The antiferromagnetic state in an optical lattice

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Abstract

In an optical lattice, atoms are trapped in a periodic lattice created by counter-propagating laser beams. At low temperatures, only the spin interactions between the atoms are relevant. The system is in the antiferromagnetic state, where spins are pointing alternatingly up and down. An imbalance in the spin species can also be achieved experimentally.

The topic of this thesis is the antiferromagnetic state in an optical lattice. The phase transition from an antiferromagnet to a paramagnet is investigated. In particular, the imbalanced case is considered, where there is a spin magnetization. The mean field phase diagram for the imbalanced case is presented. Then spin waves are treated. The dispersion relations are given, and investigated. Finally, in two dimensions topological excitations, or merons, are discussed. The famous Kosterlitz-Thouless phase transition investigated.
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Introduction

In 1968 it was first suggested that it might be possible to trap atoms using standing waves of light [7]. This turned out to be true, and in 1987, the first experimental realization of such a system was obtained using cesium atoms [10]. Today these systems are called optical lattices, and are a hot research topic. Since optical lattices resemble crystals in many ways, they can be used to study solids in a controlled way, by using the high degree to which parameters such as lattice spacing and interaction strength can be adjusted. These systems can be accurately described by the Hubbard model. When one particle is present per lattice site, there is a Mott-insulator phase. For fermions this phase has only recently been observed [5, 11], and for bosons the superfluid to Mott insulator phase transition has been observed [3]. The Hubbard model is also thought to describe superconductivity at higher temperatures [1]. The ground state of this model is antiferromagnetic, and significant effort is going into trying to obtain this state experimentally. Another topic into which a lot of experimental effort is going, is imbalance in two component Fermi gases, where there is control over the separate components of the gas [9, 17]. This is important in a large number of fields including condensed matter, nuclear, high energy and astroparticle physics. In this thesis we investigate the effect of imbalance on the antiferromagnetic ground state of the Mott insulator phase.

First we will show that at low temperatures in an optical lattice only spin degrees of freedom are relevant. Then we will describe the phase transition from the antiferromagnetic to the paramagnetic state. After that we will determine how spin waves, or low level excitations, behave. Next, we will discuss topological excitations, known as merons, and finally, the Kosterlitz-Thouless phase transition is described.
Chapter 1

Optical lattices

In this chapter some background will be given to the material treated in the coming chapters. First we will see what optical lattices are. It will be explained how particles can be confined in lattices, which leads us to use the Hubbard model describing such systems. In particular, we will look at fermions trapped in lattices, such that there will be no hopping of the particles. This is described by a special case of the Hubbard model known as the Heisenberg model.

1.1 Atom laser interaction

Optical lattices are created by a set of counter propagating laser beams. The electric field of one such beam can in general be written as

$$\mathbf{E}(x, t) = \epsilon E_0 \cos(kz - \omega t) \exp\left\{ -\frac{x^2 + y^2}{2w^2(z)} \right\}. \quad (1.1)$$

Here, the frequency for photons of wavelength $\lambda$ is $\omega = \frac{2\pi c}{\lambda}$, and the wavenumber is $k = \frac{2\pi}{\lambda}$. $\epsilon$ is the polarization of the beam, which can be either constant or a function of space and time. We will take it to be constant. This electric field describes a wave travelling in the $z$-direction. In the $x$- and $y$-direction, it falls of exponentially. How quickly it falls of is determined by $w(z)$, which we will also take as a constant. If we now add a second laser beam, travelling in the opposite direction, we obtain a standing wave of light. The electric field can be written as

$$\mathbf{E}(x, t) = 2\epsilon E_0 \cos(kz) \cos(\omega t) \exp\left\{ -\frac{x^2 + y^2}{2w^2} \right\}. \quad (1.2)$$

Rewriting this as,

$$\mathbf{E}(r, t) = \epsilon E(x) \left( \frac{e^{i\omega t} + e^{-i\omega t}}{2} \right), \quad (1.3)$$

this can be quantized by writing the annihilation operator as $\hat{a} = \sqrt{\langle N_{ph} \rangle} e^{-i\omega t}$. The electric field operator is then given by

$$\hat{\mathbf{E}}(x) = \epsilon E(x) \left( \frac{\hat{a} + \hat{a}^\dagger}{2\sqrt{\langle N_{ph} \rangle}} \right). \quad (1.4)$$
This then describes what the optical lattice looks like.

If we now add a gas of atoms to the lattice, we need to know how these particles interact with the photons of the lattice. The main contribution is the quadratic Stark effect. An electric dipole moment is induced, which is classically given by, $d(x) = \alpha(\omega)E(x)$. Since other contributions to the coupling can usually be neglected, the potential can be written as

$$V^{ex}(x) = d(x) \cdot E(x) = -\alpha E^2(x).$$  \hspace{1cm} (1.5)

We can actually do better than this, by considering the quantum mechanical dipole operator. In its simplest form, we can consider an alkali atom, which has two states, the ground state $|g\rangle$, and an excited state $|e\rangle$, with energy $E_g$ and $E_e$ respectively. The interaction between the atom and the laser light is the same as it is classically:

$$\hat{H}_I = -\hat{d} \cdot \hat{E}(x),$$  \hspace{1cm} (1.6)

but now the dipole operator is given by $\hat{d} = -e \sum_i \hat{r}_i$. Here $e$ is the electron charge, and the sum is over all electrons of the alkali atom. Only the electrons in the outer shell are important though, and the alkali atoms have only one electron in their outer shells. Now we use perturbation theory, which for completeness is given appendix A. We write $\hat{H} = \hat{H}_0 + \hat{H}_I$, and assume that $\hat{H}_I$ is a weak perturbation. In the ground state the electronic orbital angular momentum is zero, therefore the first order correction vanishes:

$$\langle g | \hat{H}_I | g \rangle = 0.$$  \hspace{1cm} (1.7)

The second order correction is given by

$$E^{(2)} = \sum_{\nu \neq \nu'} \frac{|\langle \nu' | \hat{H}_I | \nu \rangle|^2}{E^{(0)}_{\nu} - E^{(0)}_{\nu'}}$$

$$= \sum_{\nu \neq \nu'} \frac{|\langle \nu' | \hat{d} \cdot \epsilon (\hat{a} + \hat{a}^\dagger) | \nu \rangle|^2}{4(N_{ph})} \frac{E^2(x)}{E^{(0)}_{\nu} - E^{(0)}_{\nu'}}$$

$$= \frac{|\langle g | \hat{d} \cdot \epsilon | e \rangle|^2}{4} \left( \frac{1}{E_g - E_e - \hbar \omega} + \frac{1}{E_g - E_e + \hbar \omega} \right) E^2(x),$$  \hspace{1cm} (1.8)

where the $\hat{a}$ and $\hat{a}^\dagger$ act on the states, which implicitly depend on the number of photons, $|\nu\rangle = |\nu, (N_{ph})\rangle$. We identify this contribution with the potential energy $V^{ex}$ for atoms in a laser trap. We now introduce the Rabi frequency

$$\hbar \Omega = \langle g | \hat{d} \cdot \epsilon | e \rangle E_0,$$  \hspace{1cm} (1.9)

which contains the information about the coupling of the atom with the laser light. Furthermore, we define the detuning from resonance $\delta$ as

$$\delta = \omega - (E_e - E_g)/\hbar.$$  \hspace{1cm} (1.10)

We assume the detuning to be small, so that the difference in energy between the two energy levels is more or less $E_e - E_g \sim \hbar \omega$. The potential for the atoms then becomes

$$V^{ex} = \frac{\Omega^2}{\delta} \cos^2(2\pi z/\lambda) \exp \left( -\frac{x^2 + y^2}{w^2} \right),$$  \hspace{1cm} (1.11)
Although this gives a good idea of how atoms are trapped in optical lattices, this is not the whole story. In some cases it may be necessary to consider the fine structure or even the hyperfine structure of the atoms. This can be calculated by writing out the total angular momentum states in the orbital angular momentum and the spin angular momentum states, by using the Clebsch-Gordan coefficients. We will just state the result. The potential the atoms will feel will look like

\[ V^{\text{ex}}(r) = \frac{(\hbar \Omega)^2}{3} \cos^2(2\pi z/\lambda) \exp \left\{ -\frac{x^2 + y^2}{w^2} \right\} \left( \frac{1}{E_g - E_{D1} + \hbar \omega} + \frac{1}{E_g - E_{D1} - \hbar \omega} + \frac{2}{E_g - E_{D2} + \hbar \omega} + \frac{2}{E_g - E_{D2} - \hbar \omega} \right) \].

(1.12)

In the limit \( \hbar \delta \gg |E_{D1} - E_{D2}| \) this result coincides with the result (1.11).

For a somewhat more elaborate discussion, see the book by Stoof, Gubbels and Dickerscheid [13].

1.1.1 Band structure

The wavefunction of a free atom is given by \( e^{ik \cdot x}/\sqrt{V} \), with a dispersion relation \( \epsilon_k = \hbar^2 k^2 / 2m \). The wavefunctions for noninteracting atoms in optical lattices remarkably resembles this to a high degree. From Bloch’s theorem [16], we know that the wavefunctions can be written

\[ \chi_{n,k}(x) = e^{ik \cdot x} u_{n,k}(x), \]

(1.13)

where \( u_{n,k}(x) \) is a function periodic in the lattice spacing. The dispersion relations will also be periodic. Each period is called a Brillouin zone, and each Brillouin zone will show a gap, where it goes over into the next zone. Since it costs more energy to be in the consecutive Brillouin zones, the energy will jump past the gaps, therefore there are different energy bands. The momentum of an atom can then be specified by the band index \( n \), and a value that is in the first Brillouin zone \( k \). Using the terminology, the Bloch wavefunctions can be written as

\[ \chi_{n,k}(x) = \sum_i e^{ik \cdot x} w_n(x - x_i) , \]

(1.14)

where the \( w_n(x - x_i) \) are the Wannier functions, which are orthogonal for the different bands, as well as for different sites. The minima of the lattice are denoted by \( x_i \). We will not need the specific form of these functions so we will not be bothered with that here.

1.2 The Hubbard model

Now that we know what the potential for fermions in an optical lattice looks like, we can try to describe the behavior of the particles in such a system. The action that describes a gas of atoms in an optical lattice is given by

\[
S[\psi^*, \psi] = \int_0^\hbar d\tau \int d\mathbf{x} \psi^*(\mathbf{x}, \tau) \left( \hbar \frac{\partial}{\partial \tau} - \frac{\hbar^2 \nabla^2}{2m} + V^{\text{ex}}(\mathbf{x}) \right) \psi(\mathbf{x}, \tau)
+ \frac{1}{2} \int_0^\hbar d\tau \int d\mathbf{x} \psi^*(\mathbf{x}, \tau) \psi^*(\mathbf{x}', \tau) V(\mathbf{x} - \mathbf{x}') \psi(\mathbf{x}', \tau) \psi(\mathbf{x}, \tau).
\]
The external potential here is that of an optical lattice:

\[ V_{\text{ex}}(x) = \sum_i V_0 \cos^2\left(\frac{2\pi x_i}{\lambda}\right), \tag{1.16} \]

where \( \lambda \) is the wavelength of the laser beams. The field operators can be expanded as

\[ \psi(x, \tau) = \sum_{n,i} a_{n,i}(\tau) w_n(x - x_i), \tag{1.17} \]

where the expansion coefficients \( a_{n,i}(\tau) \) correspond to the annihilation operators for the atoms, and \( w_n(x - x_i) \) denotes the Wannier wavefunction at site \( i \). If the lattices are sufficiently deep, that is, the laser intensity is large (tight-binding limit), the Wannier wavefunctions can be approximated by harmonic potentials. If we look additionally at sufficiently low temperatures, and at small interaction energies, the atoms will only occupy the ground states of the optical lattice, i.e., \( n = 0 \).

