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

\[ H = J \sum_{i=1}^{N} S_i \cdot S_{i+1} = J \sum_{i=1}^{N} \left[ S_i^x S_{i+1}^x + S_i^y S_{i+1}^y + S_i^z S_{i+1}^z \right], \]

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

Simplest way; enumerate the states
• construct the hamiltonian matrix using bits

\[ |0\rangle = |\downarrow, \downarrow, \downarrow, \ldots, \downarrow\rangle \quad (= 0 \ldots 000) \]
\[ |1\rangle = |\uparrow, \downarrow, \downarrow, \ldots, \downarrow\rangle \quad (= 0 \ldots 001) \]
\[ |2\rangle = |\downarrow, \uparrow, \downarrow, \ldots, \downarrow\rangle \quad (= 0 \ldots 010) \]
\[ |3\rangle = |\uparrow, \uparrow, \downarrow, \ldots, \downarrow\rangle \quad (= 0 \ldots 011) \]

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 \( \sim M^3 \)
Pseudocode; construction of the Hamiltonian matrix

Let \( a[i] \) refer to the \( i:th \) bit of an integer \( a \)

Define a function \( \text{flip}(a,i,j) \)
- “flips” \( 0 \leftrightarrow 1 \) bits \( i \) and \( j \) of the integer \( a \)
- In F90 the bit-level function \( \text{ieor}(a,2**i) \) can be used to flip bit \( i \) of \( a \)
- Bits \( i \) and \( j \) can be flipped using \( \text{ieor}(a,2**i+2**j) \)

\[
\begin{array}{cccccccc}
  & & & \text{i} & & \text{j} & & & \\
\text{a} & 0 & 1 & 0 & 1 & 0 & 0 & 1 & 1 \\
2^i + 2^j & 0 & 0 & 0 & 1 & 1 & 0 & 0 & 0 \\
\text{ieor}(a, 2^i + 2^j) & 0 & 1 & 0 & 0 & 1 & 0 & 1 & 1 \\
\end{array}
\]
The S=1/2 Heisenberg chain hamiltonian can be constructed according to

- $j$ is the “right” nearest-neighbor of $i$
- periodic boundary conditions

```plaintext
do $a = 0, 2^N - 1$
  do $i = 0, N - 1$
    $j = \text{mod}(i + 1, N)$
    if ($a[i] = a[j]$) then
      $H(a, a) = H(a, a) + \frac{1}{4}$
    else
      $H(a, a) = H(a, a) - \frac{1}{4}$
    endif
    $b = \text{flip}(a, i, j); H(a, b) = \frac{1}{2}$
  enddo
endo
dendo
```
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, $N \approx 40$ is max)
Simplest example; magnetization conservation

\[ m_z = \sum_{i=1}^{N} S^z_i \]

- 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 $\uparrow$

Store state-integers in ordered list $s_a$, $a=1,\ldots,M$

```
do $s = 0, 2^N - 1$
    if ($\sum_i s[i] = n_\uparrow$) then $a = a + 1; s_a = s$ endif
endo
$M = a$
```

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)

Finding the location $b$ of a state-integer $s$ in the list
- using bisection in the ordered list
Hamiltonian construction

\begin{verbatim}
\textbf{do} \ a = 1, \ M
    \textbf{do} \ i = 0, \ N - 1
        \ j = \text{mod}(i + 1, \ N)
        \textbf{if} (s_a[i] = s_a[j]) \textbf{ then}
            \ H(a, a) = H(a, a) + \frac{1}{4}
        \textbf{else}
            \ H(a, a) = H(a, a) - \frac{1}{4}
            \ s = \text{flip}(s_a, i, j)
            \textbf{call findstate}(s, b)
            \ H(a, b) = H(a, b) + \frac{1}{2}
        \textbf{endif}
    \textbf{enddo}
\textbf{enddo}
\end{verbatim}
Momentum states (translationally invariant systems)

