Kapitel 3

Collective magnetism

In this chapter, we will investigate the effect of the interaction between particles on magnetism. Magnetic phase transitions cannot be explained without including interactions. We will show that the Coulomb repulsion is fundamentally important for understanding collective magnetism.

3.1 Dipole-dipole interaction

Let us first consider the magnetostatic energy between two magnetic dipoles $\vec{\mu}_1$ and $\vec{\mu}_2$:

$$U_{\text{dipole-dipole}} = \frac{1}{r^3}\left[\vec{\mu}_1 \cdot \vec{\mu}_2 - 3(\vec{\mu} \cdot \vec{n})(\vec{\mu}_2 \cdot \vec{n})\right],$$

where $r\vec{n}$ is the position vector between the two magnetic dipoles. Approximately,

$$U_{\text{dipole-dipole}} \approx \frac{\mu_1 \mu_2}{r^3}.$$

With

$$\mu_1 \sim \mu_2 \sim g\mu_B \sim \frac{e\hbar}{m} \qquad \text{and} \qquad r \approx 2\ \mathring{A},$$

one obtains ($a_0 = \frac{\hbar^2}{me^2}$ is the Bohr radius):

$$U \sim \frac{(g\mu_B)^2}{r^3} \sim \left(\frac{e^2}{\hbar c}\right)^2 \left(\frac{a_0}{r}\right)^3 \frac{e^2}{a_0} \sim 10^{-4}\ \text{eV} \sim 1\ \text{K}.$$

This interaction is too weak to explain magnetic ordering!

3.2 Hubbard Model and Mott Insulators

In previous chapters, you have seen that the Hamiltonian for electrons interacting via the Coulomb interaction is written:

$$\hat{H} = -\frac{\hbar^2}{2m}\sum_{\alpha}\nabla_{\alpha}^2 + \frac{1}{2}\sum_{i\neq j}\frac{e^2}{|\vec{r}_\alpha - \vec{r}_\beta|}$$

An approximation of this Hamiltonian was motivated by John Hubbard in a series of papers from 1963 to 1967 entitled "Electron Correlations in Narrow Energy Bands".

Consider a crystal of Hydrogen atoms, where there is only one electron per atom (on average), and only the lowest electronic band is half-filled. Hubbard asked what would happen as we increase the distance between atoms by stretching the lattice? In this limit, the electron density would become increasingly localized around the atomic cores, which we label by an index i. Since the strength Coulomb repulsion decreases with distance between electrons as $1/|r_\alpha - r_\beta|$, the interaction is much stronger for two electrons occupying the same atomic site, compared to electrons occupying different sites.

This motivates an approximation, known as the Hubbard model, where we consider only short-ranged on-site Coulomb interactions:

$$\begin{aligned}\hat{H} &= \sum_{\vec{k},\sigma} \varepsilon_{\vec{k}} c^\dagger_{\vec{k}\sigma} c_{\vec{k}\sigma} + U \sum_i c^\dagger_{i\uparrow} c_{i\uparrow} c^\dagger_{i\downarrow} c_{i\downarrow} \\ &= t \sum_{i,\sigma} \sum_{\text{n.n. } \delta} c^\dagger_{i\sigma} c_{i+\delta,\sigma} + U \sum_i c^\dagger_{i\uparrow} c_{i\uparrow} c^\dagger_{i\downarrow} c_{i\downarrow},\end{aligned}$$

where

$$c_{i\sigma} = \frac{1}{\sqrt{N}} \sum_{\vec{k}} e^{i\vec{k}\vec{R}_i} c_{\vec{k}\sigma}, \qquad c^\dagger_{i\sigma} = \frac{1}{\sqrt{N}} \sum_{\vec{k}} e^{-i\vec{k}\vec{R}_i} c^\dagger_{\vec{k}\sigma}$$

Let us consider the ground state of this Hamiltonian in different limits.

1. Limit $U/t \to 0$:

   In the limit of weak electron-electron interactions, the ground state is analogous to the non-interacting electron gas. We fill the single-particle states up to the Fermi wavevector:

   $$|\Psi_0\rangle = \prod_{k \le k_F} c^\dagger_{k\uparrow} c^\dagger_{k\downarrow} |\text{Vacuum}\rangle$$

   Note that this ground state is unique. Since there are no interactions between electrons, their positions are not correlated with eachother. Each atomic site has a 1/4 probability of being either (i) empty, (ii) occupied with a single spin-up electron, (iii) occupied with a single spin-down electron, or (iv) occupied with two electrons. For this reason $\langle c^\dagger_{i\uparrow} c_{i\uparrow} c^\dagger_{i\downarrow} c_{i\downarrow} \rangle = 1/4$, and the average interaction energy is $NU/4$. The variational energy of this state with respect to the Hubbard model is:

   $$E_0 \equiv \langle \Psi_0 | \hat{H} | \Psi_0 \rangle = 2 \sum_{k < k_F} \varepsilon_k + \frac{NU}{4}$$

2. Limit $U/t \to \infty$:

   In the limit of strong electron-electron interactions, the ground state is now different. Since it is very expensive to place two electrons at the same atomic site, the ground state should contain no sites that are doubly occupied. Instead, every (Hydrogen)

site should contain exactly one electron. The ground state wavefunction should now be written:

$$|\Psi_\infty\rangle = \prod_{i,\sigma_i} c^\dagger_{i,\sigma_i} |\text{Vacuum}\rangle$$

where we have now used electron operators in real space, instead of k-space. The variational energy of this state is:

$$E_\infty \equiv \langle \Psi_\infty | \hat{H} | \Psi_\infty \rangle = 0$$

Both the kinetic and potential energies are zero.

Note that this wavefunction is not unique! We have placed one electron at each site, but we have not specified their spin orientation. In the limit $U/t \to \infty$, all spin configurations are degenerate, so the ground state has an overall degeneracy 2^N.

We will see later that this degeneracy is lifted by magnetic interactions!

Before continuing, let us consider the electronic properties of the above states.

In the limit $U/t \to 0$, the solution describes a metal, which may have a finite electrical conductivity.

For the limit $U/t \to \infty$, interactions make the transport of electrons energetically costly, and the model describes an electrical insulator with vanishing electrical conductivity. This type of insulator is known as a "Mott insulator" after the work of Sir Nevill Francis Mott, who was one of the first to recognize the possibility of insulators driven by electronic repulsion. He shared the 1977 Nobel prize in Physics for "fundamental theoretical investigations of the electronic structure of magnetic and disordered systems".

We can estimate the critical value of U where there is a phase transition between the metallic and Mott insulating states by setting $E_0 = E_\infty$. Thus, we can estimate:

$$U_c \approx \frac{8}{N} \sum_{k \leq k_F} \varepsilon_k \approx W$$

where $W = \max(\varepsilon_k) - \min(\varepsilon_k)$ is the electronic bandwidth.

