

Elements of Magnetism

This is another section where we will barely scratch the surface – one could take multiple courses devoted to just this topic and the myriad ways in which magnetic properties arise in solids and their consequences.

We have already seen some examples of how magnetic properties can arise. In metals, we saw that ferromagnetism may be favored at low carrier concentrations (at least within Hartree-Fock approximation) because of the exchange potential between like-spins. This type of mechanism for magnetic order is called **itinerant exchange**, itinerant because it is due to electrons that are in Bloch-states, i.e. free to move through the entire metal, and exchange because it is due to the exchange interaction. Although one has to be a bit careful with the nomenclature here, because we also use **exchange** for any type of magnetic coupling, whatever its origin, even if it has nothing to do with the exchange potential as such.

The second example that we encountered was for the 2-electron, 2-site Hubbard model, where we saw that in the limit $U \gg t$, each electron becomes localized at one site and there is anti-ferromagnetic (AFM) coupling between them with $J = 4t^2/U$, because of virtual hopping of one electron to the other site and back. AFM was favored because only if the spins are antiparallel can these virtual hoppings occur. Such coupling is called **direct exchange**. We then saw that this generalizes to any type of lattice because in the limit $U \gg t$, the Hubbard model at half-filling maps into a Heisenberg model that would usually lead to a magnetically ordered state at low-enough T . This is a very different kind of magnetism from the one discussed above for metals, because this comes from what is known as **local moments**, i.e. each ion has its own spin due to its own electron. By contrast, in magnetic metals all electrons responsible for magnetism are delocalized in the entire sample.

One can also have mixed models, where there are local moments – for instance, one species of the ions making up the crystal has a partially filled core shell with some resulting spin, as given by Hundt's rules: eg, Mn^{2+} has a half-filled $3d$ shell and therefore a spin $S = 5/2$ associated with it. Other ions in the solid may contribute valence electrons that occupy extended states and form a metal. Because these electrons also have spins, there will be magnetic interactions between the itinerant electrons and the local spins. There are many possibilities depending on details. One example is the RKKY exchange (Ruderman - Kittel - Kasuya - Yosida) that arises between impurity local moments in a metal. Think about having any normal robust metal, with some small concentration of magnetic impurities in it (such as Mn^{2+}). As we've seen, the presence of any local potential is responsible for the appearance of Friedel oscillations in the surrounding density of electrons (as they re-arrange to screen it), that go like $\cos(2k_F r)/(k_F r)^3$. If the impurity has spin, because it interacts differently with spin-up vs. spin-down electrons from the Fermi sea, it results into somewhat different phases for the Friedel oscillations associated with them. If there are two such impurities, each sets up its own Friedel oscillations. This may lead to constructive or destructive interference depending on the distance between impurities and their spin orientations. The end result is an **indirect RKKY exchange** $J(\vec{R}_{12})\vec{S}_1 \cdot \vec{S}_2$ where \vec{R}_{12} is the distance between the two impurity spins and $J(r) \sim \cos(2k_F r)/(k_F r)^3$. The name “indirect” is to show that the exchange is mediated through the Fermi sea electrons, this is not a direct interaction between the two impurity spins. There are many other such examples.

Finally, even for an insulator with local moments, other mechanism can give rise to exchange between them. For instance, in the undoped cuprates, there is one hole localized in the $3d$ orbital of each Cu ion, meaning each Cu has a spin $1/2$. However, between two neighbor Cu there is a bridging O^{2-} which has a full $2p^6$ shell. So the exchange between the Cu spins is not direct,

because the holes from Cu cannot virtually hop directly to the other Cu. Instead, they hop through the intermediary O. This also leads to an AFM coupling, which is called a **superexchange**.

However, the coupling in this case is AFM because of the orientation of the orbitals involved, see the next figure. In particular, we know that the Cu holes occupy the $3d_{x^2-y^2}$ orbital, meaning that they can only hybridize with (hop onto) the ligand $2p$ O orbital, i.e. the one whose lobes point toward the two Cu. You can now see why AFM coupling would be favored: this allows either hole to hop through the O and go visit the other Cu hole (again, virtually); or both Cu holes can hop onto the common O and then go back. Either way, either hole can return to either Cu, so the overall spins can be flipped, which is the signature of magnetic exchange. None of this could happen if the Cu spins were parallel, because of Pauli's principle.

However, if there was a 90° angle between the two bonds, then holes with either spin could hop onto the common O because they would hop into different $2p$ orbitals and Pauli's principle is not active. You might think that this means no magnetism, but that is not quite true: now the ferromagnetic order is favored because Hundt's rule lowers the cost of having two holes with the same spin on the O, vs. two holes with antiparallel spin. So in this case we get a weak ferromagnetic coupling from the superexchange just because of the different spatial orientation which means that different orbitals are involved. These and many other possibilities are described by the Goodenough-Anderson-Kanamori rules.

