Utrecht University

Institute of Theoretical Physics

Bachelor Thesis

Phase diffusion in a Bose-Einstein condensate of magnons

Author:
Quint-Hein Enneking

Supervisor:
Dr. R.A. Duine

Abstract

Research on the phase transition and phase diffusion between the Mott-insulator and superfluid phase has not yet been done extensively for the case of magnons. In this thesis we start from a model Hamiltonian for an easy-plane magnetic insulator and construct the phase diagram describing the transition between the Mott insulator and superfluid phase. Finally, we consider phase diffusion of the Bose-Einstein condensate in the superfluid phase and find that phase diffusion indeed occurs in a finite-sized system.

January 14, 2015

Contents

1 Introduction

Magnons are quasiparticles, meaning they do not consist of ordinary matter, but instead correspond to collective excitations in the magnetization. They were first introduced by Felix Bloch [1] in order to better understand the appearance of ordered spin states in ferromagnets at zero applied magnetic field and zero temperature. At absolute zero temperature, a system of atomic particles in a ferromagnet has its spin completely aligned to maximize the net magnetization and minimize the exchange interactions. When the temperature is increased, spins start to deviate randomly from the common direction defined by the ground state of the system. If one were to treat the perfectly magnetized state at $T = 0$ as the vacuum state of the system, the $T \neq 0$ state with increased internal energy and decreased net magnetization can be treated as a gas of quasiparticles, i.e. magnons. According to the laws of quantum mechanics, the change of a single particle's spin angle is equal to the partial shift of the spin angles of all particles in the system. This partial disturbance then travels through the lattice like a wave of discrete energy transferal. We may call this wave a spin wave, because the magnetization is induced by the spins of the particles. This concept is illustrated in Fig.1 below, where is shown how the spins align with the magnetic field after a strong pulse and induce changes in orientation of the surrounding spins, effectively creating a spin wave. Thus we can conclude that magnons are quantized spin waves. Holstein and Primakoff [2] then showed that magnons behave like weakly interacting quasiparticles (bosons) obeying Bose-Einstein statistics, a feature we will be using later on.

The kind of phase transition we are interested in, are quantum phase transitions. These are defined as phase transitions between two quantum phases, which are phases of matter at zero temperature. Accessing a quantum phase transition can only be done by varying a physical parameter of the system at zero temperature. A quantum phase transition typically describes a sudden change in the ground state of a many-particle system, i.e. a spontaneous break of symmetry in the Hamiltonian, due to the fact that thermal fluctuations are frozen out and quantum fluctuations prevail [3][4]. The latter is an important requirement, as we will see later on.

Since magnons can be considered bosons and obey Bose-Einstein statistics, it is theoretically possible to achieve Bose-Einstein condensation of magnons cooled to temperatures near abso-

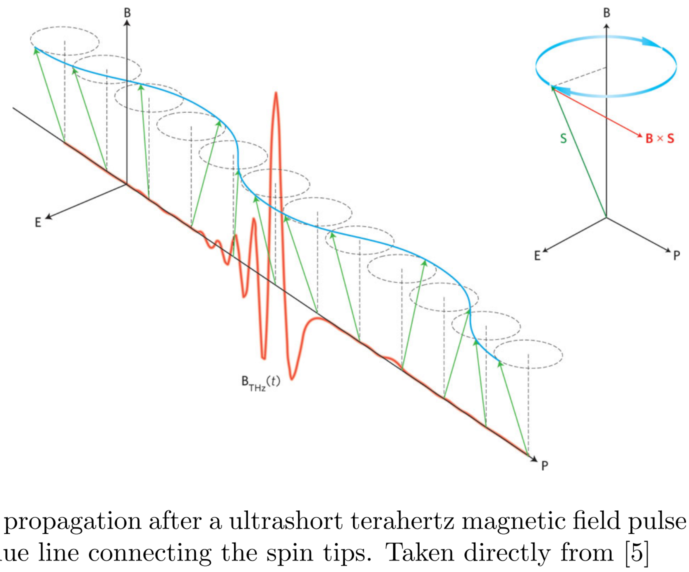

Figure 1: Magnon propagation after a ultrashort terahertz magnetic field pulse (red)- the magnon is shown by the blue line connecting the spin tips. Taken directly from [5]

lute zero. A Bose-Einstein condensate is described as a coherent state in which the quantum mechanical operators have nonzero expectation values and has a fixed phase [6]. Especially the latter argument is of importance in our section concerning phase diffusion. In this condensate, the magnons occupy the same lowest energy state which results in the fact that quantum phenomena become apparent at a macroscopic scale.

One of such macroscopic phenomena that could become apparent is the quantum phase transition between the Mott insulator and superfluid phase. As described earlier, this phase transition is induced at zero temperature and can only be accessed through varying the magnetic field B (our adjustable physical parameter). This has been done before for a system of cold atoms, but it has never been shown in the particular case of magnons [7]. Therefore one of the goals of this thesis is to create such a phase diagram in the case of magnons. Another goal of this thesis is researching phase diffusion in a magnon Bose-Einstein condensate. Typically, phase diffusion is only measurable indirectly by determining the phase difference obtained through an interference pattern. However, as will become apparent in the last section, the number of magnons in our system and the phase of those magnons are conjugate variables and and for our model the magnon phase corresponds to the spin direction in the x-y plane. This gives the oppurtunity to measure the phase directly.

This thesis will be divived into several sections, starting with the theoretical model showing what Hamiltonian governs our system and how this must be transformed to aptly describe the occurence of magnons. Next we research the effects of Bose-Einstein condensation of magnons followed by a couple of phase diagrams which are consistent with making particular approximations to the earlier derived Hamiltonian. In the following section we go into further detail on the construction of the phase diagram of the Mott insulator to superfluid phase transition. In the final chapter we discuss the phenomenon called phase diffusion in Bose-Einstein condensates and derive the equations of motion for the phase of the condensate. Finally we finish with the conclusion, extracting the most important discoveries throughout this thesis.

2 Model

In this section we determine several representations of our magnon system. This way, we express the dynamics of our system in terms of different variables, allowing us to apply this model in various situations.

2.1 The Holstein-Primakoff transformation

The model we use throughout this thesis is the easy-plane ferromagnet described by the Hamiltonian given in Eq.1. This Hamiltonian describes a three-dimensional lattice of spin particles subject to an external magnetic field B pointing in the $-z$ direction.

$$\hat{H} = -\frac{J}{2\hbar^2}\sum_{\langle i,j\rangle}\vec{S}_i\cdot\vec{S}_j + \frac{K}{2\hbar^2}\sum_i (S_i^z)^2 + \frac{B}{\hbar}\sum_i S_i^z. \tag{1}$$

Where i, j denote positions on the lattice, $\langle i, j\rangle$ describes a neighbouring pair of spins. The parameters J and K, both real and positive, correspond respectively to the interaction energies between sites and per site.

Since we are interested in the behaviour of magnons, we have to transform $\hat{H}$ in such a way that it is expressed in terms of particle rather than spin operators. To that end we apply the Holstein-Primakoff transformation to our $\hat{H}$ in order to map the angular momentum operators (corresponding to spin) to the bosonic creation and annihilation operators, where the latter describe the creation and annihilation of magnons, respectively. We introduce the following relations:

$$S_i^+ = \hbar a_i^\dagger \sqrt{2S - a_i^\dagger a_i}, \qquad S_i^- = \hbar a_i \sqrt{2S - a_i^\dagger a_i}, \qquad S_i^z = \hbar(a_i^\dagger a_i - S), \tag{2}$$

where a_i and $a_j^\dagger$ satisfy the commutation relation $[a_i, a_j^\dagger] = \delta_{i,j}$, with $\delta_{i,j}$ being the familiar Kronecker delta. We can write: $[a_i, a_i^\dagger] = 1$, which is a result we will be using later on.

Because S is relatively large compared to $a_i^\dagger a_i$ in the case we are interested in, we can Taylor expand the expressions for S_i^+ and S_i^- up to first order in powers of $\frac{1}{S}$ to obtain:

$$S_i^+ = \hbar a_i^\dagger \sqrt{2S} \sqrt{1 - \frac{a_i^\dagger a_i}{2S}} \approx \hbar\sqrt{2S} a_i^\dagger, \qquad S_i^- = \hbar a_i \sqrt{2S} \sqrt{1 - \frac{a_i^\dagger a_i}{2S}} \approx \hbar\sqrt{2S} a_i. \tag{3}$$