3.3 Exchange interaction between localized spins

In the previous section, we saw that the ground states of the Mott insulator in the $U/t \to \infty$ limit has a 2^N-fold spin degeneracy. These states correspond to all possible states with exactly one electron at every site, with different spin configurations.

In this section, we consider how this degeneracy is lifted by "exchange interactions" between spins. These interactions are completely quantum mechanical effects that arise from the fact that electrons are fermions.

Our strategy will be to divide the Hubbard Hamiltonian as:

$$\hat{H} = \hat{H}_0 + \hat{H}_1 \quad , \quad \hat{H}_0 = U \sum_i c^\dagger_{i\uparrow} c_{i\uparrow} c^\dagger_{i\downarrow} c_{i\downarrow} \quad , \quad \hat{H}_1 = t \sum_{i,\sigma} \sum_{\text{n.n. } \delta} c^\dagger_{i\sigma} c_{i+\delta,\sigma}$$

and treat the hopping as a perturbation. We will calculate the corrections to the energies of the 2^N ground states up to second order in $\hat{H}_1$. The wavefunctions $|\Phi_n\rangle$ are eigenstates of $\hat{H}_0$, with zeroth order energies $E^0_n = \langle\Phi_n|\hat{H}_0|\Phi_n\rangle$. The perturbed energies are:

$$E_n \approx \langle\Phi_n|\hat{H}_0 + \hat{H}_1|\Phi_n\rangle + \sum_{m\neq n} \frac{\langle\Phi_n|\hat{H}_1|\Phi_m\rangle\langle\Phi_m|\hat{H}_1|\Phi_n\rangle}{E^0_n - E^0_m} + ...$$

where $E^0_n = 0$ and $\langle\Phi_n|\hat{H}_1|\Phi_n\rangle = 0$ for all states with exactly one electron per site.

Why do we expect the second order correction to split the spin degeneracy?

Note that $\hat{H}_1$ hops an electron to a neighbor site. If we apply this operator to a state with all spins parallel (i.e. $\langle S^z_{tot}\rangle = \pm N/2$), it annihilates the state, because two electrons with the same spin cannot occupy the same atomic site since they are fermions. For example:

$$\hat{H}_1|\uparrow\uparrow\uparrow ... \uparrow\rangle \quad \equiv \quad \hat{H}_1 \prod_{i=1}^{N} c^\dagger_{i,\uparrow}|\text{Vacuum}\rangle = 0$$

Therefore, there is no second order energy correction for such states. In contrast, if we apply the hopping operator to a state with spins antiparallel along a particular bond, we can access an excited state with a double occupancy (with zeroth order energy $= U$). For example:

$$c^\dagger_{1,\uparrow}c_{2,\uparrow}|\downarrow\uparrow\uparrow ... \uparrow\rangle = c^\dagger_{1,\uparrow}c_{2,\uparrow}c^\dagger_{1,\downarrow}\prod_{i=2}^{N} c^\dagger_{i,\uparrow}|\text{Vacuum}\rangle = c^\dagger_{1,\downarrow}c^\dagger_{1,\uparrow}\prod_{i=3}^{N} c^\dagger_{i,\uparrow}|\text{Vacuum}\rangle \neq 0$$

As a result, states with antiparallel spins do have finite energy corrections. This differencer generates an effective interaction between the spins and splits the spin degeneracy.

In order to calculate directly the Hamiltonian for the effective spin interactions, we first start with a more general formulation of perturbation theory where we put everything in terms of operators. Formally,

$$\hat{H}_{\text{spin}} \approx \mathbb{P}(\hat{H}_0 + \hat{H}_1)\mathbb{P} + \mathbb{P}\hat{H}_1\mathbb{Q}(E_0 - \hat{H}_0)^{-1}\mathbb{Q}\hat{H}_1\mathbb{P} + ...$$

$$\mathbb{P} = \sum_{n=1}^{2^N} |\Phi_n\rangle\langle\Phi_n| \quad , \quad \mathbb{Q} = 1 - \mathbb{P} = \sum_{n>2^N} |\Phi_n\rangle\langle\Phi_n|$$

Here, $\mathbb{P}$ is a projection operator, which sums only over the degenerate ground states of $\hat{H}_0$ which have exactly one electron at every site, and $E_0 = 0$. Therefore, similar to above, we find that $\mathbb{P}(\hat{H}_0 + \hat{H}_1)\mathbb{P} = 0$. This leads to:

$$\hat{H}_{\text{spin}} \approx \sum_{n,m>2^N} \sum_{i,\delta,\sigma} \sum_{j,\delta',\sigma'} \mathbb{P}\ (t c^\dagger_{i\sigma} c_{i+\delta,\sigma})\ |\Phi_n\rangle\langle\Phi_n|\ (0 - \hat{H}_0)^{-1}\ |\Phi_m\rangle\langle\Phi_m|\ (t c^\dagger_{j\sigma'} c_{j+\delta',\sigma'})\ \mathbb{P}$$

Since $|\Phi_n\rangle$ are eigenstates of $\hat{H}_0$, we have $n = m$. All excited states that are accessed by a single hop have $n > 2^N$, and have one site that is doubly occupied. For this reason, we may use $\langle\Phi_n|\hat{H}_0|\Phi_n\rangle = U$. This leads to:

$$\hat{H}_{\text{spin}} \approx -\frac{t^2}{U}\sum_{i,\delta,\sigma}\sum_{j,\delta',\sigma'} \mathbb{P}\ (c^\dagger_{i\sigma}c_{i+\delta,\sigma})\ (c^\dagger_{j\sigma'}c_{j+\delta',\sigma'})\ \mathbb{P}$$

We can only connect back to the ground states if $i = j + \delta'$ and $i + \delta = j$. This leads to:

