Magnans

The Heisenberg interaction

In these notes we are going to consider the interaction among spins in a crystal. We assume the electrons are localized in the atomic sites, as in an insulator. This means we will be concerned with localized magnetism, in contrast to the itinerant magnetism that occurs in metals, which we will discuss later.

Each atom may have a spin contribution from several of its electrons. To account for this, we will assume each atom can be described by a spin S, not necessarily $1/2$. To each atom we therefore attribute 3 spin operators S_i^x, S_i^y, S_i^z, where $i = 1, \dots, N$ labels the atoms in the crystal. Spins of different sites commute and spins of the same site satisfy the canonical algebra

$$[S_i^x, S_j^y] = i \delta_{ij} S_i^x \qquad (1)$$

(plus cyclic permutations).

As a convenient basis, we choose the states which diagonalize each S_i^z,

$$|\vec{m}\rangle = |m_1, \dots, m_N\rangle \qquad (2)$$

where $m_i = -S, -S+1, \dots, S-1, S$

Each spin Hilbert space has dimension $(2S+1)$, so the total space will have dimension $(2S+1)^N$.

The difference between spin operators and Bosonic/Fermionic operators

Consider 2nd quantized Boson operators b_m for a lattice. They satisfy $[b_m, b_n^\dagger] = \delta_{mn}$. Now Fourier transform them

$$b_k^\dagger = \frac{1}{\sqrt{N}} \sum_m e^{-i k \cdot R_m} b_m^\dagger$$

we already know that $[b_k, b_q^\dagger] = \delta_{k,q}$.

But now try to do the same for spin operators. We start with S_m^x, S_m^y, S_m^z satisfying $[S_m^x, S_n^y] = i S_m^z \delta_{mn}$. Then we Fourier transform

$$S_k^\alpha = \frac{1}{\sqrt{N}} \sum_m e^{i k \cdot R_m} S_m^\alpha$$

We then get

$$[S_k^x, S_q^y] = \frac{1}{N} \sum_{m,n} e^{i (k \cdot R_m)} e^{i q \cdot R_n} \underbrace{[S_m^x, S_n^y]}_{i \delta_{mn} S_m^z}$$

$$= \frac{i}{N} \sum_m e^{i (k+q) \cdot R_m} S_m^z$$

Thus

$$\boxed{[S_k^x, S_q^y] = \frac{i}{\sqrt{N}} S_{k+q}^z}$$

This is not $S_k^z \delta_{k,q}$. In fact, this is no longer the algebra of angular momentum. For Bosons/Fermions, Fourier transforms preserve the algebra. For spin operators the algebra is completely messed up.

Now let's discuss how the spins interact with each other. The interaction can be either long ranged or short ranged. the long-ranged interaction is dipolar: each spin acts like a tiny magnetic dipole and therefore creates a magnetic field

$$\vec{B}_i(\mathbf{r}) = \frac{\mu}{4\pi}\left\{ \frac{3[(\mathbf{r}-\mathbf{R}_i)\cdot \mathbf{S}_i](\mathbf{r}-\mathbf{R}_i)}{|\mathbf{r}-\mathbf{R}_i|^5} - \frac{\mathbf{S}_i}{|\mathbf{r}-\mathbf{R}_i|^3}\right\} \qquad (3)$$

This is the field at position $\mathbf{r}$ produced by spin $\mathbf{S}_i$, which is at position $\mathbf{R}_i$. Every atom in the crystal feels this field. For instance, the energy of interaction between this field and spin $\mathbf{S}_j$ would be

$$-\mu\, \mathbf{S}_j \cdot \mathbf{B}_i(\mathbf{R}_j)$$

where μ is the magnetic moment.

The total energy will then be

$$U = -\mu \sum_{i \neq j} \mathbf{S}_j \cdot \mathbf{B}_i(\mathbf{R}_j)$$

or, written explicitly

$$U = -\frac{\mu^2}{8\pi} \sum_{i \neq j} \left\{ \frac{3[(\mathbf{R}_j-\mathbf{R}_i)\cdot \mathbf{S}_i][(\mathbf{R}_j-\mathbf{R}_i)\cdot \mathbf{S}_j]}{|\mathbf{R}_i-\mathbf{R}_j|^5} - \frac{\mathbf{S}_i\cdot \mathbf{S}_j}{|\mathbf{R}_j-\mathbf{R}_i|^3} \right\} \qquad (4)$$

As you can see, the dipolar interaction is very complicated. Not only is it a long ranged interaction, but it also has a very low symmetry. Moreover, even though the interaction decays as $1/r^3$, there is no simple criteria for when the interaction stops becomming significant.

Lucky for us, the dipolar interaction is not the most important interaction in magnetism. If it were, we would know much less about magnetism than we do nowadays.

Despite not being essential to magnetism, the dipolar interaction does play a role. In particular, it introduces a dependence on the shape of the particles. It is, for instance, the interaction responsible for making U-shaped magnets more stable than other shapes (this effect is called shape anisotropy).

The important interactions in magnetism are actually short ranged and are fully quantum mechanical in nature. they are related to the overlap between the localized wave-functions of the electrons. Hence, they fall very quickly with the distance and, most of the times, it suffices to consider only nearest neighbors.

There are several such interactions, which appear depending on the symmetries of your crystal. the most important are

$$\text{Heisenberg}: \quad \vec{S}_i \cdot \vec{S}_j \tag{5a}$$

$$\text{Ising}: \quad S_i^z S_j^z \tag{5b}$$

$$\text{XY}: \quad S_i^x S_j^x + S_i^y S_j^y \tag{5c}$$

$$\text{Dzyaloshinskii Moriya}: \quad \vec{D} \cdot (\vec{S}_i \times \vec{S}_j) \tag{5d}$$

(It took me 5 minutes to write the last one).