If we use this, the action can be written as

\[ S[a^*, a] = S_0[a^*, a] + S_{\text{int}}[a^*, a], \tag{1.18} \]

where,

\[ S_0[a^*, a] = \int_0^{\beta} d\tau \left\{ \sum_i a_i^*(\tau) \left( \frac{\hbar}{\partial \tau} + \varepsilon_i - \mu \right) a_i(\tau) - \sum_{i \neq j} a_i^*(\tau) t_{i,j} a_i(\tau) \right\}, \tag{1.19} \]

and the on site energy is given by

\[ \varepsilon_i = \int dx w_0^*(x - x_i) \left\{ -\frac{\hbar^2}{2m} \nabla^2 + V_{\text{ex}}(x) \right\} w_0(x - x_i). \tag{1.20} \]

Tunneling and hopping is described by

\[ t_{i,j} = -\int dx w_0^*(x - x_i) \left\{ -\frac{\hbar^2}{2m} \nabla^2 + V_{\text{ex}}(x) \right\} w_0(x - x_j), \tag{1.21} \]

which is almost the same as for the on site energy, but relates different sites. In principle, hopping can occur between all sites of the lattice, as indicated by the sum over \( i \neq j \) in equation (1.19), but in the tight binding limit hopping between not adjacent sites will be exponentially suppressed, so that in this limit the sum will be only over nearest neighbor pairs, indicated by \( \langle i, j \rangle \). The tunneling amplitude is now the same for all sites, so the subscript \( i, j \) can be dropped. The interaction term is given by

\[ S_{\text{int}}[a^*, a] = \int_0^{\beta} d\tau \frac{U}{2} \sum_i a_i^*(\tau) a_i^*(\tau) a_i(\tau) a_i(\tau), \tag{1.22} \]

with the interaction energy \( U \) given by

\[ U = \int dx \int dx' w_0^*(x - x_i) w_0^*(x - x_i) V(x - x') w_0(x' - x_i) w_0(x - x_i). \tag{1.23} \]
Now we are ready to introduce the Hubbard Hamiltonian. For bosons this is called the Bose-Hubbard model. We are interested in fermions only though. Due to the Pauli exclusion principle, in our case the Hamiltonian can be written as

\[ H = -\sum_{\alpha=\uparrow,\downarrow} t_{\alpha} \sum_{\langle ij \rangle} a_{i,\alpha}^\dagger a_{j,\alpha} + \sum_{\alpha=\uparrow,\downarrow} \sum_{i} (\varepsilon_{i,\alpha} - \mu_{\alpha}) a_{i,\alpha}^\dagger a_{i,\alpha} + U \sum_{i} a_{i,\uparrow}^\dagger a_{i,\uparrow} a_{i,\downarrow} a_{i,\downarrow}. \] (1.24)

This is the Hubbard Hamiltonian for fermions in an optical lattice. The first term describes tunneling between neighboring sites. The second term describes a possible imbalance between the different spin species. The last term describes the on site interaction between the particles.

Although this result was derived for fermions in an optical lattice, this model applies to other systems as well. For instance, using the concept of pseudo spin, we can describe double layer quantum Hall systems. Pseudo spin means that the spin label does not refer to the actual spin of a particle, but instead to some other quantity. For example, MacDonald et al. treat the case of bilayer systems. Here the spin label is used to refer to the layer the particle is in \[8\].

### 1.3 The Heisenberg Model

The following is a derivation taken from notes by Jan Zaanen \[14\]. We will now look at a special case of the Hubbard model. We will assume that there is no imbalance, so that the second term in equation (1.24) is absent. At very low temperatures, it is favorable to occupy each lattice site only once. If there are two particles on a site, one with spin up and one with spin down, this will cost energy due to the interaction term. Furthermore, we will assume that tunneling is kept to a minimum. This leads to the condition \( U \gg t \). The Hamiltonian can be written

\[ H = H_0 + T_+ + T_- \] (1.25)

\[ H_0 = V + T_0 \] (1.26)

\[ V = U \sum_{i} n_{i,\uparrow} n_{i,\downarrow} \] (1.27)

\[ T_0 = -t \sum_{\langle i,j \rangle,\alpha} \{(1 - n_{i,\bar{\alpha}}) a_{i,\alpha}^\dagger a_{j,\alpha}(1 - n_{j,\bar{\alpha}}) + n_{i,\bar{\alpha}} c_{i,\alpha}^\dagger c_{j,\alpha} n_{j,\bar{\alpha}}\} \] (1.28)

\[ T_+ = -t \sum_{\langle i,j \rangle,\alpha} n_{i,\bar{\alpha}} a_{i,\alpha}^\dagger a_{j,\alpha}(1 - n_{j,\bar{\alpha}}) \] (1.29)

\[ T_- = -t \sum_{\langle i,j \rangle,\alpha} (1 - n_{i,\bar{\alpha}}) a_{i,\alpha}^\dagger a_{j,\alpha} n_{j,\bar{\alpha}} \] (1.30)

Here we introduced the number operator \( n_{i,\alpha} = a_{i,\alpha}^\dagger a_{i,\alpha} \), and used the convention \( \bar{\alpha} = \uparrow, \downarrow \) when \( \alpha = \downarrow, \uparrow \). Next, we do a canonical transformation:

\[ H_{\text{eff}} = e^{S} H e^{-S} = H + [S, H] + \frac{1}{2} [S, [S, H]] + \mathcal{O}(S^3). \] (1.31)

Requiring this to vanish quickly, we have \( S \sim t/U \). To first order this transformation then becomes

\[ H^{(1)}_{\text{eff}} = H_0 + T_+ + T_- + [S^{(1)}, H] + \mathcal{O}(S^2). \] (1.32)
Now we demand that $H_0 = H_{\text{eff}}^{(1)}$. This then is equivalent to the condition

$$T_+ + T_- = -[S^{(1)}, H] = -[S^{(1)}, V],$$

(1.33)

where the last step follows from $S^{(1)} \sim t/U$. This can be solved to find $S^{(1)}$. First we calculate the commutators of $T_\pm$ and $V$:

$$[T_+, V] = -Ut \sum_{\langle ij \rangle k, \alpha} n_{i, \alpha} a_{i, \alpha}^\dagger a_{j, \alpha} n_{k, \uparrow} n_{k, \downarrow} (1 - n_{j, \bar{\alpha}})$$

(1.34)

$$= -Ut \sum_{\langle ij \rangle \alpha} n_{i, \alpha} (a_{i, \alpha}^\dagger a_{j, \alpha} n_{j, \uparrow} \delta_{\alpha, \uparrow} + a_{i, \alpha}^\dagger a_{j, \alpha} \delta_{\alpha, \downarrow} + a_{i, \alpha} n_{j, \uparrow} a_{j, \alpha} \delta_{\alpha, \uparrow} + a_{i, \alpha} n_{j, \downarrow} a_{j, \alpha} \delta_{\alpha, \downarrow})$$

$$+ n_{j, \bar{\alpha}} (a_{i, \alpha}^\dagger a_{j, \alpha} \delta_{\alpha, \downarrow})(1 - n_{j, \bar{\alpha}})$$

$$= -Ut \sum_{\langle ij \rangle \alpha} n_{i, \alpha} (a_{i, \alpha}^\dagger a_{j, \alpha} n_{j, \bar{\alpha}} + a_{i, \alpha}^\dagger a_{j, \alpha} n_{j, \bar{\alpha}} a_{j, \alpha} (1 - n_{j, \bar{\alpha}}).$$

Realizing that $n_{i, \alpha}^2 = n_{i, \alpha}$, the last line equals $-UT_+$. For $T_-$ a similar calculation can be made. We find

$$[T_+, V] = \mp UT_\pm.$$  

(1.35)

From this we can find $S^{(1)}$. We have

$$T_+ + T_- = -\frac{1}{U}(T_+ - T_-), V],$$

(1.36)

so that

$$S^{(1)} = \frac{1}{U}(T_+ - T_-).$$

(1.37)

Now up to second order, we write

$$H_{\text{eff}}^{(2)} = H_0 + H',$$

(1.38)

$$S^{(2)} = S^{(1)} + S'.$$

Comparing this to (1.31),

$$H_{\text{eff}}^{(2)} = H_0 + T_+ + T_- + [S^{(1)} + S', H] + \frac{1}{2}[S^{(1)}, [S^{(1)}, H]],$$

(1.39)

$$H' = [S^{(1)}, T_0] + [S^{(1)}, T_+] + [S', V] + \frac{1}{2}[S^{(1)}, [S^{(1)}, H]]$$

(1.40)

$$= \frac{1}{U}[T_+ - T_-] + [S^{(1)}, T_0] + [S', V].$$

Here we used that $S' \sim (t/U)^2$, and because of this, we have up to $O(t^3/U^2)$, that $[S', H] = [S', V]$. All higher powers are discarded. Analogous to the first order expansion, we now have

$$[S^{(1)}, T_0] = -[S', V],$$

(1.41)

so that to second order, to hamiltonian becomes

$$H_{\text{eff}}^{(2)} = H_0 + \frac{1}{U}[T_+, T_-].$$

(1.42)
If we now assume that there are no doubly occupied sites on the lattice, this simplifies even further. In this case we have $V = 0$. Furthermore, the combination $a_{i,\alpha}n_{i,\bar{\alpha}}$ is also zero. If there is a particle of spin $\bar{\alpha}$ on site $i$, $n_{i,\bar{\alpha}} = 1$, but $a_{i,\alpha}$ gives zero, since there is no particle of spin $\alpha$. If on the other hand, there is a particle of spin $\alpha$, then $n_{i,\bar{\alpha}} = 0$. Therefore, in this case, $T_+T_- = 0$ and the second term of $T_0$ is zero as well and $H^{(2)}_{\text{eff}}$ reduces to

$$H^{(2)}_{\text{eff}} = -\frac{J}{4} \sum_{\langle ij \rangle, \alpha, \alpha'} (1 - n_{i,\bar{\alpha}}) a_{i,\alpha}^\dagger a_{j,\alpha'}(1 - n_{j,\bar{\alpha}}). \quad (1.43)$$

Here we introduced $J = 4t^2/U$, called the superexchange interaction constant. It is the energy cost for virtual hops, or spin flips. In a virtual hop, particles hopping to adjacent sites are still allowed, but the particles have to hop back to the empty sites, so that in the end there are no doubly occupied sites. If we now make the final assumption that there is one particle for each lattice site, the first term in (1.43) is zero, since each hopping of a particle would leave the system with a doubly occupied site, which is not allowed. Furthermore, we must have $i = i'$ and $j = j'$, otherwise again there would be doubly occupied sites. For the same reason we have $(1 - n_{i,\bar{\alpha}})c_{i,\sigma}^\dagger = c_{i,\sigma}^\dagger$. We then have

$$H^{(2)}_{\text{eff}} = -\frac{J}{4} \sum_{\langle ij \rangle, \alpha, \alpha'} a_{i,\alpha}^\dagger a_{j,\alpha} n_{j,\bar{\alpha}} n_{i,\bar{\alpha}}', a_{i,\alpha'}^\dagger a_{j,\alpha'}(1 - n_{j,\bar{\alpha}}). \quad (1.44)$$

If we now introduce the spin operators for spin $\frac{1}{2}$ particles

$$\hat{S}_i^z = \frac{1}{2} \left( a_{i\uparrow}^\dagger a_{i\uparrow} - a_{i\downarrow}^\dagger a_{i\downarrow} \right)$$

$$\hat{S}_i^+ = a_{i\uparrow}^\dagger a_{i\downarrow}$$

$$\hat{S}_i^- = a_{i\downarrow}^\dagger a_{i\uparrow}, \quad (1.45)$$

the Hamiltonian becomes

$$H^{(2)}_{\text{eff}} = J \sum_{\langle ij \rangle} \left( \hat{S}_i \cdot \hat{S}_j - \frac{1}{4} \right). \quad (1.46)$$

This is the Heisenberg Hamiltonian. We see that in contrast to the Hubbard model, only spin degrees of freedom are relevant. At energies $\ll U$, the following virtual hop could occur: $|\uparrow_i\downarrow_{i+\delta}\rangle \rightarrow |0\rangle |\downarrow_i\uparrow_{i+\delta}\rangle \rightarrow |\downarrow_i\uparrow_{i+\delta}\rangle$. Effectively, this is a spin flip. For the state $|\uparrow_i\downarrow_{i+\delta}\rangle$ virtual hoppings are forbidden by the Pauli exclusion principle. Fluctuations of this state lead to an energy gain. Therefore anti-parallel alignment is more favorable. This then justifies taking $J > 0$. 
Chapter 2

The phase transition

The aim of this chapter is to derive where the phase transition from antiferromagnet to paramagnet occurs. We will see that only for zero magnetic field, a pure antiferromagnet can occur. For non zero magnetic field, and below a certain critical temperature, the system will be in the canted phase, in which the spin degrees of freedom of the system tend to align due to the presence of the magnetic field, but also tend to anti align due to the repulsive nature of the interaction. Therefore, in the ground state the spins will be pointing in two directions alternatingly. It will be convenient to divide the lattice in two sublattices, called the A and the B lattice, where the particles in one sublattice only have neighbors in the other sublattice, so that all particles in one sublattice point in the same direction. For a two dimensional lattice, this is shown in picture 2.1.

