Plan for today

1. More on ions in a crystalline environment
2. Comments on quantum magnetism
3. Quantum spin liquids

Examples of ionic electronic structure in a crystal

1. MnO - A Mott insulator

\[ \text{Mn}^{2+}\text{O}^{2-} : \text{Mn has atomic # 25 and electronic structure [Ar]3d}^54s^2 \]

Mn\(^{2+}\) has configuration [Ar]3d\(^5\)

\[ \uparrow \uparrow \downarrow \downarrow \text{ e}_g \]

It turns out that strong Hund's energy overwhelms crystal
Field energy and Mn$^{2+}$ has $S = \frac{5}{2}$

2) La$_2$CuO$_4$ (parent of high $T_c$ SC)
   A F Mott insulator

La$^{3+}$Cu$^{2+}$O$_4^-$: Cu has atomic # 29
   2 electronic configuration
   $1s^2 2s^2 2p^6 3s^2 3p^6 3d^{10} 4s^1 = [Ar]3d^{10}$

Cu$^{2+}$ has the configuration

$[Ar]3d^9$

In La$_2$CuO$_4$, the Cu$^{2+}$ is in a (distorted) octahedral environment $\rightarrow$ d-orbital split

into $t_{2g} < e_g$.

$\begin{align*}
&\begin{array}{c}
t_{2g} \\
e_g
\end{array} \\
&\begin{array}{c}
t_{2g} \\
e_g
\end{array}
\end{align*}$
Magnetism comes from the single $e$ in the $d_{x^2-y^2}$ orbital.

$\Sigma \La_2CuO_4$ is a spin-$\frac{1}{2}$ system.

Quantum magnetism

Energy scale $U \propto$ charge gap - local moments form

$J \propto U^2$: Moments interact with each
Typically in a Mott insulator,

$$H = \sum \xi_i \cdot \xi_j + \cdots$$

with $J > 0$, i.e., antiferromagnetic.

Standard lattice (e.g., square lattice
with nearest-neighbor exchange
in $d=2$ or $d=3$);

Ground state has Neel 2RO.

Caricature:

Break spin $SO(3)$ symmetry down
to a $U(1)$ subgroup.

Low energy excitations: spin waves (a.k.a. magnons)

- Goldstone bosons of the broken symmetry.

Seen in many materials.

More interesting possibilities if

1. lattice is frustrated
2. spatial dimension is low
3. $t/J$ is not too small

$\Rightarrow$ effective spin Hamiltonian has higher order terms in the $t/J$ expansion which are not small.
Eg: Frustration

Ising spins on a $\Delta$ with AF interactions

Quantum fluctuations of the spins can play a role in determining the ground state.

Extreme example: Atom fluctuations prevent any magnetic ordering even at $T=0$ K.

(Analogy: He-4 or He-3 at $T=0$ at ambient pressure; quantum zero point motion "melts" crystal order)
Terminology: Quantum paramagnets

Actually there are many different kinds of quantum paramagnets, so we need a more refined language to describe them.

Some simple quantum paramagnets

1. $d = 1$ quantum XY chain

$$H = J \sum_i (s_i^+ s_{i+1}^- + h.c.)$$

for spin-$\frac{1}{2}$ operators $s_i^+$ at each site $i$.

From exact solution, we know that this does not order, and is gapless.
2. d = 1 2-leg ladder

\[
H = J_{ll} \sum_i \left( \vec{S}_i \cdot \vec{S}_{i+1} + \frac{\vec{S}_{2i} \cdot \vec{S}_{2i+1}}{2} \right) + J_1 \sum_i \vec{S}_i \cdot \vec{S}_{i+1}
\]

(J_{ll}, J_1 \gg 0).

If \( J_1 \gg J_{ll} \), first diagonalize the \( J_1 \) term.

For each \( i \), form a rung singlet

\[
\frac{1}{\sqrt{2}} \left( |1_{2i} \rangle \langle 1_{2i}| - |1_{2i} \rangle \langle 1_{2i}| \right)
\]
Ground state of each ring is unique (energy $-3\frac{3}{4}$).

Excited state is a kink
with energy $\frac{3}{4}$.

Now perturb with $J_{41}$; for $J_{41} < 1$,

expect nothing dramatic happens.

& perturbation theory converges.

$\Rightarrow$ Get a unique paramagnetic
ground state with a gap to
all excitations.

3. Quantum paramagnetic with broken
translation symmetry (known as
"Spin Peierls" or "Valence Bond Solids"

\[ E_1 \]

\[ d = 1 \]

or

Realized by
\[ H = J_1 \sum \vec{S}_i \cdot \vec{S}_{i+1} + J_2 \sum \vec{S}_i \cdot \vec{S}_{i+2} \]

(with \( \vec{S}_i = \text{spin-1/2} \)) for

\[ \frac{T_2 \pi}{J_1} \approx 0.24 \]