We can now rewrite our $\hat{H}$ in terms of S^+ and S^- after which we can substitute the above mentioned equations to eventually yield the following expressions:

$$\hat{H} = -\frac{J}{2\hbar^2} \sum_{\langle i,j \rangle} \Big(\frac{1}{2}(S_i^+ S_j^- + S_i^- S_j^+) + S_i^z S_j^z \Big) + \frac{K}{2\hbar^2} \sum_i (S_i^z)^2 + \frac{B}{\hbar} \sum_i S_i^z \tag{4a}$$

$$\approx -\frac{J}{2\hbar^2} \sum_{\langle i,j \rangle} \hbar^2 \Big(S(a_i^\dagger a_j + a_i a_j^\dagger) + (a_i^\dagger a_i - S)(a_j^\dagger a_j - S) \Big) + \frac{K}{2\hbar^2} \sum_i \hbar^2 (a_i^\dagger a_i - S)^2 \tag{4b}$$

$$+ \frac{B}{\hbar} \sum_i \hbar (a_i^\dagger a_i - S).$$

Which can be further simplified to yield:

$$\hat{H} = -\frac{J}{2} \sum_{\langle i,j \rangle} \Big(S(a_i^\dagger a_j + a_i a_j^\dagger) + a_i^\dagger a_i a_j^\dagger a_j - S(a_i^\dagger a_i + a_j^\dagger a_j) + S^2 \Big) \tag{5}$$

$$+ \frac{K}{2} \sum_i \Big(a_i^\dagger a_i a_i^\dagger a_i - 2S a_i^\dagger a_i + S^2 \Big) + B \sum_i \Big(a_i^\dagger a_i - S \Big)$$

$$= -\frac{J}{2} \sum_{\langle i,j \rangle} \Big(2S(a_i^\dagger a_j - a_i^\dagger a_i) + a_i^\dagger a_i a_j^\dagger a_j \Big) + \frac{K}{2} \sum_i \Big(a_i^\dagger a_i a_i^\dagger a_i - 2S a_i^\dagger a_i \Big) + B \sum_i a_i^\dagger a_i \tag{6}$$

$$- \frac{1}{2} J N_s (N_s - 1) S^2 + \frac{1}{2} K N_s S^2 - B N_s S.$$

Here N_s equals the total number of lattice sites. If we now neglect the constant terms and rearrange the remaining ones, we retrieve in essence the Bose-Hubbard Hamiltonian:

$$\hat{H} = -\frac{J}{2} \sum_{\langle i,j \rangle} \Big(2S(a_i^\dagger a_j - a_i^\dagger a_i) + a_i^\dagger a_j^\dagger a_i a_j \Big) + \Big(\frac{K}{2}(1 - 2S) + B \Big) \sum_i a_i^\dagger a_i \tag{7}$$

$$+ \frac{K}{2} \sum_i a_i^\dagger a_i^\dagger a_i a_i.$$

Where we've made use of the relation following from $[a_i, a_j^\dagger] = \delta_{i,j}$, in particular that $a_i a_i^\dagger = 1 + a_i^\dagger a_i$, in order to arrange the terms according to the normal ordering convention. In this convention the creation operators are ordered left of their annihilation counterparts.

2.2 Fourier transform

We are now ready to Fourier transform this equation for our system using the identities $a_i = \frac{1}{\sqrt{N}}\sum_k a_{\vec{k}} e^{i\vec{k}\cdot\vec{R}_i}$ and $a_i^\dagger = \frac{1}{\sqrt{N}}\sum_{\vec{k}} a_{\vec{k}}^\dagger e^{-i\vec{k}\cdot\vec{R}_i}$, where $\vec{R}_i$ is a three-dimensional vector representing the position in Cartesian coordinates of a particle on lattice site i and $\vec{k}$ is the three-dimensional wave vector. Therefore we can write $\vec{R}_i = \alpha_i a\hat{x} + \beta_i a\hat{y} + \gamma_i a\hat{z}$ $(\alpha,\beta,\gamma \in \mathbb{Z})$ and $\vec{k} = k_x\hat{x} + k_y\hat{y} + k_z\hat{z}$. The constant a represents the spacing between the lattice points. Writing out our terms separately we obtain:

$$\sum_{\langle i,j\rangle} a_i^\dagger a_j = \frac{1}{2N}\sum_{\alpha,\beta,\gamma}\sum_{\vec{k},\vec{k}'} a_{\vec{k}}^\dagger a_{\vec{k}'} e^{-ia(k_x\alpha+k_y\beta+k_z\gamma)} \tag{8a}$$

$$\Big(e^{-ia(k_x(\alpha+1)+k_y\beta+k_z\gamma)} + e^{-ia(k_x(\alpha-1)+k_y\beta+k_z\gamma)} + e^{-ia(k_x\alpha+k_y(\beta+1)+k_z\gamma)}$$
$$+ e^{-ia(k_x\alpha+k_y(\beta-1)+k_z\gamma)} + e^{-ia(k_x\alpha+k_y\beta+k_z(\gamma+1))} + e^{-ia(k_x\alpha+k_y\beta+k_z(\gamma-1))}\Big)$$

$$= \frac{1}{2N}\sum_{\alpha,\beta,\gamma}\sum_{\vec{k},\vec{k}'} a_{\vec{k}}^\dagger a_{\vec{k}'} e^{i\alpha a(k_x'-k_x)} e^{i\beta a(k_y'-k_y)} e^{i\gamma a(k_z'-k_z)} \tag{8b}$$

$$\big(e^{ik_x'a} + e^{-ik_x'a} + e^{ik_y'a} + e^{-ik_y'a} + e^{ik_z'a} + e^{-ik_z'a}\big)$$

$$= \frac{1}{2}\sum_{\vec{k},\vec{k}'} a_{\vec{k}}^\dagger a_{\vec{k}'} \delta_{\vec{k},\vec{k}'} \big(e^{ik_x'a} + e^{-ik_x'a} + e^{ik_y'a} + e^{-ik_y'a} + e^{ik_z'a} + e^{-ik_z'a}\big) \tag{8c}$$

$$= \sum_{\vec{k}} a_{\vec{k}}^\dagger a_{\vec{k}} \big(\cos(k_x a) + \cos(k_y a) + \cos(k_z a)\big). \tag{8d}$$

Note that we used that $\sum_{\langle i,j\rangle} a_i^\dagger a_j = \sum_i a_i^\dagger(a_{i-1} + a_{i+1})$ in order to reduce the sum over neighbouring pairs to one dependent only on lattice site i. We also used the following relation in Eq.8b: $\sum_{\alpha,\beta,\gamma} e^{i\alpha a(k_x'-k_x)} e^{i\beta a(k_y'-k_y)} e^{i\gamma a(k_z'-k_z)} = N\delta_{\vec{k},\vec{k}'}$. The next term gives us:

$$\sum_{\langle i,j\rangle} a_i^\dagger a_i = \frac{3}{N}\sum_{\alpha,\beta,\gamma}\sum_{\vec{k},\vec{k}'} a_{\vec{k}}^\dagger a_{\vec{k}'} e^{-ia(k_x\alpha+k_y\beta+k_z\gamma)} e^{-ia(k_x'\alpha+k_y'\beta+k_z'\gamma)} \tag{9a}$$

$$= \frac{3}{N}\sum_{\alpha,\beta,\gamma}\sum_{\vec{k},\vec{k}'} a_{\vec{k}}^\dagger a_{\vec{k}'} e^{i\alpha a(k_x'-k_x)} e^{i\beta a(k_y'-k_y)} e^{i\gamma a(k_z'-k_z)} \tag{9b}$$

$$= 3\sum_{\vec{k},\vec{k}'} a_{\vec{k}}^\dagger a_{\vec{k}'} \delta_{\vec{k},\vec{k}'} = 3\sum_{\vec{k}} a_{\vec{k}}^\dagger a_{\vec{k}}. \tag{9c}$$

Where the factor 3 in the foregoing equations arises due to the fact that in three dimensions the sum runs over 6 pairs of spins and, in order to avoid double contributions, has to be divided through by 2 resulting in a factor equal to 3. Analogous to the above, we can also write:

$$\sum_i a_i^\dagger a_i = \frac{1}{N}\sum_{\alpha,\beta,\gamma}\sum_{\vec{k},\vec{k}'} a_{\vec{k}}^\dagger a_{\vec{k}'} e^{i\alpha a(k_x'-k_x)} e^{i\beta a(k_y'-k_y)} e^{i\gamma a(k_z'-k_z)} \tag{10a}$$

$$= \sum_{\vec{k},\vec{k}'} a_{\vec{k}}^\dagger a_{\vec{k}'} \delta_{\vec{k},\vec{k}'} = \sum_{\vec{k}} a_{\vec{k}}^\dagger a_{\vec{k}}. \tag{10b}$$

Now that we have Fourier-transformed every term seperately, we can write down Eq.7 again, but now in terms of $a_k^\dagger$ and a_k. In this expression we have chosen to neglect the fourth-order terms in J and K.

$$\hat{H} = \sum_{\vec{k}} \Big(\hbar\omega_{\vec{k}} + \frac{K}{2}(1-2S) + B\Big) a^\dagger_{\vec{k}} a_{\vec{k}}, \tag{11}$$

where $\hbar\omega_{\vec{k}} = \cos(k_x a) + \cos(k_y a) + \cos(k_z a) - 3.$

3 Bose-Einstein condensation of magnons and phase diagrams

In this chapter, we construct a phase diagram for Bose-Einstein condensation occurring in our magnon system. We also study the behaviour of our system when we neglect the magnon-magnon hopping and consider only a single spin of a lattice site. In this chapter, we

3.1 Constructing the phase diagram for BEC

Now that we have succesfully Fourier transformed our Hamiltonian, we can construct a BEC-phase diagram of our system of magnons. This is accomplished by examining the behaviour of the chemical potential μ of the system. Since it is not *a priori* clear what μ is, we have to calculate the distribution function of our system first and compare it to the Bose-Einstein distribution function (which governs bosons i.e. magnons) in order to identify the chemical potential in Eq.11. To achieve this we introduce the dispersion relation $\Omega_{\vec{k}} = \hbar\omega_{\vec{k}} + \frac{K}{2}(1-2S) + B$, our Hamiltonian can then be written as:

$$\hat{H} = \sum_{\vec{k}} \Omega_{\vec{k}} a^\dagger_{\vec{k}} a_{\vec{k}}, \tag{12}$$

where we note that this expression is actually reminiscent of a sum over many harmonic oscillators with frequencies $\frac{\Omega_{\vec{k}}}{\hbar}$. We can then derive the energy states ϵ_n to be equal to:

$$\epsilon_{n_k} = \sum_{\vec{k}} \Omega_{\vec{k}}(n_k + \frac{1}{2}), \tag{13}$$

where n_k takes on integer values. We shift out the ground-state energy so our energy states are given by $\epsilon_{n_k} = \sum_{\vec{k}} \Omega_{\vec{k}} n_k$.