\begin{figure}[h]
\centering
\includegraphics[width=0.5\textwidth]{lattice_division.png}
\caption{It is shown how a lattice can be divided in two sublattices, such that all sites only have neighbors in the other sublattice.}
\end{figure}

2.1 The free energy

The easiest way to find the critical temperature, at which the phase transition occurs, is by looking at the behavior of the free energy of the system. Starting from the Heisenberg hamiltonian in the presence of a magnetic field,

\begin{equation}
H = J \sum_{(ij)} \hat{S}_i \cdot \hat{S}_j - \sum_i \hat{S}_i \cdot \mathbf{B},
\end{equation}

where \( J \) is the exchange integral and \( \mathbf{B} \) is the magnetic field.
it is straightforward to calculate the free energy. In this expression $J$ is the superexchange constant that determines the strength of the repulsive interaction between the spins, $\mathbf{S}_i$ is the spin operator at site $i$ with expectation value $\pm \frac{1}{2}$. $\mathbf{B}$ is the magnetic field and $\langle ij \rangle$ denotes all nearest neighbor pairs. To treat the hamiltonian in mean field theory, we write

$$\hat{\mathbf{S}}_i = M_i + \delta \hat{\mathbf{S}}_i,$$  \hspace{1cm} (2.2)

where $M_i = \langle \hat{\mathbf{S}}_i \rangle$. Since all particles in one sublattice point in the same direction, we write $M_i = M_{A,B}$, where $i$ is in the $A$ or in the $B$ sublattice respectively. The mean field theory consists of linearizing in the fluctuations $\delta \hat{\mathbf{S}}_i$. The first term of (2.1) becomes

$$J \sum_{\langle ij \rangle} (\mathbf{M}^A \cdot \mathbf{M}^B + \mathbf{M}^A \cdot \delta \hat{\mathbf{S}}_j^B + \mathbf{M}^B \cdot \delta \hat{\mathbf{S}}_j^A + \delta \hat{\mathbf{S}}_i^A \cdot \delta \hat{\mathbf{S}}_j^B).$$  \hspace{1cm} (2.3)

Neglecting terms $\delta S^2$ this equals

$$J \sum_{\langle ij \rangle} (-\mathbf{M}^A \cdot \mathbf{M}^B + \mathbf{M}^A \cdot \delta \hat{\mathbf{S}}_j^B + \mathbf{M}^B \cdot \delta \hat{\mathbf{S}}_j^A).$$  \hspace{1cm} (2.4)

We find

$$H = -\frac{1}{2} J z N \mathbf{M}^A \cdot \mathbf{M}^B + J z \sum_i (\mathbf{M}^A \cdot \delta \hat{\mathbf{S}}_i^B + \mathbf{M}^B \cdot \hat{\mathbf{S}}_i^A) - \sum_i \mathbf{B} \cdot (\hat{\mathbf{S}}_i^A + \hat{\mathbf{S}}_i^B)$$  \hspace{1cm} (2.5)

$$= -\frac{1}{2} J z N \mathbf{M}^A \cdot \mathbf{M}^B - \sum_i (B - J z \mathbf{M}^A) \cdot \hat{\mathbf{S}}_i^B - \sum_i (B - J z \mathbf{M}^B) \cdot \hat{\mathbf{S}}_i^A.$$  \hspace{1cm} (2.6)

The partition function is found by summing $\exp \{-\beta H_s\}$ over all possible states $s$:

$$Z = e^{\beta J z N \mathbf{M}^A \cdot \mathbf{M}^B / 2} \prod_s \prod_i \exp \left\{ \beta (\mathbf{B} - J z \mathbf{M}^A) \cdot \hat{\mathbf{S}}_i^B + \beta (\mathbf{B} - J z \mathbf{M}^B) \cdot \hat{\mathbf{S}}_i^A \right\}.$$  \hspace{1cm} (2.7)

This expression can be simplified by realizing that $\sum_s \prod_i = \prod_i \sum_s$, and $s_i$ are the possible states on one site, which is just $\pm \frac{1}{2}$. We find

$$Z = e^{\beta J z N \mathbf{M}^A \cdot \mathbf{M}^B / 2} \left( 4 \cosh \left\{ \frac{\beta}{2} |\mathbf{B} - J z \mathbf{M}^A| \right\} \cosh \left\{ \frac{\beta}{2} |\mathbf{B} - J z \mathbf{M}^B| \right\} \right)^{N/2}.$$  \hspace{1cm} (2.8)

The free energy is now given by

$$F = -\frac{1}{\beta} \log Z,$$  \hspace{1cm} (2.9)

where $\beta$ is $1/k_BT$ is the inverse temperature. Using the expression for $Z$, the free energy is

$$F = -\frac{J z N}{2} \mathbf{M}^A \cdot \mathbf{M}^B - \frac{N}{2\beta} \log \left( 4 \cosh \left\{ \frac{\beta}{2} |\mathbf{B} - J z \mathbf{M}^A| \right\} \cosh \left\{ \frac{\beta}{2} |\mathbf{B} - J z \mathbf{M}^B| \right\} \right).$$  \hspace{1cm} (2.10)

We define the total magnetization $\mathbf{m}$ and the Néel parameter $\mathbf{n}$ by

$$z \mathbf{M}^A = \mathbf{m} + \mathbf{n}, \quad z \mathbf{M}^B = \mathbf{m} - \mathbf{n}.$$  \hspace{1cm} (2.11)
The magnetization describes the amount of imbalance in the system. At full magnetization, all spins are pointing in the same direction. At zero magnetization, all spins are alternatingly pointing up and down. At other values of the magnetization, the spin species populations are not equally sized when measured, that is, there is an imbalance. The Néel parameter describes the amount of anti alignment, or the anti parallel component of the spins on the two sublattices. It is convenient to use this notation, because the Néel parameter turns out to be the order parameter of the phase transition. If \( n = 0 \), then \( M^A = M^B \), and the system is in the ferromagnetic phase. The phase transition then occurs at the point where \( n \) becomes non-zero. Rescaling \( F/J, \beta \) and \( B \) by \( J \),

\[
\frac{F}{J} \rightarrow F, \quad J\beta \rightarrow \beta, \quad \frac{B}{J} \rightarrow B,
\]

the free energy per particle\(^1\) becomes

\[
F = \frac{n^2 - m^2}{2z} - \frac{1}{2\beta} \log \left( 4 \cosh \left( \frac{\beta}{2} |B - m - n| \right) \cosh \left( \frac{\beta}{2} |B - m + n| \right) \right). \tag{2.13}
\]

It is more convenient however to write it a bit differently. If we write

\[
\tilde{F} = \frac{n^2 - m^2}{2z} - \frac{1}{2\beta} \log \left( 4 \cosh \left( \frac{\beta}{2} |B - m - n| \right) \cosh \left( \frac{\beta}{2} |B - m + n| \right) \right) + \frac{1}{z} m \cdot B, \tag{2.14}
\]

we have the same equations provided that they are subject to the constraint

\[
\nabla_B \tilde{F} = 0. \tag{2.15}
\]

This allows us to solve for \( B \) and put the expression for \( B \) back in the free energy. To see that this is correct, we write the hamiltonian as

\[
H = H_I - \sum_i \hat{S}_i \cdot B. \tag{2.16}
\]

We see that

\[
\nabla_B F = -\frac{1}{\beta} \nabla_B \log Z = -\frac{1}{\beta Z} \sum_s \beta \sum_i \hat{S}_i \exp \{ -\beta H_s \} = -\sum_i \langle \hat{S}_i \rangle = -\frac{m}{z}, \tag{2.17}
\]

or

\[
\nabla_B \tilde{F} = \nabla_B (F + \frac{1}{z} m \cdot B) = 0. \tag{2.18}
\]

From this expression, the similarity with the difference between a canonical and a grand canonical ensemble is apparent. Working backwards from this expression, we have

\[
\tilde{F} = -\frac{1}{\beta} \log \left[ \text{Tr} \exp \left\{ \beta \left( \frac{1}{z} m \cdot B - H_s \right) \right\} \right]. \tag{2.19}
\]

Taking the analogy with the grand canonical ensemble, we have that the magnetization plays the role of the number of particles, and the magnetic field that of the chemical potential. This makes sense since the magnetization can be written \( m = S(N_\uparrow - N_\downarrow)/(N_\uparrow + N_\downarrow) \), so it is expressed not in the number of particles, but in the number of different spin orientations. Since the spins tend to align to the magnetic field, changing the magnetic field changes the number of spins pointing in one direction, which is what the chemical potential tells one about two systems of particles.

Since in the remainder, we will only use \( \tilde{F} \), we will simply call it \( F \) from now on.

---

\(^1\)It does not matter how the free energy is scaled, as we are only interested in the minimum of the free energy.
2.2 Phase transition

Now that we have the free energy, we can calculate where the phase transition occurs. The value of the Néel parameter is found by minimizing the free energy. We want to find the point where this value becomes non-zero. Since we are looking at the minimum of the free energy, there will be no linear term. If the coefficient of the second order term is negative, the minimum will not be at \( n = 0 \), since it is leading order\(^2\). If the second order term is positive on the other hand, the minimum will be at \( n = 0 \). The phase transition then occurs when the coefficient of the second order term in the expansion of \( F \) is zero. Therefore, we expand the free energy in \( n \) and only keep terms of \( O(n^2) \).

For this approach to work properly, it is important that we are dealing with a second-order phase transition. One can check this by plotting the total free energy surface as a function of the magnetization and the Néel parameter, and then checking at different temperatures that the minima are that of a mexican hat: one can find minima on circles centered at \( n = 0 \) and \( m = 0 \). For increasing temperatures, these circles shrink until there is only one minimum at \( n = 0 \) and \( m = 0 \). This shows that the order parameter is a continuous function.

2.2.1 The Ising model

We will first do the calculations for the Ising model. Although we will see that the results for the Ising model are more complicated than for the Heisenberg model, the calculation itself is much less involved. The difference between the Ising model and the Heisenberg model is that in the Ising model, the Néel parameter and the magnetization are restricted to be along the same axis, while in the Heisenberg model there is no such restriction. This simplifies the problem considerably since now we no longer need vector expressions. The Ising model can be written

\[
H = J \sum_{\langle ij \rangle} S_i^z S_j^z, \tag{2.20}
\]

and the free energy for the Ising model is given by

\[
F = \frac{n^2 - m^2}{2z} - \frac{1}{2\beta} \log[4 \cosh[\frac{\beta}{2}(b - m - n)] \cosh[\frac{\beta}{2}(b - m + n)]] + \frac{mb}{z}. \tag{2.21}
\]

Here \( m \) is the magnetization, \( n \) is the Néel parameter, \( b \) is the magnetic field and \( \beta \) is the inverse temperature. This expression can be obtained either by calculating it directly from the hamiltonian, or by noting that the Ising free energy is just a scalar version of the Heisenberg free energy. The constraint on the free energy is \( \partial_b F = 0 \), or

\[
\frac{4m}{z} = \tanh[\frac{\beta}{2}(b - m + n)] + \tanh[\frac{\beta}{2}(b - m - n)]. \tag{2.22}
\]

This expression can be solved for small \( n \), to derive the constrained magnetic field. Since we are solving to find the minimum, we only need \( b \) up to order \( O(n^2) \). We write \( b = b_0 + b_2 n^2 \). Using

\(^2\)If this pre-factor is negative, \( n = 0 \) will be a local maximum of the free energy, whereas when this factor is positive, this will be a local minimum.
this in the constraint and expanding to $O(n^2)$ gives

$$\frac{4m}{z} = 2 \tanh \left[ \frac{\beta}{2} (b_0 - m) \right] + \frac{\beta \left[ 2b_2 - \beta \tanh \left[ \frac{\beta}{2} (b_0 - m) \right] \right]}{2 \cosh^2 \left[ \frac{\beta}{2} (b_0 - m) \right]} n^2. \quad (2.23)$$

To find $b_0$ from this expression, we put $n$ to zero and solve for $b_0$:

$$b_0 = m + \frac{2}{\beta} \arctanh \left[ \frac{2m}{z} \right]. \quad (2.24)$$

Plugging this back in, we can solve for $b_2$:

$$b_2 = \frac{m \beta}{z}. \quad (2.25)$$

Therefore $b$ is, up to order $O(n^2)$, given by

$$b = m + \frac{2}{\beta} \arctanh \left[ \frac{2m}{z} \right] + \frac{m \beta}{z} n^2. \quad (2.26)$$

This we can use in the free energy. Since we are only interested in the quadratic term in the expansion of the free energy, we take the second derivative of the free energy, with respect to $n$. Putting this to zero, we find

$$z^2 \beta = 4z + 4m^2 \beta, \quad (2.27)$$

or

$$T_{\text{crit}} = \frac{z^2 - 4m^2}{4z}. \quad (2.28)$$

The results are shown in figure 2.2, along with the results for the Heisenberg model derived in the following section.