$$\begin{aligned}
\hat{H}_{\text{spin}} \approx\ & -\frac{t^2}{U}\sum_{i,\delta\sigma,\sigma'} \mathbb{P}\ c^\dagger_{i\sigma}c_{i+\delta,\sigma}c^\dagger_{i+\delta,\sigma'}c_{i,\sigma'}\ \mathbb{P} \\
=\ & -\frac{t^2}{U}\sum_{i,\delta\sigma,\sigma'} \mathbb{P}\ c^\dagger_{i\sigma}c_{i,\sigma'}(\delta_{\sigma,\sigma'} - c^\dagger_{i+\delta,\sigma'}c_{i+\delta,\sigma})\ \mathbb{P} \\
=\ & -\frac{t^2}{U}\sum_{i,\delta} \mathbb{P}\ (n_{i\uparrow} + n_{i\downarrow} - n_{i\uparrow}n_{i+\delta,\uparrow} - n_{i\downarrow}n_{i+\delta,\downarrow} \\
& \qquad - c^\dagger_{i\uparrow}c_{i,\downarrow}c^\dagger_{i+\delta,\downarrow}c_{i+\delta,\uparrow} - c^\dagger_{i\downarrow}c_{i,\uparrow}c^\dagger_{i+\delta,\uparrow}c_{i+\delta,\downarrow})\ \mathbb{P} \\
=\ & -\frac{t^2}{U}\sum_{i,\delta} \mathbb{P}\ (n_{i\uparrow} + n_{i\downarrow} - \frac{1}{2}(n_{i\uparrow} + n_{i\downarrow})(n_{i+\delta,\uparrow} + n_{i+\delta,\downarrow}) \\
& \qquad - \frac{1}{2}(n_{i\uparrow} - n_{i\downarrow})(n_{i+\delta,\uparrow} - n_{i+\delta,\downarrow}) \\
& \qquad - c^\dagger_{i\uparrow}c_{i,\downarrow}c^\dagger_{i+\delta,\downarrow}c_{i+\delta,\uparrow} - c^\dagger_{i\downarrow}c_{i,\uparrow}c^\dagger_{i+\delta,\uparrow}c_{i+\delta,\downarrow})\ \mathbb{P}
\end{aligned}$$

Let's rewrite these operators in terms of spin operators. We define:

$$c^\dagger_{i,\uparrow}c_{i,\downarrow} \equiv S^+_i \quad , \quad c^\dagger_{i,\downarrow}c_{i,\uparrow} \equiv S^-_i \quad , \quad S^x_i = \frac{1}{2}(S^+_i + S^-_i) \quad , \quad S^y_i = \frac{1}{2i}(S^+_i - S^-_i)$$
$$S^z_i = \frac{1}{2}(n_{i,\uparrow} - n_{i,\downarrow}) \quad , \quad n_i = n_{i,\uparrow} + n_{i,\downarrow}$$

This gives:

$$\begin{aligned}
\hat{H}_{\text{spin}} \approx\ & -\frac{t^2}{U}\sum_{i,\delta} \mathbb{P}\ (n_i - \frac{1}{2}n_i n_{i+\delta} - 2S^z_i S^z_{i+\delta} - S^+_i S^-_{i+\delta} - S^-_i S^+_{i+\delta})\ \mathbb{P} \\
=\ & -\frac{t^2}{U}\sum_{i,\delta} \mathbb{P}\ (n_i - \frac{1}{2}n_i n_{i+\delta} - 2S^z_i S^z_{i+\delta} - 2S^x_i S^x_{i+\delta} - 2S^y_i S^y_{i+\delta})\ \mathbb{P}
\end{aligned}$$

At this point, we can note that $\mathbb{P}n_i\mathbb{P} = 1$, since all spin states have exactly one electron per site. In the summation, each pair of sites is double counted. If we sum over each nearest neighbour pair only once, we get:

$$\boxed{\hat{H}_{\text{spin}} \approx \tfrac{4t^2}{U}\textstyle\sum_{\langle ij\rangle}\left(\vec{S}_i \cdot \vec{S}_j - \tfrac{1}{4}\right)}$$

which is called the Heisenberg Hamiltonian. If we consider the different spin configurations for a pair of sites, it is easy to see that this Hamiltonian favors singlet configurations since

$$\left\{ \begin{array}{c} |\uparrow\uparrow\rangle \\ (|\uparrow\downarrow\rangle + |\downarrow\uparrow\rangle)\frac{1}{\sqrt{2}} \\ |\downarrow\downarrow\rangle \end{array} \right\} \quad \rightarrow \quad \langle \vec{S}_i \cdot \vec{S}_j \rangle = +\frac{1}{4},$$

$$(|\uparrow\downarrow\rangle - |\downarrow\uparrow\rangle)/\sqrt{2} \quad \rightarrow \quad E_{\rm s} = \langle \vec{S}_i \cdot \vec{S}_j \rangle = -\frac{3}{4}.$$

We can generalize the Heisenberg model:

$$H = -J \sum_{\langle ij \rangle} \vec{S}_i \cdot \vec{S}_j.$$

In the one-orbital Hubbard model at half-filling, the magnetic interactions are antiferromagnetic, corresponding to $J < 0$. For more elaborate models, it is also possible to have ferromagnetic interactions with $J > 0$.

For typical Mott insulator materials, $U \sim 1 - 10$ eV, and $t \sim 0.1 - 1$ eV. This leads to interactions $|J| \sim 10 - 1000$ K. These are strong enough to explain magnetic ordering!!

Apart from the exchange interaction, there are other possible interactions that are also important for magnetism, like the so-called RKKY interaction. This interaction acts between localized magnetic moments through conduction electrons, namely, a localized spin couples to the spins of conduction electrons and the second localized spin "sees" the induced spin-polarization of the conduction electrons. The sign of this interaction can be both ferromagnetic and antiferromagnetic.

3.4 Heisenberg model and related lattice models for collective magnetism

We consider a Bravais lattice described by vectors $\{\vec{R}_i\}$. At each lattice site, we have a spin $\vec{S}$ and a total momentum $\vec{J} = \vec{L} + \vec{S}$. This situation is characteristic to systems with partially filled f-shells, like Gd, EuO, *etc.*, or partially filled d-shells, like MnO, TiOCl, *etc.* (insulators and semiconductors). This does not apply to Fe, Co, Ni, *etc.*, since in those systems the $3d$ electrons are not localized and the collective magnetism is discussed in terms of band magnetism.

As was shown in the previous section, localized spins are described by the Hamiltonian

$$H = -\sum_{\langle ij \rangle} J_{ij} \vec{S}_i \cdot \vec{S}_j + g\mu_B \sum_i \vec{B} \cdot \vec{S}_i.$$

- For $J > 0$ the system favors ferromagnetism and for $J < 0$ antiferromagnetism.
- In one dimension (1D), there is no phase transition to an ordered magnetic state due to quantum fluctuations.

- In one and two dimensions (2D), at finite temperatures the system doesn't show long range order (Mermin-Wagner theorem).
- concepts like frustration and spin glass behavior can be described by this Hamiltonian.

Let us consider special cases of the model.

(1) Ising model:

$$H = -\sum_{\langle ij \rangle} J_{ij} S_i^z S_j^z + g\mu_B B \sum_i S_i^z.$$

This model can be solved exactly in 1D and 2D. There is no phase transition in 1D at finite T, but the system undergoes a phase transition to an ordered state in 2D.

(2) XY-model:

$$H = -\sum_{ij} J_{ij} (S_i^x S_j^x + S_i^y S_j^y) + g\mu_B \vec{B} \sum_i \vec{S}_i.$$

The classical 2D XY-model has been much discussed because it does not exhibit long range order at finite T, but instead displays a "Berezinskii-Kosterlitz-Thouless transition" related to the behavior of topological defects. This discovery was partly the subject of the 2016 Nobel Prize in Physics.

