Numerical diagonalization studies of quantum spin chains

Introduction to computational studies of 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

Lanczos diagonalization (ground state, low excitations)

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
Quantum spins
Spin magnitude $S$; basis states $|S^z_1, S^z_2, ..., S^z_N>$; $S^z_i = -S, ..., S-1, S$

Commutation relations:

$$[S^x_i, S^y_i] = i\hbar S^z_i \quad \text{(we set $\hbar = 1$)}$$

$$[S^x_i, S^y_j] = [S^x_i, S^z_j] = \ldots = [S^z_i, S^z_j] = 0 \quad (i \neq j)$$

Ladder (raising and lowering) operators:

$$S^+_i = S^x_i + iS^y_i, \quad S^-_i = S^x_i - iS^y_i$$

$$S^+_i |S^z_i\rangle = \sqrt{S(S + 1) - S^z_i(S^z_i + 1)} |S^z_i + 1\rangle,$$

$$S^-_i |S^z_i\rangle = \sqrt{S(S + 1) - S^z_i(S^z_i - 1)} |S^z_i - 1\rangle,$$

Spin (individual) squared operator: $S^2_i |S^z_i\rangle = S(S + 1) |S^z_i\rangle$

S=1/2 spins; very simple rules

$$|S^z_i = +\frac{1}{2}\rangle = |\uparrow_i\rangle, \quad |S^z_i = -\frac{1}{2}\rangle = |\downarrow_i\rangle$$

$$S^z_i |\uparrow_i\rangle = +\frac{1}{2} |\uparrow_i\rangle \quad S^z_i |\downarrow_i\rangle = -\frac{1}{2} |\downarrow_i\rangle$$

$$S^+_i |\uparrow_i\rangle = 0 \quad S^-_i |\uparrow_i\rangle = 0 \quad S^+_i |\downarrow_i\rangle = 0 \quad S^-_i |\downarrow_i\rangle = 0$$
Quantum spin models

Ising, XY, Heisenberg hamiltonians
• the spins always have three (x,y,z) components
• interactions may contain 1 (Ising), 2 (XY), or 3 (Heisenberg) components

\[ H = \sum_{\langle ij \rangle} J_{ij} S^z_i S^z_j = \frac{1}{4} \sum_{\langle ij \rangle} J_{ij} \sigma_i \sigma_j \]  (Ising)

\[ H = \sum_{\langle ij \rangle} J_{ij} [S^x_i S^x_j + S^y_i S^y_j] = \frac{1}{2} \sum_{\langle ij \rangle} J_{ij} [S^+_i S^-_j + S^-_i S^+_j] \]  (XY)

\[ H = \sum_{\langle ij \rangle} J_{ij} \vec{S}_i \cdot \vec{S}_j = \sum_{\langle ij \rangle} J_{ij} [S^z_i S^z_j + \frac{1}{2} (S^+_i S^-_j + S^-_i S^+_j)] \]  (Heisenberg)

Quantum statistical mechanics

\[ \langle Q \rangle = \frac{1}{Z} \text{Tr} \left\{ Q e^{-H/T} \right\} \]
\[ Z = \text{Tr} \left\{ e^{-H/T} \right\} = \sum_{n=0}^{M-1} e^{-E_n / T} \]

Large size M of the Hilbert space; \( M = 2^N \) for \( S = 1/2 \)
- difficult problem to find the eigenstates and energies
- we are also interested in the ground state (\( T \rightarrow 0 \))
  - for classical systems the ground state is often trivial
Why study quantum spin systems?

**Solid-state physics**
- localized electronic spins in Mott insulators (e.g., high-Tc cuprates)
- large variety of lattices, interactions, physical properties
- search for “exotic” quantum states in such systems (e.g., spin liquid)

**Ultracold atoms (in optical lattices)**
- some spin hamiltonians can be engineered (ongoing efforts)
- some bosonic systems very similar to spins (e.g., “hard-core” bosons)

**Quantum information theory / quantum computing**
- possible physical realizations of quantum computers using interacting spins
- many concepts developed using spins (e.g., entanglement)
- quantum annealing

**Generic quantum many-body physics**
- testing grounds for collective quantum behavior, quantum phase transitions
- identify “Ising models” of quantum many-body physics

**Particle physics / field theory / quantum gravity**
- some quantum-spin phenomena have parallels in high-energy physics
  - e.g., spinon confinement-deconfinement transition
- spin foams, string nets: models to describe “emergence” of space-time and elementary particles
Prototypical Mott insulator; high-Tc cuprates (antiferromagnets)

CuO$_2$ planes, localized spins on Cu sites
- Lowest-order spin model: S=1/2 Heisenberg
- Super-exchange coupling, J\(\approx\)1500K

Many other quasi-1D and quasi-2D cuprates
• chains, ladders, impurities and dilution, frustrated interactions, ...

