PY 502, Computational Physics, Fall 2024
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Numerical studies of quantum spin systems

Introduction to computational studies of spin systems

Using basis states incorporating conservation laws (symmetries)
- magnetization conservation, momentum states, parity, spin inversion
- discussion without group theory (1D)
  - only basic quantum mechanics and common sense needed

Lanczos diagonalization (ground state, low excitations)

Dynamics; quantum annealing

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 $|S^z_1, S^z_2, \ldots, S^z_N\rangle$, $S^z_i = -S, \ldots, S-1, S$

Commutation relations:

$$[S_i^x, S_i^y] = i\hbar S_i^z \quad (\text{we set } \hbar = 1)$$

$$[S_i^x, S_j^y] = [S_i^x, S_j^z] = \ldots = [S_i^z, S_j^z] = 0 \quad (i \neq j)$$

Ladder (raising and lowering) operators:

$$S_i^+ = S_i^x + iS_i^y, \qquad S_i^- = S_i^x - iS_i^y$$

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

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

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

S=1/2 spins; very simple rules

$$|S_i^z = +\tfrac{1}{2}\rangle = |\uparrow_i\rangle, \qquad |S_i^z = -\tfrac{1}{2}\rangle = |\downarrow_i\rangle$$

$$S_i^z|\uparrow_i\rangle = +\tfrac{1}{2}|\uparrow_i\rangle \qquad S_i^-|\uparrow_i\rangle = |\downarrow_i\rangle \qquad S_i^+|\uparrow_i\rangle = 0$$

$$S_i^z|\downarrow_i\rangle = -\tfrac{1}{2}|\downarrow_i\rangle \qquad S_i^+|\downarrow_i\rangle = |\uparrow_i\rangle \qquad S_i^-|\downarrow_i\rangle = 0$$

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

$$H = \sum_{\langle ij \rangle} J_{ij} S_i^z S_j^z = \frac{1}{4} \sum_{\langle ij \rangle} J_{ij} \sigma_i \sigma_j$$ **(Ising)**

$$H = \sum_{\langle ij \rangle} J_{ij} [S_i^x S_j^x + S_i^y S_j^y] = \frac{1}{2} \sum_{\langle ij \rangle} J_{ij} [S_i^+ S_j^- + S_i^- S_j^+]$$ **(XY)**

$$H = \sum_{\langle ij \rangle} J_{ij} \vec{S}_i \cdot \vec{S}_j = \sum_{\langle ij \rangle} J_{ij} [S_i^z S_j^z + \tfrac{1}{2}(S_i^+ S_j^- + S_i^- S_j^+)]$$ **(Heisenberg)**

Quantum statistical mechanics

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

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→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

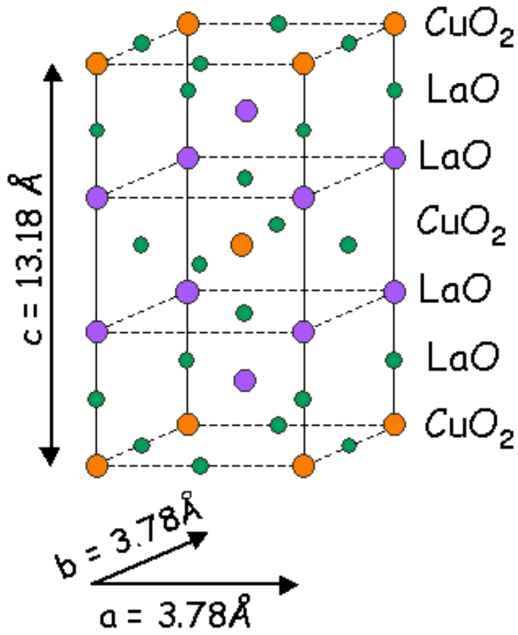
Generic quantum many-body physics

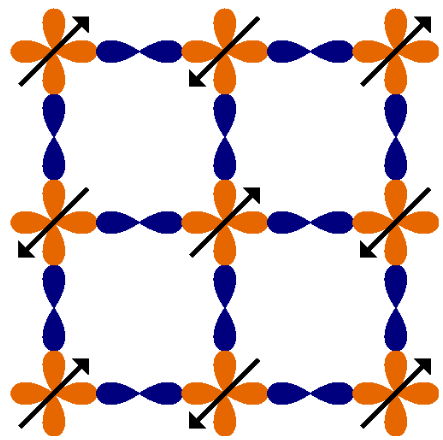
- testing grounds for collective quantum behavior, quantum phase transitions
- identify “Ising models” of quantum many-body physics