Now we start by calculating the partition function of our system. We use the partition function to find an expression for $\langle U\rangle$, which is obtained through the relation: $\langle U\rangle = -\frac{\partial}{\partial\beta}\ln Z$.

$$Z = \sum_{n_k} e^{-\beta\epsilon_{n_k}} = \sum_{n_k} e^{-\beta\sum_{\vec{k}}\Omega_{\vec{k}} n_k} = \prod_{\vec{k}}\sum_{n} e^{-(\beta\Omega_{\vec{k}})n} = \prod_{\vec{k}} \frac{1}{1-e^{-\beta\Omega_{\vec{k}}}}, \tag{14}$$

$$\begin{aligned}\langle U\rangle &= -\frac{\partial}{\partial\beta}\ln\Big(\prod_{\vec{k}}\frac{1}{1-e^{-\beta\Omega_{\vec{k}}}}\Big) = -\frac{\partial}{\partial\beta}\left(\sum_{\vec{k}}\ln\Big(\frac{1}{1-e^{-\beta\Omega_{\vec{k}}}}\Big)\right) \\ &= \sum_{\vec{k}}\Omega_{\vec{k}} e^{-\beta\Omega_{\vec{k}}}\frac{1-e^{-\beta\Omega_{\vec{k}}}}{(1-e^{-\beta\Omega_{\vec{k}}})^2} = \sum_{\vec{k}}\frac{\Omega_{\vec{k}} e^{-\beta\Omega_{\vec{k}}}}{1-e^{-\beta\Omega_{\vec{k}}}} = \sum_{\vec{k}}\frac{\Omega_{\vec{k}}}{e^{\beta\Omega_{\vec{k}}}-1}.\end{aligned} \tag{15}$$

Due to the fact that the distribution function $\langle N_{\vec{k}}\rangle$ of a system is directly related to its average energy through the relation $\langle U\rangle = \sum_{\vec{k}}\langle N_{\vec{k}}\rangle\Omega_{\vec{k}}$, we can immediately extract that the distribution function of our system is given by:

$$\langle N_{\vec{k}}\rangle = \langle a^\dagger_{\vec{k}} a_{\vec{k}}\rangle = (e^{\beta\Omega_{\vec{k}}}-1)^{-1} = (e^{\beta(\hbar\omega_{\vec{k}}+\frac{K}{2}(1-2S)+B)}-1)^{-1}. \tag{16}$$

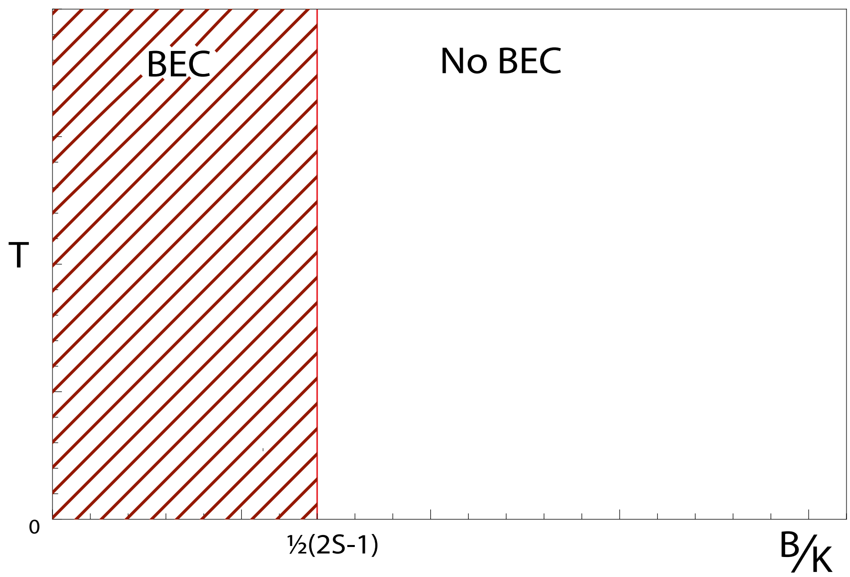

Figure 2: BEC phase diagram of magnon system after Holstein-Primakoff transformation, without magnon-magnon interactions

Now we compare our calculated distribution function to the one which should govern all bosons, namely the Bose-Einstein distribution: $f(\epsilon_{\vec{k}}) = (e^{\beta(\epsilon_{\vec{k}}-\mu)} - 1)^{-1}$. Matching this with Eq.16 and taking $\epsilon_{\vec{k}} = \hbar\omega_{\vec{k}}$ we find that our chemical potential μ is given by:

$$\mu = -\frac{K}{2}(1-2S) - B. \tag{17}$$

Since the conditions for Bose-Einstein condensation of a purely bosonic system obeying Bose-Einstein statistics depend on the chemical potential, we now have all the necessary information to construct our phase diagram. When the chemical potential is greater than or equal to the lowest single-particle energy state, which equals $\hbar\omega_{\vec{k}=0} = 0$ in our case, Bose-Einstein condensation occurs. If μ is less than 0, no Bose-Einstein condensation will take place. To summarize what that means for our system of magnons, we write down the conditions followed by the phase diagram below.

$$\mu = \begin{cases} \geq 0 \quad \text{if} \quad \frac{B}{K} \leq -\frac{1}{2}(1-2S) \Rightarrow \text{BEC} \\ \\ < 0 \quad \text{if} \quad \frac{B}{K} > -\frac{1}{2}(1-2S) \Rightarrow \text{No BEC} \end{cases} \tag{18}$$

Therefore we have established a threshold for $\frac{B}{K}$ at which Bose-Einstein condensation of our system of magnons will occur. We note that this depends on spin only and is therefore indepedent of temperature. The result is shown in Fig.2

3.2 Magnon behaviour in a single-spin problem at $J = 0$

In this section we are interested in how our system of magnons behaves when there are no magnon-magnon interactions between lattice sites, thus taking $J = 0$. In doing this, we actually only have to look at a single lattice site, since the sites are now uncoupled. Therefore it is sufficient to consider a single spin in our calculation and multiplying the final result by N_s, yielding the correct answer for our uncoupled system of magnons.

As we saw in the previous calculations, the chemical potential μ is dependent on the magnetic field B. Since B is a parameter which is experimentally easily adjustable, we can vary B to observe the changes in behaviour of our system. We already know that, according to the approximations made in section 3.1, our system collapses to a Bose-Einstein condensate once a certain threshold of $\frac{B}{K}$ is passed. For that reason we construct another diagram, but now for $J = 0$, expressed in terms of $\frac{B}{K}$ for the sake of comparison.

The Hamiltonian for a single lattice site is given by:

$$\hat{H} = \frac{K}{2\hbar^2}(S^z)^2 + \frac{B}{\hbar}S^z. \tag{19}$$

Let us first consider $T = 0$. Since the Holstein-Primakoff transformation defines a relation between the the spin and number of magnons, we want to make a diagram where we somehow express the expectation value of the spin in the $\hat{z}$-direction in terms of $\frac{B}{K}$. That way we can translate that diagram to obtain what we are after, namely a plot of the number of magnons in our system. We know the eigenvalue equation for S^z: $S^z|S, m_s\rangle = \hbar m_s|S, m_s\rangle$. Using this, we can evaluate our spin-Hamiltonian in this basis.

$$\begin{aligned}\hat{H}|S, m_s\rangle =& \frac{K}{2\hbar^2}(S^z)^2|S, m_s\rangle + \frac{B}{\hbar}S^z|S, m_s\rangle \\ =& \left(\frac{K}{2}(m_s)^2 + Bm_s\right)|S, m_s\rangle.\end{aligned} \tag{20}$$

Here m_s is the secondary quantum number which ranges from $-S$ to S in integer steps.

Since we are interested in the expecation value of S^z at $T = 0$, we have to find the ground state of our system, which we denote as $|\Psi_0\rangle$. Thus in order to evaluate $\langle S^z\rangle_{T=0}$, we must find the value of $m_{s,0}$, since $\langle S^z\rangle_{T=0} = \langle\Psi_0|S^z|\Psi_0\rangle = \hbar m_{s,0}\langle\Psi_0|\Psi_0\rangle = \hbar m_{s,0}$. However, this ground state is not the same in all regimes of B and therefore has different values of $m_{s,0}$ corresponding to the ground state in each of the domains.

