

Introduction to Quantum Spins

- Properties of $s = \frac{1}{2}$ quantum spins
- Spin-spin interactions - ferro and antiferro
- Ferro and Neel-ordered states
- Valance bonds
- Where does J come from?
- Beyond $s = \frac{1}{2}$ and the one-band Hubbard model

Classical and Quantum Spins

Classical Two-State Systems:

- Ising spins - \uparrow, \downarrow or $+1, -1$
- Bits - $0, 1$
- Lattice Gas - 0 (empty), 1 (occupied)

Quantum States: $|\psi\rangle = a|\uparrow\rangle + b|\downarrow\rangle$

where a and b are complex

$$|\psi\rangle = a|\uparrow\rangle + b|\downarrow\rangle$$

where:

$$a = e^{i\varphi/2} \cos \theta/2$$

$$b = e^{-i\varphi/2} \sin \theta/2$$

Pauli matrices

$$\sigma_x = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}, \quad \sigma_y = \begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix}, \quad \sigma_z = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}$$

Define

$$\vec{S} = \frac{\hbar}{2} (\sigma_x, \sigma_y, \sigma_z) \quad (\text{Hereafter, } \hbar = 1)$$

Then

$$[S_x, S_y] = iS_z \text{ and cyclic permutations}$$

- \vec{S} is an angular momentum operator
- \vec{S} is the generator of rotations for the spin state $|\psi\rangle$.

Given that $|\psi\rangle = a|\uparrow\rangle + b|\downarrow\rangle$, then

$$\begin{aligned}\langle \vec{S} \rangle_\psi &= \langle \psi | \vec{S} | \psi \rangle \\ &= \frac{1}{2} (\sin \theta \cos \varphi, \sin \theta \sin \varphi, \cos \theta)\end{aligned}$$

Relates SU(2) to O(3).

Raising and lowering operators:

$$S^+ = S_x + iS_y = \frac{1}{2}(\sigma_x + i\sigma_y) = \frac{1}{2} \left[\begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix} + i \begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix} \right]$$

$$= \begin{pmatrix} 0 & 1 \\ 0 & 0 \end{pmatrix} = \sigma^+$$

Similarly

$$S^- = S_x - iS_y = \sigma^-$$

Spin-Spin Interactions

Ising Interaction

$$H = \pm J \sum_{(i,j)} s_i s_j, \quad s_i = \pm 1$$

 Sum over nearest
neighbour pairs

$-J$ favours $s_i s_j > 0$ parallel spins

$+J$ favours $s_i s_j < 0$ antiparallel spins

Interactions Between Quantum Spins

$$H = -J \sum_{(i,j)} \vec{S}_i \cdot \vec{S}_j \text{ the Heisenberg Interaction}$$

What are the eigenstates of H ?

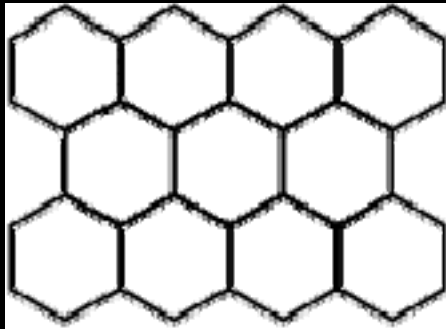
$$\begin{aligned} \vec{S}_i \cdot \vec{S}_j &= S_i^x S_j^x + S_i^y S_j^y + S_i^z S_j^z \\ &= 1/2 (S_i^+ S_j^- + S_i^- S_j^+) + S_i^z S_j^z \end{aligned}$$

$$\vec{S}_i \cdot \vec{S}_j |\uparrow\uparrow\uparrow\uparrow \dots\rangle = 1/4 |\uparrow\uparrow\uparrow\uparrow \dots\rangle \text{ an eigenstate!}$$