Particle physics / field theory / quantum gravity

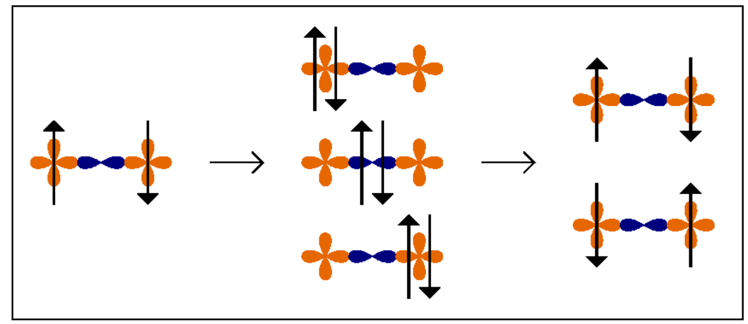
- some quantum-spin phenomena have parallels in high-energy physics
  - e.g., spinon confinement-deconfinement transition
- spin foams, string nets: models to describe “emergence” of space-time and elementary particles

Prototypical Mott insulator; high-Tc cuprates (antiferromagnets)





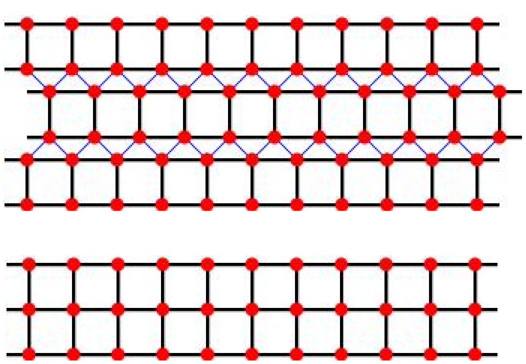
superexchange mechanism

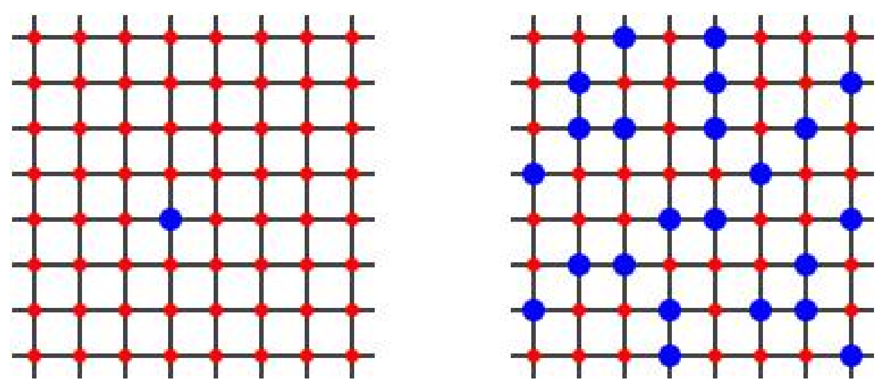


CuO_2 planes, localized spins on Cu sites
- Lowest-order spin model: S=1/2 Heisenberg
- Super-exchange coupling, J≈1500K

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

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





Cu (S = 1/2)
Zn (S = 0)

