PERIMETER SCHOLARS INTERNATIONAL
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Quantum spin simulations

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Part 1: Introduction to quantum spin systems

- what they are, where they come from, why study them
- some simple analytical calculations (details in tutorials)
- related classical physics (phase transitions)

Part 2: Exact diagonalization studies (small systems)

- use of symmetries
- full diagonalization (all states), the Lanczos method (low-energy states)
- Physics of spin chains

Part 3: Quantum Monte Carlo methods and applications

- T>0: path integrals (background), stochastic series expansion (algorithms)
- studying ground states in the valence-bond basis
- quantum phase transitions in two-dimensional systems

Classical spin models

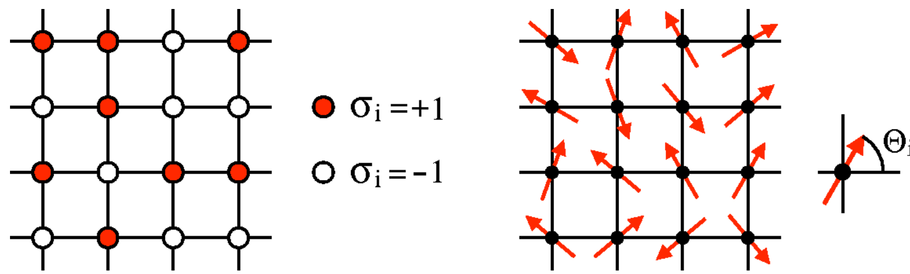
Lattice models with “spin” degrees of freedom at the vertices

Classified by type of spin:

- **Ising model:** discrete spins, normally two-state $\sigma_i = -1, +1$
- **XY model:** planar vector spins (normally of length S=1)
- **Heisenberg model**: 3-dimensional vector spins (S=1)

Statistical mechanics

- spin configurations C
- energy E(C)
- some quantity Q(C)
- temperature T (k_B=1)



$$\langle Q \rangle = \frac{1}{Z} \sum_C Q(C) e^{-E(C)/T}$$

$$Z = \sum_C e^{-E(C)/T}$$

$$E = \sum_{\langle ij \rangle} J_{ij} \sigma_i \sigma_j \qquad \textbf{(Ising)}$$

$$E = \sum_{\langle ij \rangle} J_{ij} \vec{S}_i \cdot \vec{S}_j = \sum_{\langle ij \rangle} J_{ij} \cos(\Theta_i - \Theta_j) \qquad \textbf{(XY)}$$

$$E = \sum_{\langle ij \rangle} J_{ij} \vec{S}_i \cdot \vec{S}_j \qquad \textbf{(Heisenberg)}$$

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

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

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

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

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)

- spin hamiltonians can (?) be engineered
- 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)

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 (?)

➤ Learning about quantum spin physics and computations will be very useful for research in many subfields of theoretical physics

Lecture contents and goals

Quantum spin systems discussed from a computational perspective

- Thorough introduction before details of computational methods
  - including some analytical calculations and related classical physics

Models

- S=1/2 Heisenberg model and its extensions, 1D, 2D lattices

Methods

- finite-lattice methods; exact diagonalization, quantum Monte Carlo
- primarily focusing on “unbiased” (numerically exact) methods
- some discussion of variational methods
- algorithms and implementations in detail