So there is a zoo of possibilities for generating spin-dependent interactions, for instance I haven't even mentioned hyperfine couplings. In the following we will discuss the simplest cases with local moments, to get a feeling for what we can expect to happen in magnetically ordered phases. But before moving on, let me re-emphasize something we already discussed when we discovered the direct exchange, in the 2-site Hubbard model: all these magnetic exchanges arise as consequence of the Coulomb interactions and this makes them strong (they have rather large energy scales). There are also dipole-dipole interactions between the magnetic moments associated with the electron spins, but those are usually much weaker and we usually ignore them. However, as I will comment in a bit, sometimes they actually also play an important role because of their long-range nature.

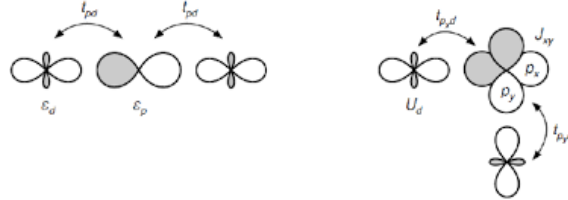


Figure 1: Left: Two Cu $3d_{x^2-y^2}$ orbitals bridged by a $2p$ ligand O orbital. In this case, holes localized on the Cu will prefer AFM order. Right: Same situation but now at a right-angle, meaning that both in-plane $O2p$ orbitals become relevant. Two holes localized on the Cu will now prefer FM order. I found this image online, hence the poor quality. Why do you think the Cu orbitals are so distorted (these are nominally $d_{x^2-y^2}$ states), is that a mistake or is it something meaningful?

1 Hamiltonians

For simplicity, let us assume that we have a lattice, with a local moment of spin S at each site. The most common model to describe their magnetic properties is the **Heisenberg model**:

$$\mathcal{H} = - \sum_{i,j} J_{ij} \hat{\vec{S}}_i \cdot \hat{\vec{S}}_j \approx -J \sum_{\langle i,j \rangle} \hat{\vec{S}}_i \cdot \hat{\vec{S}}_j \quad (1)$$

Because the exchange integrals J_{ij} decrease fast (usually exponentially) with the distance between sites, normally we only keep the nearest-neighbor terms, as I did in the second equality. Of course, we can add more terms if need be.

If $J > 0$, this Hamiltonian favors FM order because the energy is minimized when neighbor spins are parallel. If $J < 0$, then it favors AFM order. We will briefly discuss these two cases for simple cubic lattices. Let me mention that for 1D chains, this model can be solved exactly for any J using the Bethe ansatz. In higher dimensions, we do not have exact results so we are forced to either used approximations or numerical simulations.

Before discussing them, let me introduce a few more well-known magnetic Hamiltonians. The **Ising model** is:

$$\mathcal{H} = - \sum_{i,j} J_{ij} \hat{S}_i^z \cdot \hat{S}_j^z \approx -J \sum_{\langle i,j \rangle} \hat{S}_i^z \cdot \hat{S}_j^z \quad (2)$$

In other words, only the z -axis projections of the spins are coupled, not the whole spin operator. This is a much simpler Hamiltonian, obviously. In practice it arises in situations where the local environment of the ions is anisotropic in such a way that the spin is forced to be oriented along one axis (which we call the z -axis). Here “forced” means that it is much more energetically expensive for the spin to point in other directions, so we just ignore those possibilities.

This model can be solved exactly in 1D – you’ve probably done this in a stat mech course. It has magnetic order at $T = 0$ but is disordered at all finite- T . The 2D solution was found by Onsager, who showed that magnetic order survives up to a finite T_C . This result is one of the crowning glories of exactly solvable models. By the way, I hope you’re familiar with the Mermin-Wagner theorem from your undergraduate physics course (if not, do some reading!) – is the finite T_C in this 2D case contradicting that theorem? In higher dimensions we need again to use approximations or numerics.

We also have the **xy model**:

$$\mathcal{H} = - \sum_{i,j} J_{ij} \left[\hat{S}_i^x \cdot \hat{S}_j^x + \hat{S}_i^y \cdot \hat{S}_j^y \right] \approx -J \sum_{\langle i,j \rangle} \left[\hat{S}_i^x \cdot \hat{S}_j^x + \hat{S}_i^y \cdot \hat{S}_j^y \right] \quad (3)$$

which arises when the local environment is such that the spin prefer to lie in a plane (this is called an easy-plane anisotropy, in contrast to the easy-axis that leads to Ising coupling). This model can also be solved exactly in 1D, and I hope you’ll have a look at that very entertaining solution. For a 2D system there is also very nice physics having to do with vortices and the Kosterling-Thouless transition (which got the Nobel prize very recently!), but that is something to be left for another course.

