tau(k)|H_j|a^\sigma(k)\rangle = \tau^{(\sigma-\tau)/2} h_a^j \sqrt{\frac{N_{b_j}}{N_a}} C_k^{\sigma\tau}(l_j)$$

σ is mot a conserved quantum number

- H and T mix σ=+1 and σ=–1 states
- the H matrix is twice as large as for momentum states

Why are the semi-momentum states useful then?

Because we can construct a real-valued basis:

Semi-momentum states with parity

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

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

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

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

P,T transformations

example: N=8;note that

- **$T^5P|a\rangle=|a\rangle$**

such P,T relationships will affect normalization and H-elements

Normalization: We have to check whether or not

$$T^m P|a\rangle = |a\rangle \quad \text{for some } m \in \{1, \ldots, N-1\}$$

Simple algebra gives

$$N_a^\sigma = \frac{N^2}{R_a} \times \begin{cases} 1, & T^m P|a\rangle \neq |a\rangle \\ 1 + \sigma p \cos(km), & T^m P|a\rangle = |a\rangle \end{cases}$$

In the latter case the σ=-1 and σ=+1 states are not orthogonal

- calculation of the overlap gives

$$\langle a^{\mp}(k,p)|a^{\pm}(k,p)\rangle = -p, \quad (T^m P|a\rangle = |a\rangle \text{ for some } m)$$

Then only one of them should be included in the basis

- convention: **use σ=+1 if 1+*σp*cos(*km*)≠0, else σ=+1**

If both σ=+1 and σ=–1 are present:

- **we store 2 copies of the same representative**
- we will store the σ value along with the periodicity of the representative

Pseudocode: semi-momentum, parity basis construction

```
do s = 0, 2^N − 1
    call checkstate(s, R, m)
    do σ = ±1 (do only σ = +1 if k = 0 or k = N/2)
        if (m ≠ −1) then
            if (1 + σp cos(ikm2π/N) = 0) R = −1
            if (σ = −1 and 1 − σp cos(ikm2π/N) ≠ 0); R = −1
        endif
        if R > 0 then a = a + 1; s_a = s; R_a = σR; m_a = m endif
    enddo
enddo
```

In the subroutine **checkstate**(), we now find whether

$$T^m P|a\rangle = |a\rangle \quad \text{for some } m \in \{1, \ldots, N-1\}$$

m=–1 if there is no such transformation

if σ=–1 we check whether the σ=+1 state is orthogonal to the σ=–1 state or not

- if not orthogonal use σ=+1
- R=–1 for not including

the subroutine **checkstate**()
is modified to gives us:

- periodicity R (R=–1 if incompatible)
- m>0 if T^m|s>=|s>
- m=–1 if no such relationship

check all translations of |s>

construct reflected state |Ps>

check all translations of |Ps>

```
subroutine checkstate(s, R, m)
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; exit
    endif
enddo
t = reflectbits(s, N); m = −1
do i = 0, R − 1
    if (t < s) then
        R = −1; return
    elseif (t = s) then
        m = i; return
    endif
    t = cyclebits(t, N)
enddo
```

Hamiltonian : Act with an operator H_j on a representative state:

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

We can write H acting on a basis state as

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

Using the properties (trigonometry) of the C-functions:

$$H|a^\sigma(k,p)\rangle = \sum_{j=0}^{N} h_a^j (\sigma p)^{q_j} \sqrt{\frac{N_{b_j}^\sigma}{N_a^\sigma}} \times$$

$$\left(\cos(kl_j)|b_j^\sigma(k,p)\rangle - \sigma\sqrt{\frac{N_{b_j}^{-\sigma}}{N_{b_j}^\sigma}}\sin(kl_j)|b^{-\sigma}(k,p)\rangle\right)$$

If, for some m, $T^m P|b_j\rangle = |b_j\rangle$ then

$$\sqrt{\frac{N_{b_j}^{-\sigma}}{N_{b_j}^\sigma}} = \sqrt{\frac{1-\sigma p\cos(km)}{1+\sigma p\cos(km)}} = \frac{|\sin(km)|}{1+\sigma p\cos(km)}$$

$$\langle b_j^{\mp}(k,p)|b_j^{\pm}(k,p)\rangle = -p$$

else the ratio is one and the + and – states are orthogonal

The matrix elements are

diagonal in σ

$$\langle b_j^\sigma(k,p)|H_j|a^\sigma(k,p)\rangle = h_a^j(\sigma p)^{q_j}\sqrt{\frac{N_{b_j}^\sigma}{N_a^\sigma}}\times$$

$$\begin{cases} \cos(kl_j), & P|b_j\rangle \neq T^m|b_j\rangle \\ \frac{\cos(kl_j)+\sigma p\cos(k[l_j-m])}{1+\sigma p\cos(km)}, & P|b_j\rangle = T^m|b_j\rangle \end{cases}$$

off-diagonal in σ

$$\langle b_j^{-\sigma}(k,p)|H_j|a^\sigma(k,p)\rangle = h_a^j(\sigma p)^{q_j}\sqrt{\frac{N_{b_j}^{-\sigma}}{N_a^\sigma}}\times$$

$$\begin{cases} -\sigma\sin(kl_j), & P|b_j\rangle \neq T^m|b_j\rangle, \\ \frac{-\sigma\sin(kl_j)+p\sin(k[l_j-m])|}{1-\sigma p\cos(km)}, & P|b_j\rangle = T^m|b_j\rangle, \end{cases}$$