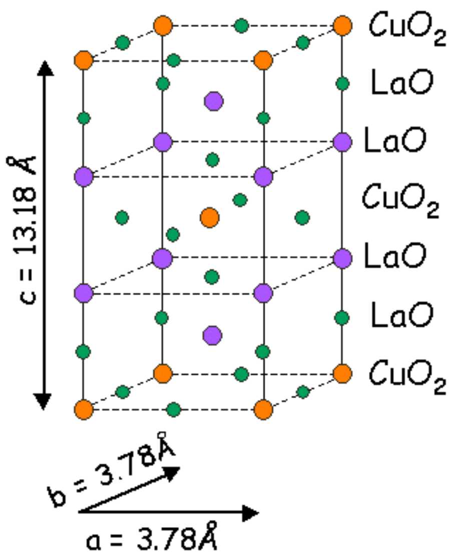
Physics

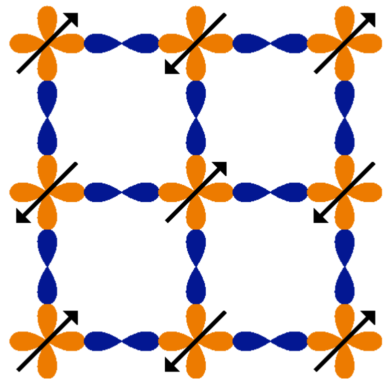
- illustrative results for key models and phenomena
- various types of ordered and disordered ground states
- quantum phase transitions

Goals

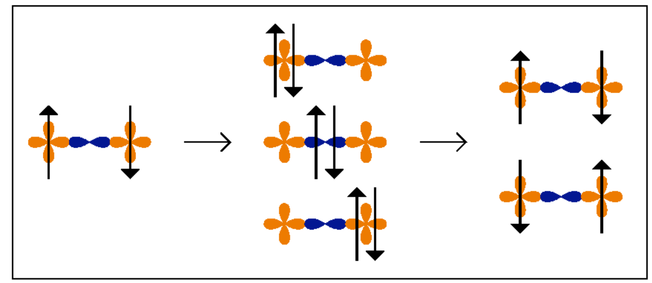
- introduce essential spin models and physical phenomena
- to cover enough computational details to write your own code
- overview of the field; from the basics to current research

Prototypical Mott insulator; high-Tc cuprates (antiferromagnets)





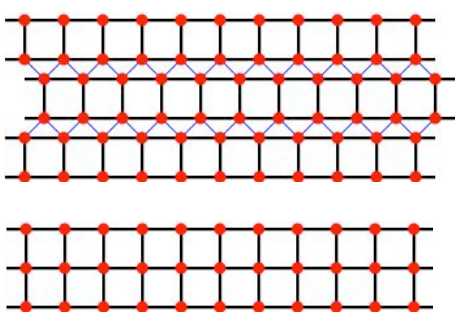
superexchange mechanism

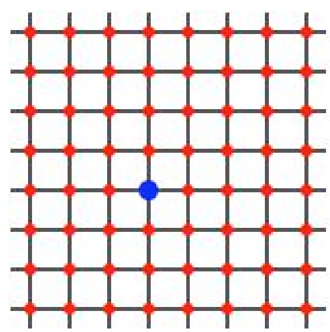


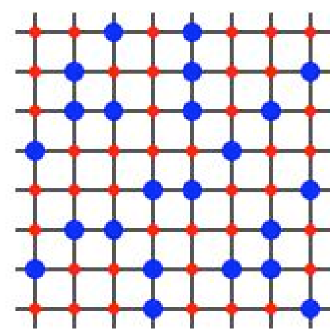
CuO_2 planes, localized spins on Cu sites
- Lowest-order spin model: S=1/2 Heisenberg
- Super-exchange coupling, J≈1500K

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

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







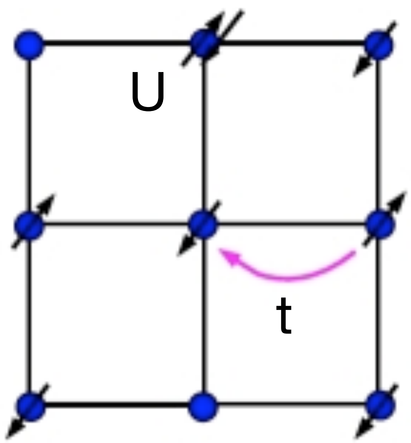
- Cu (S = 1/2)
- Zn (S = 0)