A periodic chain (ring) is translationally invariant
• the eigenstates have a momentum (crystal momentum )
• quantum number k

\[ T | n \rangle = e^{i k} | n \rangle \quad k = m \frac{2\pi}{N}, \quad m = 0, \ldots, N - 1, \]

The operator T translates the state by one lattice spacing
• for a spin basis state

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

\[ [T, H] = 0 \rightarrow \text{momentum blocks of H} \]
• can use eigenstates of T with given k as basis
A momentum state can be constructed from any representative state

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

Construct ordered list of representatives

If $|a\rangle$ and $|b\rangle$ are representatives, then

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

The sum can contain several copies of the same state

If $T^R |a\rangle = |a\rangle$ for some $R$

• the total weight for this component is

\[ 1 + e^{-ikR} + e^{-i2kR} + \ldots + e^{-i(N-R)} \]

• vanishes (state incompatible with k) unless $kR = n2\pi$

• the total weight of the representative is then $N/R$

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

4-site examples

- $|0011\rangle \rightarrow |0110\rangle, |1100\rangle, |1001\rangle$
- $|0101\rangle \rightarrow |1010\rangle$
\[ |a(k)\rangle = \frac{1}{\sqrt{N_a}} \sum_{r=0}^{N-1} e^{-ikr T^r} |a\rangle \]

Normalization of a state \( |a(k)\rangle \) 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

\begin{verbatim}
do s = 0, 2^N - 1
   call checkstate(s, R)
   if R ≥ 0 then a = a + 1; s_a = s; R_a = R endif
endo
M = a
\end{verbatim}

\( M = \text{size of the H-block} \)

Uses a subroutine \textbf{checkstate}(s, R)

- \( R = \text{periodicity if state-integer } s \text{ is a new representative} \)
- store in list \( R_a, a=1,...,M \)
- \( R = -1 \text{ if some translation of } |s\rangle \text{ gives a smaller integer} \)
**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**

```plaintext
subroutine checkstate(s, R)
    R = −1
    if (∑ᵢ s[i] ≠ n₁) 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
enddo
```

The representative is the lowest integer among all translations
The Hamiltonian matrix. Write \( S = 1/2 \) chain hamiltonian as

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

Act with \( H \) on a momentum state

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

\( H_j|a\rangle \) is related to some representative: \( H_j|a\rangle = h^j_a T^{-l_j} |b_j\rangle \)

\[
H|a(k)\rangle = \sum_{j=0}^{N} \frac{h^j_a}{\sqrt{N_a}} \sum_{r=0}^{N-1} e^{-ikr T^{(r-l_j)}} |b_j\rangle
\]

Shift summation index \( r \) and use definition of momentum state

\[
H|a(k)\rangle = \sum_{j=0}^{N} h^j_a e^{-ikl_j} \sqrt{\frac{N_{b_j}}{N_a}} |b_j(k)\rangle \quad \rightarrow \text{matrix elements}
\]

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

\[
\langle b_j(k)|H_{j>0}|a(k)\rangle = e^{-ikl_j} \frac{1}{2} \sqrt{\frac{R_a}{R_{b_j}}}, \quad |b_j\rangle \propto T^{-l_j} H_j|a\rangle,
\]
Pseudocode; hamiltonian construction

First, some elements needed; recall

\[ H_j |a\rangle = h_j^a T^{-l_j} |b_j\rangle \]

Finding the representative \( r \) of a state-integer \( s \)

```plaintext
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
```