### 2.2.2 The Heisenberg model

#### Solving the constraint

To find the phase transition for the Heisenberg model, we use the same approach as for the Ising model. First we will need to evaluate the constraint. We have

$$\nabla_B F(n) = -\frac{1}{2\beta} \left( \nabla_B \cosh \left\{ \frac{\beta}{2} |B - m + n| \right\} + \frac{\nabla_B \cosh \left\{ \frac{\beta}{2} |B - m - n| \right\}}{\cosh \left\{ \frac{\beta}{2} |B - m - n| \right\}} \right) + \frac{m}{z} = 0, \quad (2.29)$$

$$\nabla_B \cosh \left\{ \frac{\beta}{2} |B - m \pm n| \right\} = \frac{\beta}{2} \sinh \left\{ \frac{\beta}{2} |B - m \pm n| \right\} \frac{B - m \pm n}{|B - m \pm n|}. \quad (2.30)$$

If we define

$$g_\sigma = g(B - m + \sigma n) = \frac{\tanh \left\{ \frac{\beta}{2} |B - m + \sigma n| \right\}}{|B - m + \sigma n|}, \quad (2.31)$$
the constraint can be rewritten as
\[ B = \frac{4}{z} \frac{m}{g_+ + g_-} + m - n \frac{g_+ - g_-}{g_+ + g_-}. \]  
(2.32)
The \( g_\pm \) are still a function of \( B \) though. Next, we expand \( B \) in \( n \)
\[ B = B_0 + B_{2,0} n^2 m + B_{2,1} (m \cdot n)^2 m + B_{2,2} (m \cdot n) n + H.O. \]  
(2.33)
From (2.32) we can see directly that
\[ B_0 = B|_{n=0} = \left( \frac{2}{zg_0} + 1 \right) m \equiv (B_0 + 1)m, \]  
(2.34)
with
\[ g_\pm|_{n=0} = g_0 = \frac{2}{zB_0}. \]  
(2.35)
Expanding \( g_\pm \) in orders of \( |n| \) gives
\[ g_\pm = g_0 \pm (n \cdot m)B_0 g_1 + \frac{A_1}{2} n^2 + \frac{A_2}{2} (n \cdot m)^2, \]  
(2.36)
with
\[ A_1 = g_1 (1 + 2B_0 B_{2,0} m^2), \]  
(2.37)
\[ A_2 = (B_0^2 g_2 + 2g_1 B_0 (B_{2,1} m^2 + B_{2,2})). \]  
(2.38)
Plugging this in the expression for \( B \) allows us to solve for the coefficients of \( B \). The results are
\[ B_{2,0} = -g_1 B_0^2 z \frac{1 + 2B_0 B_{2,0} m^2}{4}, \]  
(2.39)
\[ B_{2,1} = \frac{zB_0^4(zB_0 g_1^2 - g_2)}{4 + 2zB_0 g_1 m^2}, \]  
(2.40)
\[ B_{2,2} = -\frac{zB_0^2 g_1}{2}, \]  
(2.41)
with
\[ B_0 = \frac{2}{\beta |m|} \arctanh \left( \frac{2|m|}{z} \right), \]  
(2.42)
\[ g_1 = -\frac{2}{B_0^2 m^2 z} + \frac{\beta}{2B_0^2 m^2} - \frac{2\beta}{B_0^2 z^2}, \]  
(2.43)
\[ g_2 = \frac{6}{B_0^3 m^4 z} - \frac{3\beta}{2B_0^3 m^4} + \frac{6\beta}{B_0^3 m^2 z^2} + \frac{4\beta^2}{B_0^3 z^3} - \frac{\beta^2}{B_0^3 m^2 z}, \]  
(2.44)
thus finding \( B \) up to second order.
Expanding the free energy

Now that we have a small \( n \) expression for the constrained \( B \), we can expand the free energy. Since this expansion can be written as

\[
F(n) = F\bigr|_{n=0} + \nabla F\bigr|_{n=0} \cdot n + \frac{1}{2} \nabla \otimes \nabla F\bigr|_{n=0} : n \otimes n + O(n^3),
\]

this boils down to calculating derivatives. Since we are only interested in the minimum of the free energy, the zeroth order term does not concern us. Therefore we proceed to calculate \( \nabla F \):

\[
\nabla F = \frac{n}{z} - \frac{1}{2\beta} \sum_{\sigma = \pm} \tanh \left\{ \frac{\beta}{2} |B - m + \sigma n| \right\} \frac{\beta}{2} \nabla |B - m + \sigma n| + \frac{1}{z} \nabla (m \cdot B).
\]

In the following we will use an index notation and summation convention, because otherwise it will be hard to follow what different kinds of products mean. We have \((\nabla)_i = \partial_i\) and

\[
\partial_i |B - m + \sigma n| = \frac{(B_j - m_j + \sigma n_j)}{|B - m + \sigma n|} (\partial_i B_j + \sigma \delta_{ij}),
\]

\[
\partial_i B_j = 2B_{2,0} n_i m_j + 2B_{2,1} m_k n_k m_j + B_{2,2} (m_i n_j + m_k n_k \delta_{ij}).
\]

From this we can see directly that \( \nabla F\bigr|_{n=0} = 0 \), as it should be at the minimum. For the second order term, we need to calculate

\[
\nabla \otimes \nabla F\bigr|_{n=0} = \frac{1}{z} - \frac{1}{4} \sum_{\sigma} \partial_j \left[ \frac{\tanh \left\{ \frac{\beta}{2} |B - m + \sigma n| \right\}}{|B - m + \sigma n|} (B_k - m_k + \sigma n_k) (\partial_i B_k + \sigma \delta_{ik}) \right] \big|_{n=0}
\]

\[
+ \frac{1}{z} m_k \partial_i \partial_j B_k \big|_{n=0}
\]

\[
= \frac{1}{z} - \frac{1}{2} g_1 B_0^2 m \otimes n - \frac{1}{2} g_0.
\]

If we now choose coordinates such that \( n = (0, 0, n) \) and \( m \cdot n = mn \cos \alpha \), with \( m = |m| \), we find

\[
\nabla \otimes \nabla F\bigr|_{n=0} : n \otimes n = \frac{\beta (2mn + (4m^2 - z^2) \arctanh \left\{ \frac{2m}{z} \right\}) m^2 \cos^2 \alpha - 2m^2z (m\beta - 2\arctanh \left\{ \frac{2m}{z} \right\})}{4m^2z^2 \arctanh \left\{ \frac{2m}{z} \right\}} n^2.
\]

Next, we can minimize this expression with respect to the angle \( \alpha \). We find that \( \cos \alpha = 0 \) and, by putting the result equal to zero,

\[
T_{\text{crit}} = \frac{m}{2 \arctanh \left\{ \frac{2m}{z} \right\}}.
\]

Using this in the expression we had for the constrained magnetic field, we find

\[
B_{\text{crit}} = 2m.
\]

Now we have found where the phase transition occurs.
Figure 2.2: Phase diagrams plotted for the Heisenberg model (solid line) and the Ising model (dashed line). The reentrant behavior is absent in the Heisenberg case, which can be seen in the plot of B as a function of T. Also shown is B as a function of m.

2.2.3 The phase diagram

It is interesting to compare the Heisenberg model with the Ising model. For both models the phase transition from paramagnet to antiferromagnet is shown in figure 2.2. The Ising model is a well studied model, which can also be described by the Heisenberg hamiltonian, but in which the Néel parameter and the magnetization are restricted to be parallel. In our case, this state is in principle allowed, but it turns out that it is not favorable energetically. This can be seen as follows. At zero temperature, the expectation value of the spins is $\pm \frac{1}{2}$. Now if there is a magnetic field, all spins tend to align to the magnetic field, but at the same time anti align to each other. In the Heisenberg model, the system can go into the canted phase, in which the spins compromise between the two, while maintaining expectation value $\pm \frac{1}{2}$, but in the Ising model, this is not possible, since when the expectation value is $\pm \frac{1}{2}$, the spins are either fully aligned, or fully anti aligned. Therefore, the Ising model can never describe the groundstate of the Heisenberg model.

It is important to notice, that the reentrant behavior that was present in the Ising case, is absent. This was a peculiar feature of the Ising model, which meant that you could go from the paramagnetic phase, to the antiferromagnetic phase by raising the temperature.

Now that we know where the transition from paramagnet to antiferromagnet occurs, we would like to know what happens below the critical temperature. We can follow the same procedure as before, that is minimize the free energy with respect to the Néel vector, and then solve for the angle $\alpha$ between the Néel vector and the magnetization. The difference is that now we have to expand around an arbitrary value of $\mathbf{n}$. For the constraint this would involve solving for a hyperbolic tangent, so there are no analytic solutions to this problem. It is however possible to do
Figure 2.3: The phase diagram is shown again, but with the magnitude of $n$ given at each point. The red line shows the phase diagram as plotted in figure 2.2

This numerically. The phase diagram with for every point the value for $|n|$ is given in figure 2.3.

It turns out that the magnetization and the Néel vector are perpendicular everywhere in the phase diagram, and that the magnetization is always parallel to the magnetic field. This means that there is an imbalance in the spin species populations, and the system is always in the canted phase: the spin-vectors on the two sublattices parallel part in the direction of the magnetic field, and an anti-parallel part perpendicular to the magnetic field.
Chapter 3

Spin waves

In the previous chapter the phase diagram was determined in mean field theory. Now we would like to calculate how excitations of the system behave. We will look at spin waves travelling through the lattice, first starting from the Heisenberg hamiltonian, and then using a spin path integral formalism. Then we will look at the dispersion relations, corresponding to the spin waves in the system.

3.1 Dispersion relations

We start again with the Heisenberg hamiltonian

\[ H = J \sum_{\langle ij \rangle} \hat{S}_i \cdot \hat{S}_j. \] (3.1)

The magnetic field term is absent here, and we choose instead to take this into account by putting a constraint on the free energy, as was done in the previous chapter. Using the Heisenberg equation, we can compute the time-evolution of operators:

\[ \frac{d}{dt} \hat{S} = \hat{S} = \frac{1}{i\hbar} \left[ \hat{S}, H \right]. \] (3.2)

We also need the spin commutation relations,

\[ [\hat{S}_i, \hat{S}_j] = i\hbar \epsilon_{ijk} \hat{S}_k. \] (3.3)

We find

\[ \frac{d}{dt} \hat{S}_k^\alpha = \frac{J}{i\hbar} \sum_{\langle \mu \nu \rangle} \left[ \hat{S}_k^\alpha, \hat{S}_\mu^\beta \hat{S}_\nu^\beta \right], \] (3.4)
where the upper greek indices label the sites, the lower latin indices are used to label the vector components, and there is summation convention over the latin indices. We then have

$$\frac{d}{dt} \hat{S}_k^\alpha = J \sum_{\langle \mu \nu \rangle} \epsilon_{klm} \left( \langle S_m^\mu \rangle \delta_{\alpha \mu} + \langle S_m^\mu \rangle \delta_{\nu \alpha} \right)$$

(3.5)

$$= J \sum_{\langle \mu \nu \rangle} \epsilon_{klm} \langle S_l^\mu \rangle \langle S_m^\nu \rangle (-\delta_{\alpha \mu} + \delta_{\alpha \nu}).$$

At this point, we can easily see that for the total magnetization, we have

$$\frac{d}{dt} M = \frac{d}{dt} \sum_\alpha \hat{S}_k^\alpha = 0.$$  

(3.6)

So the magnetization is a constant of the motion, and therefore it also does not fluctuate. This makes sense, as we have seen in the last chapter that the Néel parameter is the order parameter of the system, and the magnetization is directly related to the magnetic field.