Ladder systems
- even/odd effects

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

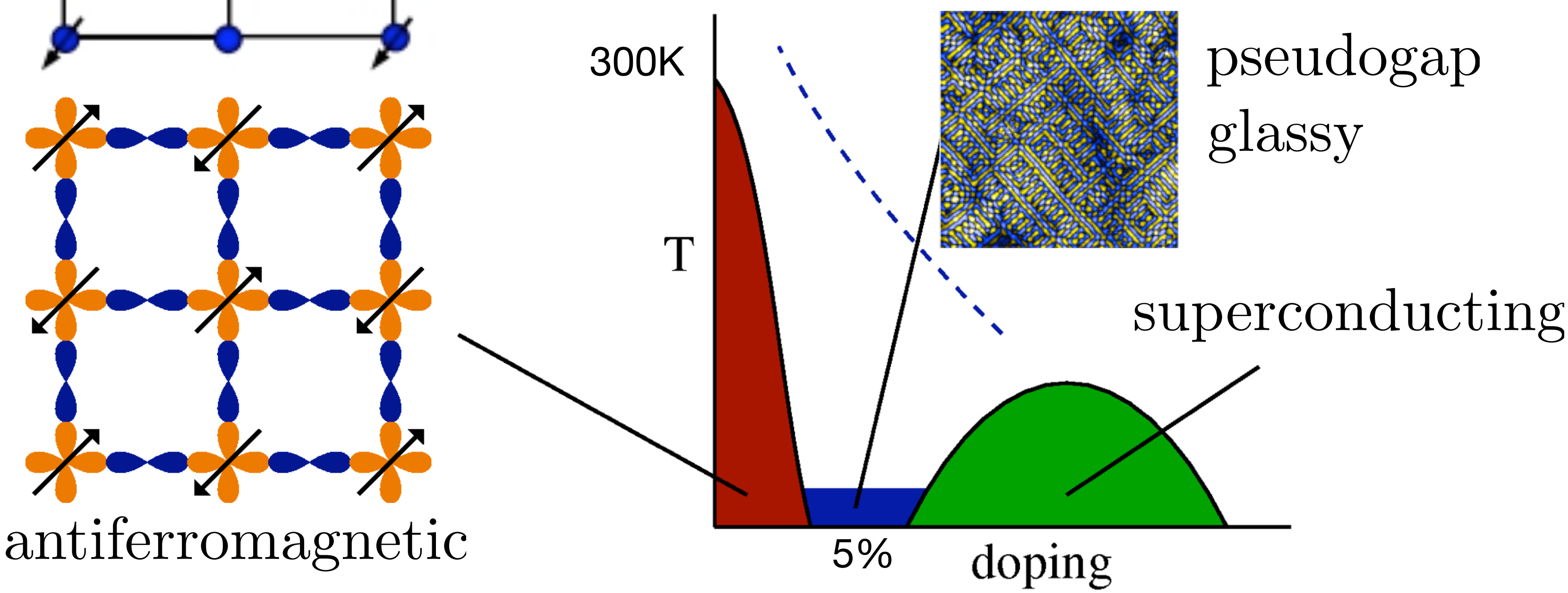
Doping the cuprates (e.g., La→Sr) ⇒ holes in the copper-oxygen planes

- **Hubbard model**; "hopping" t, doubly-occupied site costs energy U
- **t-J model**; U large, exclude doubly-occupied sites ⇒ spin interaction
- Do we have to keep the O sites? ⇒ **3-band Hubbard model**
- **Very difficult quantum many-body problems; no consensus yet**



Hubbard $$H = -t \sum_{\langle i,j \rangle} \sum_{\sigma=\uparrow,\downarrow} c^{+}_{i,\sigma} c_{j,\sigma} + U \sum_{i} n_{i,\uparrow} n_{i,\downarrow}$$