Let us try to understand them a bit. the most important one is the Heisenberg interaction. It is reasonable to expect that an interaction will be bilinear in S_i^α. that is, we expect to be able to write it as

$$\sum_{\alpha\beta} A_{\alpha\beta} S_i^\alpha S_j^\beta$$

All interactions in (5) are particular cases of this.

The reason why the Heisenberg interaction is the most important is because it is the only one which is isotropic: it depends only on the angle between the spins. An interaction like the Ising term $S_i^z S_j^z$ highlights z as a particular direction in space. Thus, interactions like Ising, XY or DM require a crystal effect to break the isotropy of space

It is also useful to think about them as if $\vec{S}_i$ was a classical vector with length S. Then $\vec{S}_i \cdot \vec{S}_j = S^2 \cos\theta_{ij}$ will depend only on the relative angle between the vectors. The Heisenberg interaction does not care about where the spins lie. All it cares about is their relative orientation.

To determine the GS, we need to know the sign of the interaction. We usually write the Heisenberg Hamiltonian as

$$\mathcal{H}_{ij} = -J \, \mathbf{S}_i \cdot \mathbf{S}_j$$

If $J > 0$ then we can lower the energy by making the spins parallel to each other. This is the ferromagnetic interaction. If $J < 0$ then we lower the energy by making the spins anti-parallel to each other, which is the anti-ferromagnetic case.

Ferromagnetic magnons

Let us consider ferromagnetic interactions between nearest neighbors in a d-dimensional hypercubic lattice

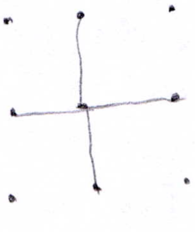
$$\boxed{\mathcal{H} = -J \sum_{\langle i,j\rangle} \mathbf{S}_i \cdot \mathbf{S}_j} \qquad (6)$$

where $J>0$. Here $\langle i,j\rangle$ means a sum over all nearest neighbors, without double counting.

Or we can write

$$\boxed{\mathcal{H} = -\frac{J}{2} \sum_{i} \sum_{j\in\Gamma_i} \mathbf{S}_i \cdot \mathbf{S}_j} \qquad (7)$$

where Γ_i stands for "the neighborhood of site i". Now I divided by 2 because we are double counting each term



Let us change the Heisenberg interaction a bit. Let

$$S_i^x = \frac{S_i^+ + S_i^-}{2}$$

$$S_i^y = \frac{S_i^+ - S_i^-}{2i} \qquad (8)$$

or

$$S_i^\pm = S_i^x \pm i S_i^y \qquad (9)$$

Now we write

$$\mathbf{S}_i \cdot \mathbf{S}_j = S_i^x S_j^x + S_i^y S_j^y + S_i^z S_j^z$$

$$= \frac{1}{4}(S_i^+ + S_i^-)(S_j^+ + S_j^-) - \frac{1}{4}(S_i^+ - S_i^-)(S_j^+ - S_j^-) + S_i^z S_j^z$$

$$= \frac{1}{2}(S_i^+ S_j^- + S_i^- S_j^+) + S_i^z S_j^z$$

Thus, we may also write the Hamiltonian as

$$\boxed{\mathcal{H} = -J \sum_{\langle ij \rangle} \left\{ \frac{S_i^+ S_j^- + S_i^- S_j^+}{2} + S_i^z S_j^z \right\}} \qquad (10)$$

Oops: I forgot to say. the $S_i^\pm$ satisfy the following algebra

$$\boxed{[S_i^z, S_j^\pm] = \pm \delta_{ij} S_i^\pm \qquad [S_i^+, S_j^-] = 2\delta_{ij} S_i^z} \qquad (11)$$

which is a direct consequence of (1).

The GS of this Hamiltonian is easy to figure out, classically we minimize the energy by making all spins parallel to each other. The actual direction does not matter, as long as they are parallel. We therefore expect that the GS will be highly degenerate. We can lift this degeneracy by adding a magnetic field

$$\boxed{\mathcal{H} = -J\sum_{\langle ij\rangle}' \mathbf{S}_i\cdot\mathbf{S}_j - h\sum_i' S_i^z} \qquad (12)$$

Now (at least classically) the GS will be around the z direction.

Let us then check if this continues to be true quantum mechanically. We define the FM state [cf. Eq (2)].

$$|FM\rangle = |S, S, \dots\rangle \quad (\text{all } m_i = S) \qquad (13)$$

This state satisfies

$$S_i^z\,|FM\rangle = S\,|FM\rangle \qquad (14)$$

Moreover, S_i^+ annihilates this state since S_i^+ is a ladder operator. Thus

$$(S_i^+ S_j^- + S_i^- S_j^+)|FM\rangle = 0 \qquad (15)$$

Hence, we conclude that

$$\mathcal{H}|FM\rangle = (-dJNS^2 - JSN)|FM\rangle = \mathcal{E}_{gs}|FM\rangle \qquad (16)$$

The FM state is therefore an eigenstate of $\mathcal{H}$. We can know it is also the GS because the spin operators are bounded, so there is no way of making the energy smaller.

For the FM Heisenberg model we therefore know the GS. Now let us try to describe the <u>excitations</u> <u>above</u> <u>the</u> <u>GS</u>. To do that we shall use a method developed by <u>Holstein</u> and <u>Primakoff</u>. It consists in mapping the spin operators into Boson operators.

The idea is that the two are quite similar, with one main difference: the spin ladder is bounded on both sides, whereas the boson ladder is only bounded on one side:

Bosons : $m = 0, 1, 2, 3, \ldots$

Spin : $m = S, S-1, S-2, \ldots, -S$

But suppose we are only interested in staying close to $m=S$, then what happens at $-S$ is irrelevant, specially when S is large.

The HP transformation maps the excitations away from $m=S$ into Boson excitations. The transformation is

$$\boxed{\begin{aligned} S^z &= S - a^\dagger a & (17a)\\ S^+ &= \sqrt{2S - a^\dagger a}\; a & (17b)\\ S^- &= a^\dagger \sqrt{2S - a^\dagger a} & (17c)\end{aligned}}$$

where $[a, a^\dagger] = 1$.