To make this comprehensible, we compute the eigenvalues for $S = 1$ and $S = 2$ and highlight the minimum values in each domain. For practical reasons, we divide through by K and immediately use those eigenvalues to plot our diagram in terms of $\frac{B}{K}$. Since the magnetic field is an easily adjustable parameter

Table 1: Eigenvalues for S=1

	$\frac{B}{K}$	0	$(0, \frac{1}{2})$	$\frac{1}{2}$	$> \frac{1}{2}$
m_s					
-1		$\frac{1}{2}$	$\frac{1}{2} - \frac{B}{K}$	0	$\frac{1}{2} - \frac{B}{K}$
0		0	0	0	0
1		$\frac{1}{2}$	$\frac{1}{2} + \frac{B}{K}$	1	$\frac{1}{2} + \frac{B}{K}$

Now that we know the ground states and corresponding values of m_s in every domain, we can evaluate $\langle S^z\rangle_{T=0}$ for each one. As mentioned before, we can translate this result to obtain a diagram for the number of magnons, $\langle a^\dagger a\rangle$.

$$\langle a^\dagger a\rangle = \frac{\langle S^z\rangle}{\hbar} + S. \tag{21}$$

Table 2: Eigenvalues for S=2

	$\frac{B}{K}$	0	$(0,\frac{1}{2})$	$\frac{1}{2}$	$(\frac{1}{2},1)$	1	$(1,\frac{3}{2})$	$\frac{3}{2}$	$>\frac{3}{2}$
m_s									
-2		2	$2-2\frac{B}{K}$	1	$2-2\frac{B}{K}$	0	$2-2\frac{B}{K}$	-1	$2-2\frac{B}{K}$
-1		$\frac{1}{2}$	$\frac{1}{2}-\frac{B}{K}$	0	$\frac{1}{2}-\frac{B}{K}$	$-\frac{1}{2}$	$\frac{1}{2}-\frac{B}{K}$	-1	$\frac{1}{2}-\frac{B}{K}$
0		0	0	0	0	0	0	0	0
1		$\frac{1}{2}$	$\frac{1}{2}+\frac{B}{K}$	1	$\frac{1}{2}+\frac{B}{K}$	$\frac{3}{2}$	$\frac{1}{2}+\frac{B}{K}$	2	$\frac{1}{2}+\frac{B}{K}$
2		2	$2+2\frac{B}{K}$	3	$2+2\frac{B}{K}$	4	$2+2\frac{B}{K}$	5	$2+2\frac{B}{K}$

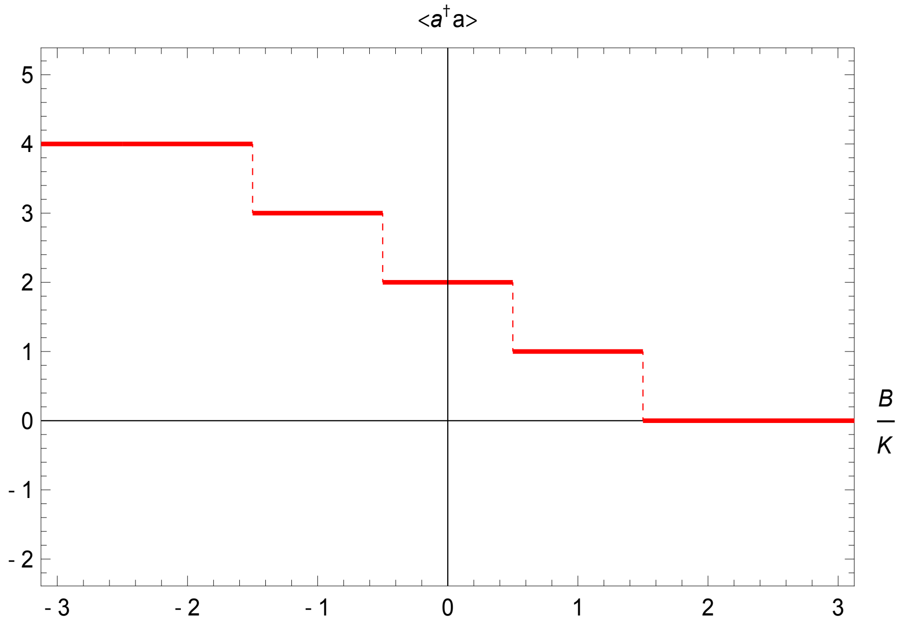

Figure 3: $\langle a^\dagger a\rangle$ at $T=0$ for a single spin-2 particle

In Fig.3, we plot our results for the case where $S=2$.

In the diagram we can see that when $\frac{B}{K} > \frac{3}{2}$, $\langle a^\dagger a\rangle = 0$ which means that there are no magnons when $\frac{B}{K}$ reaches a certain threshold. Recall that this is due to the fact that when the magnetic field is strong enough, it completely aligns the spin in the negative $\hat{z}$-direction. When the magnetic field is not so strong, the spin will not be aligned so forcibly and therefore gains some freedom in varying its spin angle. This implies the increase in the number of magnons in proportion with the decrease in magnetic field strength up to a maximum of $2S$ magnons per spin particle.

We are now interested in the behaviour of our magnon system when $T\neq 0$. We therefore attempt to find the eigenvalues of $\langle S^z\rangle$ and divide them through by K again. Since we now have a nonzero temperature, we can also vary the temperature in order to induce changes in the behaviour of our system. Varying the temperature corresponds to changing the value of βK. If we use Eq.20 and calculate the expectation value through the related partition function, we

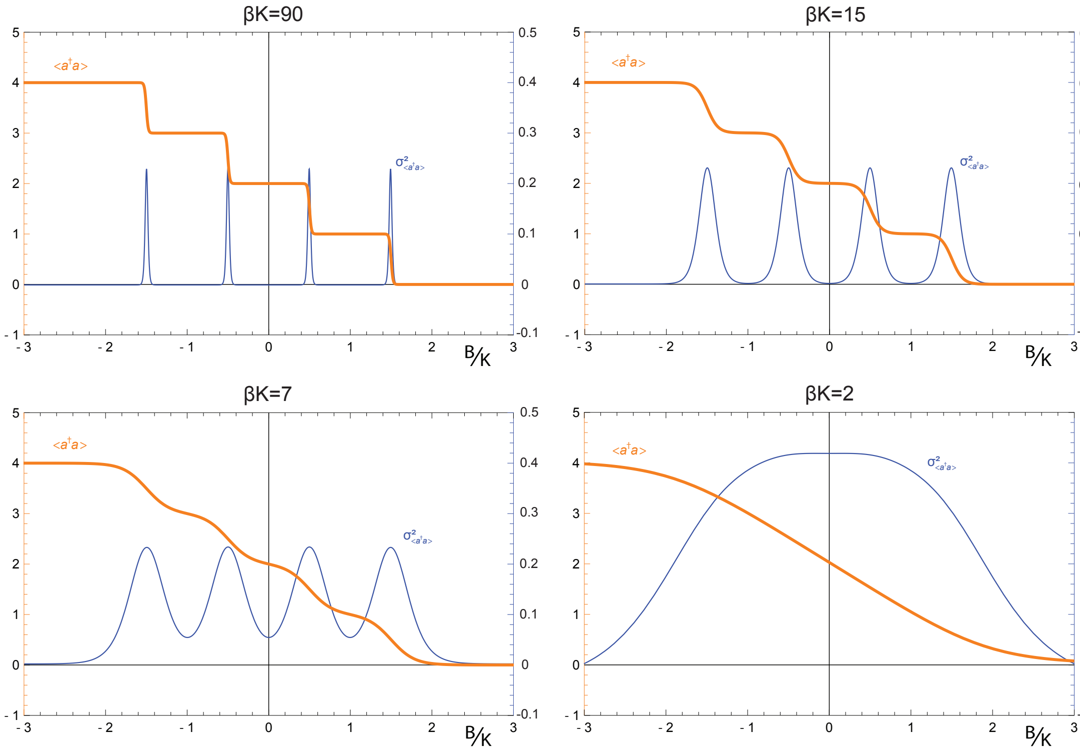

Figure 4: $\langle a^\dagger a\rangle$ and $\sigma^2_{\langle a^\dagger a\rangle}$ at $T{\neq}0$ for a single spin-2 particle

obtain:

$$\langle S^z\rangle = \frac{1}{Z}\sum_{m_s=-S}^{S} m_s\hbar e^{-\beta\left(\frac{K}{2}m_s^2+Bm_s\right)} = \frac{1}{Z}\sum_{m_s=-S}^{S} m_s\hbar e^{-\beta K\left(\frac{1}{2}m_s^2+\frac{B}{K}m_s\right)}, \tag{22}$$

$$\text{where } Z = \sum_{m_s=-S}^{S} e^{-\beta K\left(\frac{1}{2}m_s^2+\frac{B}{K}m_s\right)}.$$

As before, we translate this using the Holstein-Primakoff transformation to obtain a plot for $\langle a^\dagger a\rangle$ in terms of $\frac{B}{K}$. However, since the temperature is now greater than zero, the number of magnons (per lattice site) will not be well-defined i.e. our system will have a nonzero variance $\sigma^2_{\langle a^\dagger a\rangle}$ at each lattice site. We calculate the variance through:

$$\sigma^2_{\langle a^\dagger a\rangle} = \langle (a^\dagger a)^2\rangle - \langle a^\dagger a\rangle^2 = \left\langle\left(\frac{S^z}{\hbar}-S\right)^2\right\rangle - \left\langle\left(\frac{S^z}{\hbar}-S\right)\right\rangle^2 = \frac{\langle (S^z)^2\rangle - \langle S^z\rangle^2}{\hbar^2}. \tag{23}$$

So now we can plot $\langle a^\dagger a\rangle$ and $\sigma^2_{\langle a^\dagger a\rangle}$ for several values of βK, which is depicted in the diagrams above. As is clear from the plots, thermal fluctuations become increasingly more important when the temperature is high (i.e. low value of βK). For low temperatures, the variance peaks sharply when shifts in magnon quantity occurs. This uncertainy in magnon quantity becomes more and more 'smeared' out as we further increase temperature, until it does not even reach

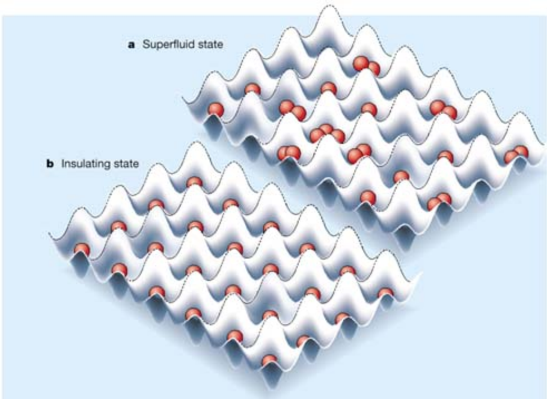

Figure 5: Schematic display of Mott insulator and superfluid phase; red spheres represent magnons

zero anymore on the magnon plateaus. By then the magnon plateaus have become so flattened that the discrete ladder depicted in Fig.3 is just barely recognizable. If we take $\beta K = 2$, the magnon quantity is essentially reduced to a straight line accompanied by a very high uncertainty which implies that thermal fluctuations dominate this particular regime.