Pseudocode: semi-momentum, parity hamiltonian

If 2 copies of the same representative, σ=–1 and σ=+1:

- do both in the same loop iteration
- examine the previous and next element
- carry out the loop iteration only if representative found for the first time

```
do a = 1, M
    if (a > 1 and s_a = s_{a-1}) then
        cycle
    elseif (a < M and s_a = s_{a+1}) then
        n = 2
    else
        n = 1
    endif
    ...
enddo
```

n is the number of copies of the representative

```
do i = a, a + n - 1
    H(a, a) = H(a, a) + E_z
enddo
```

diagonal matrix elements

- E_z = diagonal energy

```
s = flip(s_a, i, j)
call representative(s, r, l, q)
call findstate(r, b)
if (b ≥ 0) then
    if (b > 1 and s_b = s_{b-1}) then
        m = 2; b = b − 1
    elseif (b < M and s_b = s_{b+1}) then
        m = 2
    else
        m = 1
    endif
    do j = b, b + m − 1
    do i = a, a + n − 1
        H(i, j) = H(i, j) + helement(i, j, l, q)
    enddo
    enddo
endif
```

construct
off-diagonal
matrix elements

helement()
computes the
values based on
- stored info
- and l,q

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

find the
representative r of s
- translation and
  reflection numbers l,q

Using 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

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

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

Normalization: must check how a representative transforms under Z,P,T

$$\begin{array}{lllll}
1) & T^m P|a\rangle \neq |a\rangle, & T^m Z|a\rangle \neq |a\rangle & & T^m PZ|a\rangle \neq |a\rangle \\
2) & T^m P|a\rangle = |a\rangle, & T^m Z|a\rangle \neq |a\rangle & & T^m PZ|a\rangle \neq |a\rangle \\
3) & T^m P|a\rangle \neq |a\rangle, & T^m Z|a\rangle = |a\rangle & & T^m PZ|a\rangle \neq |a\rangle \\
4) & T^m P|a\rangle \neq |a\rangle, & T^m Z|a\rangle \neq |a\rangle & & T^m PZ|a\rangle = |a\rangle \\
5) & T^m P|a\rangle = |a\rangle, & T^n Z|a\rangle = |a\rangle & \Rightarrow & T^{m+n} PZ|a\rangle = |a\rangle
\end{array}$$

For cases 2,4,5 only σ=+1 or σ=–1 included

$$N_a^\sigma = \frac{2N^2}{R_a} \times \begin{cases} 1, & 1) \\ 1+\sigma p\cos(km), & 2) \\ 1+z\cos(km), & 3) \\ 1+\sigma pz\cos(km), & 4) \\ [1+\sigma p\cos(km)][1+z\cos(kn)], & 5) \end{cases}$$

Hamiltonian: acting on a state gives a transformed representative

$$H_j|a\rangle = h_a^j P^{q_j} Z^{g_j} T^{-l_j} |b_j\rangle$$

$$q_j \in \{0,1\}, \quad g_j =\in \{0,1\}, \quad l_j = \{0,1,\ldots,N-1\}$$

After some algebra .... we can obtain the matrix elements

diagonal in σ

$$\langle b_j^\sigma(k,p)|H_j|a^\sigma(k,p)\rangle = h_a^j(\sigma p)^{q_j} z^{g_j} \sqrt{\frac{N_{b_j}^\tau}{N_a^\sigma}} \times$$

$$\begin{cases} \cos(kl_j), & 1),3) \\ \frac{\cos(kl_j)+\sigma p\cos(k[l_j-m])}{1+\sigma p\cos(km)}, & 2),5) \\ \frac{\cos(kl_j)+\sigma pz\cos(k[l_j-m])}{1+\sigma pz\cos(km)}, & 4) \end{cases}$$

off-diagonal in σ

$$\langle b_j^{-\sigma}(k,p)|H_j|a^\sigma(k,p)\rangle = h_a^j(\sigma p)^{q_j} z^{g_j} \sqrt{\frac{N_{b_j}^\tau}{N_a^\sigma}} \times$$

$$\begin{cases} -\sigma\sin(kl_j), & 1),3) \\ \frac{-\sigma\sin(kl_j)+p\sin(k[l_j-m])}{1-\sigma p\cos(km)}, & 2),5) \\ \frac{-\sigma\sin(kl_j)+pz\sin(k[l_j-m])}{1-\sigma pz\cos(km)}, & 4) \end{cases}$$

Example: block sizes

k=0, m_z=0 (largest 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)**

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

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

Full diagonalization; expectation values

shorthand block label: **j=(m_z,k,p)** or **j=(m_z=0,k,p,z)**

$$D_j^{-1} H_j D_j = E_j, \quad \langle n_j|A|n_j\rangle = [D_j^{-1} A D_j]_{nn}$$

T>0: sum over all blocks j and states in block n=0,M_j–1

$$\langle A\rangle = \frac{1}{Z}\sum_j \sum_{n=0}^{M_j-1} \mathrm{e}^{-\beta E_{j,n}} [D_j^{-1} A_j U_j]_{nn}, \qquad Z = \sum_j \sum_{n=0}^{M_j-1} \mathrm{e}^{-\beta E_{j,n}}$$

