

Lecture 10: Introduction to quantum antiferromagnets

In the last two lectures, we have developed a nice path integral representation of the d dimensional quantum Heisenberg antiferromagnet, with Hamiltonian

$$H = J \sum_{\langle ij \rangle} \vec{S}(\vec{r}_i) \cdot \vec{S}(\vec{r}_j) \quad (1)$$

where $\langle ij \rangle$ denote nearest neighbour bonds of the d dimensional lattice. \vec{r}_i are the lattice positions, and $\vec{S}(\vec{r}_i)$ are quantum mechanical spins representing the magnetic moments that reside on these lattice sites. Now, we ask: Where does a Hamiltonian like this actually arise in practice, *i.e.*, what real-life systems are actually described by such an effective Hamiltonian?

To answer this, we start with the observation that spins are nothing but electrons that have “lost the ability to move”. To see what I mean by this, let us begin by reviewing some simple background material from your Solid State Physics course. The first thing I would like you to recall is the fact that energy eigenstates of non-interacting electrons in crystals organize themselves into “energy bands” $\epsilon_\mu(\vec{k})$, where \vec{k} is a momentum label that lies in the first “Brillouin zone” (roughly speaking, the cell in \vec{k} space needed to completely specify a function with real-space periodicity corresponding to that of the underlying crystal structure), and μ is a band index. For example, for a simple cubic lattice with lattice spacing a in all three directions, the Brillouin zone is the cubic cell defined by $0 \leq k_x \leq 2\pi/a$, $0 \leq k_y \leq 2\pi/a$, $0 \leq k_z \leq 2\pi/a$.

In materials where electron-electron repulsion (Coulomb interaction) can be ignored, these bands control all the electronic properties of the crystal. To obtain predictions, one has to know the number of electrons contributed by each atom in a real-space unit cell of the crystal and then use the Pauli principle and the resulting Fermi-Dirac distribution to decide on the Fermi energy ϵ_F , and the average occupation of each single-electron energy eigenstate $\epsilon_\mu(\vec{k})$. Properties of this free-electron gas can then be computed in the standard way.

As you know, in this free-electron, or band-theory picture, a material in which all bands are either completely filled or completely empty at zero temperature becomes an insulator, and a material in which there are some partially occupied bands becomes a metal.

All of this ignores electron-electron interactions. If their effects are “mild”, then a more sophisticated version of this approach, called the “Landau Fermi Liquid Theory”, can be used. In the Fermi liquid picture, one imagines that each electron is “dressed” by its interactions with other electrons to form a “Landau quasiparticle” which has the same spin and same charge as an electron. In principle, each energy band of these Landau quasiparticles needs to be calculated by including the effects of the occupation of bands by the quasiparticles, *i.e.* self-consistently. However, in practice, this does not modify the fundamental identification of partially filled band systems with metals and fully filled and empty band systems with insulators. Thus, although details may differ, there is no qualitative change from the free-electron picture in this class of materials that obey Fermi-liquid theory.

However, band-theory and Fermi-liquid theory both break down dramatically in a class of materials called Mott Insulators. These are insulators which should, according to the predictions of band-theory and Fermi-liquid theory, have actually been excellent metals with half-filled bands. The reason for this breakdown is that electron-electron interactions actually dominate the physics of such materials and lead to a freezing of the electron motion.

Such localized electrons only have their spin degree of freedom as a dynamical variable, and form magnetic moments that live on individual ions of the lattice. The low energy physics is dominated by these magnetic moments and interactions between them induced by virtual hopping of electrons to nearby ions and back. It is these interactions that are encapsulated by the Heisenberg Hamiltonian that we started this lecture with.

To put some flesh on this bare-bones outline, we now consider a specific and very well-known example, which has been responsible for much of the interest in quantum antiferromagnetism. This is the example of La_2CuO_4 , the parent compound of one family of high temperature superconductors. For our purposes here, it is sufficient to focus on the Copper-Oxygen (Cu-O) planes, in which the Copper ions form a square lattice, with the Oxygen at the centers of the links of this lattice—those of you who remember your solid state physics class well and would like some more detail on the actual crystal structure should refer to Fig 1 for a somewhat more “realistic” portrait of this compound. Nine electrons (or one hole) live in the $3d$ orbitals on each of these Cu sites in the parent undoped compound, and there is a large Coulomb energy cost U_d for reducing the number of electrons to eight (*i.e.* adding an additional hole) at any Cu site. As a result, although the crystal-field split Cu orbitals should have resulted in one half-filled d -band, and therefore metallic