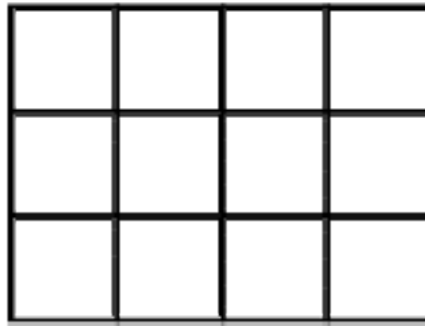
$$\text{So } H|\uparrow\uparrow\uparrow \dots\rangle = -\frac{J}{4} \left(\frac{Nz}{2} \right) |\uparrow\uparrow\uparrow \dots\rangle$$

Number of nearest neighbour pairs

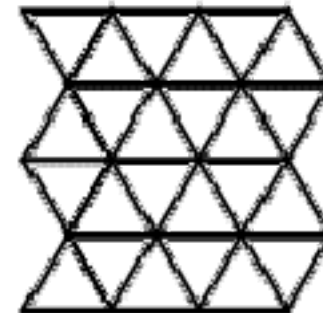
z = number of nearest neighbours



Honeycomb
 $z=3$



Square
 $z=4$



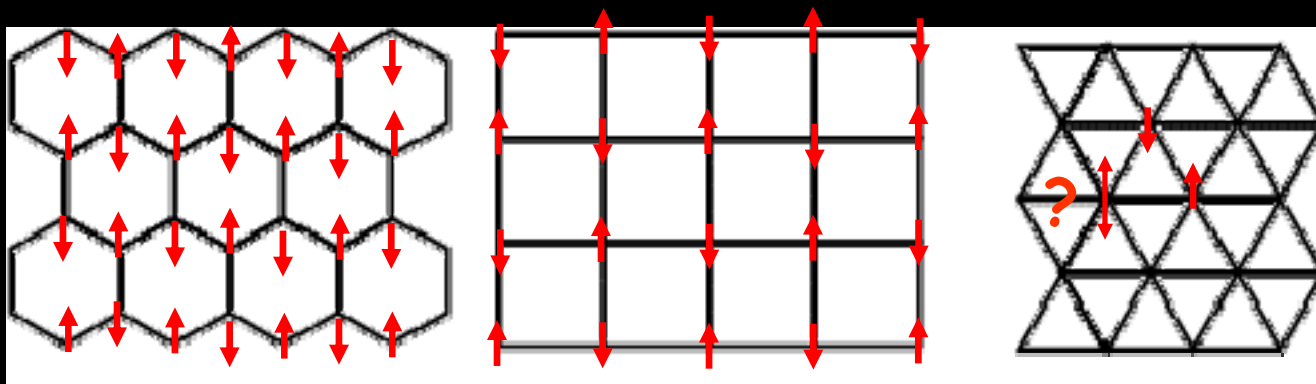
Triangular
 $z=6$

Simple Cubic: $z=6$, BCC: $z=8$, FCC: $z=12$
 $z=2$ for (1-D) chain

Antiferromagnetic Interactions

$$H = J \sum_{(i,j)} \vec{S}_i \cdot \vec{S}_j, \quad \text{with } J > 0$$

$$\text{Neel state } |\psi_N\rangle = |\uparrow\downarrow\uparrow\downarrow\dots\rangle$$



Works best on bipartite lattices.

$$E_{Neel} = -\frac{J}{4} \frac{N_z}{2} \text{ for a bi-partite lattice but}$$

Neel state $|\psi_N\rangle = |\uparrow\downarrow\uparrow\downarrow\dots\rangle$ NOT an eigenstate.