E_j = diagonal (energy) matrix, $E_{j,n}$ = energies, n=0,...,M_j–1

Full diagonalization limited to small N; N=20-24

Example: Thermodynamics

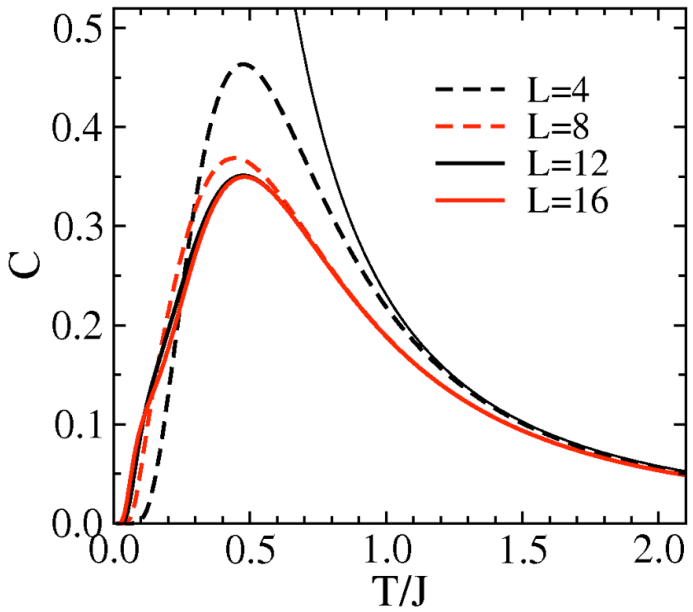
some quantities can be computed using only the magnetization m_z=0 sector

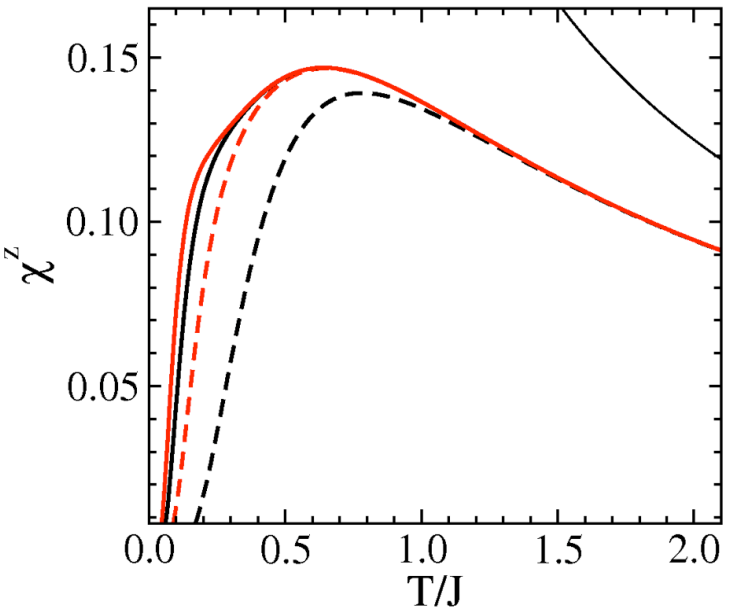
- spin-inversion symmetry can be used, smallest blocks
- spin-S state is **(2S+1)**-fold degenerate (no magnetix field) → weight factor
- possible spin dependence of expectation value → average over **m_z=–S,...,S**

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

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

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





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, *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

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

The next state and its overlaps with the previous states

$$|f_2\rangle = H|f_1\rangle - a_1|f_1\rangle - b_0|f_0\rangle$$

$$\langle f_2 | f_1 \rangle = H_{11} - a_1 N_1, \quad \langle f_2 | f_0 \rangle = N_1 - b_0 N_0$$

For orthogonal states

$$a_1 = H_{11}/N_1, \quad b_0 = N_1/N_0$$

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

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

Potential problem:

The normalization constants N_m can become very large (think of E_0^)

Solution:

generate the normalized basis directly

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

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

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

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

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

Lanczos basis generation in practice

Here: generate the orthogonal basis **{ϕ_m}** directly

$$|\phi_m\rangle = \sum_{a=1}^{M} \phi_m(a)|a\rangle, \quad m = 0, \ldots, \Lambda$$

in a given symmetry block of size M

The coefficients **$\phi_m(a)$** are stored as Λ+1 vectors of size M

- may store only the vectors **ϕ_{m-1}** and **ϕ_m** to generate **ϕ_{m+1}**
  - but basis has to be re-generated when computing expectation values
- stabilization by "re-orthogonalization" (later) requires storage of all **ϕ_m**

The main computational effort is in acting with the hamiltonian; **H|ϕ_m>**

- implement as a subroutine **hoperation**(ϕ,γ), where |γ>=H|ϕ>
- state normalization implemented as **normalize**(ϕ,n)
  - ϕ = vector to normalize, n = <ϕ|ϕ> before normalization

Pseudocode; Lanczos basis generation

Initial random state

```
do i = 1, M
    φ_0(i) = randomfloat(0, 1)
enddo
call normalize(φ_0, n_0)
```

second state

```
call hoperation(φ_0, φ_1)
a_0 = ⟨φ_0|φ_1⟩; φ_1 = φ_0 − a_0|φ_1⟩
call normalize(φ_1, n_1)
```

Generate the rest of the states

```
do m = 1, Λ − 1
    call hoperation(φ_m, φ_{m+1})
    a_m = ⟨φ_m|φ_{m+1}⟩
    φ_{m+1} = φ_{m+1} − a_m φ_m − n_m φ_{m−1}
    call normalize(φ_{m+1}, n_{m+1})
enddo
```

Note: the H-matrix can be constructed and diagonalized after each step

- follow evolution of energy versus Λ
- stop based on some convergence criterion on E_0 (or higher energy)
- expectation values converge slower than energies