The Heisenberg model and related models cannot be exactly solved in many cases. It is therefore useful to consider some approximations.

3.5 Mean-field theory for the Heisenberg model

We consider the ferromagnetic Heisenberg model in the presence of a magnetic field:

$$H = \sum_i \left(-\sum_j J_{ij} \vec{S}_j + g\mu_B \vec{B} \right) \cdot \vec{S}_i.$$

Formally, it has the form

$$H = g\mu_B \sum_i \vec{\mathcal{B}} \cdot \vec{S}_i,$$

which corresponds to a system of "non-interacting" spins in the presence of a magnetic field $\vec{\mathcal{B}}$ given by

$$\vec{\mathcal{B}} = -\sum_j \frac{J_{ij} \vec{S}_j}{g\mu_B} + \vec{B},$$

with the peculiarity that $\vec{\mathcal{B}}$ contains the operators $\vec{S}_j$. In order to be able to treat the spins as "non-interacting", we substitute the operators $\vec{S}_j$ by their average values $\langle \vec{S}_j \rangle$ so that

$$H_{\text{eff}} = \sum_i g\mu_B \vec{\mathcal{B}}_{\text{eff}} \cdot \vec{S}_i,$$

with

$$\boxed{\vec{\mathcal{B}}_{\text{eff}} = \vec{B} - \sum_j \frac{J_{ij}}{g\mu_B} \langle \vec{S}_j \rangle}\,.$$

The idea behind this approximation is to consider the effect of interacting spins with a given spin as a mean-field effect (Fig. 3.1). Instead of having to deal with a complex problem

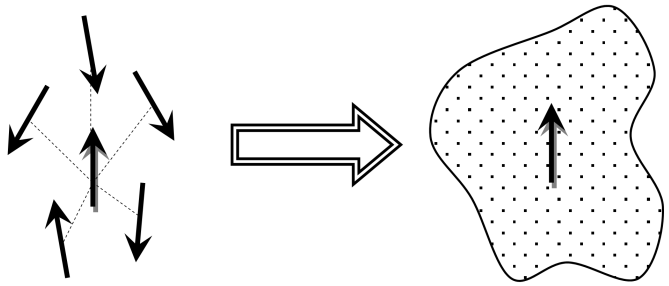

Abbildung 3.1: Mean-field approximation for interacting spins.

of two-body interactions (interacting spins), we consider the case of a spin interacting with a "mean field"created by the interaction with the other spins.

The effective magnetic field has to be found self-consistently. We define the magnetization $\vec{M}$ as the expectation value of the spin operator:

$$\vec{M} = N\langle \vec{\mu} \rangle = -Ng\mu_B \langle \vec{S}_i \rangle.$$

We consider $\vec{B} = (0, 0, B)$ and, as a special case, $S = \frac{1}{2}$. Then (see previous chapter),

$$\begin{aligned} M &= N\mu_B \tanh(\beta\mu_B \mathcal{B}_{\text{eff}}) \\ &= N\mu_B \tanh\left[\beta\mu_B \left(B - \sum_j \frac{J_{ij}}{g\mu_B} \langle S_{jz} \rangle\right)\right] \\ &= N\mu_B \tanh\left[\beta\mu_B \left(B + \frac{ZJ}{N(g\mu_B)^2} M\right)\right], \end{aligned}$$

with Z being the number of nearest neighbors as we assumed that spin-spin interactions take place only between nearest neighbors. Then, the magnetization per site is

$$\boxed{m = \frac{M}{N} = \mu_B \tanh\left[\frac{\mu_B}{k_B T}(B + Am)\right]}\,.$$

This is a self-consistent equation, with

$$A = \frac{ZJ}{g^2\mu_B^2}.$$

Without an external magnetic field, the equation reduces to

$$\boxed{m = \mu_B \tanh\left(\frac{\mu_B A}{k_B T} m\right)}.$$

We can solve this equation graphically, as shown in Fig. 3.2. We consider the function

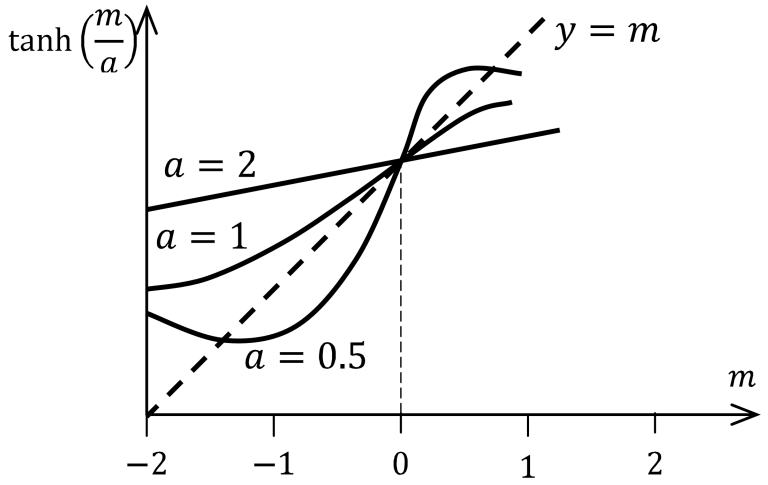

Abbildung 3.2: The self-consistent equation for magnetization solved graphically.

$$f(x) = \tanh \frac{\mu_B^2 A}{k_B T} x,$$

and introduce

$$\frac{1}{a} = \frac{\mu_B^2 A}{k_B T}.$$

For $a \geq 1$ there is only one solution $m = 0$, but for $a < 1$ there are three solutions. Fig. 3.2 shows that non-trivial solutions are only possible if the derivative of $f(x)$ at $x = 0$ is bigger than 1:

$$f'(0) > 1,$$

$$\frac{\mu_B^2 A}{k_B T} \frac{1}{\cosh^2 \frac{\mu_B^2 A}{k_B T} x\Big|_{x=0}} = \frac{\mu_B^2 A}{k_B T}.$$

This gives a critical temperature between the solutions $m = 0$ and $m \neq 0$:

$$k_B T_c = \mu_B^2 A = \frac{ZJ}{g^2}.$$

T_c is called the Curie temperature. For $T < T_c$, $m \neq 0$ even though the external magnetic field is zero. The system orders *spontaneously*, which is accompanied by a spontaneous breaking of rotational symmetry. The Heisenberg model is rotationally invariant as $\vec{S}_i \cdot \vec{S}_j$ is a scalar product. The solution $m \neq 0$ breaks the rotational symmetry since the system orders in a given direction, in our case, the z-direction. M is the order parameter of the ferromagnetic phase transition.