Next, we work in mean field theory: $\hat{S}_i^\mu = \langle S_i^\mu \rangle + \delta \hat{S}_i^\mu$, and neglect terms of $O(\delta S^2)$,

$$\hat{S}_i^\mu \hat{S}_m^\nu = (\langle S_i^\mu \rangle + \delta \hat{S}_i^\mu)(\langle S_m^\nu \rangle + \delta \hat{S}_m^\nu)$$

$$= \langle S_i^\mu \rangle \langle S_m^\nu \rangle + \langle S_i^\mu \rangle \delta \hat{S}_m^\nu + \delta \hat{S}_i^\mu \langle S_m^\nu \rangle + O(\delta S^2).$$

(3.7)

By taking the expectation value on both sides, we see that

$$\langle \hat{S}_i^\mu \hat{S}_m^\nu \rangle = \langle \hat{S}_i^\mu \rangle \langle \hat{S}_m^\nu \rangle.$$  

(3.8)

We find

$$\frac{d}{dt} \delta \hat{S}_k^\alpha = J \sum_{\langle \mu \nu \rangle} \epsilon_{klm} \langle \delta \hat{S}_m^\nu \rangle - \langle \delta \hat{S}_k^\mu \rangle (-\delta_{\alpha \mu} + \delta_{\alpha \nu}).$$

(3.9)

If we plug the expression for the total spin back in, we see that up to a constant term, the equation of motion for the fluctuations is the same as that for the total spin. Next, we can write out the summation. Since every spin pair is contained in the sum once, we can choose $\mu = \alpha$ and sum $\nu$ over all neighboring sites:

$$\frac{d}{dt} \hat{S}_k^\alpha = J \sum_{\delta} \epsilon_{klm} (-\langle S_l^\alpha \rangle \hat{S}_m^{\alpha+\delta} + \langle S_l^{\alpha+\delta} \rangle \hat{S}_m^\alpha).$$

(3.10)

Here the sum over $\delta$ indicates the sum over neighboring sites. In vector notation this can be written as

$$\frac{d}{dt} \mathbf{S}^\alpha = J \sum_{\delta} (\mathbf{S}^\alpha \times \mathbf{S}^{\alpha+\delta} + \mathbf{S}^{\alpha+\delta} \times \mathbf{S}^\alpha).$$

(3.11)

1This constant term however, does not contribute to the equations of motion, because if you apply mean field theory to the Hamiltonian, this term drops out in the commutator. Therefore the equations of motion are equivalent for the spin operators and the variations of the spin operators.
Next, we perform a Fourier transformation,

$$\hat{S}^{\alpha \in A,B} = \int d\omega \sum_{k} u_{A,B} \exp \{ i(x_{\alpha} \cdot k - \omega t) \},$$

(3.12)

where $u_{A,B} = u_{A,B}(k,\omega)$. Plugging this into the equation of motion and using the completeness of the exponentials gives

$$-i\omega u_{A,B} = J \sum_{\delta} (-\langle S^{\alpha} \rangle \times u_{B,A} e^{i\delta \cdot k} + \langle S^{\alpha+\delta} \rangle \times u_{A,B})$$

$$= Jz(-\gamma(k) \langle S^{A,B} \rangle \times u_{B,A} + \langle S^{B,A} \rangle \times u_{A,B}),$$

(3.13)

where $\gamma(k) = z^{-1} \sum_{\delta} e^{i\delta \cdot k}$. If we now use $u = (u_{A}, u_{B})$, the problem can be recast in matrix form,

$$-i\omega u = M u,$$

(3.14)

where $M$ is a 6 by 6 matrix given by

$$M = Jz \begin{pmatrix}
0 & -\langle S^{B} \rangle & \langle S^{B} \rangle & 0 & \gamma \langle S^{A} \rangle & -\gamma \langle S^{A} \rangle \\
-\langle S^{B} \rangle & 0 & -\langle S^{B} \rangle & -\gamma \langle S^{A} \rangle & 0 & \gamma \langle S^{A} \rangle \\
\langle S^{B} \rangle & -\gamma \langle S^{B} \rangle & 0 & \gamma \langle S^{A} \rangle & -\gamma \langle S^{A} \rangle & 0 \\
\langle S^{B} \rangle & -\gamma \langle S^{B} \rangle & -\gamma \langle S^{B} \rangle & 0 & -\langle S^{A} \rangle & \langle S^{A} \rangle \\
\gamma \langle S^{B} \rangle & 0 & -\gamma \langle S^{B} \rangle & -\langle S^{A} \rangle & 0 & -\langle S^{A} \rangle \\
\gamma \langle S^{B} \rangle & 0 & -\gamma \langle S^{B} \rangle & -\langle S^{A} \rangle & 0 & -\langle S^{A} \rangle \\
\end{pmatrix}.$$  

(3.15)

We can simplify this expression by relating the $\langle S^{\alpha} \rangle$ corresponding to the canted phase,

$$\langle S^{B}_{z} \rangle = \langle S^{A}_{z} \rangle$$

$$-\langle S^{B}_{y} \rangle = \langle S^{A}_{y} \rangle$$

$$\langle S^{B}_{x} \rangle = \langle S^{A}_{x} \rangle = 0,$$

(3.16)

so that the Néel vector and the magnetization are perpendicular. If we now do a transformation to $u' = (m_{x}, m_{y}, n_{z}, n_{x}, n_{y}, m_{z})$, where $m = u^{A} + u^{B}$ and $n = u^{A} - u^{B}$, the matrix becomes block diagonal,

$$M' = \begin{pmatrix}
M_{1} & 0 \\
0 & M_{2}
\end{pmatrix},$$

(3.17)

and we are left with two 3 by 3 matrices $M_{1}$ and $M_{2}$ given by

$$M_{1} = Jz \begin{pmatrix}
0 & -(S^{A}_{z})(1 - \gamma) & -(S^{A}_{y})(1 - \gamma) \\
(S^{A}_{z})(1 + \gamma) & 0 & 0 \\
(S^{A}_{y})(1 + \gamma) & 0 & 0
\end{pmatrix},$$

(3.18)

$$M_{2} = Jz \begin{pmatrix}
0 & -(S^{A}_{z})(1 + \gamma) & -(S^{A}_{y})(1 + \gamma) \\
(S^{A}_{z})(1 - \gamma) & 0 & 0 \\
(S^{A}_{y})(1 - \gamma) & 0 & 0
\end{pmatrix}.$$  

(3.19)
We now have two copies of the same problem. If we send \( \gamma \) to \(-\gamma\), then \( M_1 \) goes to \( M_2 \), and \( \gamma(k + \pi) = -\gamma(k) \), so the two are related by a \( \pi \)-shift in \( k \). We will now concentrate on \( M_1 \). There is one zero eigenvalue and the others are
\[
\pm i Jz \sqrt{(S_y^A)^2(1 - \gamma^2) + (S_z^A)^2(1 - \gamma^2)}.
\]
(3.20)
The dispersion relation for the spin waves therefore reads
\[
\omega = Jz \sqrt{(S_y^A)^2(1 - \gamma^2) + (S_z^A)^2(1 - \gamma^2)}.
\]
(3.21)
If we put \( \langle S_A^z \rangle = 0 \), which is the case for the pure antiferromagnet, this reduces to
\[
\omega = Jz S \sqrt{1 - \gamma^2},
\]
(3.22)
which is a well known result.

### 3.1.1 Path integral formalism

Using a path integral formalism for spin systems, we can derive the same dynamics as we did from the Heisenberg Hamiltonian. In appendix B, it is shown how the expression for the path integral can be obtained from the Hamiltonian. In our case the total action reads
\[
S_E = \int_0^{\hbar \beta} d\tau \left[ \sum_i i S A(\Omega_i(\tau)) \cdot \partial_\tau \Omega_i(\tau) + JS \sum_{(ij)} \Omega_i(\tau) \cdot \Omega_j(\tau) \right].
\]
(3.23)
Varying this gives
\[
\delta S_E = S \int_0^{\hbar \beta} d\tau \left[ \sum_i \left( \frac{\delta A(\Omega_i(\tau))}{\delta \Omega_i(\tau)} \cdot \delta \Omega_i(\tau) \cdot \partial_\tau \Omega_i(\tau) \right) + JS \sum_{(ij)} \delta \Omega_i(\tau) \cdot \Omega_j(\tau) \right].
\]
(3.24)
Using index notation, the dot products in the first two terms are more clear,
\[
\delta S_E = S \int_0^{\hbar \beta} d\tau \left[ \sum_i \left( i \frac{\delta A_{\mu}(\Omega_i(\tau))}{\delta \Omega_i(\tau)} \delta \Omega_i^\mu \partial_\tau \Omega_i^\mu - i \frac{\delta A_{\mu}(\Omega_i(\tau))}{\delta \Omega_i(\tau)} \partial_\tau \Omega_i^\mu \delta \Omega_i^\mu \right) + JS \sum_{(ij)} \delta \Omega_i(\tau) \cdot \Omega_j(\tau) \right].
\]
(3.25)
The claim is now that
\[
\partial_\nu A_{\mu} \delta \Omega^\nu \hat{\Omega}^\mu - \partial_\nu A_{\mu} \hat{\Omega}^\nu \delta \Omega^\mu = \epsilon_{\mu\nu\lambda} \hat{\Omega}^\mu \Omega^\nu \delta \Omega^\lambda,
\]
(3.26)
where the convention \( \partial_\nu = \partial / \partial \Omega^\nu \) was used. This can be seen by writing this equation as
\[
(\partial_\lambda A_{\mu} \hat{\Omega}^\mu - \partial_\mu A_{\lambda} \hat{\Omega}^\mu) \delta \Omega^\lambda = \epsilon_{\mu\nu\lambda} \hat{\Omega}^\mu \Omega^\nu \delta \Omega^\lambda.
\]
(3.27)
Now we rewrite equation (B.22) using index notation and multiply by \( \epsilon_{\alpha\beta\gamma} \) on both sides. We find
\[
\epsilon_{\alpha\beta\gamma}\Omega^\gamma = \epsilon_{\alpha\beta\gamma}\epsilon^{\mu\nu\delta}\partial_\mu A_\nu = \partial_\alpha A_\beta - \partial_\beta A_\alpha.
\] (3.28)

Using this, the left hand side of equation (3.27) becomes
\[
\epsilon_{\lambda\mu\nu}\Omega^\nu \dot{\Omega}^\mu \delta \Omega^\lambda,
\] (3.29)
which is exactly the right hand side of equation (3.27). So the equality holds and therefore we can write the variation of the action as
\[
\delta S_E = S \int_0^{\beta} d\tau \left[ \sum_i i(\dot{\Omega}_i \times \Omega_i) \cdot \delta \Omega_i + 2JS \sum_{(ij)} \Omega_j \cdot \delta \Omega_i \right].
\] (3.30)

At this point we can write down the equations of motion or use mean field theory. Let’s write down the equations of motion to compare with the EOM’s obtained previously. We have, using \( \partial_\tau \Omega = -i\partial_t \Omega \), that
\[
\partial_t \Omega_i \times \Omega_i = -2JS \sum_\delta \Omega_{i+\delta},
\] (3.31)
or, taking the crossproduct with \( \Omega_i \) on both sides,
\[
|\Omega|^2 \partial_t \Omega_i - \frac{1}{2} \Omega_i \partial_t |\Omega|^2 = -2JS \sum_\delta \Omega_i \times \Omega_{i+\delta},
\] (3.32)

\[
|\Omega|^2 \partial_t \Omega_i = -2JS \sum_\delta \Omega_i \times \Omega_{i+\delta},
\] (3.33)
This indeed is the same result as obtained previously, since \( |\Omega| \) has unit length. That it indeed describes the same physics, follows from taking the expectation value on both side of the expression for the spin operators,
\[
\frac{d}{dt} S_i = -2J \sum_\delta S_i \times S_{i+\delta}.
\] (3.34)

If we now use mean field theory in the varied action (eq. (3.30)) by writing \( \Omega = \langle \Omega \rangle + \delta \Omega \), and keep terms proportional to \( \delta \Omega^2 \) we obtain\(^2\)
\[
\delta S_E = S \int_0^{\beta} d\tau \left[ \sum_i i(\dot{\langle \Omega_i \rangle} \times \langle \Omega_i \rangle) \cdot \delta \langle \Omega_i \rangle + 2JS \sum_{(ij)} \langle \delta \Omega_i \cdot \delta \Omega_j + \langle \Omega_i \rangle \cdot \delta \Omega_j \rangle \right].
\] (3.35)