2 Ferromagnetic order

We begin by studying a Heisenberg ferromagnet. For simplicity we consider only nn coupling, although extension to longer range (if all exchanges are FM) is absolutely trivial. So our Hamiltonian

is:

$$\mathcal{H} = -J \sum_{\langle i,j \rangle} \hat{\vec{S}}_i \cdot \hat{\vec{S}}_j \quad (4)$$

where $J > 0$.

2.1 Ground-state

Intuition tells us that all spins want to be parallel to minimize energy, so we might guess that $|GS\rangle = | + S, \dots, + S \rangle$. Indeed, it is straightforward to verify that this is an eigenstate of the Hamiltonian. For this, we rewrite:

$$\hat{\vec{S}}_i \cdot \hat{\vec{S}}_j = \hat{S}_i^z \cdot \hat{S}_j^z + \frac{1}{2} [\hat{S}_i^+ \cdot \hat{S}_j^- + \hat{S}_i^- \cdot \hat{S}_j^+]$$

where $\hat{S}^\pm = \hat{S}^x \pm i\hat{S}^y$ are raising and lowering operators: $\hat{S}^\pm |S, m\rangle = \sqrt{(S \mp m)(S \pm m + 1)} |S, m \pm 1\rangle$ for any $m = -S, -S+1, \dots, S-1, S$ (I set $\hbar = 1$, but of course that is the unit for spin). Clearly, when acting on a pair of spins $| + S, + S \rangle$, the first term gives S^2 and the second one vanishes, because no spin can be further raised. Thus:

$$\mathcal{H}|GS\rangle = -\frac{Nz}{2}JS^2|GS\rangle = E_{GS}|GS\rangle$$

where N is the number of sites and z is the coordination number (number of nn neighbors of each site). For a simple cubic lattice $z = 6$. As usual, we assume PBCs so we don't need to worry that surface sites have fewer neighbors.

To prove that this is the ground-state, we must show that this is the lowest possible energy of any eigenstate. This is achieved by proving that $\langle \hat{\vec{S}}_i \cdot \hat{\vec{S}}_j \rangle \leq S^2$, no matter what state we use to take the expectation value (You should be able to prove this, but let me know if you need a pointer). The energy for $|GS\rangle$ hits this extremum value for each bond, therefore it has the lowest possible value and hence it is the true ground-state.

So far so good, but you should notice something a bit weird. All we showed, in fact, is that all spins must have maximum projection along some axis, but that axis can be any axis. So this GS is infinitely degenerate, because we could rotate the z -axis as we please. In practice, ferromagnetic systems do chose one direction, in other words the GS breaks the rotational symmetry of the Hamiltonian. One way to understand how this happens is to think of starting with a small system. As discussed, all its fully polarized states such as $|\uparrow, \dots, \uparrow\rangle, |\rightarrow, \dots, \rightarrow\rangle, |\downarrow, \dots, \downarrow\rangle, \dots$ are degenerate, and in time the system will tunnel between them. So for a small system, the average spin at any site will vanish because of sampling of all these orientations. However, as the system grows, the tunneling time between two ground-state with different orientation becomes longer and longer because more and more spins have to rotate. As the system goes to the thermodynamic limit, this time becomes so long as to be effectively infinite and basically the system remains locked into one FM order, which we'll call $| + S, \dots, + S \rangle$.

2.2 Goldstone modes: the magnons

We already discussed that if the GS of the system breaks a continuous symmetry, we expect to find gapless bosonic excitations = Goldstone modes, which try to restore the full symmetry (think phonons for lattice that breaks the full translations symmetry). Let's see how this works in this context.

We are looking for low-energy excitations. Clearly, the simplest thing we can do to increase the energy is to have one spin not quite fully parallel. Let me call

$$|n\rangle = \frac{S_n^-}{\sqrt{2S}}|GS\rangle = |S, \dots, S-1, \dots, S\rangle$$

as the state where the n th spin is lowered by 1 (the sqrt is there for normalization reasons). This clearly will have a higher energy than $|GS\rangle$ because the bonds involving spin n aren't maximized, but it is also clear that this is not an eigenstate. Part of the problem is that it breaks translational symmetry: there is nothing special about spin n so why should it be the one that's lowered? Of course, a true eigenstate will have translational symmetry; to regain it we note that any spin is equally likely to be lowered, or if you wish, that we better have a solution with a Bloch-type structure:

$$|\vec{k}\rangle = \sum_n \frac{e^{i\vec{k}\vec{R}_n}}{\sqrt{N}}|n\rangle = Q_{\vec{k}}^\dagger|GS\rangle$$