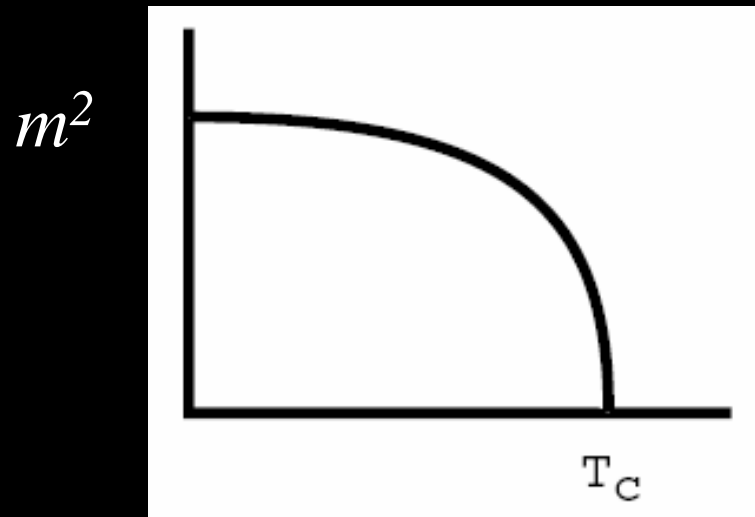
$$\text{because } (\vec{S}_i \cdot \vec{S}_j) |\uparrow\downarrow\rangle = -\frac{1}{4} |\uparrow\downarrow\rangle + \frac{1}{2} |\downarrow\uparrow\rangle$$

$$\therefore E_0 < E_{Neel}$$

Order Parameters

For ferromagnet at $T = 0$,

$$m^2 = \frac{1}{s^2} \lim_{|i-j| \rightarrow \infty} \langle F | \vec{S}_i \cdot \vec{S}_j | F \rangle = 1$$



Antiferromagnetic Order Parameter

For Neel state at $T = 0$,

$$m_S^2 = \frac{1}{S^2} \lim_{|i-j| \rightarrow \infty} \langle \psi_N | e^{-\vec{Q} \cdot (\vec{R}_i - \vec{R}_j)} \vec{S}_i \cdot \vec{S}_j | \psi_N \rangle = 1$$

For the exact ground state,

$$m_S < 1$$

If Neel order exists, $1 > m_S > 0$.

Otherwise, $m_S = 0$.

Singlets and Triplets

Two spins: $|\uparrow\downarrow\rangle, |\downarrow\uparrow\rangle, |\uparrow\uparrow\rangle, |\downarrow\downarrow\rangle$

$$\vec{S}_1 \cdot \vec{S}_2 |\uparrow\uparrow\rangle = \frac{1}{4} |\uparrow\uparrow\rangle, \quad \vec{S}_1 \cdot \vec{S}_2 |\downarrow\downarrow\rangle = \frac{1}{4} |\downarrow\downarrow\rangle \text{ eigenstates!}$$

$$\vec{S}_1 \cdot \vec{S}_2 |\uparrow\downarrow\rangle = -\frac{1}{4} |\uparrow\downarrow\rangle + \frac{1}{2} |\downarrow\uparrow\rangle$$

$$\vec{S}_1 \cdot \vec{S}_2 |\downarrow\uparrow\rangle = -\frac{1}{4} |\downarrow\uparrow\rangle + \frac{1}{2} |\uparrow\downarrow\rangle$$

$$\therefore \vec{S}_1 \cdot \vec{S}_2 (|\uparrow\downarrow\rangle \pm |\downarrow\uparrow\rangle) = \left(-\frac{1}{4} \pm \frac{1}{2}\right) (|\uparrow\downarrow\rangle \pm |\downarrow\uparrow\rangle)$$

Singlet and Triplet States

$$S = 0, \vec{S}_1 \cdot \vec{S}_2 = -\frac{3}{4} \quad \frac{1}{\sqrt{2}} (|\uparrow\downarrow\rangle - |\downarrow\uparrow\rangle) \quad \text{Singlet}$$

$$S = 1, \vec{S}_1 \cdot \vec{S}_2 = \frac{1}{4} \quad \left\{ \begin{array}{l} |\uparrow\uparrow\rangle \\ \frac{1}{\sqrt{2}} (|\uparrow\downarrow\rangle + |\downarrow\uparrow\rangle) \\ |\downarrow\downarrow\rangle \end{array} \right. \quad \text{Triplet}$$

For $H = J\vec{S}_1 \cdot \vec{S}_2$, $E_{\text{Singlet}} = -\frac{3}{4}J$, $E_{\text{Triplet}} = \frac{1}{4}J$

↖ A much lower energy!