This mapping is exact, but we will see in a second that it is only useful if used as an approximation.

The spin quantum number m is now mapped into

$$m = S - n, \qquad n = 0, 1, 2, \dots \tag{18}$$

Thus, zero Boson excitations mean we are in the $m = +S$ state and the larger is the number of Boson excitations the further we are from $m = +S$.

We can check that (17) is exact by checking that they preserve the algebra (11). For instance

$$\begin{aligned}[S^+, S^-] &= \sqrt{2S - a^\dagger a}\; a\, a^\dagger \sqrt{2S - a^\dagger a} \quad + \\ &\quad - a^\dagger \sqrt{2S - a^\dagger a}\,\sqrt{2S - a^\dagger a}\; a\end{aligned}$$

In the first term, $a a^\dagger = 1 + a^\dagger a$ which commutes with $\sqrt{2S - a^\dagger a}$. Thus

$$\begin{aligned}[S^+, S^-] &= a a^\dagger (2S - a^\dagger a) - a^\dagger (2S - a^\dagger a) a \\ &= 2S \underbrace{(a a^\dagger - a^\dagger a)}_{1} - a a^\dagger a^\dagger a + a^\dagger a^\dagger a a \\ &= 2S + a^\dagger a^\dagger a a - (1 + a^\dagger a) a^\dagger a \\ &= 2S + a^\dagger a^\dagger a a - a^\dagger a - a^\dagger (1 + a^\dagger a) a \\ &= 2S - 2 a^\dagger a \\ &= 2 (S_z)\end{aligned}$$

I will leave the other commutation as an exercise.

The fact that the HP transformation contains the square root of an operator makes it very difficult to make exact calculations. It's usefulness lies in approximating the square root when $2S \gg a^\dagger a$. We use the Taylor expansion

$$\sqrt{1-x} \simeq 1 - \frac{x}{2} - \frac{x^2}{8} + \dots \qquad (19)$$

to write

$$\sqrt{2S - a^\dagger a} = \sqrt{2S}\sqrt{1 - \frac{a^\dagger a}{2S}}$$

$$\simeq \sqrt{2S}\left\{1 - \frac{1}{2}\frac{a^\dagger a}{2S} - \frac{1}{8}\frac{(a^\dagger a)^2}{(2S)^2} + \dots\right\}$$

or

$$\boxed{\sqrt{2S - a^\dagger a} \simeq \sqrt{2S} - \frac{1}{2}\frac{a^\dagger a}{\sqrt{2S}} - \frac{1}{8}\frac{(a^\dagger a)^2}{(2S)^{3/2}} - \dots} \qquad (20)$$

If $2S$ is large we see that higher order terms will become smaller and smaller. Funny enough, sometimes even $S = 1/2$ (with $2S = 1$) can be considered large!

Going back to (17), we now have

$$S^{+} \simeq \sqrt{2S}\, a - \frac{1}{2}\frac{a^{\dagger} a a}{\sqrt{2S}}$$

$$S^{-} \simeq \sqrt{2S}\, a^{\dagger} - \frac{1}{2}\frac{a^{\dagger} a^{\dagger} a}{\sqrt{2S}} \qquad (21)$$

Now let us go back to the full Hamiltonian (10) or (12). We do a HP transformation for each spin. Thus, to each site we attribute a Boson operator a_i. We then get

$$S_i^z S_j^z = (S - a_i^{\dagger} a_i)(S - a_j^{\dagger} a_j)$$

$$= S^2 - S(a_i^{\dagger} a_i + a_j^{\dagger} a_j) - a_i^{\dagger} a_i a_j^{\dagger} a_j$$

$$S_i^{+} S_j^{-} = \left\{ \sqrt{2S}\, a_i - \frac{1}{2}\frac{a_i^{\dagger} a_i a_i}{\sqrt{2S}} \right\}\left\{ \sqrt{2S}\, a_j^{\dagger} - \frac{1}{2}\frac{a_j^{\dagger} a_j^{\dagger} a_j}{\sqrt{2S}} \right\}$$

$$= 2S\, a_i a_j^{\dagger} - \frac{1}{2}\left[a_i a_j^{\dagger} a_j^{\dagger} a_j + a_i^{\dagger} a_i a_i a_j^{\dagger} \right]$$

$$+ \frac{1}{4}\frac{a_i^{\dagger} a_i a_i a_j^{\dagger} a_j^{\dagger} a_j}{2S}$$

Notice how the terms in both results are ordered by $2S$. Terms which are quadratic in a have a factor $2S$. Quartic terms have have $(2S)^0$ and sextic terms (no sex joke implied) have $(2S)^{-1}$.

If we stop at quadratic terms, the Hamiltonian (12) becomes

$$\mathcal{H} = -dJS^2N - hSN - JS\sum_{\langle i,j\rangle}\left\{ a_i^\dagger a_j + a_j^\dagger a_i - a_i^\dagger a_i - a_j^\dagger a_j \right\} + h\sum_i a_i^\dagger a_i$$

We see here the GS energy $\mathcal{E}_{gs}$ in (16). Let us also organize this a bit. For instance

$$JS\sum_{\langle i,j\rangle} a_i^\dagger a_i = \frac{JS}{2}\sum_i \sum_{j\in\Gamma_i} a_i^\dagger a_i = \frac{JS}{2}(2d)\sum_i a_i^\dagger a_i$$

where I used the fact that, in a d-dimensional hypercubic lattice, the neighborhood of a site has $2d$ neighbors (for instance $d=2$ has 4 neighbors). Similarly, the term $a_j^\dagger a_j$ will give the same result. Thus we can write

$$\boxed{\mathcal{H} = \mathcal{E}_{gs} + (h + 2JdS)\sum_i a_i^\dagger a_i - JS\sum_{\langle i,j\rangle}(a_i^\dagger a_j + a_j^\dagger a_i)} \tag{22}$$

This is nothing but a tight-binding Hamiltonian!