$t - J$ $$H = -t \sum_{\langle i,j \rangle} \sum_{\sigma=\uparrow,\downarrow} c^{+}_{i,\sigma} c_{j,\sigma} + J \sum_{\langle i,j \rangle} \vec{S}_i \cdot \vec{S}_j$$



Origin of antiferromagnetic interactions

Insights from a simple system: the 2-site Hubbard model

$$H_{12} = -t(c_{2\uparrow}^{\dagger}c_{1\uparrow} + c_{1\uparrow}^{\dagger}c_{2\uparrow} + c_{2\downarrow}^{\dagger}c_{1\downarrow} + c_{1\downarrow}^{\dagger}c_{2\downarrow}) + U(n_{1\uparrow}n_{1\downarrow} + n_{2\uparrow}n_{2\downarrow})$$

2-particle subspace (half-filled band)

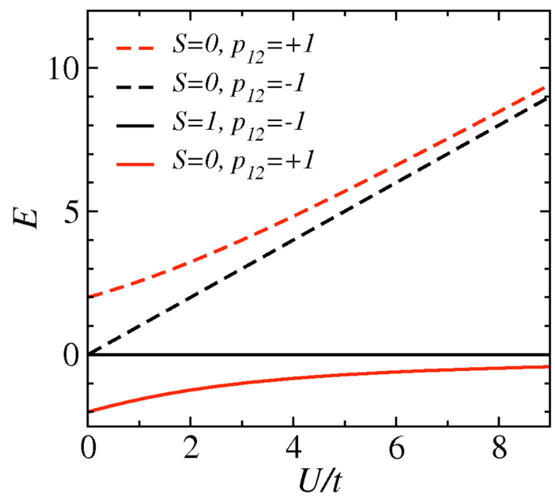
- 6 states in the Hilbert space: $|\uparrow\downarrow\rangle, \quad |\downarrow\uparrow\rangle, \quad |\uparrow\uparrow\rangle, \quad |\downarrow\downarrow\rangle, \quad |02\rangle, \quad |20\rangle$
- details of the solution in tutorial

U large, 2 lowest states

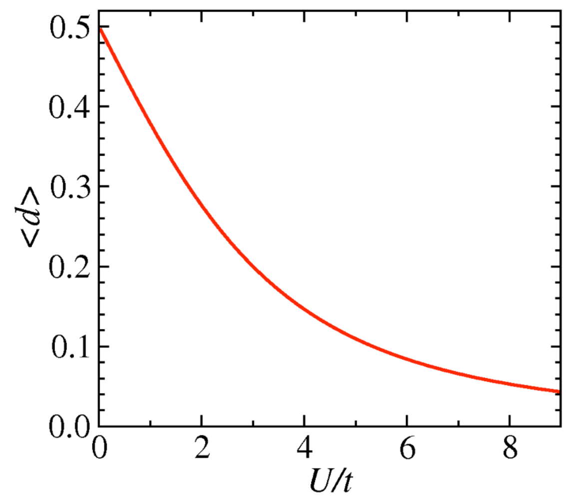
- total-spin singlet (S=0)
- small gap to S=1 states
- one-to-one with states of 2-site Heisenberg

$$\Delta = J \rightarrow \frac{4t^2}{U}$$

energies



double-occupation
in the ground state



$$|\psi_0\rangle = \frac{1}{\sqrt{2+8t^2/U^2}}\left[|\uparrow\downarrow\rangle - |\downarrow\uparrow\rangle + \frac{2t}{U}(|20\rangle + |02\rangle)\right] \longrightarrow \frac{1}{\sqrt{2}}(|\uparrow\downarrow\rangle - |\downarrow\uparrow\rangle)$$

$$|\psi_{1-}\rangle = |\downarrow\downarrow\rangle, \quad |\psi_{1+}\rangle = |\uparrow\uparrow\rangle, \quad |\psi_{10}\rangle \frac{1}{\sqrt{2}}(|\uparrow\downarrow\rangle + |\downarrow\uparrow\rangle)$$