Valence Bond (Singlet) States

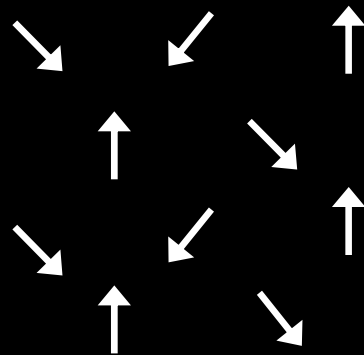


Many ways
to do this

$$E_{\text{VB}} = -\frac{3}{4}J \frac{N}{2}, \quad E_{\text{Neel}} = -\frac{1}{4}J \frac{zN}{2}$$

E_{Neel} wins for $z > 3$.

Triangular Lattice



120° Neel structure
has $E_{\text{Neel}} = -J/8$ per
pair.

For triangular lattice ($z=6$)

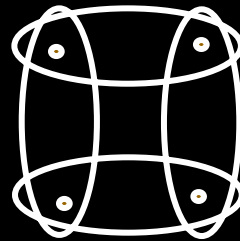
$$E_{\text{Neel}} = E_{\text{VB}} = -3JN/8$$

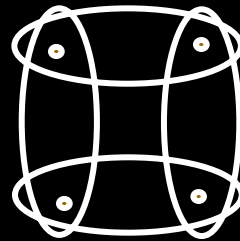
Anderson (1973) and Fazekas & Anderson (1974)

Which one wins?

Quantum Fluctuations

- For Neel ordered states, mix $|\uparrow\downarrow\rangle$ with $|\downarrow\uparrow\rangle$, reduces m_S .



- For VB states, mix  - RVB states
- So which wins depends on how quantum fluctuations stabilize both states

Where does J come from?

NOT from dipole-dipole interactions between spins













$$E_{\text{dipole}} \sim \frac{\mu_B^2}{a^3} < 1K$$

J , the "exchange interaction" arises from the Pauli Principle, kinetic energy and the Coulomb interaction. Typically, $J \gg 1K$.

The Two-Site Hubbard Model

$$H = -t \sum_{\sigma=\uparrow,\downarrow} (c_{2,\sigma}^\dagger c_{1,\sigma} + c_{1,\sigma}^\dagger c_{2,\sigma}) + U (n_{1,\uparrow} n_{1,\downarrow} + n_{2,\uparrow} n_{2,\downarrow})$$

Six states for two electrons:

$ 1\rangle =$			$ 2\rangle =$			Triplets
$ \tilde{3}\rangle =$			$ \tilde{4}\rangle =$			
$ 5\rangle =$			$ 6\rangle =$			Singlets

$$|1\rangle = c_{1\uparrow}^\dagger c_{2\uparrow}^\dagger |0\rangle, \quad |2\rangle = c_{1\downarrow}^\dagger c_{2\downarrow}^\dagger |0\rangle$$

$$|3\rangle = \frac{1}{\sqrt{2}} (c_{1\uparrow}^\dagger c_{2\downarrow}^\dagger + c_{1\downarrow}^\dagger c_{2\uparrow}^\dagger) |0\rangle \quad \text{Triplets}$$

$$|4\rangle = \frac{1}{\sqrt{2}} (c_{1\uparrow}^\dagger c_{2\downarrow}^\dagger - c_{1\downarrow}^\dagger c_{2\uparrow}^\dagger) |0\rangle \quad \text{Singlets}$$

$$|5\rangle = c_{1\uparrow}^\dagger c_{1\downarrow}^\dagger |0\rangle, \quad |6\rangle = c_{2\uparrow}^\dagger c_{2\downarrow}^\dagger |0\rangle$$

Easy to see that $H|1\rangle = H|2\rangle = 0$.