We diagonalize it like we always do:

$$a_i^\dagger = \frac{1}{\sqrt{N}} \sum_{\mathbb{k}} e^{i \mathbb{k} \cdot \mathbb{R}_i} a_{\mathbb{k}} \qquad (23)$$

Then, like we have done a million times before

$$\sum_i a_i^\dagger a_i = \sum_{\mathbb{k}} a_{\mathbb{k}}^\dagger a_{\mathbb{k}} \qquad (24)$$

and

$$\sum_{\langle i,j \rangle} a_i^\dagger a_j + a_j^\dagger a_i = \frac{1}{2} \sum_i \sum_{j \in \Gamma_i} (a_i^\dagger a_j + a_j^\dagger a_i)$$

$$= \sum_i \sum_{j \in \Gamma_i} a_i^\dagger a_j$$

$$= \sum_i \sum_{j \in \Gamma_i} \frac{1}{N} \sum_{\mathbb{k} \mathbb{q}} e^{i \mathbb{k} \cdot \mathbb{R}_i} e^{-i \mathbb{q} \cdot \mathbb{R}_j} a_{\mathbb{k}}^\dagger a_{\mathbb{q}}$$

Write $\mathbb{R}_j = \mathbb{R}_i + \mathbb{r}_j$, then

$$\sum_{\langle i,j \rangle} a_i^\dagger a_j + a_j^\dagger a_i = \sum_{\mathbb{k}} \left[2\cos k_1 a + \ldots + 2\cos k_d a \right] a_{\mathbb{k}}^\dagger a_{\mathbb{k}}$$

Thus we get

$$\boxed{\mathcal{H} = E_{gs} + \sum_{k} \epsilon_k a_k^\dagger a_k} \tag{25}$$

where

$$\boxed{\epsilon_k = h + 2JS\left(d - \sum_{i=1}^{d} \cos k_i a\right)} \tag{26}$$

We have found that the excitations above the FM ground-state behave like Bosons with a dispersion relation ϵ_k. These are the magnons, or the quanta of spin waves.

At long wavelengths we may expand

$$d - \sum_i \cos k_i a \simeq \frac{a^2}{2} |k|^2$$

thus we get

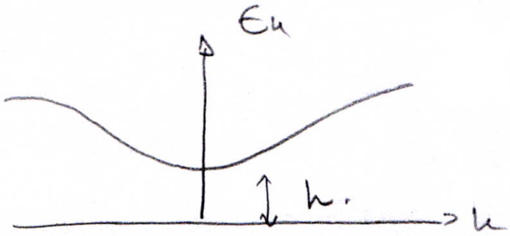
$$\boxed{\epsilon_k \simeq h + JSa^2 |k|^2} \tag{27}$$

This is a quadratic (non-relativistic) dispersion relation. Magnons therefore behave like a massive particle with

$$\frac{1}{2m} = JSa^2 \rightarrow m = \frac{1}{2JSa^2} \qquad (28)$$

Larger interaction constants J, or larger spins S, make the mass larger.

We see also that the magnetic field h plays the role of an <u>energy gap</u>.



If we had kept quartic terms in our HP expansion in page 14, we would get terms describing the interaction of magnons

$$\boxed{\mathcal{H}_{int} = J \sum_{\langle ij \rangle} \left\{ a_i^\dagger a_i a_j^\dagger a_j + \frac{1}{4} \left(a_j^\dagger a_j^\dagger a_i a_j + a_i^\dagger a_j^\dagger a_i a_i \right) \right\}} \quad (29)$$

This term describes the scattering between magnons. But note that we always have 2 annihilations and 2 creations. The Heisenberg interaction conserves the number of magnons. Other interactions, like the dipolar, do not. They therefore appear as 3 body terms, where 2 magnons go in, but only one comes out.

Thermal properties

Since magnons are bosons, the average number of magnons with momentum $\mathbb{k}$ will be given by

$$\bar{n}_{\mathbb{k}} = \frac{1}{e^{\beta \epsilon_{\mathbb{k}}} - 1} \qquad (30)$$

there is no chemical potential because the number of magnons is free to vary

the total numbers of magnons is then

$$\langle \hat{N} \rangle = \left(\frac{L}{2\pi}\right)^d \int d^d\mathbb{k} \; \bar{n}_{\mathbb{k}} \qquad (31)$$

this quantity is important because it is related to the magnetization

$$M = \sum_i \langle S_i^z \rangle \qquad (32)$$

Using (17a) we get

$$M = NS - \langle \hat{N} \rangle \qquad (33)$$

[N is the number of sites].

The integral in (31) is d-dimensional, so we may write

$$\int d^d k = \int d\Omega \, dk \, k^{d-1} \tag{34}$$

where $d\Omega$ is the d-dimensional solid angle. Let us assume that $h=0$ and approximate the dispersion by $\epsilon_k \approx k^2/2m$. We then get

$$\langle \hat{N} \rangle = \left(\frac{L}{2\pi}\right)^d S_d \int_0^\infty dk \, \frac{k^{d-1}}{e^{\beta k^2/2m} - 1} \tag{35}$$

where S_d is the surface area of a d-dimensional sphere

$$S_d = \frac{2\pi^{d/2}}{\Gamma(d/2)} \tag{36}$$

Now change variables to $x = \beta k^2/2m$. Then $k = \sqrt{\frac{2m}{\beta}}\sqrt{x}$ and

$$dk\, k^{d-1} = \left(\frac{2m}{\beta}\right)^{d/2} \frac{dx}{2\sqrt{x}} \, x^{\frac{d-1}{2}} = \left(\frac{2m}{\beta}\right)^{d/2} \frac{dx}{2} x^{\frac{d}{2}-1}$$