4 Creating a phase diagram of Mott insulator to superfluid phase transition

In this section we focus our efforts on creating a phase diagram of the so called Mott insulator to superfluid phase transition. This transition takes place within the Bose-Einstein condensation regime at zero temperature (see Fig.2) where all thermal fluctuations have died out and is thus governed by quantum fluctuations. In the following subsections we explain what a Mott insulating phase exactly is and how to construct the corresponding phase diagram.

4.1 What are Mott insulating and superfluid phases?

We consider again our lattice site in three dimensions. Let there be an integer number of particles per site i and $JS \ll K$. Then this means that the magnon-magnon hopping is significantly smaller than the on-site interaction, therefore making it energetically unfavorable for particles to move between sites, i.e. the number of magnons per lattice site is fixed. This situation is what is known as the Mott insulating phase or Mott insulator. Note that in the Mott insulating phase, the number of magnons on each site is well-defined. This implies that the fluctuation in magnon number per site is reduced which leads to increased fluctuations in the phase. Fig.5 shows the distribution of magnons on a lattice. Note that in the Mott insulating phase, the phases of the magnons fluctuate while in the superfluid phase they are coherent (see Fig.8). We discuss the latter case later on.

The other phase in which particles can reside in is the superfluid phase. In this phase, each atom is essentially spread out over the entire lattice which corresponds to the magnon-magnon hopping being more dominant than the on-site interactions. This leads to a long-range phase coherence for particles in the superfluid phase whereas particles in the insulating phase have no phase coherence across the lattice. The phase transition between these two phases only

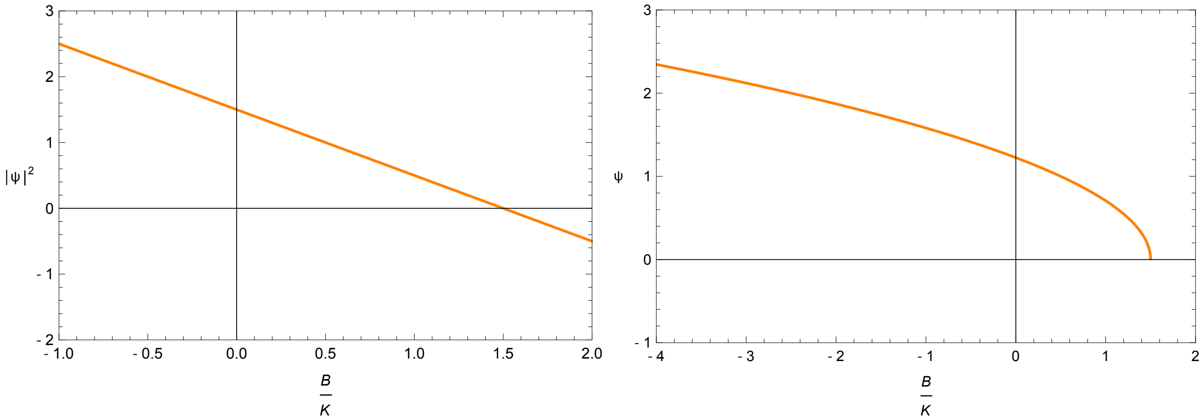

Figure 6: Ψ and $|\Psi|^2$ plotted as functions of $\frac{B}{K}$

occurs at zero temperature when the thermal fluctuations have died out completely and quantum fluctuations, which are present at $T = 0$, are strong enough to induce a phase transition. Most of the information stated above has been adapted from [7].

In order to actually describe the zero-temperature phase transition analytically in the superfluid case, we need to apply a mean-field approximation to our Hamiltonian:

$$a_i \to \langle a \rangle, \quad a_i^\dagger \to \langle a^\dagger \rangle \quad \text{and} \quad \text{substituting} \quad \Psi = \langle a \rangle = \langle a^\dagger \rangle. \tag{24}$$

Where Ψ is introduced and represents the superfluid order parameter. If we plug these expressions into our Hamiltonian defined in Eq.7 we obtain:

$$\begin{aligned} \hat{H} &= -JS \sum_{\langle i,j \rangle} \left(a_i^\dagger a_j - a_i^\dagger a_i \right) + \left(\frac{K}{2}(1 - 2S) + B \right) \sum_i a_i^\dagger a_i + \frac{K}{2} \sum_i a_i^\dagger a_i^\dagger a_i a_i \\ &\to -\mu |\Psi|^2 \sum_i + \frac{K}{2} |\Psi|^4 \sum_i = -\mu N_s |\Psi|^2 + \frac{K}{2} N_s |\Psi|^4 = E. \end{aligned} \tag{25}$$

Where we used Eq.17 to further simplify the equation. Furthermore we have set the end result equal to E to clarify that the expression must equal a constant after the mean-field approximation. If we now were to minimalise this energy E, we would obtain a non-trivial relation between the superfluid order parameter Ψ and $\frac{B}{K}$ as will be illustrated below:

$$\frac{\partial E}{\partial \Psi} = 2N_s \Psi \left(-\mu + K|\Psi|^2 \right) = 0 \quad \Rightarrow \quad |\Psi|^2 = \frac{\mu}{K} = S - \frac{B}{K} - \frac{1}{2}. \tag{26}$$

Note that in the diagram of $\Psi(\frac{B}{K})$ we only plotted one of the possibilities since any plot would be correct when multiplied by a phase factor $e^{i\theta}$. This phase diagram is in agreement with our previous phase diagram for Bose-Einstein condensation, i.e., the order parameter Ψ is nonzero if $\mu > 0$.

4.2 Constructing the phase diagram

We now determine the phase diagram including the Mott-insulator. First we take our Hamiltonian defined in Eq.7. Neglecting the fourth order magnon-magnon interaction term again and rearranging the terms, we get:

$$\hat{H} = -JS \sum_{\langle i,j \rangle} a_i^\dagger a_j + \Big(\frac{K}{2}(1-2S) + B + \frac{zJS}{2}\Big) \sum_i a_i^\dagger a_i + \frac{K}{2} \sum_i a_i^\dagger a_i^\dagger a_i a_i, \tag{27}$$

where the term $\frac{zJS}{2}\sum_i a_i^\dagger a_i$ originates from transforming $JS\sum_{\langle i,j \rangle} a_i^\dagger a_i$ to a sum over i sites and z signifies the number of nearest neighbours, so in three dimensions $z = 6$. The factor $\frac{1}{2}$ arises to prevent double counting of pairs. When we compare this Hamiltonian to the Bose-Hubbard Hamiltonian:

$$\hat{H}_{BH} = -t \sum_{\langle i,j \rangle} a_i^\dagger a_j - \mu \sum_i a_i^\dagger a_i + \frac{U}{2} \sum_i a_i^\dagger a_i^\dagger a_i a_i, \tag{28}$$

we can immediately see that $\mu = -\frac{K}{2}(1-2S) - B - \frac{zJS}{2}$, $t = JS$ and $U = K$. In order to make this Hamiltonian dimensionless, we scale all energies with a factor $\frac{1}{zt} = \frac{1}{zJS}$. So $\bar{\mu} = \frac{\mu}{zJS}$ and $\bar{K} = \frac{K}{zJS}$. This means that the chemical potential can we written in the form:

$$\bar{\mu} = -\frac{K}{2zJS}(1-2S) - \frac{B}{2zJS} - \frac{1}{2} = -\frac{\bar{K}}{2}(1-2S) - \bar{K}\frac{B}{K} - \frac{1}{2}. \tag{29}$$

The second term was multiplied by $\frac{K}{K} = 1$ in order to write $\bar{\mu}$ in terms of the now familiar parameter $\frac{B}{K}$.