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

```plaintext
subroutine findstate(s, b)
    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

\[
\text{do } a = 1, M \\
\quad \text{do } i = 0, N - 1 \\
\quad \quad j = \text{mod}(i + 1, N) \\
\quad \quad \text{if } (s_{a}[i] = s_{a}[j]) \text{ then} \\
\quad \quad \quad H(a, a) = H(a, a) + \frac{1}{4} \\
\quad \quad \text{else} \\
\quad \quad \quad H(a, a) = H(a, a) - \frac{1}{4} \\
\quad \quad \quad s = \text{flip}(s_{a}, i, j) \\
\quad \quad \quad \text{call representative}(s, r, l) \\
\quad \quad \quad \text{call findstate}(r, b) \\
\quad \quad \quad \text{if } (b \geq 0) \text{ then} \\
\quad \quad \quad \quad H(a, b) = H(a, b) + \frac{1}{2} \sqrt{R_{a}/R_{b}} e^{i2\pi kl/N} \\
\quad \quad \quad \text{endif} \\
\quad \quad \text{endif} \\
\quad \text{enddo} \\
\text{enddo}
\]
**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 \([P, T] \neq 0\)

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

\[ |a(k, p)\rangle = \frac{1}{\sqrt{N_a}} \sum_{r=0}^{N-1} e^{-i k r T^r} (1 + p P) |a\rangle, \quad p = \pm 1 \]

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

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

\[ = p \frac{1}{\sqrt{N_a}} \sum_{r=0}^{N-1} e^{i k r T^r} (1 + p P) |a\rangle = p |a(k, p)\rangle \text{ if } k = 0 \text{ or } k = \pi \]

\(k=0,\pi\) momentum blocks are split into \(p=+1\) and \(p=-1\) sub-blocks

- \([T, P]=0\) in the \(k=0,\pi\) blocks
- physically clear because \(-k=k\) on the lattice for \(k=0,\pi\)
- we can exploit parity in a different way for other \(k\) →
- **semi-momentum states**
Semi-momentum states

Mix momenta $+k$ and $-k$ for $k \neq 0, \pi$. Introduce function

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

Useful trigonometric relationships

$$C_\pm^k(-r) = \pm C_\pm^k(r),$$
$$C_\pm^k(r + d) = C_\pm^k(r)C_\mp^k(d) \mp C_\mp^k(r)C_\pm^k(d).$$

Semi-momentum state

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

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

States with same $k$, different $\sigma$ 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

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

The matrix elements are

\[ \langle b^{\tau} (k)|H_j|a^\sigma (k)\rangle = \tau^{(\sigma-\tau)/2} h^j_a \sqrt{\frac{N_{b_j}}{N_a}} C_k^{\sigma \tau} (l_j) \]

\[ \sigma \text{ is not a conserved quantum number} \]
\[ \cdot \text{H and T mix } \sigma=+1 \text{ and } \sigma=-1 \text{ states} \]
\[ \cdot \text{the H matrix is twice as large as for momentum states} \]
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 \( p = -1 \)

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

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

<table>
<thead>
<tr>
<th>( r )</th>
<th>( T^r )</th>
<th>( T^5P )</th>
</tr>
</thead>
<tbody>
<tr>
<td>0</td>
<td>27 0011011</td>
<td>216 11011000</td>
</tr>
<tr>
<td>1</td>
<td>54 00110110</td>
<td>177 10110001</td>
</tr>
<tr>
<td>2</td>
<td>108 01101100</td>
<td>99 01100011</td>
</tr>
<tr>
<td>3</td>
<td>216 11011000</td>
<td>198 11000110</td>
</tr>
<tr>
<td>4</td>
<td>177 10110001</td>
<td>141 10001101</td>
</tr>
<tr>
<td>5</td>
<td>99 01100011</td>
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</tr>
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<td>6</td>
<td>198 11000110</td>
<td>54 00110110</td>
</tr>
<tr>
<td>7</td>
<td>141 10001101</td>
<td>108 01101100</td>
</tr>
</tbody>
</table>

**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 \( \sigma=-1 \) and \( \sigma=+1 \) 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 \( \sigma=+1 \) if \( 1 + \sigma p \cos(km) \neq 0 \), else \( \sigma=+1 \)

If both \( \sigma=+1 \) and \( \sigma=-1 \) are present:

• we store 2 copies of the same representative

• we will store the \( \sigma \) value along with the periodicity of the representative
Pseudocode: semi-momentum, parity basis construction

\[
\text{do } s = 0, 2^N - 1 \\
\text{call checkstate}(s, R, m) \\
\text{do } \sigma = \pm 1 \ (\text{do only } \sigma = +1 \text{ if } k = 0 \text{ or } k = N/2) \\
\quad \text{if } (m \neq -1) \text{ then} \\
\quad \quad \text{if } (1 + \sigma p \cos(ikm2\pi/N) = 0) R = -1 \\
\quad \quad \text{if } (\sigma = -1 \text{ and } 1 - \sigma p \cos(ikm2\pi/N) \neq 0); R = -1 \\
\quad \text{endif} \\
\quad \text{if } R > 0 \text{ then } a = a + 1; s_a = s; R_a = \sigma R; m_a = m \text{ endif} \\
\text{enddo} \\
\text{enddo}
\]

In the subroutine \textbf{checkstate}(), we now find whether

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

\(m=-1\) if there is no such transformation

if \(\sigma=-1\) we check whether the \(\sigma=+1\) state is orthogonal to the \(\sigma=-1\) state or not
• if not orthogonal use \(\sigma=+1\)
• \(R=-1\) for not including
the subroutine **checkstate()**
is modified to gives us:
• periodicity R (R=−1 if incompatible)
• m>0 if T^mPls>ls>
• m=−1 if no such relationship