The subroutine **hoperation**(ϕ,γ) implements

$$H|\phi\rangle = |\gamma\rangle = \sum_{a=1}^{M}\sum_{b=1}^{M}\phi(a)\langle b|H|a\rangle|b\rangle$$

in a given symmetry block (M = block size)

We do not want to store *H* as an *M×M* matrix (too big). Two options:
- carry out the operations on the fly; only the vectors are stored
- store *H* in a compact form; only non-0 elements (sparse matrix)

Storing *H* speeds up the Lanczos iterations
- but may require a lot of memory

Compact storage of H: For each ***a=1,M***
- e_a is the number of non-0 elements $\langle \mathbf{b}|\mathbf{H}|\mathbf{a}\rangle$
- labels $i=s_a+1, s_a+e_a$ will refer to these matrix elements; $\mathbf{s_a} = \sum_{\mathbf{c=1}}^{\mathbf{a-1}} \mathbf{e_a}$
- ***H*(i)** contains the values of the matrix elements $\langle \mathbf{b}|\mathbf{H}|\mathbf{a}\rangle$
- ***B*(i)** contains the corresponding "target" state index ***b***
- The hamiltonian is symmetric
  - store only elements with b ≤ a (divide diagonal elements by 2)

Pseudocode; hamiltonian operation with compact storage

```
subroutine hoperation(φ, γ)
γ = 0; i = 0
do a = 1, M
    do j = 1, e_a
        i = i + 1
        γ(B(i)) = γ(B(i)) + H(i)φ(a)
        γ(a) = γ(a) + H(i)φ(B(i))
    enddo
enddo
```

$$H|\phi\rangle = |\gamma\rangle = \sum_{a=1}^{M}\sum_{b=1}^{M}\phi(a)\langle b|H|a\rangle|b\rangle$$

Further storage compactification possible

- small number of different elements
- use mapping $\langle \mathbf{b}|\mathbf{H}|\mathbf{a}\rangle \rightarrow \text{integer}$
- many operations on Ia> give same Ib>
  - add up all contributions before storing

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 ($<< \Lambda$) are correct eigenstates of H

To compute expectation values we normally go back to the original basis

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

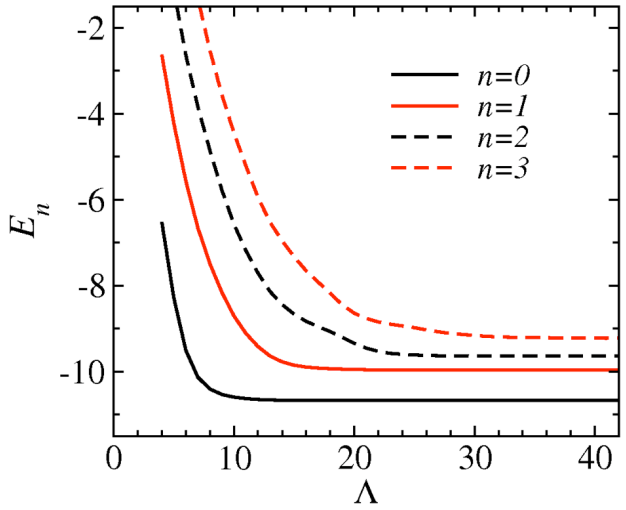
To compute $\langle\psi_\mathbf{n}|\mathbf{O}|\psi_\mathbf{n}\rangle$ first construct

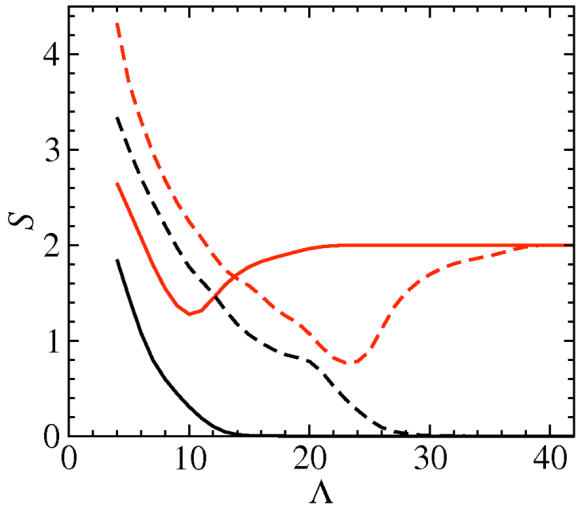
$$\begin{aligned} O|\psi_n\rangle = |\psi_n^O\rangle &= \sum_{a=1}^{M} \psi_n(a) O|a\rangle \\ &= \sum_{a=1}^{M}\sum_{b=1}^{M} \psi_n(a)|b\rangle\langle b|O|a\rangle \\ &= \sum_{b=1}^{M} \psi_n^O(b)|b\rangle \qquad \psi_n^O(b) = \sum_{a=1}^{M} \psi_n(a)\langle b|O|a\rangle \end{aligned}$$

Then evaluate the scalar product

$$\langle\psi_n|O|\psi_n\rangle = \langle\psi_n|\psi_n^O\rangle = \sum_{a=1}^{M} \psi_n(a)\psi_n^O(a)$$