Eq (35) then becomes

$$\langle \hat{N} \rangle = \frac{S_d}{2} \left(\frac{L}{2\pi}\right)^d \left(\frac{2m}{\beta}\right)^{d/2} \int_0^\infty dx \, \frac{x^{\frac{d}{2}-1}}{e^x - 1} \tag{37}$$

But now note the following. Close to $x = 0$ we may expand $e^{x} - 1 \simeq x$. Then we will be integrating $x^{\frac{d}{2}-2}$. If $d = 2$ this is an integral of x^{-1}, which is $\ln x$ and hence diverges as $x \to 0$. The same happens for $d=1$. For $d=3$ the integral remains finite. In fact

$$\int_{0}^{\infty} dx \, \frac{x^{1/2}}{e^{x}-1} = \frac{\sqrt{\pi}}{2} \zeta(3/2) = 2{,}315\,16 \qquad (38)$$

We therefore reach a very important conclusion; for $d = 1$ or 2, any thermal fluctuation would make $\langle N \rangle$ insanely high. This will break our HP approximation. and therefore completely destroy the FM order.

This is an instance of the Mermin-Wagner theorem: systems with continuous symmetries cannot present an ordered phase when $d \leqslant 2$.

For $d=3$ we do obtain an ordered phase. Indeed, plugging (38) in (37) we get $[S_3 = 4\pi]$

$$\langle \hat{N} \rangle = \frac{4\pi}{2} \frac{V}{(2\pi)^3} (2mT)^{3/2} \frac{\sqrt{\pi}}{2} \zeta(3/2) \tag{39}$$

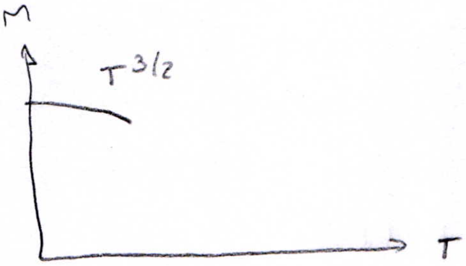
the important part of this result is the temperature dependence

$$\langle \hat{N} \rangle \sim T^{3/2} \tag{40}$$

this means that close to $T=0$ the magnetization falls as

$$M \simeq M_0 - \text{const} \times T^{3/2} \tag{41}$$

which is known as the $T^{3/2}$ - law (a very creative name).



this law is actually verified experimentally.

We can do a similar analysis for the energy, in order to compute the specific heat. We have

$$U = \langle \mathcal{H} \rangle = \frac{V}{(2\pi)^3} \int d^3k \; \frac{k^2}{2m} \; \frac{1}{e^{\beta k^2/2m} - 1}$$

$$= \frac{V}{(2\pi)^3} 4\pi \int dk \; \frac{k^4}{2m} \; \frac{1}{e^{\beta k^2/2m} - 1}$$

Again we change variables to $x = \beta k^2/2m$. Then $dk\, k^4$ will give us a factor $(2m/\beta)^{\frac{1+4}{2}}$, which means

$$U \sim T^{5/2} \tag{42}$$

the specific heat will then be

$$c \sim T^{3/2} \tag{43}$$

This is the magnon contribution to the specific heat. It can be verified experimentally.

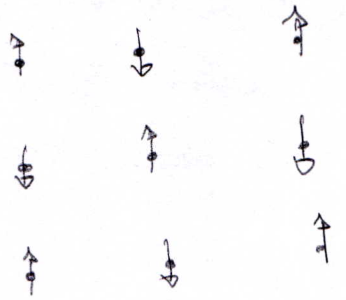
Antiferromagnetic magnons

we now consider the Heisenberg model with anti-ferromagnetic interactions

$$\mathcal{H} = \frac{J}{2}\sum_{i}\sum_{j\in\Gamma_i} \mathbf{S}_i \cdot \mathbf{S}_j \qquad (44)$$

where $J>0$. Again, we consider a d-dimensional hypercubic lattice.

Classically, each term in (44) can be minimized by making the spins anti-parallel to each other. For instance, in a square lattice we can make this happen by putting



This is called the Néel state

$$|N\rangle = |S, -S, S, -S, \ldots\rangle \qquad (45)$$

However, the Néel state is not an eigenstate of Eq (44) that can be seen by writting (44) as

$$\mathcal{H} = -\frac{J}{2}\sum_{i}\sum_{j\in\Gamma_i}\left\{\frac{S_i^+ S_j^- + S_i^- S_j^+}{2} + S_i^z S_j^z\right\} \qquad (46)$$

the terms $S_i^+ S_j^-$ and $S_i^- S_j^+$ didn't contribute when we were dealing with the FM case because they gave zero when acting on $|FM\rangle$. But they will not give zero when acting on N. For instance

$$S_1^+ S_2^- |S,-S\rangle = 0$$

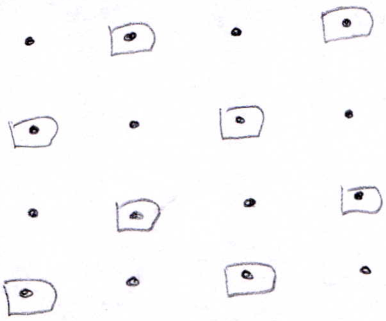
But

$$S_1^- S_2^+ |S,-S\rangle \propto |S-1,-S+1\rangle$$

Thus, the Néel state is not an eigenstate of $\mathcal{H}$. Notwithstanding, it should not be insanely far from the true GS since, at least in the classical case it works.

We will therefore take the Néel state as a starting point and expand around it using the HP method.

We proceed as follows. We take for concreteness the square lattice. The results are readily generalized to other dimensions. The square lattice is a *bi-partite* lattice, meaning it can be divided into two sub-lattices, like a *checkerboard*. We call them the even ($\underline{e}$) and odd (o) sub lattices



We assume that in $|N\rangle$ of Eq (45), $+S$ refers to $\underline{e}$ and $-S$ refers to $\underline{o}$. Of course, we could have chosen it the other way around.

