PY 502, Computational Physics, Fall 2018

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

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

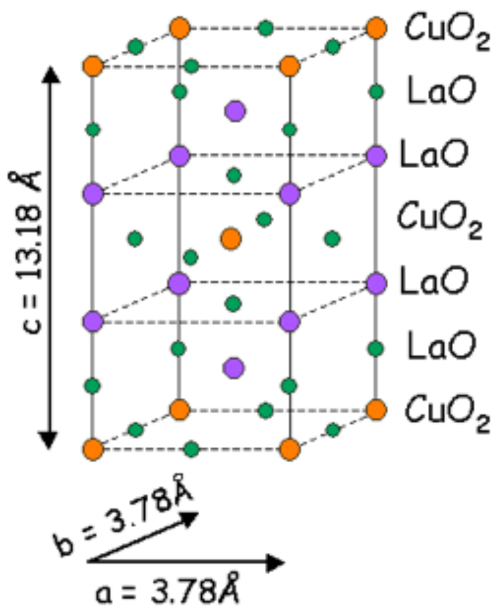
Generic quantum many-body physics

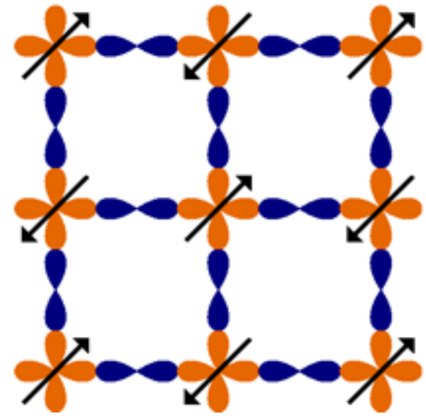
- testing grounds for collective quantum behavior, quantum phase transitions
- identify "Ising models" of quantum many-body physics

Particle physics / field theory / quantum gravity

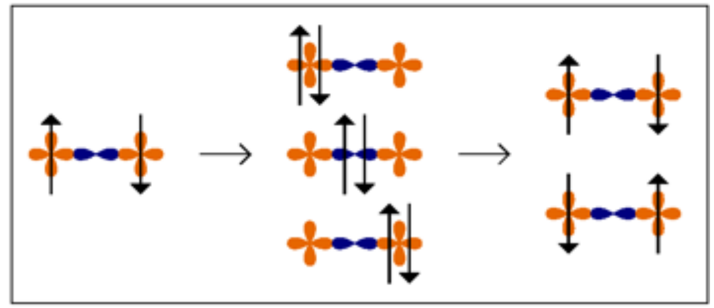
- some quantum-spin phenomena have parallels in high-energy physics
  - e.g., spinon confinement-deconfinement transition
- spin foams, string nets: models to describe "emergence" of space-time and elementary particles

Prototypical Mott insulator; high-Tc cuprates (antiferromagnets)





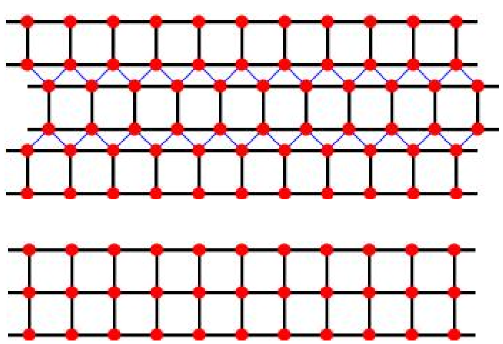
superexchange mechanism



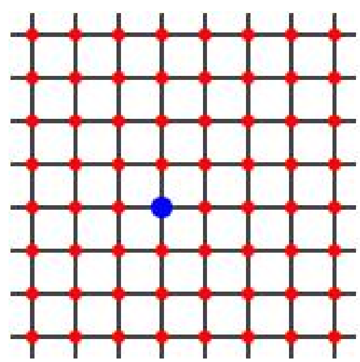
CuO_2 planes, localized spins on Cu sites
- Lowest-order spin model: S=1/2 Heisenberg
- Super-exchange coupling, J≈1500K

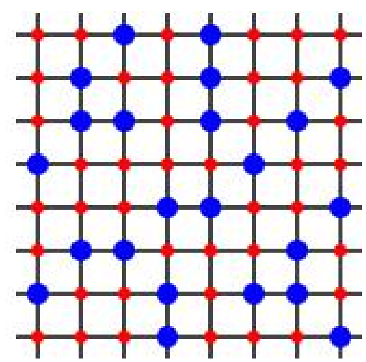
$$H = J \sum_{\langle i,j \rangle} \vec{S}_i \cdot \vec{S}_j$$

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



Ladder systems
- even/odd effects





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

● $\mathrm{Cu}\ (\mathrm{S} = 1/2)$
● $\mathrm{Zn}\ (\mathrm{S} = 0)$

The antiferromagnetic (Néel) state and quantum fluctuations

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

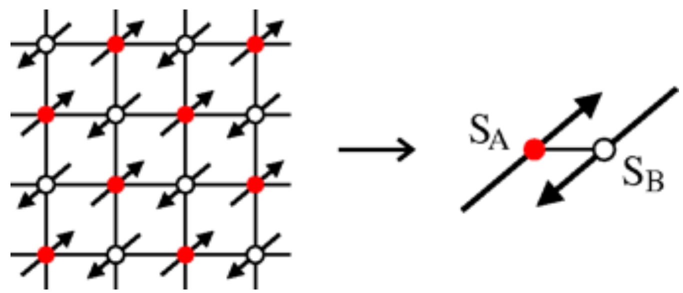
$$H = J\sum_{\langle ij\rangle} \vec{S}_i \cdot \vec{S}_j = J\sum_{\langle ij\rangle}[S^z_i S^z_j + \tfrac{1}{2}(S^+_i S^-_j + S^-_i S^+_j)]$$

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

$$\langle m_s \rangle = \frac{1}{N}\sum_{i=1}^{N} \phi_i \langle S^z_i \rangle = |\langle S^z_i \rangle|$$

- For S→∞ (classical limit) $\langle m_s \rangle \to S$
- 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

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

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

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**

- In Fortran 90 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

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

r	T^r		T^rP	
0	27	00011011	216	11011000
1	54	00110110	177	10110001
2	108	01101100	99	01100011
3	216	11011000	198	11000110
4	177	10110001	141	10001101
5	99	01100011	27	00011011
6	198	11000110	54	00110110
7	141	10001101	108	01101100