Convergence properties of the Lanczos method



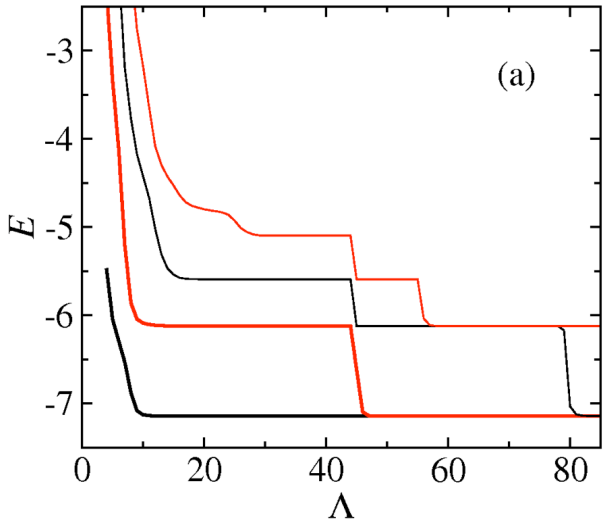


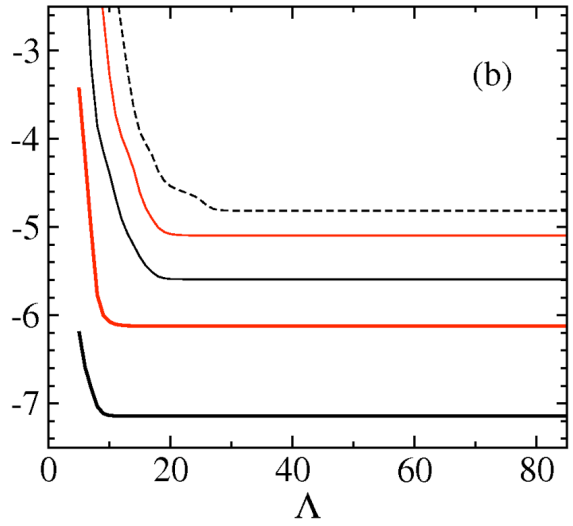
Example; 24-site chain
$m_z = 0$, $k = 0$, $p = 1$, $z = 1$
block size M=28416

Ground state converges first, then successively excited states

Loss of orthogonality: accumulation of numerical error → basis becomes non-orthogonal

- higher states collapse down onto lower ones
- can be cured with re-orthogonalization





Example; 16-site chain
$m_z = 0$, $k = 0$, $p = 1$, $z = 1$
block size M=212

- (a) non-orthogonality
- (b) re-orthogonalized

Re-orthogonalization procedure

For each state generated, remove all components of prior states, *i=1,...,m*

• easy if we work with the normalized basis and all states are stored

$$|\phi_m\rangle \rightarrow \frac{|\phi_m\rangle - q|\phi_i\rangle}{1-q^2}, \qquad q = \langle\phi_i|\phi_m\rangle$$

Pseudocode: modify state generation

```
do m = 1, Λ − 1
    call hoperation(φ_m, φ_{m+1})
    a_m = ⟨φ_m|φ_{m+1}⟩; φ_{m+1} = φ_{m+1} − a_m φ_m − n_m φ_{m−1}
    call normalize(φ_{m+1}, n_{m+1})
    do i = 1, m
        q = ⟨φ_{m+1}|φ_i⟩; φ_{m+1} = (φ_{m+1} − q φ_i)/(1 − q^2)
    enddo
enddo
```

Note: the Lanczos method can only generate a single state of a multiplet

• some random linear combination of degenerate states

Example: 2 degenerate states i, j:

$$H^\Lambda|\Psi\rangle = \sum_{m\neq i,j} c_m E^\Lambda_m|\psi_m\rangle + E^m_{i,j}(c_i|\psi_i\rangle + c_j|\psi_j\rangle)$$

The mixing of the duplet is determined by c_i, c_j of the initial state

Spin correlations in the Heisenberg chain

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

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

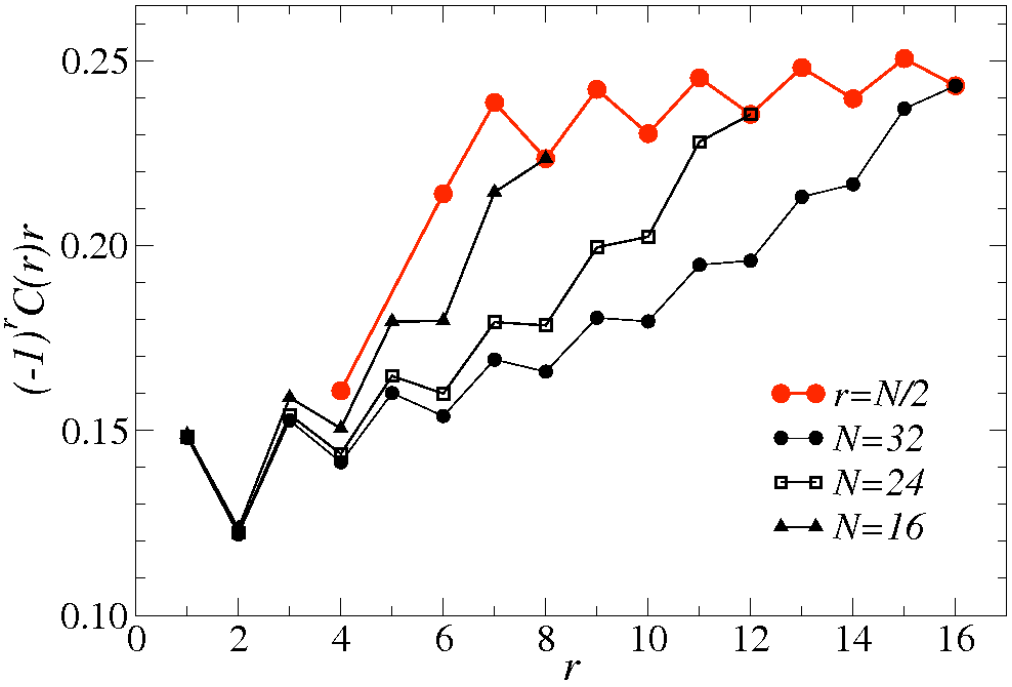
versus the distance r and at r=N/2 versus system size N