For spins in $\underline{e}$, we want to do a HP expansion around $+S$, so we set

$$i \in e \qquad \begin{aligned} S_i^z &= S - a_i^\dagger a_i \\ S_i^+ &= \sqrt{2S}\, a_i \\ S_i^- &= \sqrt{2S}\, a_i^\dagger \end{aligned} \tag{47}$$

But for spins in $\underline{o}$ we want an expansion around $-S$, so we set

$$
i \in o \qquad
\begin{aligned}
S_i^z &= -S + b_i^\dagger b_i \\
S_i^+ &= \sqrt{2S}\, b_i^\dagger \\
S_i^- &= \sqrt{2S}\, b_i
\end{aligned}
\qquad (48)
$$

Since the sum in (44) is over nearest neighbors, we will always have terms where $i \in \underline{e}$, $j \in \underline{o}$ and vice-versa. Let's sepparate (44) as

$$
\mathcal{H} = \frac{J}{2} \sum_{i \in e} \sum_{j \in \Gamma_i} \mathbf{S}_i \cdot \mathbf{S}_j + \frac{J}{2} \sum_{i \in o} \sum_{j \in \Gamma_i} \mathbf{S}_i \cdot \mathbf{S}_j \qquad (49)
$$

In the first term $i \in e$ and $j \in o$. Then we will have

$$
\begin{aligned}
\mathbf{S}_e \cdot \mathbf{S}_o &= \frac{S_e^+ S_o^- + S_e^- S_o^+}{2} + S_e^z S_o^z \\
&= \frac{2S}{2} \left(a_e b_o + a_e^\dagger b_o^\dagger \right) + \left(S - a_e^\dagger a_e \right) \left(-S + b_o^\dagger b_o \right) \\
&= -S^2 + S \left(a_e b_o + a_e^\dagger b_o^\dagger + a_e^\dagger a_e + b_o^\dagger b_o \right)
\end{aligned}
$$

Thus we get

$$\mathcal{H} = \underbrace{-\alpha J S^2 N}_{\substack{\mathcal{E}_N \\ \text{(Néel energy)}}} + \frac{JS}{2}\sum_{i\in e}\sum_{j\in\Gamma_i}\left\{a_i^\dagger a_i + b_j^\dagger b_j + a_i b_j + b_j^\dagger a_i\right\}$$

$$+ \frac{JS}{2}\sum_{i\in o}\sum_{j\in\Gamma_i}\left\{b_i^\dagger b_i + a_j^\dagger a_j + b_i a_j + a_j^\dagger b_i^\dagger\right\}$$

But if you think about it for a second, the second sum is the same as the first. So we may write

$$\boxed{\mathcal{H} = \mathcal{E}_N + JS\sum_{i\in e}\sum_{j\in\Gamma_i}\left\{a_i^\dagger a_i + b_j^\dagger b_j + a_i b_j + b_j^\dagger a_i\right\}} \quad (50)$$

Now, as always, we move to Fourier space by defining

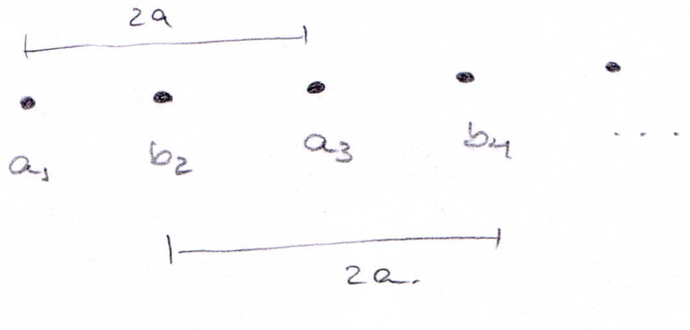
$$a_i^\dagger = \frac{1}{\sqrt{N}}\sum_{k} e^{i k\cdot R_i}\, a_k \qquad (51)$$

$$b_j^\dagger = \frac{1}{\sqrt{N}}\sum_{k} e^{-i k\cdot R_j}\, b_k$$

where we defined one with the + sign and the other with the - sign, just for convenience.

We must also ask what are the allowed values of k.

For instance in 1 D the a_i and b_i alternate

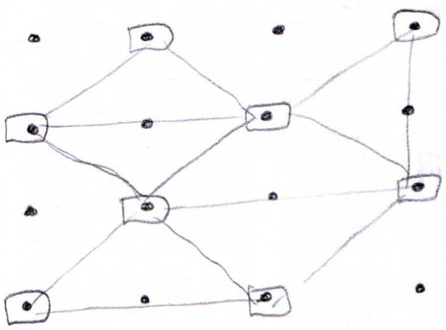


Thus, the unit cell for each interaction actually has spacing 2a. So for 1D we would get

$$k \in \left[-\frac{\pi}{2a}, \frac{\pi}{2a}\right]$$

The Brillouin zone is therefore half the size as for a regular crystal.

In 2D and 3D things are more complicated. For instance in 2D



In 2D the $\underline{c}$ sub-lattice is therefore a centered rectangular lattice. In 3D the sub-lattices of a simple cubic is an FCC.

That is all to say that the k quantization will be different. But lucky for us, we don't need to know exactly how the k's are quantized.