Ladder systems
- even/odd effects

non-magnetic impurities/dilution
- dilution-driven phase transition

\[ H = J \sum_{\langle i,j \rangle} \vec{S}_i \cdot \vec{S}_j \]

- Cu (S = 1/2)
- Zn (S = 0)
The antiferromagnetic (Néel) state and quantum fluctuations

The ground state of the Heisenberg model (bipartite 2D or 3D lattice)

\[ H = J \sum_{\langle ij \rangle} \vec{S}_i \cdot \vec{S}_j = J \sum_{\langle ij \rangle} [S_i^z S_j^z + \frac{1}{2} (S_i^+ S_j^- + S_i^- S_j^+)] \]

Does the long-range “staggered” order survive quantum fluctuations?
• order parameter: staggered (sublattice) magnetization; \([H, m_s] \neq 0\)

\[
m_s = \frac{1}{N} \sum_{i=1}^{N} \phi_i \vec{S}_i, \quad \phi_i = (-1)^{x_i+y_i} \quad (2D \text{ square lattice})
\]

\[
m_s = \frac{1}{N} \left( \vec{S}_A - \vec{S}_B \right)
\]

If there is order \((m_s > 0)\), the direction of the vector is fixed \((N=\infty)\)
• conventionally this is taken as the z direction

\[
\langle m_s \rangle = \frac{1}{N} \sum_{i=1}^{N} \phi_i \langle S_i^z \rangle = |\langle S_i^z \rangle|
\]

• For \(S \to \infty\) (classical limit) \(<m_s> \to S\)
• what happens for small \(S\) (especially \(S=1/2\))?
**Numerical diagonalization of the Hamiltonian**

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

$$H = J \sum_{i=1}^{N} S_i \cdot S_{i+1} = J \sum_{i=1}^{N} [S_x S_{x+1}^x + S_y S_{y+1}^y + S_z S_{z+1}^z],$$

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

Simplest way computationally; enumerate the states
- construct the Hamiltonian matrix using **bit-representation** of integers

$$|0\rangle = |\downarrow, \downarrow, \downarrow, \ldots, \downarrow\rangle \quad (= 0 \ldots 000)$$

$$|1\rangle = |\uparrow, \downarrow, \downarrow, \ldots, \downarrow\rangle \quad (= 0 \ldots 001)$$

$$|2\rangle = |\downarrow, \uparrow, \downarrow, \ldots, \downarrow\rangle \quad (= 0 \ldots 010)$$

$$|3\rangle = |\uparrow, \uparrow, \downarrow, \ldots, \downarrow\rangle \quad (= 0 \ldots 011)$$

bit representation perfect for $S=1/2$ systems
- use $>1$ bit/spin for $S>1/2$, or integer vector
- construct $H$ by examining/fitting 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 \( \text{ieor}(a,2**i) \) can be used to flip bit \( i \) of \( a \)
- Bits \( i \) and \( j \) can be flipped using \( \text{ieor}(a,2**i+2**j) \)

\[
\begin{array}{c|c|c|c|c|c|c|c}
  & 0 & 1 & 0 & 1 & 0 & 0 & 1 \\
\hline
a & 0 & 1 & 0 & 1 & 0 & 0 & 1 \\
2^i + 2^j & 0 & 0 & 0 & 1 & 1 & 0 & 0 \\
\text{ieor}(a, 2^i + 2^j) & 0 & 1 & 0 & 0 & 1 & 0 & 1 \\
\end{array}
\]

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

<table>
<thead>
<tr>
<th>( r )</th>
<th>( T^r )</th>
<th>( T^r_P )</th>
</tr>
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<td>11011000</td>
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<tr>
<td>1</td>
<td>00111010</td>
<td>10111000</td>
</tr>
<tr>
<td>2</td>
<td>01110110</td>
<td>01100011</td>
</tr>
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</tr>
<tr>
<td>7</td>
<td>11000110</td>
<td>00110110</td>
</tr>
</tbody>
</table>
The S=1/2 Heisenberg chain hamiltonian can be constructed according to:

\[
\text{do } a = 0, 2^N - 1 \\
\text{do } i = 0, N - 1 \\
\quad j = \text{mod}(i + 1, N) \\
\quad \text{if } (a[i] = a[j]) \text{ then} \\
\quad \quad H(a, a) = H(a, a) + \frac{1}{4} \\
\quad \text{else} \\
\quad \quad H(a, a) = H(a, a) - \frac{1}{4} \\
\quad \quad b = \text{flip}(a, i, j); H(a, b) = \frac{1}{2} \\
\text{endif} \\
\text{endo} \\
\text{endo}
\]

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

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

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; \( N \approx 20 \)
- \( M^2 \) 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, \( N \approx 40 \) is max)