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

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

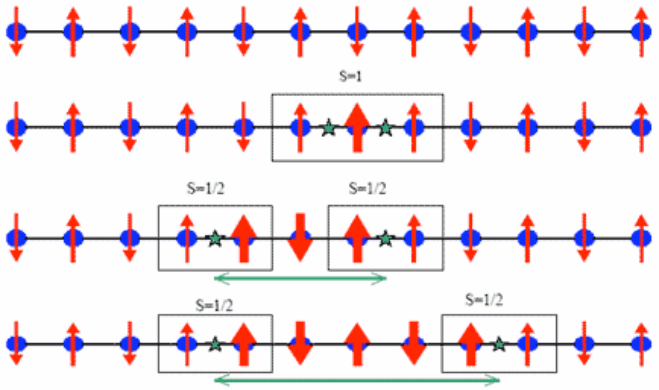
Plausible based on N up to 32
- other methods for larger N

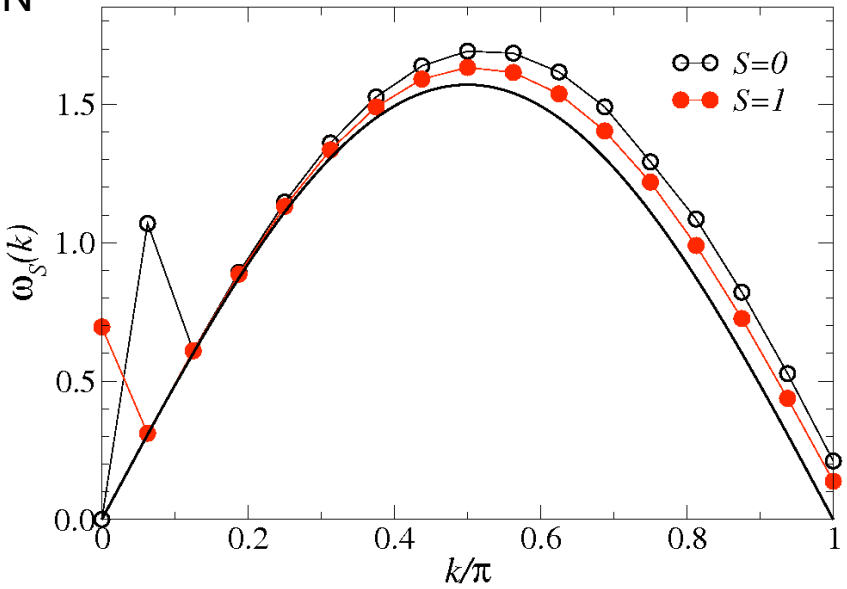
Power-law correlations are a sign of a "critical" state; at the boundary between
- ordered (antiferromagnetic)
- disordered (spin liquid)



Excitations of the Heisenberg chain

- the ground state is a singlet (S=0) for even N
- the first excited state is a triplet (S=1)
- can be understood as pair of “spinons”

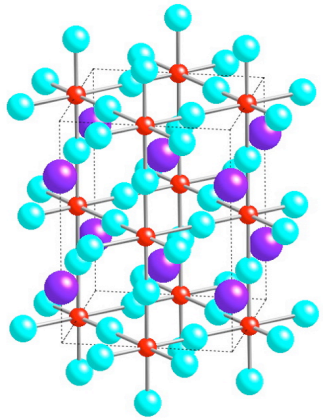


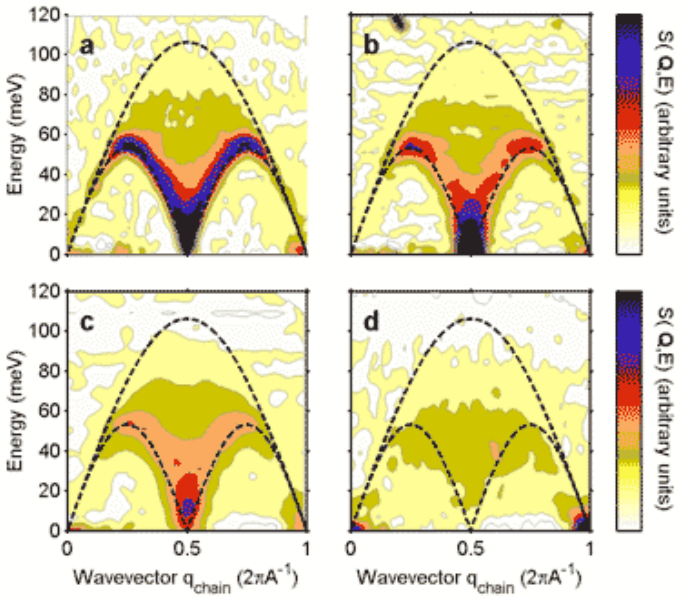


Neutron scattering experiments

- quasi-one-dimensional $KCuF_3$

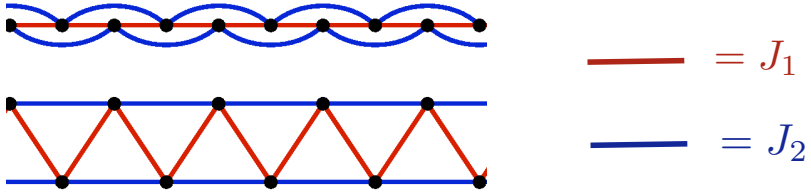
B. Lake et al., Nature Materials 4 329-334 (2005)