Now that our $\hat{H}$ is dimensionless and we have arrived at a mean-field theory capable of describing the Mott insulator phase, we can actually derive the phase diagram analytically using second-order pertubation theory [8]. Doing this we eventually discover that the ground state energy is given by:

$$E_g^{(2)} = \frac{g}{\bar{K}(g-1) - \bar{\mu}} + \frac{g+1}{\bar{\mu} - \bar{K}g}. \tag{30}$$

If the Landau procedure for second-order phase transition is followed, we write the ground state energy as an expansion in Ψ:

$$E_g(\Psi) = a_0(g, \bar{K}, \bar{\mu}) + a_2(g, \bar{K}, \bar{\mu})\Psi^2 + \mathcal{O}(\Psi^4). \tag{31}$$

When we minimize this as a function of Ψ, it is established that $\Psi = 0$ when $a_2(g, \bar{K}, \bar{\mu}) > 0$ and $\Psi \neq 0$ if $a_2(g, \bar{K}, \bar{\mu}) < 0$. This has the important implication that $a_2(g, \bar{K}, \bar{\mu}) = 0$ signifies the boundary between the Mott insulator and superfluid phase. When this is solved, it yields the relation:

$$\bar{\mu}_\pm = \frac{1}{2}\left(\bar{K}(2g-1) - 1\right) \pm \frac{1}{2}\sqrt{\bar{K}^2 - 2\bar{K}(2g+1) + 1}. \tag{32}$$

Since Eq.29 gives another expression for $\bar{\mu}$, we can plug that in:

$$-\frac{\bar{K}}{2}(1-2S) - \bar{K}\frac{B}{K} - \frac{1}{2} = \frac{1}{2}\left(\bar{K}(2g-1) - 1\right) \pm \frac{1}{2}\sqrt{\bar{K}^2 - 2\bar{K}(2g+1) + 1}. \tag{33}$$

We can solve this to find an equation that expresses $\frac{J}{K}$ in terms of $\frac{B}{K}$:

$$\frac{J}{K} = \frac{1}{zS}\left(1 + 2g - 2\sqrt{2g^2 + (S - \frac{B}{K})^2 + g(1 - 2S + 2\frac{B}{K})}\right). \tag{34}$$

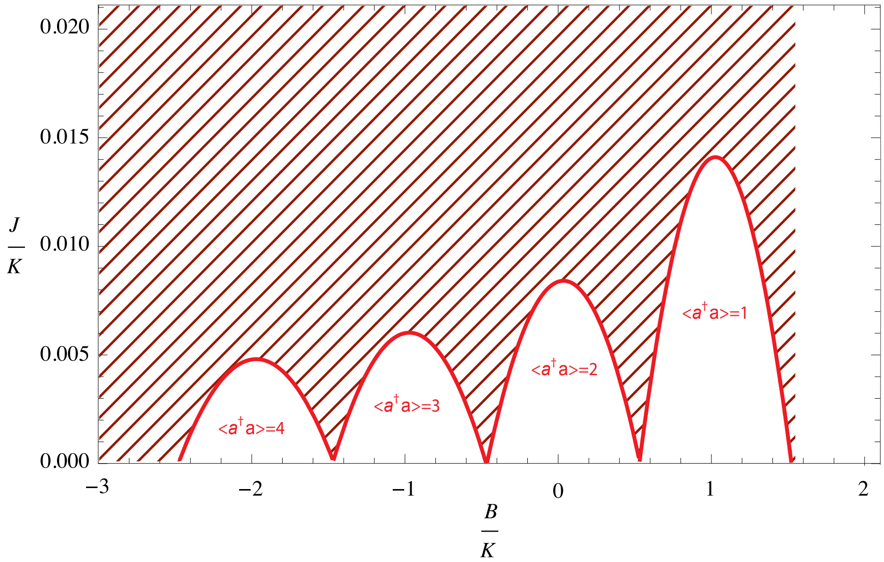

Figure 7: Phase diagram of the Mott insulator to superfluid phase transition for spin-2 particles

When we then plot this in the three dimensional case (so $z = 6$) and for a spin-2 particle, we obtain the phase diagram depicted in Fig.7. Note that the red line represents the boundary between the Mott insulating and superfluid phases. The shaded area shows Bose-Einstein condensation, within the bumps particles resides in the Mott-insulating phase. We look in particular at the right-most slope's intersection with the $\frac{J}{K} = 0$ line. As we can see, this occurs at $\frac{B}{K} = \frac{3}{2}$, which coincides with the BEC boundary determined in Fig.2 for $S = 2$: $\frac{1}{2}(4-1) = \frac{3}{2}$. This therefore validates our result, since the Mott insulating phase can only occur within the BEC regime, where the number of magnons is larger than zero.

5 Phase diffusion in the superfluid regime

We now relay our focus to the superfluid regime, where the magnon gas has the ability to flow without experiencing friction. The superfluid regime is established for $\frac{J}{K} \gg 1$ which implies that the magnon-magnon hopping is stronger than the on-site interactions, as becomes clear when looking at the height of the tallest slope in Fig.7. An interesting phenomenon occuring within this superfluid phase is phase diffusion, which is a direct consequence of the spontaneous $U(1)$ symmetry breaking and the finite size of the condensate [9]. Here $U(1)$ represents the group consisting of all complex numbers with absolute value equal to 1 under multiplication. We approach this problem by looking at the probability distribution for the quantum mechanical observables upon undergoing the phase transition. Unlike its classical counterparts, the mean value of those operators is nonzero [10]. In the context of Bose-Einstein condensation, this then means that the Hamiltonian describing our system remains invariant under global $U(1)$ transformations. These transformations are associated with the conservation of the number of magnons. Therefore the above implies the important relation, namely that the number of condensed magnons and the phase of the condensate itself are conjugate variables. It follows from Heisenberg's uncertainty principle that for a fixed number of magnons in the condensate, the phase of the condensate necassarily fluctuates [7]. However, as stated in the introduction,

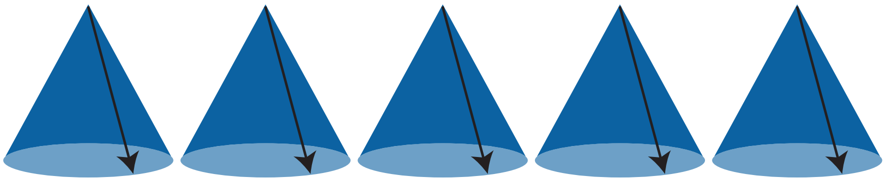

Figure 8: Illustration of phase coherence for a few magnons in the Bose-Einstein condensate

the phase of a Bose-Einstein condensate is typically fixed (as shown in Fig.8), which implies fluctuations in magnon number. Therefore, if we take a finite-sized condensate, the system can not be in a state with a definite phase. Consequently, the phase of the condensate is described by a probability distribution, which can lead to non-trivial equations of motion for the phase. This section is devoted to validating the above statements in the case of magnons. We approach this in two manners; one involves Ehrenfest's theorem applied to the spin-Hamiltonian given in Eq.1, the other method considers a given action and derives the equation of motion from it.

5.1 Spin method for deriving the equations of motion of the phase of the condensate

In this subsection, we would like to derive the equations of motion for the phase of the condensate. We begin by verifying Ehrenfest's theorem in the spin operator representation:

$$\frac{d\langle S_\alpha\rangle}{dt} = -\varepsilon_{\alpha\beta\gamma}\langle S_\beta\rangle\frac{\partial H[\langle\vec{S}\rangle]}{\partial\langle S_\gamma\rangle}, \qquad \text{where } \alpha,\beta,\gamma\in\{x,y,z\}, \tag{35}$$

and $\varepsilon_{\alpha\beta\gamma}$ is the Levi-Cevita symbol. Initially, we use the single-spin Hamiltonian $\hat{H}[\langle\vec{S}\rangle] = -g\vec{B}\cdot\langle\vec{S}\rangle$ to check whether Eq.35 indeed reproduces the known relation for the time-derivative of the expectation value of the spin operator: $\frac{d\langle\vec{S}\rangle}{dt} = g\langle\vec{S}\rangle\times\vec{B}$. This expression follows directly from Ehrenfest's theorem for any quantum mechanical operator $\hat{A}$:

$$\frac{d\langle\hat{A}\rangle}{dt} = \frac{1}{i\hbar}\langle[\hat{A},\hat{H}]\rangle + \left\langle\frac{\partial\hat{A}}{dt}\right\rangle. \tag{36}$$

We note that every component of the spin operator is time-independent which implies that the second term of Eq.36 equals zero. Thus we calculate the first term for $\hat{A} = S_x$, where we initially consider the x-component of the spin operator and deduce the result for all components analogously afterwards.

$$\begin{aligned}\frac{1}{i\hbar}\langle[S_x,\hat{H}]\rangle &= -\frac{g}{i\hbar}\big\langle\,(B_x[S_x,S_x]+B_y[S_x,S_y]+B_z[S_x,S_z])\,\big\rangle \\ &= -\frac{g}{i\hbar}\big\langle\,(B_x\cdot 0+B_y(i\hbar S_z)-B_z i\hbar S_y)\,\big\rangle = g\,(B_z\langle S_y\rangle - B_y\langle S_z\rangle)\,.\end{aligned} \tag{37}$$

This immediately gives the expression that:

$$\frac{d\langle S_x\rangle}{dt} = g\,(B_z\langle S_y\rangle - B_y\langle S_z\rangle)\,. \tag{38}$$

The corresponding expressions for the time-derivates of S_y and S_z are obtained through permutation of the indices yielding indeed the cross-product relation mentioned above. All that is left now, is to calculate the time-derivative of the x-component using Eq.35 and the fact that $\frac{\partial H[\langle\vec{S}\rangle]}{\partial\langle S_\alpha\rangle} = -gB_\alpha$:

$$\begin{aligned}\frac{d\langle S_x\rangle}{dt} &= \varepsilon_{xyz}\langle S_y\rangle gB_z + \varepsilon_{xzy}\langle S_z\rangle gB_y \\ &= gB_z\langle S_y\rangle - gB_y\langle S_z\rangle = g\left(B_z\langle S_y\rangle - B_y\langle S_z\rangle\right),\end{aligned} \tag{39}$$

which is exacty Eq.38 and can be extended analogously to all components so that we therefore may conclude that the spin representation of Ehrenfest's theorem defined in Eq.35 holds.