Now we use the constraint that the variations have to be perpendicular to the expectation value. This amounts to claiming that the length is conserved or
\[
|\Omega|^2 = \langle \Omega \rangle \cdot \langle \Omega \rangle + 2\langle \Omega \rangle \cdot \delta \Omega + \delta \Omega \cdot \delta \Omega,
\] (3.36)
\[
2\langle \Omega \rangle \cdot \delta \Omega + \delta \Omega \cdot \delta \Omega = 0,
\] (3.37)
\(^2\)We keep terms \( \delta \Omega^2 \), because the leading order here is first order. The equations of motion are then again first order in the fluctuations.
By choosing the expectation value in the plane, and corresponding to the canted phase, we have
\( \langle \Omega_z^2 \rangle = 0 \). Since the length of \( \Omega \) is conserved, at every point there are only two directions for fluctuations. This means that one of the fluctuations can be expressed in terms of the others. The constraint can be rewritten, up to second order

\[
\delta \Omega^y = \frac{\langle \Omega^2 \rangle}{\langle \Omega^y \rangle} \delta \Omega^x - \frac{(\delta \Omega^y)^2 + \alpha (\delta \Omega^z)^2}{\langle \Omega^y \rangle^2},
\]

(3.38)

\[
\alpha = \frac{\langle \Omega^y \rangle^2 + \langle \Omega^z \rangle^2}{\langle \Omega^y \rangle^2}.
\]

(3.39)

If we now write out the vector components of the fluctuations in the action explicitly, we find

\[
\delta S_E = S \int_0^{\beta} d\tau \left[ \sum_i i \alpha \langle \Omega^y_i \rangle \left\{ \delta \Omega_x^i \delta \Omega_x^i - \delta \Omega_y^i \delta \Omega_y^i \right\} \right.
\]

\[
+ 2JS \sum_{\langle ij \rangle} \delta \Omega_x^i \delta \Omega_x^j + \delta \Omega_y^i \delta \Omega_y^j \left( 1 + \frac{\langle \Omega_z^i \rangle \langle \Omega_z^j \rangle}{\langle \Omega^y_i \rangle \langle \Omega^y_j \rangle} \right) - JS \sum_{\langle ij \rangle} \frac{\langle \Omega^y_i \rangle}{\langle \Omega^y_j \rangle} \left\{ (\delta \Omega_x^i)^2 + (\delta \Omega_z^i)^2 \alpha \right\} \right].
\]

(3.40)

Using equation (3.38), this becomes

\[
\delta S_E = S \int_0^{\beta} d\tau \left[ \sum_i i \alpha \langle \Omega^y_i \rangle \left\{ \delta \Omega_x^i \delta \Omega_x^i - \delta \Omega_y^i \delta \Omega_y^i \right\} \right.
\]

\[
+ 2JS \sum_{\langle ij \rangle} \delta \Omega_x^i \delta \Omega_x^j + \delta \Omega_y^i \delta \Omega_y^j \left( 1 + \frac{\langle \Omega_z^i \rangle \langle \Omega_z^j \rangle}{\langle \Omega^y_i \rangle \langle \Omega^y_j \rangle} \right) - JS \sum_{\langle ij \rangle} \frac{\langle \Omega^y_i \rangle}{\langle \Omega^y_j \rangle} \left\{ (\delta \Omega_x^i)^2 + (\delta \Omega_z^i)^2 \alpha \right\} \right].
\]

(3.41)

Next, we Fourier transform the expression,

\[
\delta S_E = S \int d\omega \sum_k \left[ i \omega \alpha_A \langle \Omega^y_A \rangle \left\{ \delta \Omega_x^A \delta \Omega_x^A - \delta \Omega_y^A \delta \Omega_y^A \right\} + i \omega \alpha_B \langle \Omega^y_B \rangle \left\{ \delta \Omega_x^B \delta \Omega_x^B - \delta \Omega_y^B \delta \Omega_y^B \right\} \right.
\]

\[
+ 2JS \gamma(k) \left\{ \delta \Omega_x^A \delta \Omega_x^B + \delta \Omega_y^A \delta \Omega_y^B \left( 1 + \frac{\langle \Omega_z^A \rangle \langle \Omega_z^B \rangle}{\langle \Omega^y_A \rangle \langle \Omega^y_B \rangle} \right) \right\}
\]

\[
+ J_z S \{ (\delta \Omega_x^A)^2 + (\delta \Omega_z^A)^2 \alpha_A \} + JS \{ (\delta \Omega_x^B)^2 + (\delta \Omega_z^B)^2 \alpha_B \} \right].
\]

(3.42)

Using \( \langle \Omega_z^A \rangle = \langle \Omega_z^B \rangle = \langle \Omega^z \rangle \) and \( \langle \Omega^y_A \rangle = -\langle \Omega^y_B \rangle = \langle \Omega^y \rangle \), we have

\[
\delta S_E = S \int d\omega \sum_k \left[ i \omega \frac{\langle \Omega^z \rangle^2 + \langle \Omega^y \rangle^2}{\langle \Omega^y \rangle} \left\{ \delta \Omega_x^A \delta \Omega_x^A - \delta \Omega_y^A \delta \Omega_y^A \right\} \right.
\]

\[
+ J_z S \gamma(k) \left\{ \delta \Omega_x^A \delta \Omega_x^B + \delta \Omega_y^A \delta \Omega_y^B \frac{\langle \Omega^y \rangle^2 - \langle \Omega^z \rangle^2}{\langle \Omega^y \rangle^2} \right\} + J_z S \left\{ (\delta \Omega_x^A)^2 + (\delta \Omega_z^A)^2 \frac{\langle \Omega^y \rangle^2 + \langle \Omega^z \rangle^2}{\langle \Omega^y \rangle^2} \right\} \right. \\
+ (A \leftrightarrow B). \]

(3.43)
If we now take
\[
\begin{align*}
a &= \frac{\langle \Omega^2 \rangle^2 + \langle \Omega^\nu \rangle^2}{\langle \Omega^\nu \rangle^2}, \\
b &= \frac{\langle \Omega^\nu \rangle^2 - \langle \Omega^z \rangle^2}{\langle \Omega^\nu \rangle^2},
\end{align*}
\] (3.44)
(3.45)
eq \text{eq. (3.43) can be written as}
\[
\delta S_E = S \int d\omega \sum_k \left( \begin{array}{cccc}
JzS & -i\omega a & JzS\gamma & 0 \\
i\omega a \langle \Omega^\nu \rangle & JzSa & 0 & JzS\gamma b \\
JzS\gamma & 0 & JzS & i\omega a \langle \Omega^\nu \rangle \\
0 & JzS\gamma b & -i\omega a \langle \Omega^\nu \rangle & JzSa
\end{array} \right) \cdot \left( \begin{array}{c}
\delta \Omega^z_A \\
\delta \Omega^z_B \\
\delta \Omega^x_A \\
\delta \Omega^x_B
\end{array} \right).
\] (3.46)

If we take the determinant of this matrix, put it to zero and solve for \(\omega\), we find the dispersion relations,
\[
\omega = JzS \sqrt{1 \pm \gamma(k) \sqrt{a + b\gamma(k)}}/a \langle \Omega^\nu \rangle,
\] (3.47)
which are again the same as obtained previously.\(^3\)

### 3.1.2 The long wavelength limit

To study the dispersion relations, it is useful to consider the long wavelength (or small momentum) limit. Previously, we introduced \(\gamma(k)\). It is given by
\[
\gamma(k) = \frac{1}{z} \sum_i e^{i\delta \cdot k} = \frac{2}{z} \sum_i \cos k_i
\] (3.48)

Since we would like to know the limits for both dispersion relations, we expand around \(k = 0\) and \(k = \pi\). The limits are given by
\[
\omega = \sqrt{2zJn|k|},
\]
\[
\omega = 2Jzm + Jm \left( \frac{n^2}{2m^2} - 1 \right) |k|^2.
\] (3.49)

### 3.2 Plots

Now that we have the dispersion relations, we can plot the frequency of the spin waves as a function of the momentum. In figure 3.1 the dispersion relations are shown. Recall that there were two dispersion relations, and that they were related by a shift of \(\pi\) in \(k\). We then see that for \(m = 0\), the dispersions are the same. There are two zero modes, with linear momentum for small \(k\). On

\(^3\)To see this explicitly, use \(|\langle \Omega \rangle| = 1\), and \(S(\Omega) = S\)
Figure 3.1: The dispersion relations are plotted, for $m = 0$ (dashed curve), $m = 0.5$ (solid curve) and $m = 2$ (thick curve). For $m = 0$, the periodicity is $\pi$, whereas for $m \neq 0$, the periodicity is $2\pi$.

the other hand, for $m \neq 0$, this degeneracy is lifted, and one zero mode remains while the other mode now is a gapped one, which is quadratic for small momenta. The magnitude of the gap is $2Jz m$. This is just the magnitude of the magnetic field that we found in the previous chapter. This mode therefore describes motion due to the magnetic field, or Larmor precession of the spins.
Chapter 4

Merons

Up to this point all calculations were done in mean field theory. The low level excitations, were obtained by linearizing the equations of motion. Other kinds of excitations in optical lattices are topological excitations. These occur when locally, the spins are not pointing in the same direction (on one sublattice), but are pointing in the same direction at infinity. This requires energy, since as we have seen, it is most favorable to have all spins on a sublattice point in the same direction. This leads to all kinds of interesting structures. In this chapter we will look at merons, which are topological stable excitations occurring in 2d optical lattices. In the ground state, the Néel vector is pointing in the same direction on every site. In particular, it lies in a plane which is perpendicular to the direction of the magnetic field. This plane is called the easy plane. In the center of a meron, the Néel vector is tilted out of the easy plane. At infinity, it lies in the easy plane. When looking away from the center of the meron, the Néel parameter smoothly rotates into the easy plane. Now there are two possible stable configurations which obey this. In the first case, the Néel parameter always points away from the center of the meron. This would be a meron with vorticity +1. In the second case, the Néel vector points radially outwards along the y-axis, and radially inwards along the x-axis, and rotates smoothly in between. This is a meron with vorticity −1. In figure 4.1 two merons are shown. For the right meron the Néel vector is pointing radially outward and for the left meron it is not. As can be seen, far away from the merons, the contributions cancel out and the Néel vector is pointing in the same direction on each site. The texture of a meron which points radially outwards everywhere, can be parametrized by

\[ n = n \begin{pmatrix} \sqrt{1 - n_z^2} \cos \phi \\ n_v \sqrt{1 - n_z^2} \sin \phi \\ n_z(r) \end{pmatrix}, \]  

(4.1)

where, \( \phi \) is an arbitrary angle, \( n = |n| \), \( n_v = \pm 1 \) is the vorticity of the meron and \( r \) is the the distance to the center of the meron. We take

\[ n_z(r) = \pm \frac{1}{(r/\lambda)^4 + 2(r/\lambda)^2 + 1}, \]  

(4.2)

with \( \lambda \) the characteristic meron size. This is not the only ansatz that one is allowed to make. For example, it would be a nice feature if \( n_z \) would fall of exponentially at large distances. The ansatz in equation (4.2) will be good enough for our purposes though.
4.1 Meron size

We would like to calculate the characteristic size of merons occurring in an optical lattice. It is possible to capture the long wave length dynamics described in the previous chapter by making use of a non linear sigma model. We then look in the continuum limit, where the lattice spacing is small compared to the typical length scales that we are looking at. If we write down this non linear sigma model, we can put in the meron texture, and minimize to find the meron size. The non linear sigma model action \cite{4,15} is given by

\[
S[n(x, t)] = \int dt \int d^Dx \left\{ \frac{1}{4Jzn^2} \left( \hbar \frac{\partial n(x, t)}{\partial t} - 2Jz \mathbf{m} \times \mathbf{n}(x, t) \right)^2 - \frac{Jd^2}{2} [\nabla n(x, t)]^2 \right\}, \tag{4.3}
\]

with \( d \) the lattice spacing. The prefactors are chosen such that the long wavelength limit of the spin waves coincides with the dispersion relations found in chapter 3. The equilibrium is found by minimizing the Landau free energy,

\[
F[n(x, t)] = \int d^Dx \left\{ \frac{Jd^2}{2} [\nabla n(x, t)]^2 + f[n(x, t)] \right\}, \tag{4.4}
\]

where \( f[n(x, t)] \) is the on site free energy derived in chapter 2. If we now look at the first term, we can use the meron texture given in equation (4.1). The first term we write as

\[
[\nabla n(x, t)]^2 = \sum_{i=x,y,z} \sum_{\nu=1,2} (\partial_\nu n_i)^2, \tag{4.5}
\]

where

\[
\nabla = \left( \frac{\partial}{\partial x}, \sin \phi \frac{\partial}{\partial y} - \cos \phi \frac{1}{r} \frac{\partial}{\partial \phi}, \cos \phi \frac{\partial}{\partial r} + \sin \phi \frac{1}{r} \frac{\partial}{\partial \phi} \right). \tag{4.6}
\]

The contribution to the Landau free energy is then

\[
E(\lambda) = J\pi \int_0^\Lambda dr r (\nabla n)^2 = Jn^2\pi \left( \frac{511}{60} - \pi - 6 \log 2 - \log \lambda + \log \Lambda \right) + O(\Lambda^{-2}). \tag{4.7}
\]

Figure 4.1: Two merons of opposite vorticity are shown. Far away from the meron centers, the contributions cancel. In yellow the meron centers are indicated.
Figure 4.2: The core size of merons is plotted as a function of the magnetization and the temperature. For every point within the phase diagram, there is a corresponding meron size. When the magnetization goes to zero, the meron size diverges.