The previous calculation was done for spin-$\frac{1}{2}$. In the case of a system of spins S, the critical temperature is given by

$$\boxed{k_B T_c = \frac{1}{3} Z J S(S+1)}.$$

3.5.0.1 Behavior near the phase transition

We consider the Taylor expansion of

$$m = \mu_B \tanh\left(\frac{\mu_B A}{k_B T} m\right)$$

for small m:

$$\tanh x = x - \frac{1}{3}x^3 + \ldots, \quad x \ll 1.$$

Then,

$$m = \frac{\mu_B^2 A}{k_B T} m - \frac{1}{3}\frac{\mu_B^4 A^3}{(k_B T)^3} m^3 + \ldots$$

For $T < T_c$, $m \neq 0$ and ($T_c = \frac{\mu_B^2 A}{k_B}$)

$$1 = \frac{\mu_B^2 A}{k_B T} - \frac{1}{3}\frac{\mu_B^2 A^3}{(k_B T)^3} m^2 + \ldots = \frac{T_c}{T} - \frac{1}{3}\left(\frac{T_c}{T}\right)^3 \frac{m^2}{\mu_B^2} + \ldots$$

This equation can be rewritten as

$$m^2 = 3\mu_B^2 \frac{T^3}{T_c^3}\left(\frac{T_c}{T} - 1\right) \approx 3\mu_B^2 \left(\frac{T}{T_c}\right)^2 \left(1 - \frac{T}{T_c}\right),$$

which defines the behavior of the order parameter m near the phase transition:

$$\boxed{m \approx \sqrt{\frac{3\mu_B^2}{T_c}}\sqrt{T_c - T}}.$$

This shows that the critical exponent for the magnetization α, defined as

$$m \sim (T_c - T)^\alpha,$$

is

$$\alpha = \frac{1}{2}.$$

This value is commonly obtained in the mean-field approximation. We will show that the order parameter in the BCS superconductivity has a similar behavior.

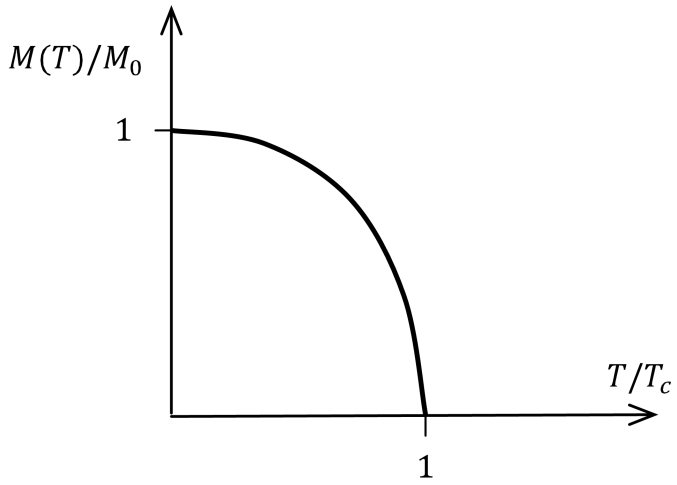

Abbildung 3.3: Magnetization m as a function of temperature T.

3.5.0.2 Behavior at small temperatures $T \ll T_c$

Let us write tanh in the following way:

$$\frac{m}{\mu_B} = \tanh\left(\frac{T_c}{T}\frac{m}{\mu_B}\right) = \frac{1 - e^{-2\frac{T_c}{T}\frac{m}{\mu_B}}}{1 + e^{-2\frac{T_c}{T}\frac{m}{\mu_B}}}.$$

Then, for $T \ll T_c$

$$\frac{m}{\mu_B} \approx 1 - e^{-2\frac{T_c}{T}\frac{m}{\mu_B}} \approx 1 - e^{-2\frac{T_c}{T}}.$$

This result deviates from observations. At small temperatures, the interactions among spins are important and cannot be accounted for in terms of a mean field.

3.5.0.3 Susceptibility in the mean-field approximation

By definition,

$$\chi = \frac{\partial M}{\partial B} = \frac{\partial M}{\partial \mathcal{B}_{\text{eff}}}\frac{\partial \mathcal{B}_{\text{eff}}}{\partial B} = N\mu_B^2\beta\frac{1}{\cosh^2\beta\mu_B\mathcal{B}_{\text{eff}}}\left(1 + \frac{ZJ}{N(g\mu_B)^2}\frac{\partial M}{\partial B}\right).$$

For $T > T_c$, $M = 0$ if $B \to 0$. Therefore, $\mathcal{B}_{\text{eff}} = 0$ and $\cosh^2\beta\mu_B\mathcal{B}_{\text{eff}} = 1$. Then,

$$\chi = \frac{N\mu_B^2}{k_BT}\left(1 + \frac{k_BT_c}{N\mu_B^2}\chi\right),$$

$$\boxed{\chi(B=0) = \frac{N\mu_B^2}{k_B}\frac{1}{T - T_c}},$$

which is the Curie-Weiss law. It should be compared with the Curie law for independent localized spins derived in the previous chapter.

3.6 Spin wave excitations: magnons

We saw in the previous section that the behavior of magnetization at low temperatures is wrongly described within a mean-field approximation. In order to describe magnetic excitations of a system of interacting spins at low temperatures, we shall introduce in this section the spin-wave theory. We will consider here the ferromagnetic case. Our starting Hamiltonian is the Heisenberg model with nearest neighbor couplings in the presence of a magnetic field:

$$H = -J \sum_i \sum_\delta \vec{S}_i \cdot \vec{S}_{i+\delta} + g\mu_B \sum_i \vec{B} \cdot \vec{S}_i,$$

where $J > 0$ and δ denotes the nearest neighbors. The wavefunction for the N-spin system can be described as

$$|\Psi\rangle = |S_1, \ldots, S_i, \ldots, S_N\rangle,$$

with $S_i = -S, -S+1, \ldots, +S$. The ground state ($T = 0$) at $B = 0$ is the ferromagnetic state:

$$|\Psi_0\rangle = |S, S, \ldots, S, \ldots, S\rangle = |\uparrow, \uparrow, \ldots, \uparrow, \ldots, \uparrow\rangle,$$

$$|\Psi_0\rangle = \prod_i |\uparrow\rangle_i \qquad \text{(for spin-}\tfrac{1}{2}\text{)}.$$

The energy of the ground state is

$$E_0 = -NZJS^2$$

since

$$H = J \sum_{i\delta} \vec{S}_i \cdot \vec{S}_{i+\delta} = J \sum_{i\delta} \left\{ S_i^z S_{i+\delta}^z + \frac{1}{2}(S_i^+ S_{i+\delta}^- + S_i^- S_{i+\delta}^+) \right\},$$

$$S_i^+ S_{i+\delta}^- |\Psi_0\rangle = 0,$$

$$S_i^z S_{i+\delta}^z |\Psi_0\rangle = \frac{1}{4}|\Psi_0\rangle,$$

and therefore

$$H|\Psi_0\rangle = -\frac{1}{4}JZN|\Psi_0\rangle = E_0|\Psi_0\rangle.$$

We consider now a local spin excitation on the ground state:

$$\begin{array}{cccccccc} \uparrow & \uparrow & \uparrow & \downarrow & \uparrow & \uparrow & \uparrow \\ & & & j & & & \end{array}$$

which, for a general spin S, corresponds to a wavefunction

$$|\Psi_j\rangle = |S, S, \ldots, S, \underbrace{S-1}_{j}, S, \ldots, S\rangle.$$