```plaintext
subroutine checkstate(s, R, m)
R = −1
if (\sum_i s[i] \neq 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) \neq 0) return
        R = i; exit
    endif
endo
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)
endo
```
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:

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

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

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

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

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

else the ratio is one and the + and − states are orthogonal
The matrix elements are

**diagonal in \( \sigma \)**

\[
\langle b^\sigma_j (k, p) | H_j | a^\sigma (k, p) \rangle = h^j_a (\sigma p)^{q_j} \sqrt{\frac{N_{b^\sigma_j}}{N^\sigma_a}} \times \left\{ \begin{array}{l}
\cos(\ell_j), \\
\frac{\cos(\ell_j) + \sigma p \cos(k[l_j - m])}{1 + \sigma p \cos(km)},
\end{array} \right.
\]

\( P |b_j\rangle \neq T^m |b_j\rangle \)

\( P |b_j\rangle = T^m |b_j\rangle \)

**off-diagonal in \( \sigma \)**

\[
\langle b^-\sigma_j (k, p) | H_j | a^\sigma (k, p) \rangle = h^j_a (\sigma p)^{q_j} \sqrt{\frac{N_{b^-\sigma_j}}{N^\sigma_a}} \times \left\{ \begin{array}{l}
-\sigma \sin(\ell_j), \\
\frac{-\sigma \sin(\ell_j) + p \sin(k[l_j - m])}{1 - \sigma p \cos(km)},
\end{array} \right.
\]

\( P |b_j\rangle \neq T^m |b_j\rangle \),

\( P |b_j\rangle = T^m |b_j\rangle \),
Pseudocode: semi-momentum, parity hamiltonian

If 2 copies of the same representative, \( \sigma = -1 \) and \( \sigma = +1 \):
• 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

\[
\text{do } a = 1, M \\
\quad \text{if } (a > 1 \text{ and } s_a = s_{a-1}) \text{ then} \\
\quad \quad \text{cycle} \\
\quad \text{elseif } (a < M \text{ and } s_a = s_{a+1}) \text{ then} \\
\quad \quad \quad n = 2 \\
\quad \text{else} \\
\quad \quad \quad n = 1 \\
\quad \text{endif} \\
\quad \ldots \\
\text{enddo}
\]

\[
\text{do } i = a, a + n - 1 \\
\quad H(a, a) = H(a, a) + E_z \\
\text{enddo}
\]

\( n \) is the number of copies of the representative

\( E_z \) = diagonal energy
subroutine representative (s, r, l, q)
... 
\( t = \text{reflectbits}(s, N); q = 0 \)
do \( i = 1, N - 1 \)
  \( t = \text{cyclebits}(t, N) \)
  if \( (t < r) \) then \( r = t; l = i; q = 1 \) endif
endo
Using spin-inversion symmetry

Spin inversion operator:  \( Z\ket{S_1^z, S_2^z, \ldots, S_N^z} = \ket{-S_1^z, -S_2^z, \ldots, -S_N^z} \)

In the magnetization block \( m_z = 0 \) we can use eigenstates of \( Z \)

\[
\ket{a^\sigma (k, p, z)} = \frac{1}{\sqrt{N_a^\sigma}} \sum_{r=0}^{N-1} C_k^\sigma (r) (1 + pP)(1 + zZ)T_r \ket{a},
\]

\[
Z\ket{a^\sigma (k, p, z)} = z\ket{a^\sigma (k, p, z)}, \quad z = \pm 1
\]

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

1) \( T^m P \ket{a} \neq \ket{a}, \quad T^m Z \ket{a} \neq \ket{a} \quad T^m PZ \ket{a} \neq \ket{a} \)
2) \( T^m P \ket{a} = \ket{a}, \quad T^m Z \ket{a} \neq \ket{a} \quad T^m PZ \ket{a} \neq \ket{a} \)
3) \( T^m P \ket{a} \neq \ket{a}, \quad T^m Z \ket{a} = \ket{a} \quad T^m PZ \ket{a} \neq \ket{a} \)
4) \( T^m P \ket{a} \neq \ket{a}, \quad T^m Z \ket{a} \neq \ket{a} \quad T^m PZ \ket{a} = \ket{a} \)
5) \( T^m P \ket{a} = \ket{a}, \quad T^n Z \ket{a} = \ket{a} \quad \Rightarrow T^{m+n} PZ \ket{a} = \ket{a} \)

For cases 2,4,5 only \( \sigma=+1 \) or \( \sigma=-1 \) 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 \(\sigma\)**

\[
\langle b_j^\sigma (k, p) | H_j | a^\sigma (k, p) \rangle = h_a^j (\sigma p)^{q_j} Z^{g_j} \sqrt{\frac{N^{\tau}_{b_j}}{N^\sigma_a}} \times \\
\begin{cases}
\cos(kl_j), & 1), 3) \\
\frac{\cos(kl_j) + \sigma p \cos(k[l_j - m])}{1 + \sigma p \cos(km)}, & 2), 5) \\
\frac{\cos(kl_j) + \sigma p z \cos(k[l_j - m])}{1 + \sigma p z \cos(km)}, & 4)
\end{cases}
\]

**off-diagonal in \(\sigma\)**

\[
\langle b_j^{-\sigma} (k, p) | H_j | a^\sigma (k, p) \rangle = h_a^j (\sigma p)^{q_j} Z^{g_j} \sqrt{\frac{N^{\tau}_{b_j}}{N^\sigma_a}} \times \\
\begin{cases}
-\sigma \sin(kl_j), & 1), 3) \\
\frac{-\sigma \sin(kl_j) + p \sin(k[l_j - m])}{1 - \sigma p \cos(km)}, & 2), 5) \\
\frac{-\sigma \sin(kl_j) + p z \sin(k[l_j - m])}{1 - \sigma p z \cos(km)}, & 4)
\end{cases}
\]
**Example: block sizes**

k=0, m_z=0 (largest block)

\[
\begin{array}{cccc}
N & (+1, +1) & (+1, -1) & (-1, +1) & (-1, -1) \\
8 & 7 & 1 & 0 & 2 \\
12 & 35 & 15 & 9 & 21 \\
16 & 257 & 183 & 158 & 212 \\
20 & 2518 & 2234 & 2136 & 2364 \\
24 & 28968 & 27854 & 27482 & 28416 \\
28 & 361270 & 356876 & 355458 & 359256 \\
32 & 4707969 & 4690551 & 4685150 & 4700500 \\
\end{array}
\]

**Total spin S conservation**

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