It is straightforward to check that:

$$\mathcal{H}|\vec{k}\rangle = [E_{GS} + \hbar\Omega(\vec{k})]|\vec{k}\rangle$$

where

$$\hbar\Omega(\vec{k}) = 4SJ \left[\sin^2 \frac{k_x a}{2} + \sin^2 \frac{k_y a}{2} + \sin^2 \frac{k_z a}{2} \right]$$

Just like we did for phonons, we interpret $|GS\rangle$ as the vacuum for excitations, and $Q_{\vec{k}}^\dagger$ as the creation operator for an excitation of energy $\hbar\Omega(\vec{k})$. The name we give to such magnetic excitations is **magnons** or **spin-waves**, and note that indeed they are gapless excitations (can you explain in a simple way why it must be so?). Also note that the magnons are **collective excitations** (like the phonons) because each involves all spins in the system. One reason for the name spin-wave is that if we calculate the in-plane angle between any two neighbor spins, we find $\langle \vec{k} | \hat{S}_{i,\perp} \hat{S}_{j,\perp} | \vec{k} \rangle = \frac{2S}{N} \cos \vec{k} \cdot (\vec{R}_i - \vec{R}_j)$, in other words the in-plane angle ϕ has a wave-like behavior.

However, there is a major difference between magnons and phonons. For phonons, any state with an arbitrary number of phonons was also an eigenstate (within the harmonic approximation). Here, it is easy to verify that only one-magnon states are true eigenstates. If there are two or more magnons in the system they interact and the eigenstates become very complicated. Another way to see that this must be so is to note that the magnon creation operator $Q_{\vec{k}}^\dagger$ defined above and its annihilation counterpart $Q_{\vec{k}}$ are not bosonic operators: they do not satisfy simple commutation relations $[Q_{\vec{k}}, Q_{\vec{k}'}^\dagger] \neq \delta_{\vec{k}, \vec{k}'}$ (more on this below).

So then what is the actual use of knowing these magnon excitations? Well, it turns out that it is a good approximation to pretend that magnons behave like non-interacting bosons, if there are few of them (so for example, if the system is at very low temperatures and therefore not likely to have many magnons excited thermally). Indeed, one can use neutron scattering to measure the low-energy excitations of ferromagnets and one gets good agreement with the magnon spectrum, at low temperatures. One can also use this to derive how the magnetization of the system decreases with increasing T , in the limit $T \ll T_C = J$:

$$M_z(T) = \frac{1}{N} \langle \sum_{n=1}^N \hat{S}_n^z \rangle \approx S - \frac{1}{N} \sum_{\vec{k}} \frac{1}{e^{\beta \hbar \Omega_{\vec{k}}} - 1}$$

where the second equality shows that each magnon decreases the total spin by 1 from its maximum NS value, and the average number of magnons (if we treat them as non-interacting bosons) is given by the Bose-Einstein distribution. The chemical potential is again zero like for phonons and all other similar bosonic collective excitations.

We do the usual tricks to transform this into an integral:

$$\Delta M_z(T) = -\frac{a^3}{(2\pi)^3} \int d\vec{k} \frac{1}{e^{\beta\hbar\Omega_{\vec{k}}} - 1}$$

At low temperatures, only magnons with small \vec{k} are likely to be excited, because they cost the least amount energy. But $\hbar\Omega(\vec{k}) \rightarrow zJSk^2a^2$ as $k \rightarrow 0$. This allows us to integrate over angles, and changing the radial variable from k to $x = \beta\hbar zJSk^2a^2$ we find that

$$\Delta M_z(T) = -\alpha T^{\frac{3}{2}}$$

where α contains the remaining integral over x , which is just a number if we send the upper limit to ∞ , which we do (why?). Indeed, it is found that this so-called **Brillouin law** is well-obeyed by ferromagnets at low- T . At higher T , however, the system is with high probability in higher and higher energy states which are worse and worse described as collections of independent magnons. To figure out what happens there, we need a different approximation. We will turn to our good friend the mean-field approximation, which is the direct analog of the Hartree-Fock approximation.

2.3 Finite temperatures: mean-field approximation

This mean-field approximation can be justified in many ways. The original one was to consider each spin as if it's interacting with the average values of its neighbors, and to ignore the fluctuations about the average. This leads to a certain factorization of the Hamiltonian and self-consistent equations, as we discuss next. However, it is important for you to realize that this is also a variational method, very similar in spirit to HFA and BCS: in all cases we try to approximate the interacting model by the “best” fit of a non-interacting model. You might want to think about how you would formulate this approximations in these terms, both using a fully variational calculation (i.e., minimizing the free energy, at finite- T) or with the equation-of-motion approach. All give the same result, when done properly.