This state is not anymore an eigenstate of the Heisenberg Hamiltonian since the terms $S_j^+ S_{j+\delta}^-$ propagate the local excitation further. $|\Psi_j\rangle$ is only an eigenstate of the Ising model but not of the Heisenberg model. In order to take into account the propagation of the local spin excitation in the Heisenberg model, we introduce the plane wave state

$$\boxed{|\Psi_{\vec{q}}\rangle = \frac{1}{\sqrt{N}} \sum_j e^{i\vec{q}\vec{R}_j} |\Psi_j\rangle},$$

also called the one-magnon state. We will show that this is an eigenstate of the ferromagnetic Heisenberg Hamiltonian. We first show that

$$H|\Psi_j\rangle = -J\left[(NZS^2 - 2ZS)|\Psi_j\rangle + 2S\sum_\delta |\Psi_{j+\delta}\rangle\right],$$

which follows from the following considerations:

$$\begin{aligned}
&\sum_i S_i^z S_{i+\delta} |S, S, \ldots, S-1, \ldots, S\rangle \\
&= \left[(N-Z-1)ZS^2 + Z(Z-1)S^2 + 2ZS(S-1)\right]|\Psi_j\rangle \\
&= (NZS^2 - 2ZS)|\Psi_j\rangle,
\end{aligned}$$

$$\begin{aligned}
&\sum_{i\delta} \left\{S_i^+ S_{i+\delta}^- + S_i^- S_{i+\delta}^+\right\} |S, S, \ldots, S-1, \ldots, S\rangle \\
&= [S(S+1) - S(S-1)] \sum_\delta |\Psi_{j-\delta}\rangle + [S(S+1) - S(S-1)] \sum_\delta |\Psi_{j-\delta}\rangle \\
&= 4S \sum_\delta |\Psi_{j+\delta}\rangle,
\end{aligned}$$

where we used

$$\begin{aligned}
S^-|S,m\rangle &= \sqrt{S(S+1) - m(m-1)}|S, m-1\rangle, \\
S^+|S,m\rangle &= \sqrt{S(S+1) - m(m+1)}|S, m+1\rangle;
\end{aligned}$$

then,

$$H|\Psi_j\rangle = -J\left[(NZS^2 - 2ZS)|\Psi_j\rangle + 2S\sum_\delta |\Psi_{j+\delta}\rangle\right]$$

and

$$\begin{aligned}
H|\Psi_{\vec{q}}\rangle &= \frac{1}{\sqrt{N}} \sum_j e^{i\vec{q}\vec{R}_j} \left[-J(NZS^2 - 2ZS)|\Psi_j\rangle - 2SJ\sum_\delta |\Psi_{j+\delta}\rangle\right] \\
&= -J(NZS^2 - 2ZS)|\Psi_{\vec{q}}\rangle - 2SJ\frac{1}{\sqrt{N}} \sum_{j\delta} e^{i\vec{q}(\vec{R}_j + \vec{\delta})} |\Psi_{j+\delta}\rangle e^{-i\vec{q}\vec{\delta}} \\
&= \left[-J(NZS^2 - 2ZS) - 2SZ\sum_\delta e^{-i\vec{q}\vec{\delta}}\right]|\Psi_{\vec{q}}\rangle.
\end{aligned}$$

$|\Psi_{\vec{q}}\rangle$ are indeed eigenstates of H:

$$H|\Psi_{\vec{q}}\rangle = (E_0 + E_{\vec{q}})|\Psi_{\vec{q}}\rangle,$$

with

$$\boxed{E_{\vec{q}} = 2S\left(ZJ - J\sum_{\delta} e^{-i\vec{q}\vec{\delta}}\right)}.$$

The one-magnon spectrum $E_{\vec{q}}$ does not have an energy gap: $E_{\vec{q}} \xrightarrow{q\to 0} E_0$. This is a special case of the Goldstone theorem, which states that all systems with a broken continuous symmetry have gapless excitations, the so-called *Goldstone modes*. The continuous symmetry broken here is the spin rotational symmetry.

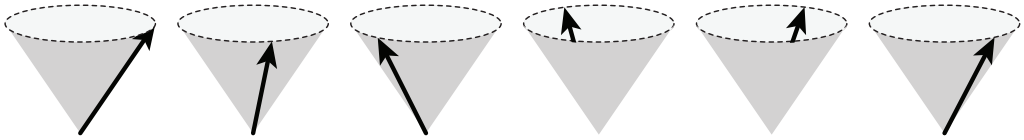

Abbildung 3.4: Representation of a spin wave.

For phononic excitations, breaking of translational invariance creates gapless excitations, which are acoustic phonons.

3.7 Quantization of spin waves

In order to characterize the magnon excitations, we can either remain in the spin space or choose a different representation for these excitations. The disadvantage of working in spin space is connected with the spin commutation relations:

$$[S^\alpha, S^\beta] = i\epsilon_{\alpha\beta\gamma}S^\gamma.$$

We can substitute the spin operators by Bose operators such that all commutation relations are preserved. Formally, the Heisenberg spin Hamiltonian will be reformulated in terms of a Hamilton operator of interacting bosons.

Instead of being described by its z component, the spin state on a site can be described by the quantum number m:

$$m = -S, \ldots, +S.$$

Here, m is the azimuthal quantum number and not the magnetization. We introduce the "occupation" number n:

$$n = 0, \ldots, 2S,$$

such that $m = +S$ corresponds to $n = 0$ and, in general, $n = S - m$. Then,

$$\begin{aligned} S^+|n\rangle &= S^+|S,m\rangle = \sqrt{S(S+1) - m(m+1)}|S,m+1\rangle \\ &= \sqrt{S^2 + S - n^2 + 2Sn - S^2 + n - S}|S,m+1\rangle \\ &= \sqrt{2S+1-n}\sqrt{n}|n-1\rangle \end{aligned}$$

and

$$\begin{aligned} S^-|n\rangle &= \sqrt{2S-n}\sqrt{n+1}|n+1\rangle, \\ S^z|n\rangle &= m|S,m\rangle = (S-n)|S,m\rangle = S|n\rangle - n|n\rangle. \end{aligned}$$