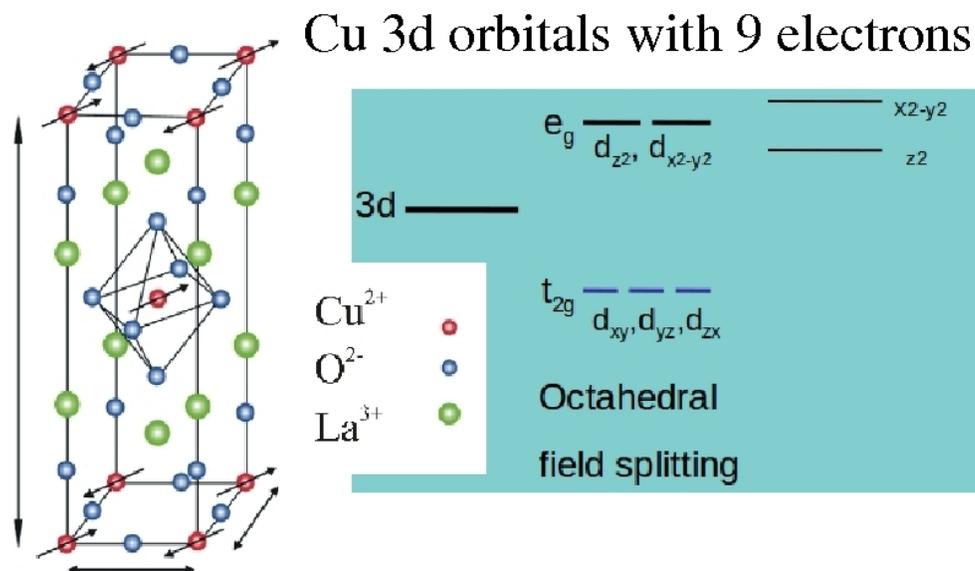


Figure 1: The La_2CuO_4 perovskite crystal structure. Note the *octahedral* environment (formed by the four in-plane Oxygen neighbours along with two out-of-plane Oxygen neighbours of each Copper ion) of each Cu^{2+} ion, which dictates the main pattern of crystal field splittings (also shown) of the Copper 3d orbitals, and the small distortion from perfect octahedral geometry responsible for the final splitting between the two orbitals with e_g symmetry (in case, you haven't studied this in your Solid State Physics course, don't worry—it is a detail that will not affect your understanding of what I am saying in this lecture).

behaviour, the system is actually a very good ceramic insulator.

This “parent-compound” can be thought of as being the first member in a series of compounds with varying Strontium doping, *i.e.* with the chemical formula $\text{La}_{(2-x)}\text{Sr}_x\text{CuO}_4$. Due to differences in the nominal valence of La and Sr (La^{3+} versus Sr^{2+}), each Strontium atom results in one additional hole added to the Copper-Oxygen plane. If the system conformed to the expectations of band-theory, the $x = 0$ parent would have had a half-filled d band, and for $x > 0$, the doped compound would have had a hole Fermi surface of “size” proportional to $1+x$ (since each Sr contributes one additional hole). However, as mentioned earlier, the $x = 0$ parent is actually an insulator with *no* Fermi surface, and at small x , the system actually has a small Fermi