Plugging (51) in (50) we get

$$\sum_{i\in e}\sum_{j\in\Gamma_i} a_i^{\dagger} a_j = 2d\sum_{\mathbf{k}} a_{\mathbf{k}}^{\dagger} a_{\mathbf{k}}$$

$$\sum_{i\in e}\sum_{j\in\Gamma_i} b_j^{\dagger} b_j = 2d\sum_{\mathbf{k}} b_{\mathbf{k}}^{\dagger} b_{\mathbf{k}}$$

$$\sum_{i\in e}\sum_{j\in\Gamma_i} a_i b_j = \sum_{i\in e}\sum_{j\in\Gamma_i}\frac{1}{N}\sum_{\mathbf{k}\mathbf{q}} e^{i(\mathbf{k}\cdot\mathbf{R}_i-\mathbf{q}\cdot\mathbf{R}_j)} a_{\mathbf{k}}^{\dagger} b_{\mathbf{q}}$$

Now we let $\mathbf{R}_j = \mathbf{R}_i + \delta_i$, where δ_i are the nearest-neighbors of i, ie, $\pm\hat{x}$, $\pm\hat{y}$, etc. then

$$\sum_{i\in e}\sum_{j\in\Gamma_i} a_i b_j = \sum_{i\in e}\sum_{\delta_i}\frac{1}{N}\sum_{\mathbf{k}\mathbf{q}} e^{i(\mathbf{k}-\mathbf{q})\cdot\mathbf{R}_i} e^{-i\mathbf{q}\cdot\delta_i} a_{\mathbf{k}} b_{\mathbf{q}}$$

$$= \sum_{\mathbf{k}}\left[\sum_{\delta_i} e^{-i\mathbf{k}\cdot\delta_i}\right] a_{\mathbf{k}} b_{\mathbf{k}}$$

we define

$$\boxed{\gamma_{\mathbf{k}} = \frac{1}{2d}\sum_{\delta_i} e^{-i\mathbf{k}\cdot\delta_i} = \frac{1}{d}(\cos k_1 a + \dots + \cos k_d a)} \qquad (52)$$

then

$$\sum_{i\in e}\sum_{j\in\Gamma_i} a_i b_j = 2d\sum_{\mathbf{k}} \gamma_{\mathbf{k}} a_{\mathbf{k}} b_{\mathbf{k}} \qquad (53)$$

Thus, the Hamiltonian becomes

$$\boxed{\mathcal{H} = \mathcal{E}_N + 2dJS\sum_{k}\left\{a_k^{+}a_k + b_k^{+}b_k + \gamma_k\left(a_k b_k + b_k^{+}a_k^{+}\right)\right\}} \qquad (54)$$

This Hamiltonian is not yet diagonal. To diagonalize it, we must now do a <u>Bogoliubov transformation</u>.

Consider the simpler Hamiltonian

$$H = a^{+}a + b^{+}b + \gamma(ab + b^{+}a^{+}) \qquad (55)$$

Now let

$$\begin{aligned} a &= u\alpha - v\beta^{+} \\ b^{+} &= v\alpha - u\beta^{+} \end{aligned} \qquad (56)$$

In order for α, β to be Bosonic operators, we require that

$$u^2 - v^2 = 1 \qquad (57)$$

Now we have

$$\begin{aligned} a^{+}a &= (u\alpha^{+} - v\beta)(u\alpha - v\beta^{+}) \\ &= u^2\alpha^{+}\alpha + v^2\beta\beta^{+} - uv(\alpha^{+}\beta^{+} + \beta\alpha) \end{aligned}$$

$$\begin{aligned} b^{+}b &= (v\alpha - u\beta^{+})(v\alpha^{+} - u\beta) \\ &= v^2\alpha\alpha^{+} + u^2\beta^{+}\beta - uv(\alpha\beta + \beta^{+}\alpha^{+}) \end{aligned}$$

$$ab = (u\alpha - v\beta^\dagger)(v\alpha^\dagger - u\beta)$$

$$= uv(\alpha\alpha^\dagger + \beta^\dagger\beta) - u^2\alpha\beta - v^2\beta^\dagger\alpha^\dagger$$

$$b^\dagger a^\dagger = uv(\alpha\alpha^\dagger + \beta^\dagger\beta) - u^2\alpha^\dagger\beta^\dagger - v^2\alpha\beta.$$

Thus

$$H = u^2\alpha^\dagger\alpha + v^2\alpha\alpha^\dagger + 2\kappa uv\,\alpha\alpha^\dagger$$

$$+ v^2\beta\beta^\dagger + u^2\beta^\dagger\beta + 2\kappa uv\,\beta^\dagger\beta$$

$$-\left[2uv + \kappa(u^2 + v^2)\right](\alpha\beta + \beta^\dagger\alpha) \qquad (57')$$

To make this diagonal we choose

$$2uv = -\kappa(u^2 + v^2)$$

we know that $\kappa > 0$ so uv must be negative. Now square this and use the fact that $u^2 = 1 + v^2$ to get

$$4(1 + v^2)v^2 = \kappa^2(1 + 2v^2)^2$$

$$= \kappa^2(1 + 4v^2 + 4v^4)$$

$$(4\kappa^2 - 4)v^4 + (4\kappa^2 - 4)v^2 + \kappa^2 = 0$$

$$v^4 + v^2 + \frac{\kappa^2}{4\kappa^2 - 4} = 0$$

Thus

$$v^2 = -\frac{1}{2} \pm \frac{1}{2}\sqrt{1 - \frac{4x^2}{4x^2-4}}$$

$$= -\frac{1}{2} \pm \frac{1}{2}\sqrt{\frac{4}{4-4x^2}} = -\frac{1}{2} \pm \frac{1}{2}\sqrt{\frac{1}{1-x^2}}$$

We must choose the positive root since we assumed v was real. We also see that we must have $x^2 < 1$, which is actually true for (52). Thus

$$v^2 = \frac{1}{2}\left\{\sqrt{\frac{1}{1-x^2}} - 1\right\} \qquad (58)$$

Then $u^2 = 1 + v^2$ so

$$u^2 = \frac{1}{2}\left\{\sqrt{\frac{1}{1-x^2}} + 1\right\} \qquad (59)$$

and

$$u^2 v^2 = \frac{1}{4}\left\{\frac{1}{1-x^2} - 1\right\} = \frac{1}{4}\left\{\frac{x^2}{1-x^2}\right\}$$