3.7.0.1 Holstein-Primakoff transformation

We define the bosonic creation and annihilation operators via

$$\begin{aligned} a|n\rangle &= \sqrt{n}|n-1\rangle, \\ a^\dagger|n\rangle &= \sqrt{n+1}|n+1\rangle, \\ a^\dagger a|n\rangle &= n|n\rangle, \end{aligned}$$

with $[a, a^\dagger] = 1$, and consider the canonical transformation

$$\boxed{\begin{aligned} S^+ &= \sqrt{2S}\sqrt{1 - \frac{a^\dagger a}{2S}}\,a \\ S^- &= \sqrt{2S}\,a^\dagger\sqrt{1 - \frac{a^\dagger a}{2S}} \\ S^z &= S - a^\dagger a \end{aligned}}$$

This transformation is canonical since the spin commutation relations are preserved:

$$[S_i^+, S_i^-] = 2S_i^z, \qquad [S_i^-, S_i^z] = S_i^-, \qquad [S_i^+, S_i^z] = -S_i^+.$$

For instance, the first relation can be confirmed in the following way:

$$[S^+, S^-]|n\rangle = S^+S^-|n\rangle - S^-S^+|n\rangle = 2(S-n)|n\rangle \equiv 2S_i^z|n\rangle.$$

Then, in terms of the newly introduced operators, the Heisenberg Hamiltonian is written as

$$\boxed{\begin{aligned} H = -J\sum_i\sum_{\delta i}\Bigg[\; & S\left(\sqrt{1 - \frac{a_i^\dagger a_i}{2S}}\,a_i a_{i+\delta}^\dagger\sqrt{1 - \frac{a_{i+\delta}^\dagger a_{i+\delta}}{2S}}\right. \\ & \left. + a_i^\dagger\sqrt{1 - \frac{a_i^\dagger a_i}{2S}}\sqrt{1 - \frac{a_{i+\delta}^\dagger a_{i+\delta}}{2S}}\,a_{i+\delta}\right) \\ & + (S - a_i^\dagger a_i)(S - a_{i+\delta}^\dagger a_{i+\delta})\;\Bigg] \end{aligned}} \tag{3.1}$$

Here, a_i and $a_i^\dagger$ obey

$$[a_i, a_j^\dagger] = \delta_{ij}, \qquad [a_i, a_j] = [a_i^\dagger, a_j^\dagger] = 0.$$

These Bose operators describe spin wave excitations that are *quantized*, called magnons. The ground state of (3.1) corresponds to the state without magnons

$$|0, 0, \ldots, 0\rangle,$$

and the ground state energy is

$$E_0 = -JNZS^2.$$

Magnons are quasiparticles that describe excitations of a spin system. They do not fulfill the particle conservation principle.

We obtained a Hamiltonian that is not simpler than the initial spin Hamiltonian due to the square roots in the definition of $a^\dagger$ and a. Therefore, we consider an approximation where all terms that are quadratic or higher in the particle number operators are neglected. With that, we get a linearized magnon Hamiltonian operator:

$$\boxed{H \approx -J \sum_i \sum_\delta S(a_i^\dagger a_{i+\delta} + a_{i+\delta}^\dagger a_i - a_{i+\delta}^\dagger a_{i+\delta} - a_i^\dagger a_i) - JNZS^2}\,.$$

This approximation neglects the magnon-magnon interaction and therefore one deals here with non-interacting bosons. Through this approximation, the Hilbert space of possible states changes: the spin Hamiltonian operator has $2S+1$ states per site while the linearized magnon Hamiltonian operator has $n \to \infty$ states per site (there is no limit for excitations). That's why the linearization makes sense only at small temperatures.

The Hamiltonian (3.1) can be diagonalized by considering the Fourier transformation

$$\begin{aligned} a_i &= \frac{1}{\sqrt{N}} \sum_{\vec{q}} e^{i\vec{q}\vec{R}} a_{\vec{q}}, \\ a_i^\dagger &= \frac{1}{\sqrt{N}} \sum_{\vec{q}} e^{-i\vec{q}\vec{R}_i} a_{\vec{q}}^\dagger. \end{aligned} \tag{3.2}$$

Then,

$$\begin{aligned} H - E_0 &= -J \sum_i \sum_\delta S \frac{1}{N} \sum_{\vec{q},\vec{q}'} \Big(e^{-i\vec{q}\vec{R}_i} e^{i\vec{q}'(\vec{R}_i+\vec{\delta})} \\ &+ e^{i\vec{q}'(\vec{R}_i+\vec{\delta})} - e^{i(\vec{q}'-\vec{q})(\vec{R}_i+\vec{\delta})} - e^{i(\vec{q}'-\vec{q})\vec{R}_i} \Big) a_{\vec{q}}^\dagger a_{\vec{q}'} \\ &= -JS \sum_{\vec{q}} \sum_{\vec{\delta}} \left(e^{i\vec{q}\vec{\delta}} + e^{-i\vec{q}\vec{\delta}} - 2 \right) a_{\vec{q}}^\dagger a_{\vec{q}} \\ &= \sum_{\vec{q}} E_{\vec{q}} a_{\vec{q}}^\dagger a_{\vec{q}}, \end{aligned}$$

with

$$E_{\vec{q}} = 2JS\left(Z - \sum_{\vec{\delta}} \cos \vec{q}\vec{\delta}\right).$$

The diagonalized Hamiltonian (3.1) looks very similar to the diagonalized Hamiltonian for phonons, but the magnon dispersion for a ferromagnetic system is quadratic in δ:

$$\begin{aligned} \cos(\vec{q}\vec{\delta}) &\approx 1 - \frac{(\vec{q}\vec{\delta})^2}{2} \\ \Rightarrow \quad E_{\vec{q}} &\approx JS\sum_{\vec{\delta}}(\vec{q}\vec{\delta})^2 = \boxed{2JSa^2q^2}, \end{aligned} \tag{3.3}$$

with a being the lattice constant. Please, note the difference with respect to the corresponding result for an antiferromagnetic system, where the dependence is linear.

Now, we can calculate the thermodynamic properties of the system. The internal energy is given by

$$U = \sum_{\vec{q}} \frac{E_{\vec{q}}}{e^{\frac{E_{\vec{q}}}{k_BT}} - 1} \approx \frac{V}{(2\pi\hbar)^3}\int d^3q \frac{2JSa^2q^2}{e^{\frac{2JSa^2q^2}{k_BT}} - 1}.$$

Out of this integral, one obtains the low-temperature temperature dependence of U

$$\boxed{U \sim T^{5/2}}$$

and of the specific heat

$$\boxed{\frac{\partial U}{\partial T} \sim T^{3/2}}.$$

For the magnetization, we get

$$\begin{aligned} M &= -g\mu_B\sum_i \langle S_i^z\rangle = -g\mu_B\sum_i\left(\langle a_i^\dagger a_i\rangle - S\right) \\ &= g\mu_B\left(NS - \sum_i \langle a_i^\dagger a_i\rangle\right) \\ &= g\mu_B\left(NS - \sum_{\vec{q}} \langle a_{\vec{q}}^\dagger a_{\vec{q}}\rangle\right), \end{aligned}$$

$$\sum_{\vec{q}}\langle a_{\vec{q}}^\dagger a_{\vec{q}}\rangle \sim \int dq \frac{q^2}{e^{E_{\vec{q}}/k_BT} - 1} \sim T^{3/2}.$$

Then,

$$\frac{m}{\mu_B} = \frac{M}{Nm_B} = gS - AT^{3/2} = \boxed{1 - AT^{3/2}},$$

which agrees with experimental observations at small temperatures.