\[
S^2 = \sum_{i=1}^{N} \sum_{j=1}^{N} S_i \cdot S_j = 2 \sum_{i<j} S_i \cdot S_j + \frac{3}{4} N
\]

**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 \( n=0,M_j-1 \)

\[
\langle A \rangle = \frac{1}{Z} \sum_j \sum_{n=0}^{M_j-1} e^{-\beta E_j,n} [D_j^{-1} A_j U_j]_{nn}, \quad Z = \sum_j \sum_{n=0}^{M_j-1} e^{-\beta E_j,n}
\]

\( E_j = \) diagonal (energy) matrix, \( E_{j,n} = \) energies, \( n=0,\ldots, M_j-1 \)

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) $\rightarrow$ weight factor
• possible spin dependence of expectation value $\rightarrow$ 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
$$\chi = \frac{1}{4}/T$$
$$C = \frac{3}{13}/T^2$$
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 $\Lambda$ 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 $\Lambda$, 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 $\Lambda$

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

- 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

\[ \langle f_{m-1}|H|f_m\rangle = b_{m-1}N_{m-1} = N_m \]
\[ \langle f_m|H|f_m\rangle = a_mN_m \]
\[ \langle f_{m+1}|H|f_m\rangle = N_{m+1} \]

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

\[ \langle \phi_{m-1}|H|\phi_m\rangle = \sqrt{b_{m-1}} \]
\[ \langle \phi_m|H|\phi_m\rangle = a_m \]
\[ \langle \phi_{m+1}|H|\phi_m\rangle = \sqrt{b_m} \]
Potential problem:
The normalization constants $N_m$ can become very large (think of $E_0^\wedge$)

**Solution:**

generate the normalized basis directly

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

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

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

The definition of $N_m$ is different, and no $b_m$:

\[
a_m = \langle \phi_m | H | \phi_m \rangle
\]

\[
N_m = \langle \gamma_m | \gamma_m \rangle^{-1/2}
\]

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

The $H$-matrix is

\[
\langle \phi_{m-1} | H | \phi_m \rangle = N_m
\]

\[
\langle \phi_m | H | \phi_m \rangle = a_m
\]

\[
\langle \phi_{m+1} | H | \phi_m \rangle = N_{m+1}
\]
Lanczos basis generation in practice

Here: generate the orthogonal basis $\{\Phi_m\}$ 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 $\Lambda+1$ vectors of size M

- may store only the vectors $\Phi_{m-1}$ and $\Phi_m$ to generate $\Phi_{m+1}$
  - but basis has to be re-generated when computing expectation values
  - stabilization by “re-orthogonalization” (later) requires storage of all $\Phi_m$

The main computational effort is in acting with the hamiltonian; $H|\phi_m\rangle$

- implement as a subroutine $\text{hoperation}(\phi, \gamma)$, where $|\gamma\rangle = H|\phi\rangle$
- state normalization implemented as $\text{normalize}(\phi, n)$
  - $\Phi = \text{vector to normalize}, \quad n = <\phi|\phi>$ before normalization
## Pseudocode; Lanczos basis generation

### Initial random state

\[
\begin{align*}
\text{do } & i = 1, M \\
\phi_0(i) & = \text{randomfloat}(0, 1) \\
\text{enddo} \\
\text{call normalize}(\phi_0, n_0)
\end{align*}
\]

### second state

\[
\begin{align*}
\text{call hoperation}(\phi_0, \phi_1) \\
a_0 & = \langle \phi_0 | \phi_1 \rangle; \ \phi_1 = \phi_0 - a_0 | \phi_1 \rangle \\
\text{call normalize}(\phi_1, n_1)
\end{align*}
\]

### Generate the rest of the states

\[
\begin{align*}
\text{do } & m = 1, \Lambda - 1 \\
\text{call hoperation}(\phi_m, \phi_{m+1}) \\
a_m & = \langle \phi_m | \phi_{m+1} \rangle \\
\phi_{m+1} & = \phi_{m+1} - a_m \phi_m - n_m \phi_{m-1} \\
\text{call normalize}(\phi_{m+1}, n_{m+1}) \\
\text{enddo}
\end{align*}
\]

Note: the H-matrix can be constructed and diagonalized after each step
- follow evolution of energy versus \( \Lambda \)
- stop based on some convergence criterion on \( E_0 \) (or higher energy)
- expectation values converge slower than energies
The subroutine \texttt{hoperation}(\phi, \gamma) 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 (\(M = \text{block size}\))

We do not want to store \(H\) as an \(M \times M\) 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)

\textbf{Storing \(H\) speeds up the Lanczos iterations}
- but may require a lot of memory

\textbf{Compact storage of \(H\):} For each \(a=1,M\)
- \(e_a\) is the number of non-0 elements \(\langle b | H | a \rangle\)
- labels \(i=s_a+1,s_a+e_a\) will refer to these matrix elements;
- \(H(i)\) contains the values of the matrix elements \(\langle b | H | a \rangle\)
- \(B(i)\) contains the corresponding “target” state index \(b\)
- The hamiltonian is symmetric
  - store only elements with \(b \leq a\) (divide diagonal elements by 2)
Pseudocode; hamiltonian operation with compact storage