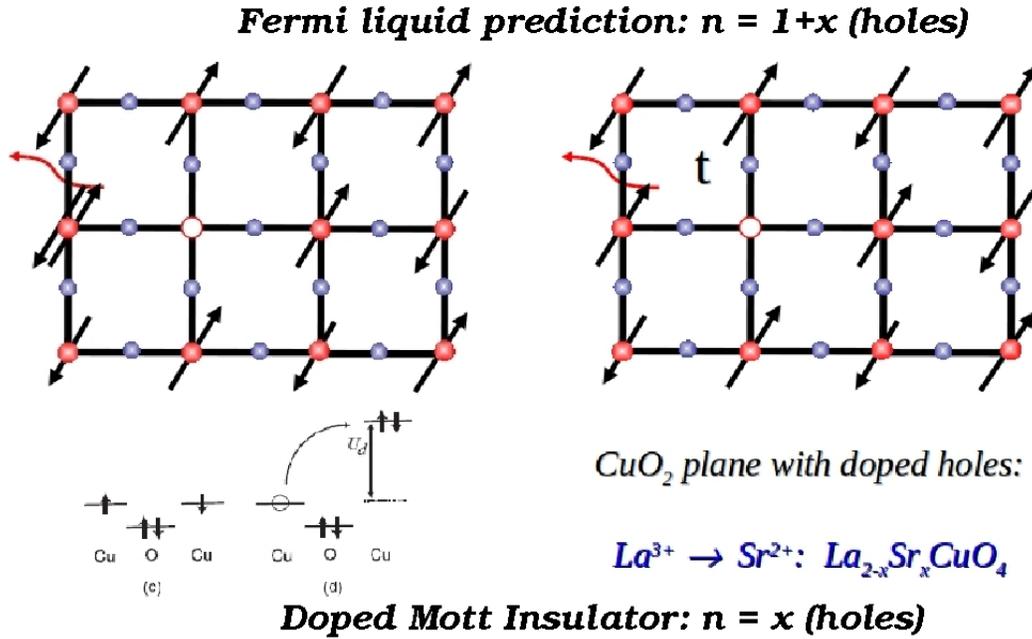


Figure 2: Depiction of the Copper-Oxide plane in $La_{2-x}Sr_xCuO_4$. The arrows represent $S = 1/2$ moments on the Copper sites. On the left panel is a depiction of an electron that has hopped to a neighbouring site costing charging energy U_d (the subscript d denotes the nature of the orbital which is doubly occupied) and leaving behind a hole. On the right is a depiction of a system with $x > 0$ in which holes are created without the need for double-occupancies.

surface of size x and behaves like a bad metal upon doping (see Fig 2).

With all of this background in mind, let us now ask just how and why the low energy physics of such a Mott Insulator (at $x = 0$) is well-described by the simple $S = 1/2$ Heisenberg antiferromagnet Hamiltonian we wrote at the beginning of this lecture.

To this end, consider a simple model that captures all the essential features of the example at hand: In the simple model, we have electrons (instead of holes, just to keep things familiar) that can live on sites of a square lattice and hop from site to neighbouring site with hopping amplitude t without changing the spin polarization of the electron (if the final state is allowed by Pauli exclusion). The total number of electrons is equal to the number of lattice sites (this models the $x = 0$ insulator described in the foregoing). Nat-

urally, two electrons with the same spin state cannot simultaneously occupy the same site (due to Pauli exclusion). However, two electrons with opposite spin polarization (one pointing up along some axis and the other pointing down) can occupy the same site simultaneously. To capture the most important effects of the Coulomb repulsion between electrons, we postulate that such double occupancy of a site costs “charging energy” U . (we drop the subscript d since our analysis is more general than the specific example of the cuprate Mott Insulator).

Our goal is to work out the *energy spectrum approximately* in the limit of very small t/U at $x = 0$, i.e with exactly one electron per site on average. This is an exercise in massively degenerate perturbation theory. To see what I mean, start with $t = 0$, *i.e.* set the electron kinetic energy to zero. The problem now becomes one of classical electrostatics. The optimum electrostatic energy, $E_0 = 0$, is obtained when each site has exactly one electron. Excited states are obtained if some sites are emptied out to produce double-occupation of other sites. Each doubly occupied site costs energy U .

How many states are there with energy $E_0 = 0$? Clearly, the answer is 2^{L^2} , since each electron can have two possible spin polarizations along some quantization axis, which we take to be the z axis—there is thus an entire ground state manifold with energy E_0 . What is the leading effect of the electron kinetic energy \hat{T} , which allows each electron to hop with hopping amplitude t from a site to any of its neighbouring sites without changing the spin polarization (if the final state is permitted by the Pauli principle)?

To answer this, note that to first order in degenerate perturbation theory, the effect of the perturbation is obtained by diagonalizing the effective Hamiltonian $\mathcal{P}_0 \hat{T} \mathcal{P}_0$ where \mathcal{P}_0 is the projector into the ground state manifold. However, since every hop of an electron creates a doubly occupied site, \hat{T} acting on any state in the ground state manifold takes the system out of this manifold due to the creation of double occupancy at a site. Therefore $\mathcal{P}_0 \hat{T} \mathcal{P}_0 = 0$, and there is no effect of the kinetic energy to linear order in t .