Ladder systems
- even/odd effects

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

The antiferromagnetic (Néel) state and quantum fluctuations

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

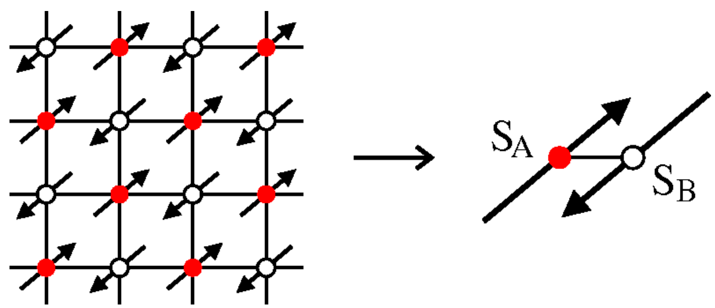
$$H = J \sum_{\langle ij \rangle} \vec{S}_i \cdot \vec{S}_j = J \sum_{\langle ij \rangle} [S_i^z S_j^z + \tfrac{1}{2}(S_i^+ S_j^- + S_i^- S_j^+)]$$

Does the long-range "staggered" order survive quantum fluctuations?

- order parameter: staggered (sublattice) magnetization; $[H, m_s] \neq 0$

$$\vec{m}_s = \frac{1}{N} \sum_{i=1}^{N} \phi_i \vec{S}_i, \qquad \phi_i = (-1)^{x_i + y_i} \quad \text{(2D square lattice)}$$

$$\vec{m}_s = \frac{1}{N} \left(\vec{S}_A - \vec{S}_B \right)$$



If there is order (m_s>0), the direction of the vector is fixed (N=∞)

- 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→∞ (classical limit) <m_s>→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

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

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

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

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

$$H_{ab} = \langle b|H|a\rangle$$
$$a,b \in \{0,1,\ldots,2^N-1\}$$

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** (i.e., not array element)

- In Julia the bit-level function **xor(a,2^i)** can be used to flip bit i of a
- bits i and j can be flipped using **xor(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 Julia bit-level functions

a << N, a <<< N
- shifts N bits to the "left"

a >> N
- shifts right

&, |
- **bit-wise and, or**

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:

$$
\begin{array}{l}
\textbf{do } a = 0, 2^N - 1 \\
\quad \textbf{do } i = 0, N-1 \\
\quad\quad j = \textbf{mod}(i+1, N) \\
\quad\quad \textbf{if } (a[i] = a[j]) \textbf{ then} \\
\quad\quad\quad H(a,a) = H(a,a) + \frac{1}{4} \\
\quad\quad \textbf{else} \\
\quad\quad\quad H(a,a) = H(a,a) - \frac{1}{4} \\
\quad\quad\quad b = \textbf{flip}(a,i,j);\ H(a,b) = \frac{1}{2} \\
\quad\quad \textbf{endif} \\
\quad \textbf{enddo} \\
\textbf{enddo}
\end{array}
$$

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

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

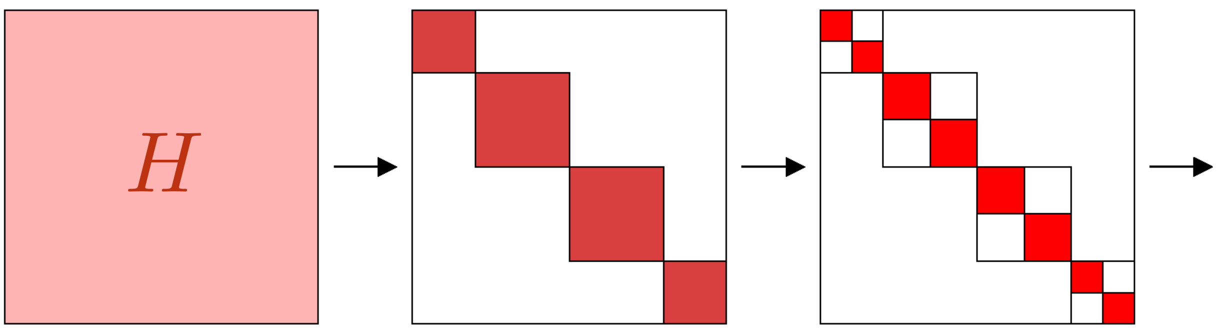
is the expectation value of some operator A in the n:th eigenstate