Since we chose uv negative, we have

$$2uv = -\frac{x}{\sqrt{1-x^2}} \qquad (60)$$

Also

$$u^2 + v^2 = -\frac{2uv}{x} = \frac{1}{\sqrt{1-x^2}} \qquad (61)$$

The Hamiltonian (57') then becomes

$$H = (u^2 + v^2 + 2\chi u v)(\alpha^\dagger\alpha + \beta^\dagger\beta) + 2v^2 + 2\chi u v$$

$$= \left\{ \frac{1}{\sqrt{1-\chi^2}} - \frac{\chi^2}{\sqrt{1-\chi^2}} \right\} (\alpha^\dagger\alpha + \beta^\dagger\beta) +$$

$$+ \left\{ \frac{1}{\sqrt{1-\chi^2}} - 1 \right\} - \frac{\chi^2}{\sqrt{1-\chi^2}}$$

$$= \sqrt{1-\chi^2}\,(\alpha^\dagger\alpha + \beta^\dagger\beta) + \left(\sqrt{1-\chi^2} - 1\right)$$

Let us summarize our result:

$$\boxed{\begin{aligned} H &= a^\dagger a + b^\dagger b + \chi(ab + b^\dagger a^\dagger) \\ &= \sqrt{1-\chi^2}\,(\alpha^\dagger\alpha + \beta^\dagger\beta) + \left(\sqrt{1-\chi^2} - 1\right) \end{aligned}} \qquad (62)$$

where

$$\boxed{\begin{gathered} a = u\alpha - v\beta^\dagger \\ b^\dagger = v\alpha - u\beta^\dagger \\ v^2 = \frac{1}{2}\left(\frac{1}{\sqrt{1-\chi^2}} - 1\right) \qquad u^2 = \frac{1}{2}\left(\frac{1}{\sqrt{1-\chi^2}} + 1\right) \\ 2uv = -\frac{\chi}{\sqrt{1-\chi^2}} \qquad u^2 + v^2 = \frac{1}{\sqrt{1-\chi^2}} \end{gathered}} \qquad (63)$$

This is the summary of a Bogoliubov transformation for Bosons. Now we go back to (54). we have

$$\mathcal{H} = \mathcal{E}_N + 2dJS\sum_{k}\left\{\sqrt{1-\gamma_k^2}\,(\alpha_k^\dagger\alpha_k + \beta_k^\dagger\beta_k) + \left(\sqrt{1-\gamma_k^2}-1\right)\right\}$$

we define

$$\boxed{\mathcal{E}_{gs} = \mathcal{E}_N + 2dJS\sum_{k}\left(\sqrt{1-\gamma_k^2}-1\right)} \tag{64}$$

and

$$\boxed{\epsilon_k = 2dJS\sqrt{1-\gamma_k^2}} \tag{65}$$

then we may finally write

$$\boxed{\mathcal{H} = \mathcal{E}_{gs} + \sum_{k}\epsilon_k\,(\alpha_k^\dagger\alpha_k + \beta_k^\dagger\beta_k)} \tag{66}$$

Woo! we did it! High 5!

Now let us analyze our result. For long wavelengths

$$\gamma_k \simeq 1 - \frac{a^2}{d}k^2$$

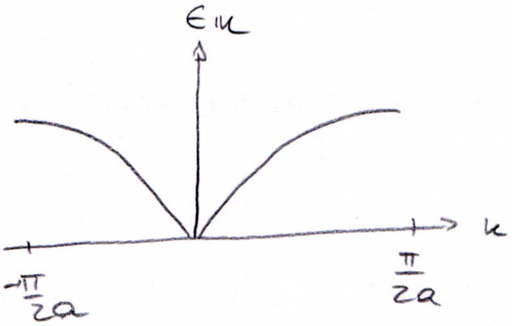
so

$$\begin{aligned} 1-\gamma_k^2 &\simeq 1-\left(1-\frac{a^2k^2}{d}\right)^2 \\ &\simeq 1-1+\frac{2a^2k^2}{d} \\ &= \frac{2a^2k^2}{d} \end{aligned}$$

Thus we conclude that

$$\epsilon_k \simeq 2dJS\sqrt{\frac{2a^2}{d}}\,|k|$$

The dispersion is now linear! This is completely different from the FM case. In fact, in 1D we now have



A linear dispersion relation is like a phonon system. Thus, antiferromagnetic magnons should contribute to the specific heat a term proportional to T^3, instead of $T^{3/2}$ as observed for FM magnons. This is indeed observable experimentally.

Another nice thing we can do is this. Consider $S=1/2$ in $d=1$. then the E_{GS} in (64) becomes

$$E_{GS} = -dJS^2N + 2dJS \sum_k{}' \left(\sqrt{1-\cos^2 k} - 1\right)$$

$$d=1,\ S=1/2$$

$$= -\frac{1}{4}NJ + \frac{NJ}{2\pi}\int_{-\pi/2}^{\pi/2} dk \left\{\sqrt{1-\cos^2 k} - 1\right\}$$

this integral can be done analytically and has the value

$$\frac{1}{2\pi}\int_{-\pi/2}^{\pi/2} dk \left\{\sqrt{1-\cos^2 k} - 1\right\} = \frac{1}{\pi} - \frac{1}{2}$$

Now, the Néel energy is

$$\frac{E_N}{NJ} = -\frac{1}{4} = -0.25$$

whereas our GS energy is

$$\frac{E_{GS}}{NJ} = -\frac{1}{4} + \frac{1}{\pi} - \frac{1}{2} = -0.43169$$

This energy can actually be found exactly (only for $S=1/2$ and only for $d=1$) and has the value -0.443147. Thus we see that our results are quite close. This is remarkable given the fact that the HP expansion should be good for $2S$ large. We are thus expanding for 1 as a large number!