PY 502, Computational Physics, Fall 2023
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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

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

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

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

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 spir
- many concepts developed using spins (e.g., entanglement)
- quantum annealing

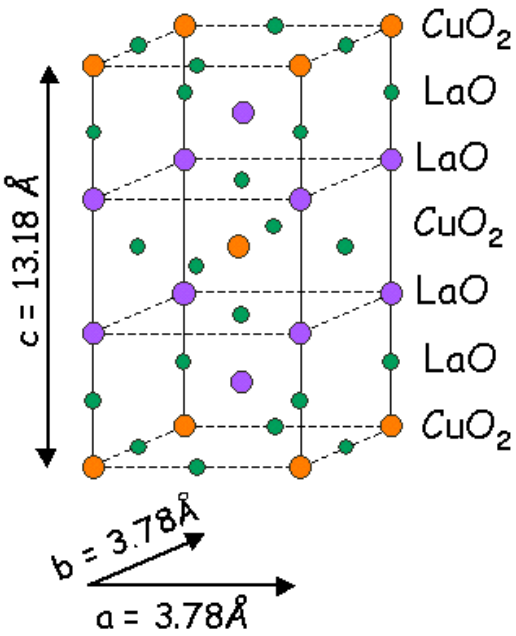
Generic quantum many-body physics

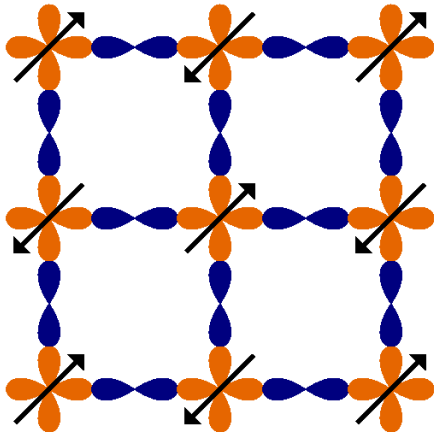
- testing grounds for collective quantum behavior, quantum phase transition
- identify “Ising models” of quantum many-body physics

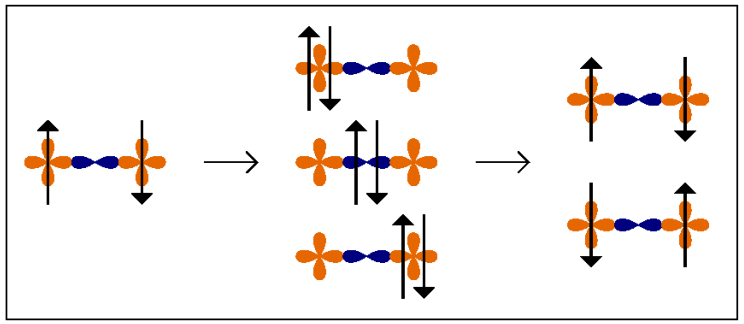
Particle physics / field theory / quantum gravity

- 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)