In principal the meron extends to infinity, so that we would have to take the limit \( \Lambda \to \infty \) to take into account the total contribution to the free energy. We can see though that the energy diverges logarithmically with \( \Lambda \). This means that a single meron cannot exits. We have seen already though that if we have a meron pair, a meron and an anti meron, with opposite vorticity, that far away from the merons, the contributions cancel out. So a meron pair can in fact exist, whereas a single meron can not. Next we minimize the Landau free energy with respect to \( \lambda \),

\[
0 = \frac{\partial}{\partial \lambda} F[n(x, t)] = \frac{\partial}{\partial \lambda} \left[ \frac{\pi}{d^2} \int_0^\Lambda dr f(r/\lambda) + E(\lambda) \right] \\
= \left[ \frac{\partial}{\partial \lambda} \frac{\pi \lambda^2}{d^2} \int_0^{\Lambda/\lambda} dx f(x) + J_n^2 \lambda \right] \\
= \left[ \frac{2\pi \lambda}{d^2} \int_0^{\Lambda/\lambda} dx x f(x) + \frac{\pi \lambda^2}{d^2} \int_0^{\Lambda/\lambda} dx x f(x) - \frac{J_n^2 \pi}{\lambda} \right].
\]

The second term can be rewritten

\[
\frac{\pi \lambda^2}{d^2} \frac{\partial}{\partial \lambda} \int_0^{\Lambda/\lambda} dx x f(x) = \frac{\pi \lambda^2 \lambda}{d^2} \frac{\partial}{\partial x} \int_0^{\Lambda/\lambda} dx x f(x) \bigg|_{x=\Lambda/\lambda} = -\frac{\pi \lambda^2}{\lambda d^2} f(\Lambda/\lambda)
\]

\[
= -\frac{2\pi \lambda}{d^2} f(\Lambda/\lambda) \int_0^{\Lambda/\lambda} dx x.
\]

If we now take the limit \( \Lambda \to \infty \), which corresponds to infinite system size, we find

\[
\lambda = n d \sqrt{\frac{J}{2} \left( \int_0^\infty dr r [f(r, m, T) - f(\infty, m, T)] \right)^{-1/2}}.
\]
The integral in this expression, is just the integral over the free energy, with the background energy (at infinity) extracted at every point. This integral can be computed numerically, which results in the meron size as a function of $m$ and $T$. The result is shown in figure 4.2.

As we have seen before, the energy of a meron is proportional to $E \sim Jn^2\pi \log(\Lambda/\lambda)$. Since $\Lambda \gg \lambda$, the maximum number of merons is roughly $(\Lambda/\lambda)^2$, and therefore the entropy can be estimated by $S = 2k\log(\Lambda/\lambda)$. The free energy is then given by

$$F = E - TS = (Jn^2\pi - 2kT)\log(\Lambda/\lambda). \quad (4.14)$$

This signals the existence of a phase transition in the system, since when the temperature is sufficiently high, the free energy will be negative, and there will be merons in the system. If the temperature is low on the other hand the free energy will be positive, and there will be no merons. This phase transition is called a Kosterlitz-Thouless phase transition.

### 4.2 The Kosterlitz-Thouless phase transition

An interesting analogy can be made between the Heisenberg model and the anisotropic $O(3)$ model, which was studied by Klomfass et al. [6]. We can write the action like

$$S = S_H + J \sum f(m_i, n_i, \beta), \quad (4.15)$$

where $S_H$ is the Heisenberg term in the action given by

$$S_H = -\int_0^{\hbar\beta} \frac{d\tau}{2Jz^2} \sum_{\langle x, x' \rangle} n(x) \cdot n(x'), \quad (4.16)$$

and $f$ is the on site free energy. If we now expand the second term in this action up to quadratic order in $n_z$, we find

$$S \simeq -\frac{J\hbar^2n^2}{2z^2} \sum_{\langle i, j \rangle} S_i \cdot S_j + J\beta n^2\gamma(m, \beta) \sum_i (S_i^z)^2, \quad (4.17)$$

where $\gamma(m, \beta)$ is some function, such that it represents the minimum of the free energy\(^1\). The action is now given by

$$S = -\beta_3 \sum_{\langle i, j \rangle} S_i \cdot S_j + \gamma_3 \sum_i (S_i^z)^2, \quad (4.18)$$

which is exactly the action of the anisotropic $O(3)$ model. This model is known to obey a phase transition. It is shown in figure 4.3.

The fit curve is given by

$$\gamma_3(\beta_3) = \frac{\beta_3}{\beta_3 - 1.06} \exp[-5.6(\beta_3 - 1.085)], \quad (4.19)$$

\(^1\)The minimum of the free energy is always quadratic in $n$, so that up to second order in $n_z$ we can always write it like this. The value of $\gamma$ can be found numerically by minimizing the free energy.
which satisfies $\beta_3 = 1.06$ for $\gamma_3 \to \infty$, and $\gamma_3 = 0$ for $\beta_3 \to \infty$. Since the coefficients $\beta_3$ and $\gamma_3$ are functions of $m$ and $T$, we can find where this phase transition occurs as a function of $m$ and $T$. It is shown in figure 4.4, where it is inserted in the phase diagram obtained with mean field theory.

The mean field result is drastically reduced, compared to the Kosterlitz-Thouless transition. In fact, not even the shape of the curve is correct. This has to do with the fact that in two dimensions, the spin fluctuations are large compared to the mean spin values, and mean field theory breaks down as a result. The shape of the Kosterlitz-Thouless phase transition line, is determined by the point where meron pairing occurs. At zero magnetization, there can be no merons. This explains why temperature goes to zero when the magnetization goes to zero in the Kosterlitz-Thouless phase diagram. In three dimensions, mean field theory is a much better approximation, and it cannot be expected that in three dimensions, spin waves and topological excitations alter the phase diagram significantly.
Figure 4.4: The phase diagram is shown, with the Kosterlitz-Thouless phase transition (solid line), and the phase transition from ferromagnet to antiferromagnet in mean field theory (dashed curve). The inset shows the behavior of the Kosterlitz-Thouless phase transition for small temperature and small magnetization. The C indicates the canted phase.
Conclusions & outlook

This masters thesis is divided in a few parts. First of all the phase transition from the antiferromagnetic state to the paramagnetic state in an optical lattices is addressed using a mean field theory. Critical values were found analytically, for the Heisenberg model and for the Ising model. The most striking difference between the two is that the peculiar re-entrant behavior of the Ising model is absent in the Heisenberg model.

Then the spin imbalance below the critical temperature was investigated. The magnetization and the Néel vector were found to be perpendicular in the whole region below the critical temperature. Again, this is a difference between the Heisenberg model and the Ising model, since in the Ising model the magnetization and the Néel vector are restricted to be along the same axis.

Next, spin waves were considered. Dispersion relations were found for collective motion of the spins, where the magnetization and the Néel vector couple to each other. At non-zero magnetization, the dispersion relations revealed the existence of magnons with a combined anti-ferromagnetic and ferromagnetic character. One of the modes is gapped, corresponding to Larmor precession in the presence of an effective magnetic field.

Finally a non linear sigma model was found which incorporates the long wave length behavior of the spin waves. Such models are known to describe topological excitations. Topological excitations in two dimensions, or merons, were considered. It was shown that at low temperatures, only meron pairs, consisting of merons with opposite vorticity, can exist, while at higher temperatures free merons occur, signalling the occurrence of a phase transition. This Kosterlitz-Thouless phase transition was investigated, improving on the mean field result.

All of the above was matter for a paper that that was send in to Physical Review Letters, and is at the time of writing under consideration for publishing.

Although we finished the subjects we wanted to treat, there remain some more topics to be addressed to further investigate the antiferromagnetic state. For example, systems of merons exhibit interesting physics as meron pairs interact with each other. It is known that merons of opposite vorticity attract each other, while merons of the same vorticity repel each other. This leads to meron dynamics, which will be similar to that of charged particles.

In the laboratory it is also possible to create 3D optical lattices. Topological excitations in these systems will not be merons, since it would require an infinite amount of energy, to stack merons in multiple layers in the lattice. Instead, the 3D equivalent of a meron will be a monopole [12]. Monopoles might exhibit quite different behavior than merons.

Then there is the issue of finite size effects. In all chapters here we assumed that the system was infinitely large, but in small systems, the spin waves for instance will suffer from scattering on the edges of the trap. This will lead to different dispersion relations.
Appendix A

Perturbation theory

Since some basic results from Rayleigh-Schrödinger perturbation theory were used in the text, it will be reviewed here how these results are obtained. We start with some hamiltonian $H_0$, which we have solved according to the Schrödinger equation

$$H_0 |\psi_0\rangle_n = E_0^n |\psi_0\rangle_n,$$

(A.1)

where the eigenstates obey $\langle \psi_0^m |\psi_0^n \rangle = \delta_{mn}$. We now want to use this result, to solve the Schrödinger equation for the perturbed hamiltonian,

$$H = H_0 + \lambda H'.$$

(A.2)

This can be done to arbitrary order, assuming that $\lambda$ is a small parameter\footnote{We will actually assume that the perturbation $H'$ is small and put $\lambda$ to 1 in the end. It just serves to keep track of different order of magnitude.}. So the perturbed hamiltonian obeys

$$H |\psi_n\rangle = E_n |\psi_n\rangle,$$

(A.3)

and we would like to find the energies $E_n$, and the states $|\psi_n\rangle$. We write them in powerseries in $\lambda$,

$$|\psi_n\rangle = |\psi_0^n\rangle + \lambda |\psi_1^n\rangle + \lambda^2 |\psi_2^n\rangle + \ldots$$

$$E_n = E_0^n + \lambda E_1^n + \lambda^2 E_2^n + \ldots.$$  

(A.4)

Putting these expressions in equation (A.3), we have

$$(H_0 + \lambda H')(|\psi_0^n\rangle + \lambda |\psi_1^n\rangle + \lambda^2 |\psi_2^n\rangle + \ldots)$$

$$= (E_0^n + \lambda E_1^n + \lambda^2 E_2^n + \ldots)(|\psi_0^n\rangle + \lambda |\psi_1^n\rangle + \lambda^2 |\psi_2^n\rangle + \ldots).$$

(A.5)

Collecting different power of $\lambda$, we find equations for the higher order corrections to $|\psi_n\rangle$ and $E_n$. For the zeroth order in $\lambda$, we have

$$H_0 |\psi_0^n\rangle = E_0^n |\psi_0^n\rangle.$$  

(A.6)

This is no news, because this is just the unperturbed Schrödinger equation (A.1). The first order gives us

$$H' |\psi_0^n\rangle + H_0 |\psi_1^n\rangle = E_1^n |\psi_0^n\rangle + E_0^n |\psi_1^n\rangle.$$  

(A.7)
Hence we find
\[ m \sum |\psi_n^1\rangle + H^0|\psi_n^0\rangle = E_n^1|\psi_n^1\rangle + E_n^0|\psi_n^0\rangle + E_n^2|\psi_n^0\rangle. \quad (A.8) \]

So for every order in \( \lambda \) we find an equation relating the increasingly higher orders of \(|\psi_n\rangle\) and \(E_n\).