Therefore, we need to go to second order in degenerate perturbation theory to understand the leading effects of the kinetic energy \hat{T} . The general prescription for the effective Hamiltonian that determines the behaviour of the system to second order is

$$H_{g',g}^{eff} = - \sum_{e \in \alpha; \alpha \neq 0} \frac{\langle g' | \hat{T} | e; \alpha \rangle \langle e; \alpha | \hat{T} | g \rangle}{E_\alpha - E_0}$$

(2)

where g and g' are states in the ground state manifold of the unperturbed Hamiltonian which has energy E_0 , $\alpha \neq 0$ labels all excited state manifolds of the unperturbed Hamiltonian with unperturbed energy E_α , and $|e; \alpha\rangle$ denotes excited states in the excited state manifold α .

We now carefully apply this to the case at hand. In our example, ground states can be labeled by their spin state, *i.e.* written as $|\sigma_1, \sigma_2, \dots, \sigma_{L^d}\rangle$, where $\sigma_i = \pm 1$ denotes the spin state of the electron on site i . The kinetic energy \hat{T} acting on any such state can produce a linear combination of excited states by hopping any one electron to one of its neighbouring singly occupied sites, if allowed by the Pauli exclusion principle. Each such excited state is produced with amplitude t and has exactly one vacant site and a doubly occupied site next to it. The doubly occupied site will have one electron on it having $\sigma = +1$ and the other having $\sigma = -1$. All other sites remain singly occupied. Any such excited state has unperturbed energy U (due to one site being doubly occupied). The second action of \hat{T} needs to bring this excited state back to the ground state manifold. This can happen in two ways: One way is for the electron that had hopped to a neighbouring site to return to the original site. The other way is for the other electron at the doubly occupied site to hop to the empty site. The second way involves an *exchange* of the two electrons, and therefore the amplitude for this process has an additional minus sign due to exchange of fermions (fermion statistics).

The first way gives a *diagonal term* in the effective Hamiltonian since the initial $|\sigma_1, \sigma_2 \dots \sigma_{L^d}\rangle$ and the final $|\sigma'_1, \sigma'_2 \dots \sigma'_{L^d}\rangle$ are the same. It acts on every pair of nearest neighbour spins (σ_1, σ_2) which are anti-aligned: $\sigma_1 = -\sigma_2$ and, by its action, lowers the system energy by $2|t|^2/U$ (the factor of two comes from the fact that there are two choices for the location of the empty site in the intermediate state). In terms of spin-half operators, it can be represented as

$$\frac{2|t|^2}{U} \sum_{\langle ij \rangle} (2S_i^z S_j^z - \frac{1}{2}) \quad (3)$$

where $\langle ij \rangle$ represents each nearest neighbour pair of sites i and j .

The second way gives an off-diagonal term, since it *exchanges* the spins on the two neighbouring sites. It too acts on each pair of nearest neighbour spins (σ_1, σ_2) which are anti-aligned, but, in contrast to the previous term,

it flips these spins:

$$|\sigma'_1 \sigma'_2\rangle = |\sigma_2, \sigma_1\rangle \quad (4)$$

The amplitude for this spin-flip is $+2|t|^2/U$. Here, the positive sign is the result of the negative sign from the fermion exchange canceling the negative sign in front of the second-order perturbation theory formula, and the factor of two is again due to the fact that there are two possibilities for the doubly occupied intermediate state.

In the language of spin-half operators, this second term can be represented as

$$\frac{2|t|^2}{U} \sum_{\langle ij \rangle} (S_i^+ S_j^- + S_i^- S_j^+) \quad (5)$$

where $\langle ij \rangle$ represents each nearest neighbour pair of sites i and j .

Putting both terms together, we obtain the effective Hamiltonian

$$H^{eff} = \frac{4|t|^2}{U} \sum_{\langle ij \rangle} [S_i^z S_j^z + \frac{1}{2}(S_i^+ S_j^- + S_i^- S_j^+) - \frac{1}{4}] \quad (6)$$

where $S_i^+ = S_i^x + iS_i^y$ and $S_i^- = S_i^x - iS_i^y$ are the spin raising and lowering operators at site i . Finally, this can be rewritten in a manifestly rotationally invariant form as

$$H^{eff} = \frac{4|t|^2}{U} \sum_{\langle ij \rangle} [\vec{S}_i \cdot \vec{S}_j - \frac{1}{4}] \quad (7)$$

In the next lecture, we will use this as starting point to discuss the spin physics of Mott insulators in more detail.