Now that we have validated the exactitude of Eq.35, we apply it to our spin Hamiltonian defined in Eq.1 so that we can derive the equations of motion subsequently. Note that our spin Hamiltonian is not yet defined in terms of expectation values as is required by Eq.35. To simplify matters, we assume that the expectation value of the inner product of two spin operators is the same as the product of the expectation values of the operators seperately. The same applies for the expectation of the square of an operator. Later on, we see that this leads to a small error in the equation of motion. Nevertheless, we choose simplicity over integrity in this particular calculation. Our Hamiltonian can thus be written in the form:

$$\hat{H} = -\frac{J}{2\hbar^2}\sum_{\langle i,j\rangle}\langle\vec{S}_i\rangle\cdot\langle\vec{S}_j\rangle + \frac{K}{2\hbar^2}\sum_i\langle S_i^z\rangle^2 + \frac{B}{\hbar}\sum_i\langle S_i^z\rangle. \tag{40}$$

Calculating the derivates required for the equations, gives us the next three expressions:

$$\begin{aligned}\frac{\partial H[\langle\vec{S}\rangle]}{\partial\langle S_i^z\rangle} &= -\frac{J}{2\hbar^2}\left(\langle S_{i-1}^z\rangle + \langle S_{i+1}^z\rangle\right) + \frac{K}{\hbar^2}\langle S_i^z\rangle + \frac{B}{\hbar} \quad, \\ \frac{\partial H[\langle\vec{S}\rangle]}{\partial\langle S_i^x\rangle} &= -\frac{J}{2\hbar^2}\left(\langle S_{i-1}^x\rangle + \langle S_{i+1}^x\rangle\right) \qquad \text{and} \qquad \frac{\partial H[\langle\vec{S}\rangle]}{\partial\langle S_i^y\rangle} = -\frac{J}{2\hbar^2}\left(\langle S_{i-1}^y\rangle + \langle S_{i+1}^y\rangle\right).\end{aligned} \tag{41}$$

Now we are ready to use Ehrenfest to calculate the time-derivatives of the spin components. Again, we start by computing the equation for the x-component, calculating the expressions for the remaining components in a similar fashion.

$$\begin{aligned}\frac{d\langle S_i^x\rangle}{dt} &= -\varepsilon_{xyz}\langle S_i^y\rangle\frac{\partial H[\langle\vec{S}\rangle]}{\partial\langle S_i^z\rangle} - \varepsilon_{xzy}\langle S_i^z\rangle\frac{\partial H[\langle\vec{S}\rangle]}{\partial\langle S_i^y\rangle} \\ &= \frac{J}{2\hbar^2}\left(\langle S_i^y\rangle\left(\langle S_{i-1}^z\rangle + \langle S_{i+1}^z\rangle\right) - \left(\langle S_{i-1}^y\rangle + \langle S_{i+1}^y\rangle\right)\langle S_i^z\rangle\right) - \frac{K}{\hbar^2}\langle S_i^y\rangle\langle S_i^z\rangle - \frac{B}{\hbar}\langle S_i^y\rangle;\end{aligned} \tag{42}$$

$$\frac{d\langle S_i^y\rangle}{dt} = \frac{J}{2\hbar^2}\left(\langle S_i^x\rangle\left(\langle S_{i-1}^x\rangle + \langle S_{i+1}^y\rangle\right) - \left(\langle S_{i-1}^z\rangle + \langle S_{i+1}^z\rangle\right)\langle S_i^x\rangle\right) + \frac{K}{\hbar^2}\langle S_i^x\rangle\langle S_i^z\rangle + \frac{B}{\hbar}\langle S_i^x\rangle; \tag{43}$$

$$\frac{d\langle S_i^z\rangle}{dt} = \frac{J}{2\hbar^2}\left(\langle S_i^x\rangle\left(\langle S_{i-1}^y\rangle + \langle S_{i+1}^y\rangle\right) - \left(\langle S_{i-1}^x\rangle + \langle S_{i+1}^x\rangle\right)\langle S_i^y\rangle\right). \tag{44}$$

We can use the Holstein-Primakoff transformation once again in order to express our relations in terms of the number operators corresponding to the creation and annihilation of magnons. Recalling that the phase of the condensate and the number of magnons are conjugate variables, we thus obtain information about the phase of the condensate indirectly. Consequently, we apply a mean-field approach to the number operators, yielding two equations of motion for the creation and annihilation operators seperately. As is to be expected, these equations of motion are conjugate to one another. We take the field operators ϕ_i^* and ϕ_i to be time-dependent, giving the following relation for our mean-field approximation: $\phi_i = \langle a_i\rangle(t)$ and $\phi_i^* = \langle a_i^\dagger\rangle(t)$.

In order to apply the abovementioned transformation, we have to derive the relations for S_j^x and S_j^y from Eq.2 using the definitions of the spin-raising and lowering operators. These are given to be: $S_j^+ = S_j^x + iS_j^y$ and $S_j^- = S_j^x - iS_j^y$. We deduce that:

$$S_j^x = \frac{1}{2}(S_j^+ + S_j^-) \approx \frac{\hbar}{2}\sqrt{2S}(a_j^\dagger + a_j) = \frac{\hbar}{2}\sqrt{2S}(\phi_j^* + \phi_j); \tag{45}$$

$$S_j^y = \frac{1}{2}(S_j^+ - S_j^-) \approx \frac{\hbar}{2i}\sqrt{2S}(a_j^\dagger - a_j) = \frac{\hbar}{2i}\sqrt{2S}(\phi_j - \phi_j^*);$$

$$S_j^z = \hbar\left(a_j^\dagger a_j - S\right) = \hbar\left(|\phi_j|^2 - S\right). \tag{46}$$

Plugging the derived expressions into Eq.42 to 44, we compute the equations of motion for the field operators. For pragmatic reasons, we initially consider Eq.44:

$$\begin{aligned}\frac{d\langle S_k^z\rangle}{dt} &= \frac{J}{2\hbar^2}\left(\langle S_k^x\rangle(\langle S_{k-1}^y\rangle + \langle S_{k+1}^y\rangle) - (\langle S_{k-1}^x\rangle + \langle S_{k+1}^x\rangle)\langle S_i^y\rangle\right) \\ &= \frac{JS}{4i}\big((\phi_k + \phi_k^*)(\phi_{k-1} - \phi_{k-1}^* + \phi_{k+1} - \phi_{k+1}^*) \\ &\quad - (\phi_k - \phi_k^*)(\phi_{k-1} + \phi_{k-1}^* + \phi_{k+1} + \phi_{k+1}^*)\big) \\ &= \frac{JS}{2i}\left(\phi_k^*(\phi_{k-1} + \phi_{k+1}) - \phi_k(\phi_{k-1}^* + \phi_{k+1}^*)\right).\end{aligned} \tag{47}$$

Here we assumed for simplicity that the lattice is one-dimensional. The actual case of three dimensions can be analogouly expanded from the one at hand. Writing out the left-hand side yields the following equation for the z-component:

$$\frac{d}{dt}|\phi_k|^2 = \frac{JS}{2i}\left(\phi_k^*(\phi_{k-1} + \phi_{k+1}) - \phi_k(\phi_{k-1}^* + \phi_{k+1}^*)\right). \tag{48}$$

However, we observe that, since we are in a BEC, it is safe to assume that the magnons are homogeneously distributed. This implies that $\phi_k = \phi$ and thus ϕ becomes independent of position. Consequently we see that the time-derivative of the z-component of the spin becomes zero. This is actually a consistent result, since S^z is directly related to the number of magnons in the homogeneous condensate approximation and therefore directly corresponds to the number of magnons being finite (i.e., fixed). Furthermore, if our condensate was not homogeneous, then Eq.48 is nonzero and would represent the density of magnons which can change locally by magnons entering and leaving a particular volume element.

Correspondingly, since the first terms of both Eq.42 and 43 are analogous to Eq.44, we see that these terms also go to zero in the homogeneous condensate approximation. The equations for the time-derivatives of the x- and y-component become:

$$\begin{aligned}\frac{d\langle S^x\rangle}{dt} &= -\frac{K}{\hbar^2}\langle S^y\rangle\langle S^z\rangle - \frac{B}{\hbar}\langle S^y\rangle \\ &= -\frac{K}{2i}\sqrt{2S}\,(\phi - \phi^*)\left(|\phi|^2 - S\right) - \frac{B}{2i}\sqrt{2S}\,(\phi - \phi^*) \\ &= \frac{\sqrt{2S}}{2i}\,(\phi - \phi^*)\left(-K|\phi|^2 + KS - B\right),\end{aligned} \tag{49}$$

$$\begin{aligned}\frac{d\langle S^y\rangle}{dt} &= \frac{K}{\hbar^2}\langle S^x\rangle\langle S^z\rangle + \frac{B}{\hbar}\langle S^x\rangle \\ &= \frac{K}{2}\sqrt{2S}\,(\phi + \phi^*)\left(|\phi|^2 - S\right) + \frac{B}{2}\sqrt{2S}\,(\phi + \phi^*) \\ &= -\frac{\sqrt{2S}}{2}\,(\phi + \phi^*)\left(-K|\phi|^2 + KS - B\right).\end{aligned} \tag{50}$$

The left-hand side of both equations are $\frac{\sqrt{2S}}{2}\hbar\left(\frac{d\phi}{dt}+\frac{d\phi^*}{dt}\right)$ and $\frac{\sqrt{2S}}{2i}\hbar\left(\frac{d\phi}{dt}-\frac{d\phi^*}{dt}\right)$ for x- and y-components respectively. To recapitulate, the expressions for both components culminate into one equation of motion comprising the two field operators. This gives us the important equation:

$$i\hbar\left(\frac{d\phi}{dt}\pm\frac{d\phi^*}{dt}\right)=(\phi\mp\phi^*)\left(-K|\phi|^2+KS-B\right). \tag{51}$$