Consider that we have a product of two operators $\hat{A}\hat{B}$ and we'd like to simplify this to have only one-operator terms. Let $\langle A \rangle, \langle B \rangle$ be the average values of the operators – if we're doing a $T = 0$ calculation then these are ground-state expectations, whereas at finite- T they are thermal averages. We can then write:

$$\hat{A}\hat{B} = [\langle A \rangle + (\hat{A} - \langle A \rangle)] [\langle B \rangle + (\hat{B} - \langle B \rangle)] = \hat{A}\langle B \rangle + \hat{B}\langle A \rangle - \langle A \rangle\langle B \rangle + (\hat{A} - \langle A \rangle)(\hat{B} - \langle B \rangle)$$

The mean-field approximation consists in setting the last term (the product of fluctuations about average) to zero. We therefore obtain:

$$\hat{A}\hat{B} \approx \hat{A}\langle B \rangle + \hat{B}\langle A \rangle - \langle A \rangle\langle B \rangle$$

in other words, we no longer have to deal with products of operators.

For our Heisenberg Hamiltonian, it is straightforward to apply this. We will assume (given our expectations about the ferromagnetic order) that $\langle \hat{S}_n \rangle = S_z(T)\hat{z}$, where I'll write $S_z(T)$ as a short

hand for the average value of the z -axis projection of any spin. Then:

$$\hat{S}_i \hat{S}_j \approx S_z(T) [\hat{S}_i^z + \hat{S}_j^z - S_z(T)]$$

Putting this into the Hamiltonian, we find (up to a constant):

$$\mathcal{H} \approx -h \sum_n \hat{S}_n^z$$

where $h = zJS_z(T)$ is as of yet unknown. Again, z is the number of nn neighbors.

This is indeed a Hamiltonian for non-interacting spins. For simplicity, let me assume that $S = 1/2$ just so I don't have to work with Brillouin functions for a general S . Then the Hamiltonian has two eigenstates with energies $\pm h/2$ and:

$$S_z(T) = \langle \hat{S}_n^z \rangle = \frac{\frac{1}{2}e^{\frac{\beta h}{2}} - \frac{1}{2}e^{-\frac{\beta h}{2}}}{e^{\frac{\beta h}{2}} + e^{-\frac{\beta h}{2}}} = \frac{1}{2} \tanh \frac{\beta h}{2}$$

(note: strictly speaking I should multiply everything by \hbar because the eigenstates of \hat{S}_z are $\hbar m$, $m = -S, \dots, S$, but we set $\hbar = 1$). Given the link between h and $S_z(T)$, we find the self-consistent equation:

$$S_z(T) = \frac{1}{2} \tanh \frac{\beta z J S_z(T)}{2}$$

Note that (up to constants), $S_z(T)$ is precisely the average density of magnetization. As $T \rightarrow 0$, $\tanh \rightarrow 1$ and we find the spins fully magnetized: $S_z(0) = +S = +\frac{1}{2}$, which is indeed what we found in the ground-state. But as T increases, the \tanh decreases and so does $S_z(T)$. The critical or **Curie** temperature T_C is the one where $S_z(T_C) \rightarrow 0$, i.e. the system loses its magnetic order. You can solve for this in various ways, the easiest I think being the graphic solution – the slope of the \tanh must be larger than unity at the origin in order for a non-trivial solution to exist. In other words, a solution $S_z(T) \neq 0$ exists so long as $\frac{1}{4}\beta z J \geq 1 \rightarrow k_B T_C = \frac{zJ}{4}$. You should check that for a general S , the answer for the Curie temperature is:

$$k_B T_C = zJ \frac{S(S+1)}{3}$$

Many other quantities can be calculated. For instance, the magnetic susceptibility above the critical temperature is found to be:

$$\chi = \frac{\chi_0}{1 - \frac{T_C}{T}}$$

where $\chi_0 = n(g\mu_B)^2 \frac{S(S+1)}{3k_B T}$ is the Curie's law for the susceptibility of a paramagnet. One can also calculate various critical exponents showing how quantities scale near T_C , etc. I hope you'll see all this analysis in a graduate stat mech course, if you haven't already encountered it in an undergraduate one.

3 Antiferromagnetic order

So now let's see what happens if we change the sign of the exchange, $J \rightarrow -J$, so that spins now favor antiparallel alignment.

Let's do first the mean-field treatment, to see what changes at this level of approximation. Of course, the main change is that we can no longer assume that $\langle \hat{S}_n \rangle = S_z(T) \hat{z}$ for all spins. Instead, we divide the sites into two sublattices, such that sites on sublattice A have only nn from sublattice B, and viceversa. Lattices that can be divided this way are called **bipartite**, and the simple cubic lattice is bipartite (for lattices that are not bipartite we usually have **frustration**, meaning there is no way to arrange the spins such that all pairs have the preferred orientation - think about 3 spins that prefer AFM order, on a triangle. In such cases all sorts of interesting things can happen, but again we won't discuss them here). Back to our bi-partite lattice: Let's say we expect spins on sublattice A to be pointing "up" and those on sublattice B to be pointing down. As a result, we should guess that $\langle \hat{S}_n \rangle = +S_z(T) \hat{z}$ if $n \in A$, and $\langle \hat{S}_n \rangle = -S_z(T) \hat{z}$ if $n \in B$. I'm taking the same magnitude because it is totally arbitrary what we call "up" and "down" and the state of the system cannot possibly depend on that choice.