Next, we try to solve this for the first order. Taking the innerproduct with \(\langle \psi_n^0 |\) on both sides of equation (A.7),
\[ \langle \psi_n^0 |H'|\psi_n^0\rangle + \langle \psi_n^0 |H^0|\psi_n^0\rangle = \langle \psi_n^0 |E_n^1|\psi_n^1\rangle + \langle \psi_n^0 |E_n^0|\psi_n^0\rangle \]
\[ \langle \psi_n^0 |H'|\psi_n^0\rangle = E_n^1\langle \psi_n^0 |\psi_n^1\rangle, \quad (A.9) \]

where we used the fact that the Hamiltonian is a Hermitian operator. For a properly normalized basis we have \(\langle \psi_n^0 |\psi_n^0\rangle = 1\), so that we find
\[ E_n^1 = \langle \psi_n^0 |H'|\psi_n^0\rangle. \quad (A.10) \]

Now we also want to find the eigenstates to first order. We rewrite equation (A.7) as
\[ (H' - E_n^1)|\psi_n^1\rangle = -(H^0 - E_n^0)|\psi_n^0\rangle, \quad (A.11) \]
and write \(|\psi_n^1\rangle\) in terms of the orthonormal basis \(|\psi_n^0\rangle\),
\[ |\psi_n^1\rangle = \sum_m c_m^{(n)}|\psi_m^0\rangle. \quad (A.12) \]

Now note that if \(|\psi_n^0\rangle\) obeys equation (A.11), so does \(|\psi_n^0\rangle + c|\psi_n^0\rangle\) for some constant \(c\), so that the sum over \(m\) can be restricted to a sum over \(m \neq n\). We now need to find the coefficients \(c_m^{(n)}\).

Substituting the expansion in (A.11), and taking the innerproduct with \(\langle \psi_k^0 |\), we obtain
\[ \langle \psi_k^0 |(H' - E_n^1)|\psi_n^0\rangle = -\sum_{m \neq n} (E_m^0 - E_n^0)c_m^{(n)}\langle \psi_k^0 |\psi_m^0\rangle. \quad (A.13) \]

Hence we find
\[ c_{k}^{(n)} = -\frac{\langle \psi_k^0 |H'|\psi_n^0\rangle}{E_k^0 - E_n^0}, \quad (A.14) \]
for \(k \neq n\), and therefore
\[ |\psi_n^1\rangle = \sum_{m \neq n} \frac{\langle \psi_m^0 |H'|\psi_n^0\rangle}{E_n^0 - E_m^0}|\psi_m^0\rangle. \quad (A.15) \]

We have now obtained the perturbation theory up to first order. With these expressions we can calculate the second order. We will now only calculate the second order energies. As before, we start by taking the innerproduct of equation (A.8) with \(\langle \psi_n^0 |\) on both sides,
\[ \langle \psi_n^0 |H'|\psi_n^1\rangle + \langle \psi_n^0 |H^0|\psi_n^0\rangle = \langle \psi_n^0 |E_n^1|\psi_n^1\rangle + \langle \psi_n^0 |E_n^0|\psi_n^0\rangle + \langle \psi_n^0 |E_n^2|\psi_n^0\rangle \]
\[ \langle \psi_n^0 |H'|\psi_n^1\rangle = E_n^1\langle \psi_n^0 |\psi_n^1\rangle + E_n^2. \quad (A.16) \]

The first term on the right hand side is zero, since
\[ \langle \psi_n^0 |\psi_n^1\rangle = \sum_{m \neq n} \frac{\langle \psi_m^0 |H'|\psi_n^0\rangle}{E_n^0 - E_m^0}\langle \psi_n^0 |\psi_m^0\rangle = 0. \quad (A.17) \]
We therefore find

\[ E_n^2 = \sum_{m \neq n} \frac{\langle \psi_0^m | H' | \psi_0^m \rangle \langle \psi_0^m | H' | \psi_0^m \rangle}{E_n^0 - E_m^0}, \]  

(A.18)

or,

\[ E_n^2 = \sum_{m \neq n} \frac{|\langle \psi_0^m | H' | \psi_0^m \rangle|^2}{E_n^0 - E_m^0}. \]  

(A.19)

In this way, one can continue to obtain corrections up to arbitrary order. The second order is good enough for our purposes though, and is actually so in many cases. It should be noted that as long as there are no degenerate eigenvalues, there are no problems, but when there are degenerate eigenvalues, the denominator in all corrections accept the first order energy become singular, and one has to resort to other techniques.
Appendix B

Spin path integral

In this appendix, we closely follow a chapter from the lecture notes from the course Spintronics given by Rembert Duine [2]. We want to derive what a path integral looks like for a system with spin $S$ particles. The Hamiltonian $\hat{H}$ is fully described in terms of the spin operators $\hat{S}$. A basis for the spin operators is given by

$$\hat{S}^2 |S,m_S\rangle = S(S+1)\hbar^2 |S,m_S\rangle$$
$$\hat{S}_z |S,m_S\rangle = m_S \hbar |S,m_S\rangle, m_S \in \{-S,-S+1,\ldots,S-1,S\}.$$  \hspace{1cm} (B.1)

The partition function is

$$Z = \text{Tr} [ e^{-\beta \hat{H}} ], \hspace{1cm} (B.2)$$

where $\beta$ is the inverse temperature, and the trace is over all states. The exponential can be interpreted as a periodic evolution operator in imaginary time. We identify the points $\tau = 0$ and $\tau = \hbar \beta$. Next, we divide this time interval in infinitesimal pieces $\Delta \tau = \hbar \beta / N$. In the end we take the limit $N \to \infty$. The partition function becomes

$$Z = \text{Tr} \left[ e^{-\sum_{i=0}^{N-1} \Delta \tau \hat{H}/\hbar} \right] \approx \text{Tr} \left[ (1 - \Delta \tau \hat{H}/\hbar)^N \right]. \hspace{1cm} (B.3)$$

At this point, we would like to insert after every time interval $\Delta \tau$, a complete set of states, so that we get rid of the operators in this expression. Therefore, we would like to find a set of states that obeys

$$\hat{S} |\Omega\rangle = \hbar S \Omega |\Omega\rangle.$$  \hspace{1cm} (B.4)

This turns out to be impossible. There does however exist a set of states that obeys

$$\langle \Omega | \hat{S} |\Omega\rangle = \hbar S \Omega.$$  \hspace{1cm} (B.5)

These are the so called spin coherent states. Here $\Omega$ is a unit vector, that can be parametrized by

$$\Omega = \begin{pmatrix} \sin \theta \cos \phi \\ \sin \theta \sin \phi \\ \cos \theta \end{pmatrix}. \hspace{1cm} (B.6)$$

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The spin coherent states are, in terms of the spin states, given by
\[
|\Omega\rangle = \sum_{m_S=-S}^{m_S=S} \left( \frac{2S}{S+m_S} \right)^{1/2} e^{-i(m_S-S)\phi} (\cos(\theta/2))^{S+m_S} (\sin(\theta/2))^{S-m_S} |S,m_S\rangle.
\] (B.7)
It is not an orthonormal basis,
\[
\langle \Omega'|\Omega \rangle = \left[ \cos(\theta'/2) \cos(\theta/2) + \sin(\theta'/2) \sin(\theta/2) e^{i(\phi-\phi')} \right]^{2S}.
\] (B.8)
When \( \theta' = \theta + d\theta \) and \( \phi' = \phi + d\phi \), this reduces to
\[
\langle \Omega'|\Omega \rangle = 1 + iS(\phi' - \phi)(\cos - 1).
\] (B.9)
Furthermore, they obey the closure relation,
\[
\frac{2S+1}{4\pi} \int d\Omega |\Omega\rangle \langle \Omega| = 1.
\] (B.10)
The angular integral measure is the standard one,
\[
\int d\Omega = \int_{-1}^{1} d(\cos \theta) \int_{0}^{2\pi} d\phi.
\] (B.11)
Using the closure relation, we can calculate the trace of an operator,
\[
\text{Tr} \hat{O} = \frac{2S+1}{4\pi} \int d\Omega |\Omega\rangle \langle \Omega| \hat{O} |\Omega\rangle.
\] (B.12)
With these expressions, we are armed to get rid of the operators in expression (B.3). By using the closure relation after each time interval, and then taking the trace of this expression, we obtain
\[
Z = \left( \frac{2S+1}{4\pi} \right)^N \left( \prod_{i=0}^{N-1} \int d\Omega_i \right) \langle \Omega_0|(1-\Delta\tau H/h)|\Omega_1\rangle \langle \Omega_1|(1-\Delta\tau H/h)|\Omega_2\rangle \ldots \langle \Omega_{N-1}|(1-\Delta\tau H/h)|\Omega_0\rangle.
\] (B.13)
Using the properties for the spin coherent states, the innerproducts in this expression, can be written
\[
\langle \Omega_i|(1-\Delta\tau H[h\hat{S}]/h)|\Omega_{i+1}\rangle \approx (1-\Delta\tau H[hS\hat{\Omega}]/h + iS(\phi_{i+1} - \phi_i)(\cos \theta_i - 1)).
\] (B.14)
After re-exponentiation, the expression look like
\[
Z = \left( \frac{2S+1}{4\pi} \right)^N \left( \prod_{i=0}^{N-1} \int d\Omega_i \right) \exp \left\{ \sum_{i=0}^{N} \Delta\tau \left[ iS \left( \frac{\phi_{i+1} - \phi_i}{\Delta\tau} \right)(\cos \theta_i - 1) - \frac{H[\Omega_i]}{h} \right] \right\},
\] (B.15)
with the periodic boundary conditions $\phi_N = \phi_0$ and $\theta_N = \theta_0$. Now we can take the continuum limit $N \to \infty$ and $\Delta \tau \to 0$, where we keep the product $N \Delta \tau = h \beta$ fixed. Using $\phi_i = \phi(\tau)$ and $\theta_i = \theta(\tau)$, and defining the path integral measure by

$$
\left(\frac{2S + 1}{4\pi}\right)^N \prod_{i=0}^{N-1} d\Omega_i = \int \mathcal{D}\Omega,
$$

(B.16)

the partition function becomes

$$
Z = \int \mathcal{D}\Omega e^{-SE[\Omega]/\hbar},
$$

(B.17)

where $S_E$ is the Euclidian action, given by

$$
S_E[\Omega] = \int_0^{h\beta} d\tau \left\{ ihS \frac{d\phi(\tau)}{d\tau} [1 - \cos \theta(\tau)] + H[\Omega] \right\}.
$$

(B.18)

The first term can be rewritten as

$$
\int_0^{h\beta} d\tau \frac{d\phi(\tau)}{d\tau} [1 - \cos \theta(\tau)] = \int_{\phi_0}^{\phi_0 + 2\pi} d\phi [1 - \cos \theta(\phi)] = \int_{\phi_0}^{\phi_0 + 2\pi} d\phi \int_0^{\theta(\phi)} d\theta \cos \theta.
$$

(B.19)

We see that it does not explicitly depend on time, but only on the parametrization given by the angles $\theta$ and $\phi$. In particular, this is just the area of the cap on the unit sphere of which the boundary is parametrized by the angles $\theta$ and $\phi$. The area of this cap can also be given without an explicit parametrization. Call the area of this cap $A$, we can write

$$
A = \int_A d\Omega \cdot \Omega,
$$

(B.20)

that is, $\Omega$ is a vector field pointing radially outward. Since it is unity everywhere on the sphere, the result is just the area. We can rewrite this expression with Stokes theorem,

$$
A = \int_{\partial A} d\Omega \cdot A(\Omega) = \int_0^{h\beta} d\tau A(\Omega) \cdot \dot{\Omega}(\tau),
$$

(B.21)

where $A(\Omega)$ is the magnetic monopole vector potential. It satisfies

$$
\nabla_{\Omega} \times A = \Omega.
$$

(B.22)

Using these expressions, the Euclidian action is given by

$$
S_E = \int_0^{h\beta} d\tau \left\{ ihS A \cdot \partial_{\tau} \Omega + H[\Omega] \right\}.
$$

(B.23)
Bibliography


[2] Rembert A. Duine. Spintronics. These are lecture notes for the course Spintronics, taught at Utrecht University, Spring 2009. They can be found at http://www.phys.uu.nl/~duine.