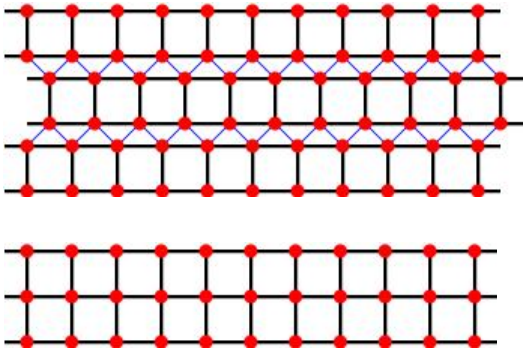




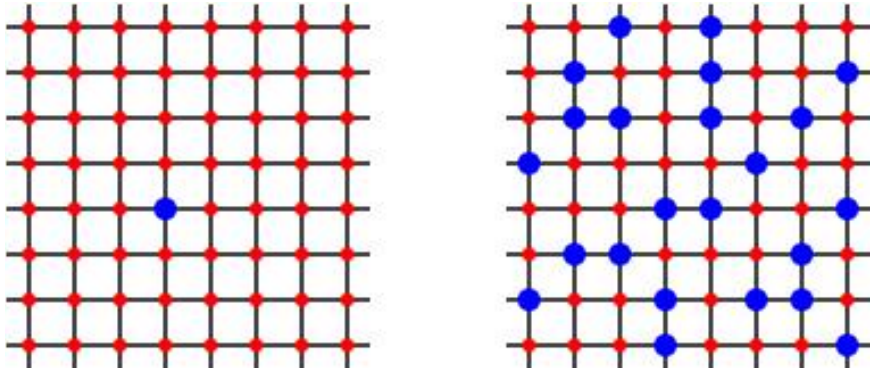
CuO_2 planes, localized spins on Cu sites
- Lowest-order spin model: S=1/2 Heisenberg
- Super-exchange coupling, J≈1500K

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

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



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)

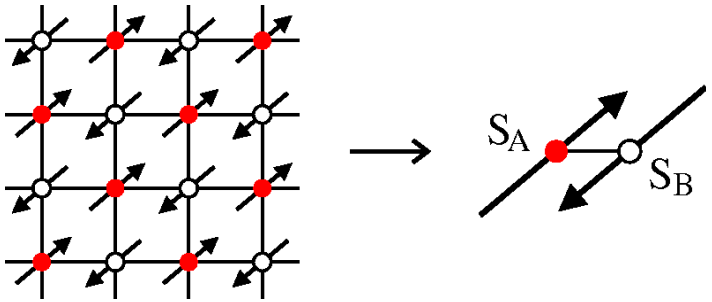
$$H = J\sum_{\langle ij\rangle}\vec{S}_i\cdot\vec{S}_j = J\sum_{\langle ij\rangle}[S_i^zS_j^z + \tfrac{1}{2}(S_i^+S_j^- + S_i^-S_j^+)]$$

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

• order parameter: staggered (sublattice) magnetization; [H,m_s] ≠ 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:

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

j is the “right” nearest-neighbor of i

- periodic boundary conditions

Diagonalizing the hamiltonian matrix

- on the computer
- gives the eigenvalues and eigenvectors

If U is the matrix whose columns are the eigenvectors of H, then

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

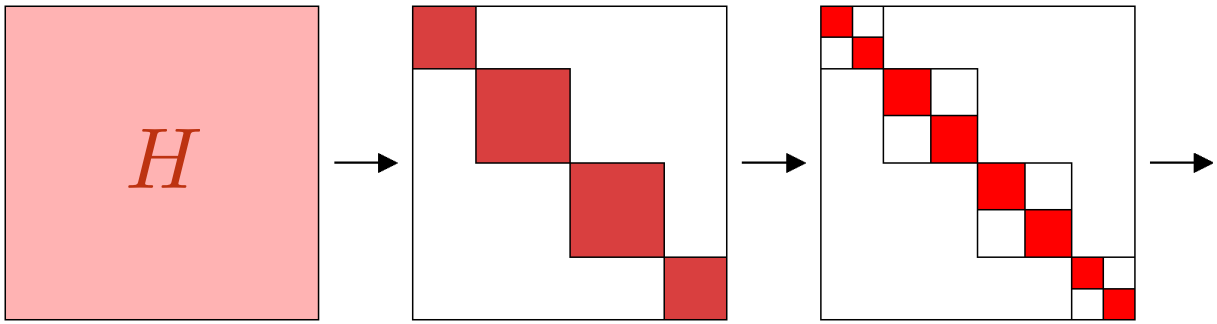
is the expectation value of some operator A in the n:th eigenstate

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

- maximum number of spins in practice; N≈20
- M^2 matrix elements to store, time to diagonalize $\propto M^3$

Using conservation laws (symmetries) for block-diagonalization

We can choose the basis in such a way that the H becomes block-diagonal



- the blocks can be diagonalized individually
- we can reach larger N (but not much larger, N≈50 is max)