```plaintext
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
enddo
```

\[
H|φ⟩ = |γ⟩ = \sum_{a=1}^{M} \sum_{b=1}^{M} φ(a)⟨b|H|a⟩|b⟩
\]

Further storage compactification possible
- small number of different elements
- use mapping \( ⟨b|H|a⟩ \rightarrow \text{integer} \)
- many operations on \( |a⟩ \) give same \( |b⟩ \)
  - add up all contributions before storing
Operator expectation values

Diagonalizing the tri-diagonal matrix → eigenstates in the Lanczos basis
• eigenvectors \( \mathbf{v}_n \), energies \( E_n \)
• only some number of low-energy states (\( \ll \Lambda \)) are correct eigenstates of \( H \)

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

\[
\psi_n(a) = \sum_{m=0}^{\Lambda} v_n(m) \phi_m(a), \quad a = 1, \ldots, M
\]

To compute \( \langle \psi_n | O | \psi_n \rangle \) first construct

\[
O | \psi_n \rangle = | \psi_n^O \rangle = \sum_{a=1}^{M} \psi_n(a) O | a \rangle
\]

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

\[
= \sum_{b=1}^{M} \psi_n^O(b) | b \rangle \quad \psi_n^O(b) = \sum_{a=1}^{M} \psi_n(a) \langle b | O | a \rangle
\]

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, \(i=1,\ldots,m\)

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

\[
|\phi_m\rangle \rightarrow \frac{|\phi_m\rangle - q|\phi_i\rangle}{1 - q^2}, \quad q = \langle \phi_i | \phi_m \rangle
\]

**Pseudocode**: modify state generation