Heisenberg chain with frustrated interactions

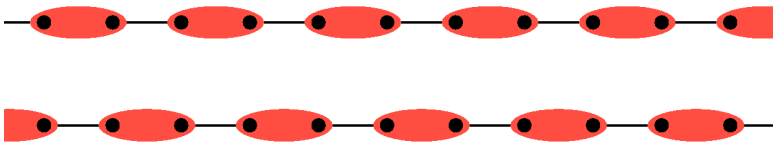
$$H = \sum_{i=1}^{N} \left[J_1 \mathbf{S}_i \cdot \mathbf{S}_{i+1} + J_2 \mathbf{S}_i \cdot \mathbf{S}_{i+2} \right]$$



For the special point $J_2/J_1=0.5$, this model has an exact solution

Singlet-product states

$$|\Psi_A\rangle = |(1,2)(3,4)(5,6)\cdots\rangle$$
$$|\Psi_B\rangle = |(1,N)(3,2)(5,4)\cdots\rangle$$



It is not hard to show that these are eigenstates of H (we will do later)

$$(a,b) = (\uparrow_a\downarrow_b - \downarrow_a\uparrow_b)/\sqrt{2}$$

The system has this kind of order (with fluctuations, no exact solution) for all $J_2/J_1>0.2411.....$ This is a **quantum phase transition** between

- a critical state
- a valence-bond-solid (VBS) state

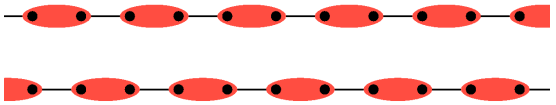
The symmetry is not broken for finite N

- the ground state is a superposition of the two ordered states

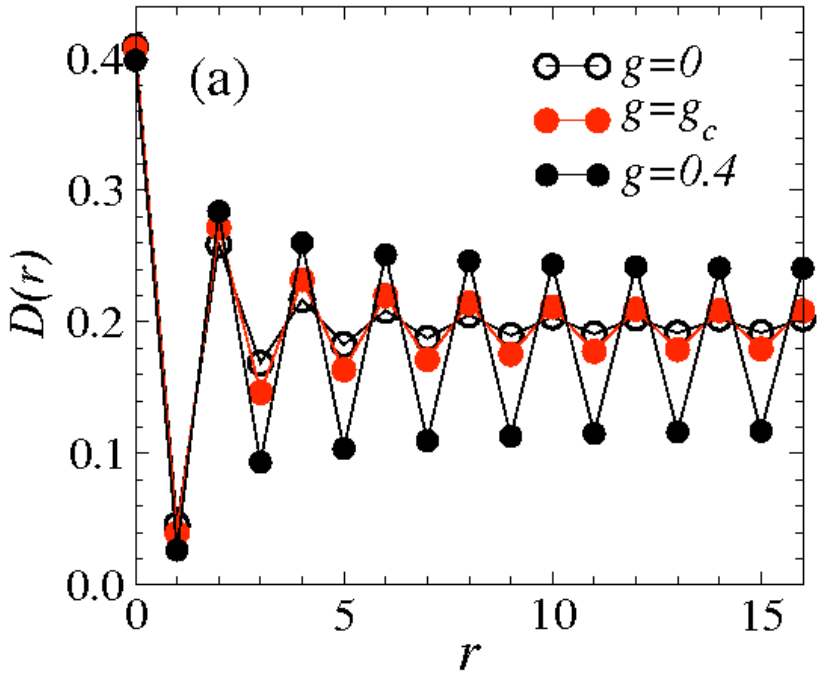
$$|\Psi_0\rangle \sim |\Psi_A\rangle + |\Psi_B\rangle, \qquad |\Psi_1\rangle \sim |\Psi_A\rangle - |\Psi_B\rangle$$

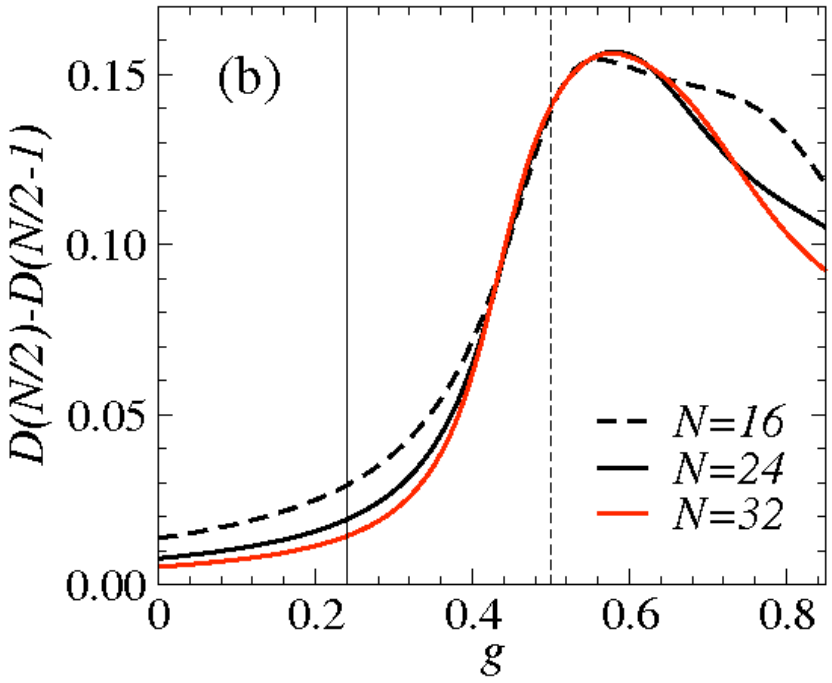
The VBS state can be detected in finite systems using “dimer” correlations