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≈50 is max)

Simplest example; magnetization conservation

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

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

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

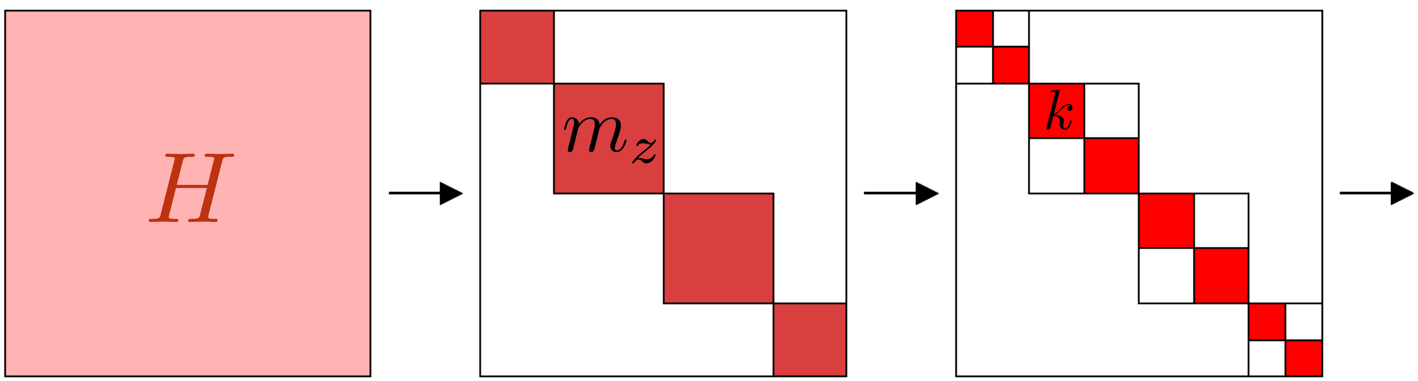
Example

N=4, m=0

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

we have to store these numbers in a vector

this is now the state label



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**

$$
\begin{aligned}
&\textbf{do}\ s = 0, 2^N - 1\\
&\qquad \textbf{if}\ (\textstyle\sum_i s[i] = n_\uparrow)\ \textbf{then}\ a = a+1;\ s_a = s\ \textbf{endif}\\
&\textbf{enddo}\\
&M = a
\end{aligned}
$$

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)

$$
\begin{aligned}
&\textbf{subroutine findstate}(s,b)\\
&b_{\min} = 1;\ b_{\max} = M\\
&\textbf{do}\\
&\qquad b = b_{\min} + (b_{\max} - b_{\min})/2\\
&\qquad \textbf{if}\ (s < s_b)\ \textbf{then}\\
&\qquad\qquad b_{\max} = b - 1\\
&\qquad \textbf{elseif}\ (s > s_b)\ \textbf{then}\\
&\qquad\qquad b_{\min} = b + 1\\
&\qquad \textbf{else}\\
&\qquad\qquad \textbf{exit}\\
&\qquad \textbf{endif}\\
&\textbf{enddo}
\end{aligned}
$$

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

$\mathbf{do}\ a = 1, M$	loop over states
$\quad \mathbf{do}\ i = 0, N-1$	loop over sites
$\quad\quad j = \mathbf{mod}(i+1, N)$	
$\quad\quad \mathbf{if}\ (s_a[i] = s_a[j])\ \mathbf{then}$	check bits of state-integers
$\quad\quad\quad H(a,a) = H(a,a) + \frac{1}{4}$	
$\quad\quad \mathbf{else}$	
$\quad\quad\quad H(a,a) = H(a,a) - \frac{1}{4}$	
$\quad\quad\quad s = \mathbf{flip}(s_a, i, j)$	state with bits i and j flipped
$\quad\quad\quad \mathbf{call\ findstate}(s, b)$	
$\quad\quad\quad H(a,b) = H(a,b) + \frac{1}{2}$	
$\quad\quad \mathbf{endif}$	
$\quad \mathbf{enddo}$	
$\mathbf{enddo}$	