```plaintext
do m = 1, \Lambda - 1
    call hoperation(\phi_m, \phi_{m+1})
    a_m = \langle \phi_m | \phi_{m+1} \rangle; \ \phi_{m+1} = \phi_{m+1} - a_m \phi_m - n_m \phi_{m-1}
    call normalize(\phi_{m+1}, n_{m+1})
    do i = 1, m
        q = \langle \phi_{m+1} | \phi_i \rangle; \ \phi_{m+1} = (\phi_{m+1} - q \phi_i) / (1 - q^2)
    enddo
endo
```

**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

\[ C(r) = \langle S_i \cdot S_{i+r} \rangle (-1)^r \]

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 KCuF₃

Heisenberg chain with frustrated interactions

\[ H = \sum_{i=1}^{N} \left[ J_1 S_i \cdot S_{i+1} + J_2 S_i \cdot S_{i+2} \right] \]

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).

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

\[ |\Psi_0\rangle \sim |\Psi_A\rangle + |\Psi_B\rangle, \quad |\Psi_1\rangle \sim |\Psi_A\rangle - |\Psi_B\rangle \]
The VBS state can be detected in finite systems using “dimer” correlations

\[ D(r) = \langle B_i B_{i+r} \rangle = \langle (S_i \cdot S_{i+1}) (S_{i+r} \cdot S_{i+1+r}) \rangle \]

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 \( g_c \)

Results from Lanczos diagonalization; different coupling ratios \( g = J_2/J_1 \)
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

The two lowest excited state should cross at $g_c$

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