From this point on, you should verify that the calculations map precisely on those we had from the FM case, because the change in sign of J is compensated by the - due to the antialignment of neighbors. So the equation for $S_z(T)$ is the same and therefore the critical temperature (now called **the Néel temperature**) has the expression, but with $J \rightarrow |J|$. The susceptibility is changed to $\chi = \frac{\chi_0}{1 + \frac{T_0}{T}}$. The sign change is because of the sign of change of J .

In any event, at this mean-field level it seems that FM and AFM are very very similar, because we could go from one to the other by flipping every second spin and changing the sign of J .

However, if we look a bit more carefully, things are in fact very different. We could formally rotate all spins on the B sublattice about their x axis, so that $\hat{S}^z \rightarrow -\hat{S}^z$; this also rotates the y component while leaving the x component unchanged. So the product $\hat{S}_i \cdot \hat{S}_j$ does not go into $-\hat{S}_i \cdot \hat{S}_j$ because we can only change the sign of 2 components (y and z), not all three! Of course, at the mean-field level where only the component z is left in the factorized Hamiltonian this is enough, but not for the full quantum model. The latter was used to find the ground-state and the magnons, so let's see what changes for AFM order.

3.1 Ground-state

The temptation here would be to guess that $|GS\rangle = |S, -S, \dots\rangle$, by which I mean that spins on sublattice A are maximally polarized "up" and those on B are maximally polarized "down". However, it is immediately apparent that this is NOT an eigenstate, because when acting on any "up-down" pair of nn spins, one of the terms in $\hat{S}_i^+ \cdot \hat{S}_j^- + \hat{S}_i^- \cdot \hat{S}_j^+$ will take it from $|\dots, +S, -S, \dots\rangle$ to $|\dots, S-1, -S+1, \dots\rangle$. In particular, for spin $S = 1/2$, this means that any pair of spin can be flipped so that the one that was up is now down, and the one that was down is now up. This shows not only that $|S, -S, \dots\rangle$ is not an eigenstate, but also makes it clear that finding the correct eigenstate is very very difficult, because the action of \mathcal{H} can flip any number of pairs of nn spins, in other words there is a huge number of components that get mixed with this $|S, -S, \dots\rangle$ state to give the true ground-state.

As I said before, in 1D and for $S = 1/2$ we can find the true ground-state using the Bethe ansatz. For higher spins and/or in higher dimensions we do not know how to solve this problem analytically (if, indeed, it is solvable). So here we are forced to use approximations to gain some understanding of the nature of the ground-state and of the low-energy excitations, which are called antiferromagnons, or simply magnons (I'll use the shorter name).

As you may suspect, lots and lots of approximations have been proposed, all with various advantages and disadvantages. I will discuss one of the most basic approaches, based on the

Holstein-Primakoff transformation.

3.2 Holstein-Primakoff transformation

The problem with spin operators is that their commutation relations are very complicated: $[\hat{S}_i^\alpha, \hat{S}_j^\beta] = i\delta_{ij}\epsilon_{\alpha\beta\gamma}\hat{S}_i^\gamma$ (where again I'll set $\hbar = 1$). Most approximation schemes aim to represent spins in terms of either bosons or fermions, because of their simpler algebra.

The Holstein-Primakoff (HP) representation is in terms of bosons. Let me consider first a single spin S , and let me introduce a pair of creation and annihilation bosons a, a^\dagger such that

$$\hat{S}^z = S - a^\dagger a.$$

In other words, we map the state with $m = +S$ in the zero-boson state; if $m = S - 1$, then we have a boson, etc. Going between different values of m means either increasing or decreasing the number of bosons, so we might guess that we should take $\hat{S}^+ = a$ and $\hat{S}^- = a^\dagger$. These would do the trick, except they do not stop the sequence of possible eigenstates at $m = -S$, instead one could create bosons for ever and have any $m \leq S$ as an allowed value. Some thinking and experimenting shows that the correct choice is:

$$\hat{S}^+ = \sqrt{2S - a^\dagger a} \cdot a \quad \hat{S}^- = a^\dagger \sqrt{2S - a^\dagger a}$$

This now insures that we cannot have more than $2S$ bosons in the system, i.e. $m \geq -S$ as well. Of course, the way to derive this is to find what function $f(a^\dagger a)$ should be used in $\hat{S}^+ = f(a^\dagger a)a$ and $\hat{S}^- = a^\dagger f(a^\dagger a)$ so that all spin commutation relations are obeyed. Try that and you'll find that this is the answer. Note: because $[f(a^\dagger a), a] \neq 0$, the order in which we write these terms is important!