Similarly $H|3\rangle = 0$ (because of antisymmetry).

In the space of singlet states:

$$H = \begin{pmatrix} 0 & -t\sqrt{2} & -t\sqrt{2} \\ -t\sqrt{2} & U & 0 \\ -t\sqrt{2} & 0 & U \end{pmatrix}$$

which has energy eigenvalues:

$$E_1 = \frac{1}{2} \left(U - \sqrt{U^2 + 16t^2} \right) \approx -4t^2/U \quad \text{Lowest singlet state}$$

$$E_2 = U, \quad E_3 = \frac{1}{2} \left(U + \sqrt{U^2 + 16t^2} \right) \approx U + 4t^2/U$$

Question: What are states for $U = 0$?

Ignoring states with energy $\sim U$

$$E_{\text{Singlet}} = -4t^2/U,$$

$$E_{\text{Triplet}} = 0 \quad \text{so}$$

$$H = J(\vec{S}_1 \cdot \vec{S}_2 - 1/4) \text{ where } J = 4t^2/U$$

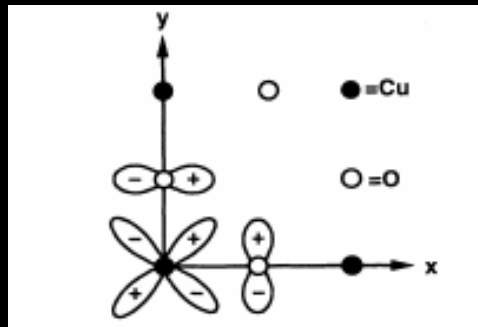
J can range from a fraction of a K
to fractions of an eV.

Beyond Spin 1/2

d-orbitals in transition metals

- Cu^{++} , $s = \frac{1}{2}$ (d^9)
- Ni^{++} , $s = 1$ (d^8) Hund's coupling - Coulomb interaction favours antisymmetric spatial state - enforces $s=1$
- Transition metal oxides involve O^{--} .

Superexchange



J is 4th order in Cu-O hopping

Sign of J depends on Cu-O-Cu bond angle -
becomes ferromagnetic for bond angles
less than about 95° .

Anisotropy

- Anisotropy results from spin-orbit coupling
- D-orbitals are oriented by crystal field, due to electrostatic potential and covalency
- Spins feel $H_{so} = \lambda \vec{L} \cdot \vec{S}$
- Single-ion anisotropy possible for $s > \frac{1}{2}$

$$H_A = \Delta \sum_i (S_i^z)^2$$

(Does nothing for $s = \frac{1}{2}$.)

Anisotropic Spin-Spin Interactions

$$H(i, j) = J(i, j) \vec{S}_i \cdot \vec{S}_j + \vec{D}(i, j) \cdot \vec{S}_i \times \vec{S}_j + \vec{S}_i \cdot \vec{M} \cdot \vec{S}_j$$

where $\vec{D}(i, j)$ is the Dzyaloshinskii - Moriya coupling constant and \vec{M} is a symmetric traceless tensor describing anisotropic exchange. Allowed even for $s = 1/2$.

J , \vec{D} , and \vec{M} are 0^{th} , 1^{st} , and 2^{nd} order in the spin - orbit coupling constant.

Comments

- Spin $\frac{1}{2}$ great for modeling quantum fluctuations, spin liquids, etc.
- Transition metal oxides much richer but much more complicated
- Superexchange paths provide mechanisms for competing interactions
- Progress requires streamlining theory

Reference for anisotropic superexchange: T. Yildirim, A.B. Harris, A. Aharony, and O. Entin-Wohlman, Phys. Rev. B52, 10239 (1995).

The End