The description of excitations in an antiferromagnetic spin system is considered in the presentation. We shall consider now *itinerant magnetism.*

3.8 Itinerant magnetism

Itinerant magnetism occurs in $3d$ systems (systems that contain atoms with partially filled $3d$ electronic shells), like Fe, Co or Ni. There, collective magnetism of itinerant electrons is possible due to the Coulomb interaction and Pauli principle.

As a model for itinerant electrons with Coulomb repulsion, we consider the Hubbard model

$$\begin{aligned} H &= \sum_{\vec{k},\sigma} \varepsilon_{\vec{k}} c^\dagger_{\vec{k}\sigma} c_{\vec{k}\sigma} + U \sum_i c^\dagger_{i\uparrow} c_{i\uparrow} c^\dagger_{i\downarrow} c_{i\downarrow} \\ &= \sum_{i,\sigma} \sum_{\text{n.n. } \delta} t c^\dagger_{i\sigma} c_{i+\delta,\sigma} + U \sum_i c^\dagger_{i\uparrow} c_{i\uparrow} c^\dagger_{i\downarrow} c_{i\downarrow}, \end{aligned}$$

where

$$c_{i\sigma} = \frac{1}{\sqrt{N}} \sum_{\vec{k}} e^{i\vec{k}\vec{R}_i} c_{\vec{k}\sigma}, \qquad c^\dagger_{i\sigma} = \frac{1}{\sqrt{N}} \sum_{\vec{k}} e^{-i\vec{k}\vec{R}_i} c^\dagger_{\vec{k}\sigma}$$

and

$$\varepsilon_{\vec{k}} = t \sum_{\text{n.n. } \delta} e^{i\vec{k}\vec{\delta}} = 2t(\cos k_x a + \cos k_y a + \cos k_z a)$$

for a cubic lattice. In the presence of a magnetic field, the Hamiltonian becomes

$$\boxed{H = \sum_{\vec{k},\sigma} (\varepsilon_{\vec{k}} + g\mu_B B\sigma) c^\dagger_{\vec{k}\sigma} c_{\vec{k}\sigma} + U \sum_i c^\dagger_{i\uparrow} c_{i\uparrow} c^\dagger_{i\downarrow} c_{i\downarrow}} \,.$$

In order to treat the problem, we can consider the following mean-field approximation:

$$\begin{aligned} H_{\text{eff}} &= \sum_{\vec{k}} \left(\varepsilon_{\vec{k}} - \mu_B B + U \langle c^\dagger_{i\uparrow} c_{i\uparrow} \rangle \right) c^\dagger_{\vec{k}\downarrow} c_{\vec{k}\downarrow} \\ &+ \sum_{\vec{k}} \left(\varepsilon_{\vec{k}} + \mu_B B + U \langle c^\dagger_{i\downarrow} c_{i\downarrow} \rangle \right) c^\dagger_{\vec{k}\uparrow} c_{\vec{k}\uparrow} \\ &- U \sum_i \langle c^\dagger_{i\uparrow} c_{i\uparrow} \rangle \langle c^\dagger_{i\downarrow} c_{i\downarrow} \rangle, \end{aligned}$$

$$
\begin{aligned}
m &= -\mu_B \left(\langle c^\dagger_{i\uparrow} c_{i\uparrow} \rangle - \langle c^\dagger_{i\downarrow} c_{i\downarrow} \rangle \right) \\
&= -\frac{\mu_B}{N} \sum_{\vec{k}} \left(\langle c^\dagger_{\vec{k}\uparrow} c_{\vec{k}\uparrow} \rangle - \langle c^\dagger_{\vec{k}\downarrow} c_{\vec{k}\downarrow} \rangle \right) \\
&= -\mu_B \int_{-\infty}^{\infty} d\varepsilon \, f(\varepsilon) \Big\{ \rho_0(\varepsilon + \mu_B B + U \langle c^\dagger_{i\downarrow} c_{i\downarrow} \rangle) \\
&\qquad\qquad - \rho_0(\varepsilon - \mu_B B + U \langle c^\dagger_{i\uparrow} c_{i\uparrow} \rangle) \Big\} \\
&= -\mu_B \int_{-\infty}^{\infty} d\varepsilon \, f(\varepsilon) \rho_0'(\varepsilon) \left\{ 2\mu_B B - U \left(\langle c^\dagger_{i\uparrow} c_{i\uparrow} \rangle - \langle c^\dagger_{i\downarrow} c_{i\downarrow} \rangle \right) \right\}
\end{aligned}
$$

$$
\begin{aligned}
\chi(T, B=0) &= \frac{\partial m}{\partial B} \\
&= \mu_B \int_{-\infty}^{\infty} d\varepsilon \left(-\frac{\partial f}{\partial \varepsilon} \right) \rho_0(\varepsilon) \left\{ 2\mu_B + \frac{U}{\mu_B} \chi(T, B=0) \right\} \\
&= 2\mu_B^2 \rho_0(\varepsilon_F) \left\{ 1 + \frac{U}{2\mu_B^2} \chi(T, B=0) \right\}. \qquad (3.4)
\end{aligned}
$$

The first term in the above susceptibility expression is the Pauli susceptibility for non-interacting electrons in a magnetic field, and the second term is present only for an interacting system. Finally,

$$
\chi(T, B=0) = \frac{\chi_0}{1 - \frac{U}{2\mu_B^2} \chi_0},
$$

with

$$
\chi_0 = 2\mu_B^2 \frac{1}{N} \sum_{\vec{k}} \left(-\frac{\partial f}{\partial \varepsilon_{\vec{k}}} \right) = 2\mu_B^2 \int_{-\infty}^{\infty} d\varepsilon \, \rho_0(\varepsilon) \left(-\frac{\partial f}{\partial \varepsilon} \right) \overset{T \to 0}{=} 2\mu_B^2 \rho_0(E_F).
$$

The derived result demonstrates an enhancement of susceptibility due to correlations, which is known as "Stoner enhancement". There is ferromagnetic instability for

$$
\frac{U}{2\mu_B^2} \chi_0 \geq 1 \quad \rightarrow \quad U_c \rho_0(E_F) \geq 1,
$$

which results in the exchange splitting of the two bands.