So far, this is exact. You can easily convince yourselves that using this in the Heisenberg Hamiltonian (where we introduce a pair of bosons a_n, a_n^\dagger for each site n), will not help because the sqrt make the result extremely ugly. So we need an approximation, to simplify things. The idea is that if we're interested in low-energy states, and if we chose our HP bosons correctly (see below) then there shouldn't be too many bosons in the system at low energies. To make this more clear, let's consider first using HP for a ferromagnet, even though its GS and one-magnon states can be solved exactly. There we saw that in the GS we had zero bosons (all spins were up), and the one-magnon states had just one boson in the entire system (only one spin was lowered by one). Because the magnon is a collective excitation, $\langle a_n^\dagger a_n \rangle = \frac{1}{N}$ at any site, i.e. indeed it is a small number. We can therefore use this as a justification to expand the sqrt $\sqrt{2S - a^\dagger a} \approx \sqrt{2S}(1 - \frac{a^\dagger a}{4S} + \dots)$ and keep only the lowest order contribution. We thus obtain a much simpler Hamiltonian, but one that is only valid so long as the number of bosons is indeed very small! By the way, you might want to try doing this for a FM: you should be able to verify both the magnon spectrum, and to understand a bit better why magnons are interacting excitations, unlike the phonons (well, we have to be careful. Phonons also interact with one another if we go beyond the harmonic approximation, but the point is that for magnons there is no equivalent of the harmonic approximation, they definitely interact with one another).

How can we use these ideas for an AFM? Clearly, we cannot use HP as written above, because all spins "down" (or mostly down) would require the maximum number of magnons to be present there and we'd have lots of magnons in the system. The solution is to use HP like above for spins up the A sublattice, i.e. those that are (mostly) "up":

$$\hat{S}_n^z = S - a_n^\dagger a_n \quad \hat{S}_n^+ = \sqrt{2S - a_n^\dagger a_n} \cdot a_n \quad \hat{S}_n^- = a_n^\dagger \sqrt{2S - a_n^\dagger a_n}$$

whereas for spins on the B sublattice, the magnons will count how far they are from their “down” state, in other words here we define:

$$\hat{S}_n^z = -S + b_n^\dagger b_n \quad \hat{S}_n^+ = b_n^\dagger \sqrt{2S - b_n^\dagger b_n} \quad \hat{S}_n^- = \sqrt{2S - b_n^\dagger b_n} \cdot b_n$$

and I will use a and b operators for the spins on the two sublattices, to remember which is which. If we implement HP this way, then indeed we can hope that there are rather few bosons in the ground-state and we are allowed to Taylor-expand the sqrts to simplify the Hamiltonian.

We do all this, and we also define the Fourier transforms: $a_{\vec{k}}^\dagger = \frac{1}{N'} \sum_{n \in A} e^{i\vec{k}\vec{R}_n} a_n^\dagger$ and similarly for b operators. Note that now $N' = N/2$ counts the number of sites on each sublattice, and the quasimomenta \vec{k} are restricted to the magnetic Brillouin zone whose size is half of that of the full Brillouin zone (this is because we now have a 2-site basis, one from A and one from B).

After some algebra we find:

$$\mathcal{H} = 2JzS \sum_{\vec{k}} \left[a_{\vec{k}}^\dagger a_{-\vec{k}} + b_{\vec{k}}^\dagger b_{-\vec{k}} + \gamma_{\vec{k}} (a_{\vec{k}}^\dagger b_{-\vec{k}}^\dagger + b_{-\vec{k}} a_{\vec{k}}) \right]$$

where $\gamma_{\vec{k}} = \gamma_{-\vec{k}} = \frac{1}{z} \sum_{\delta} e^{i\vec{k}\vec{\delta}}$ is the sum over all nn of a site. For a cubic lattice, $z = 6$ and $\gamma_{\vec{k}} = \frac{1}{3} [\cos(k_x a) + \cos(k_y a) + \cos(k_z a)]$.

The first two terms in the Hamiltonian are due to the $S^z S^z$, while the third one comes from the $S^+ S^- + S^- S^+$ parts, where we approximated the sqrt by $\sqrt{2S}$ only. We could keep the next corrections as well; they will lead to quadratic terms, so they introduce interactions between magnons. Ignoring them allows us to find the magnon dispersion while pretending that these interactions are negligible.