$$D(r) = \langle B_i B_{i+r} \rangle = \langle (\mathbf{S}_i \cdot \mathbf{S}_{i+1})(\mathbf{S}_{i+r} \cdot \mathbf{S}_{i+1+r}) \rangle$$



Results from Lanczos diagonaization; different coupling ratios ***g=J₂/J₁***

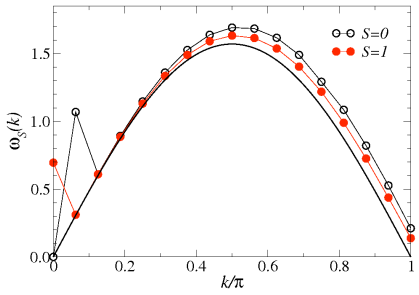




It is not easy to detect the transition this way

- much larger systems are needed for observing a sharp transition
- other properties can be used to accurately determine the critical point g_c

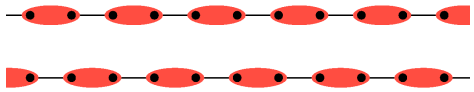
Determining the transition point using level crossings



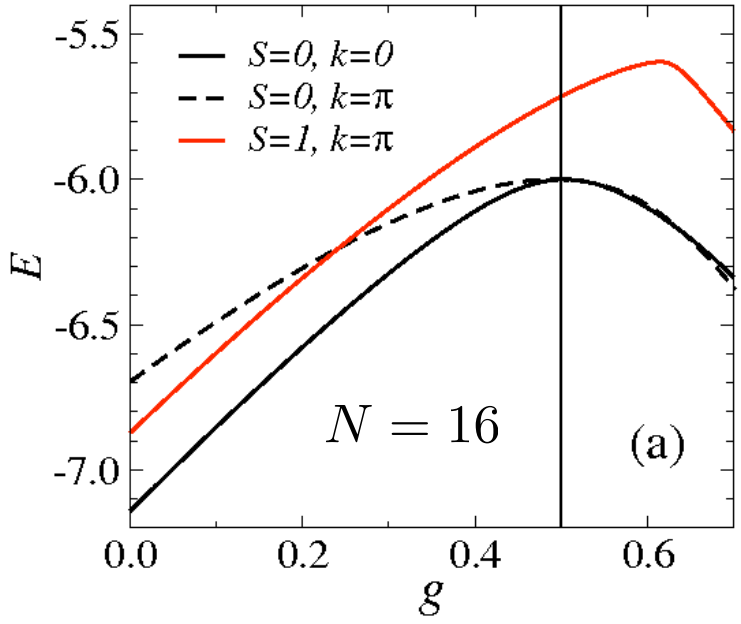
Lowest excitation for the g=0 Heisenberg chain is a triplet
- this can be expected for all $g<g_c$

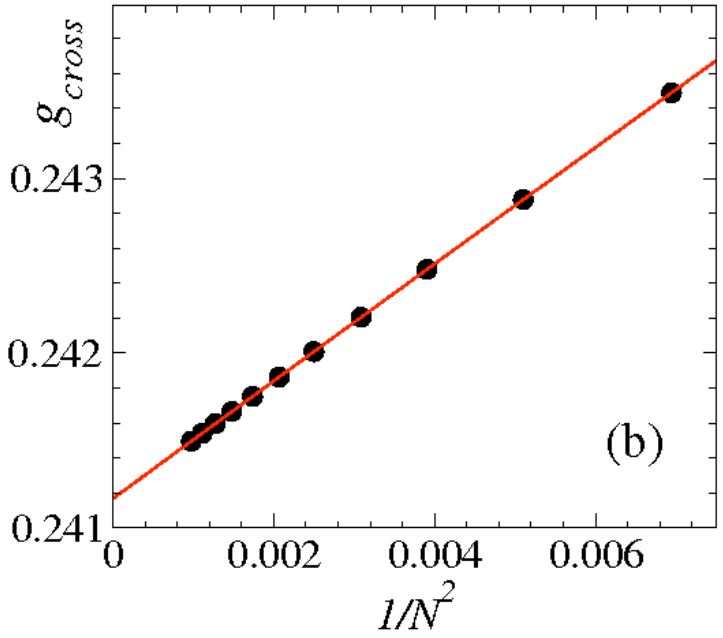
The VBS state is 2-fold degenerate for infinite N
- and for any N at g=1/2
- these two states are singlets
- gap between them closes exponentially as $N\to\infty$
- the lowest excitation is the second singlet

$$|\Psi_0\rangle \sim |\Psi_A\rangle + |\Psi_B\rangle$$
$$|\Psi_1\rangle \sim |\Psi_A\rangle - |\Psi_B\rangle$$



The two lowest excited state should cross at g_c





Extrapolating point for different N up to 32 gives g_c=0.2411674(2)