So let's diagonalize this Hamiltonian and find its GS and excitations (the magnon spectrum). Because it is quadratic, we can do this exactly (if we're ignoring the interaction terms). We'll do this precisely like we proceeded before. If we can diagonalize it, it means we can write it like:

$$\mathcal{H} = E_0 + \sum_{\vec{k}\alpha} \hbar \Omega(\vec{k}) Q_{\vec{k},\alpha}^\dagger Q_{\vec{k},\alpha}$$

where $\alpha = 1, 2$ is an index because I expect 2 solutions for each value of \vec{k} (why?). Again, we chose $\Omega(\vec{k}) > 0$ because these are energies of excitations out of the ground-state $|GS\rangle$, which is defined by $Q_{\vec{k},\alpha}|GS\rangle = 0$. This should all remind you a lot about the BCS solution and indeed the solution we'll get here is its direct analog, except now it is for bosons, not fermions.

Because momentum is a good quantum number but the number of bosons is not conserved by the Hamiltonian, we guess:

$$Q_{\vec{k},+} = u_{\vec{k}} a_{\vec{k}} + v_{\vec{k}} b_{-\vec{k}}^\dagger$$

Because the new operators are also bosonic, we must have $[Q_{\vec{k},+}, Q_{\vec{k},+}^\dagger] = 1 \rightarrow u_{\vec{k}}^2 - v_{\vec{k}}^2 = 1$ (note that the sign was “-” for fermions). This means that we could chose $u_{\vec{k}} = \cosh \theta_{\vec{k}}, v_{\vec{k}} = \sinh \theta_{\vec{k}}$. Just like we did for BCS, we'll define the second operator so as to make it easy to fulfill the “cross” commutation rules $[Q_{\vec{k},+}, Q_{\vec{k},-}] = 0$:

$$Q_{\vec{k},-} = u_{\vec{k}} b_{-\vec{k}} + v_{\vec{k}} a_{\vec{k}}^\dagger$$

Now we find these coefficients using the usual tricks: $[Q_{\vec{k},+}, \mathcal{H}] = \hbar\Omega(\vec{k})Q_{\vec{k},+}^\dagger \rightarrow u_k[a_k, \mathcal{H}] + v_k[b_{-k}^\dagger, \mathcal{H}] = \hbar\Omega(\vec{k})[u_{\vec{k}}a_{\vec{k}} + v_{\vec{k}}b_{-\vec{k}}^\dagger] \rightarrow$

$$\hbar\Omega(\vec{k})u_{\vec{k}} = u_k[[a_k, \mathcal{H}], a_k^\dagger] + v_k[[b_{-k}^\dagger, \mathcal{H}], a_k^\dagger] = u_kC - C\gamma_kv_k$$

$$\hbar\Omega(\vec{k})v_{\vec{k}} = u_k[b_{-k}, [a_k, \mathcal{H}]] + v_k[b_{-k}, [b_{-k}^\dagger, \mathcal{H}]] = u_kC\gamma_k - Cv_k$$

where $C = 2JzS$.

From this, we find immediately the (antiferro)magnon spectrum:

$$\hbar\Omega(\vec{k}) = 2JzS\sqrt{1 - \gamma_{\vec{k}}^2}$$

This spectrum is gapless: $\Omega(\vec{k}) \rightarrow 0$ when $k \rightarrow 0$ as expected, because these are also Goldstone modes which aim to restore the broken spin rotational symmetry. However, while the (ferro)magnons have quadratic dispersion for small k , note that the antiferromagnons have linear dispersion, $\hbar\Omega(\vec{k}) \sim JSka$. As a result, one can show that the sublattice magnetization decreases from its maximum $T = 0$ value like T^2 instead of $T^{\frac{3}{2}}$ for FM. Interestingly, it is now fairly easy to show that the maximum sublattice spin is not S or $-S$ (for the two sublattices) but instead it is reduced to $S - \frac{1}{N} \sum_{\vec{k}} v_{\vec{k}}^2$ (prove this!) This is because the GS does contain a finite concentration of bosons a and b , and indeed we already know that the GS is not $|+S, -S, \dots\rangle$ but has flipped spins present.

Another interesting difference is that we have 2 degenerate magnons for each \vec{k} whereas in the FM case there was one per \vec{k} value. We can understand this simply from counting: the Brillouin zone is here twice as small (because the unit cell is twice as big), so we must have twice as many modes. But we can also see this must be so because of the sub-lattice symmetry. The $+$ mode either removes an a boson, or adds a b boson. The first means raising an A spin, the second means raising a B spin. So this type of excitation increase the total S_z spin by $+1$. Similarly, we can see that the “ $-$ ” mode decreases the total spin by 1. For a ferromagnet we could only have magnons that lowered the total spin because we started with all spins up. However, here we have two sublattices, one (mostly) down and one (mostly) up). If we think in terms of the A sublattice, the magnons ought to decrease its spin, meaning they would be $-$ type; but then we must have the counterpart modes that “decrease the down spins” of B sublattice, in other words they raise spin, hence the $+$ modes.