The above equations describe the dynamics at a single lattice site. The reason we point out that this is actually one equation of motion for both field operators, is that when we seperate Eq.51 into its real and imaginary parts, we obtain the same equations for each operator twice. In other words, it does not matter whether we extract the upcoming equations of motion from the one obtained through the x-component or via the y-component. The result is as follows:

$$i\hbar\frac{d\phi}{dt}=(KS-B)\,\phi-K|\phi|^2\phi \quad \text{and} \quad i\hbar\frac{d\phi^*}{dt}=-\,(KS-B)\,\phi^*+K|\phi|^2\phi^*. \tag{52}$$

5.2 Action method for deriving the equations of motion of the phase of the condensate

In this section, we derive the equations of motion through a different, more comprehensive method in order to obtain a completer result compared to one derived in Eq.52. We begin with a given action, with the field operators as its argument, describing the dynamics of our magnon system:

$$S[\phi^*,\phi]=\int \mathrm{d}t\left\{i\hbar\phi^*\frac{\partial\phi}{\partial t}-H[\phi^*,\phi]\right\}. \tag{53}$$

Clearly we have to transform our Hamiltonian in terms of the field operators first in order to be able to derive the equations of motion using the Euler-Lagrange equations applied to the defined action. To do this we take the Hamiltonian after the Holstein-Primakoff transformation (neglecting fourth-order terms regarding the magnon-magnon interactions) Eq.27 and convert that using the aforementioned mean-field approxamation to yield:

$$\hat{H}[\phi,\phi^*]=-JS\sum_{\langle i,j\rangle}\phi_i^*\phi_j+\left(\frac{K}{2}(1-2S)+B+\frac{zJS}{2}\right)\sum_i|\phi_i|^2+\frac{K}{2}\sum_i|\phi_i|^4. \tag{54}$$

We define $\mu'=-\left(\frac{K}{2}(1-2S)+B+JS\right)$, where we again considered our lattice to be one-dimensional implying that $z=2$. Inserting this back into the action and maintaining the Einstein summation convention, we are left with:

$$S[\phi^*,\phi]=\int \mathrm{d}t\left\{i\hbar\phi_j^*\frac{\partial\phi_j}{\partial t}+JS\phi_j^*\left(\phi_{j-1}+\phi_{j+1}\right)+\mu'|\phi_j|^2-\frac{K}{2}|\phi_j|^4\right\}. \tag{55}$$

From this it can be derived that the Lagrangian density is of the form:

$$\mathcal{L}[\phi,\phi^*]=i\hbar\phi_j^*\frac{\partial\phi_j}{\partial t}+JS\phi_j^*\left(\phi_{j-1}+\phi_{j+1}\right)+\mu'|\phi_j|^2-\frac{K}{2}|\phi_j|^4. \tag{56}$$

Now that we have obtained an expression for the Lagragian density, we can apply the Euler-Langrange equations and derive the equations of motion. The Euler-Lagrange equations are given by the formula:

$$\frac{\partial\mathcal{L}}{\partial\phi_k}=\frac{\partial}{\partial t}\left(\frac{\partial\mathcal{L}}{\partial\left(\partial_t\phi_k\right)}\right). \tag{57}$$

We compute the equations for ϕ_j first and follow up with the expressions for ϕ_j^*:

$$\begin{aligned}
\frac{\partial \mathcal{L}}{\partial \phi_k} &= JS\phi_j^*\left(\delta_k^{j-1}+\delta_k^{j+1}\right)+\mu'\phi_j^*\delta_k^j-K\left(\phi_j^*\right)^2\phi_j\delta_k^j && (58)\\
&= JS\phi_j^*\left(\delta_{k+1}^{j}+\delta_{k-1}^{j}\right)+\mu'\phi_k^*-K\left(\phi_j^*\right)^2\phi_k\\
&= JS\left(\phi_{k+1}^*+\phi_{k-1}^*\right)+\mu'\phi_k^*-K|\phi_k|^2\phi_k^*\\
\frac{\partial}{\partial t}\left(\frac{\partial \mathcal{L}}{\partial\left(\partial_t\phi_k\right)}\right) &= \frac{\partial}{\partial t}\left(i\hbar\phi_j^*\delta_k^j\right)=i\hbar\frac{\partial\phi_k^*}{\partial t} && (59)\\
\frac{\partial \mathcal{L}}{\partial \phi_k^*} &= i\hbar\delta_k^j\frac{\partial\phi_j}{\partial t}+JS\phi_j\left(\delta_k^{j-1}+\delta_k^{j+1}\right)+\mu'\phi_j\delta_k^j-K\phi_j^2\phi_j^*\delta_k^j && (60)\\
&= i\hbar\frac{\partial\phi_k}{\partial t}+JS\left(\phi_{k+1}+\phi_{k-1}\right)+\mu'\phi_k-K|\phi_k|^2\phi_k\\
\frac{\partial}{\partial t}\left(\frac{\partial \mathcal{L}}{\partial\left(\partial_t\phi_k^*\right)}\right) &= 0 && (61)
\end{aligned}$$

Putting together all of the above, we arrive at the equations descbribing the change over time of our field operators:

$$\left.\begin{aligned}
i\hbar\tfrac{\partial\phi_k}{\partial t} &= -JS\left(\phi_{k+1}+\phi_{k-1}\right)-\mu'\phi_k+K|\phi_k|^2\phi_k\\
i\hbar\tfrac{\partial\phi_k^*}{\partial t} &= JS\left(\phi_{k+1}^*+\phi_{k-1}^*\right)+\mu'\phi_k^*-K|\phi_k|^2\phi_k^*
\end{aligned}\right\} \qquad (62)$$

However, since the fact that the condensate is homogeneous must be accounted for, we have to use that $\phi_k=\phi$. Applying the approximation means that the expressions become independent of J as those terms cancel out with similar ones comprised within μ'. To recap, we denote the final equations of motion for the field operators below:

$$\left.\begin{aligned}
i\hbar\tfrac{\partial\phi}{\partial t} &= -\mu\phi+K|\phi|^2\phi\\
i\hbar\tfrac{\partial\phi^*}{\partial t} &= \mu\phi^*-K|\phi|^2\phi^*
\end{aligned}\right\}\text{Equations of motion for } \phi \text{ and } \phi^*. \qquad (63)$$

Here we identified $\mu=-\left(\frac{K}{2}(1-2S)+B\right)$, which is exactly the chemical potential defined in Eq.17. Furthermore we take special note of the fact that the magnon-magnon interactions do not contribute to the change over time of the field operators and therefore the rate of creation or annihilation of magnons.

When we compare this to the equations of motion derived through the spin method, we note that the action method actually gives us an extra term. We can easily identify this term to be $\frac{K}{2}\phi$ and $\frac{K}{2}\phi^*$ for the real and imaginary field equation respectively. This can be explained due to the assumption concerning the dependence of expectation values in our Hamiltonian. In doing so, we transformed our operators into numbers, disregarding the extra term these two operators produce when commutating for the normal ordering convention. These terms turn out to be exactly the missing terms in our equations obtained through the spin-method.

In order to obtain information about the phase of the condensate, we transform our field operators to density and phase variables by the following relation: $\phi\to\sqrt{n}e^{i\theta}$ and $\phi^*\to\sqrt{n}e^{-i\theta}$. Here n signifies the magnon density in the Bose-Einstein condensate and θ represents the phase.

Plugging this into Eq.55, we obtain the following expressions for the action and Lagrangian density:

$$S[n,\theta] = \int \mathrm{d}t \left\{ i\hbar\sqrt{n}e^{-i\theta}\partial_t\left(\sqrt{n}e^{i\theta}\right) + \mu n - \frac{K}{2}n^2 \right\}, \tag{64}$$

$$\begin{aligned}\mathcal{L}[n,\theta] &= i\hbar\sqrt{n}\left(e^{i\theta}(\partial_t\sqrt{n}) + \sqrt{n}(\partial_t e^{i\theta})\right) + \mu n - \frac{K}{2}n^2 \\ &= \frac{i\hbar}{2}\partial_t n - n\hbar\partial_t\theta + \mu n - \frac{K}{2}.\end{aligned} \tag{65}$$

Now we calculate the Euler-Langrange equations in terms of our new variables. Doing so imposes restrictions on the variables which are used to describe the Lagrangian density solely in terms of the phase θ:

$$\frac{\partial\mathcal{L}}{\partial\theta} = 0,\ \frac{\partial}{\partial t}\left(\frac{\partial\mathcal{L}}{\partial(\partial_t\theta)}\right) = -\hbar\partial_t n \quad\Rightarrow\quad \partial_t n = 0, \tag{66}$$

$$\frac{\partial\mathcal{L}}{\partial n} = -\hbar\partial_t\theta + \mu - Kn,\quad \frac{\partial}{\partial t}\left(\frac{\partial\mathcal{L}}{\partial(\partial_t n)}\right) = \frac{\partial}{\partial t}\left(\frac{i\hbar}{2}\right) = 0 \quad\Rightarrow\quad \hbar\partial_t\theta = \mu - Kn. \tag{67}$$

However, combining these two equations by taking the second time-derivative of the last expression we obtain the following relation:

$$\hbar\frac{\partial^2\theta}{\partial t^2} = -K\partial_t n = 0. \tag{68}$$

The Lagrangian is given by $L = \int \mathrm{d}^s x\,\mathcal{L}$, where s is the number of spatial dimenions, i.e. in our case $s = 3$. Since our condensate is homogeneously distributed, the variables are indepent of position. We can therefore write, using the equations derived above, that the Lagrangian takes on the form:

$$L[n,\theta] = \int \mathrm{d}^3x\,\mathcal{L}[n,\theta] = V\left(-n\hbar\partial_t\theta + \mu n - \frac{K}{2}n^2\right). \tag{69}$$

Here V is the volume of our condensate. In order to express the Lagrangian in terms of just the phase, we integrate out the density. This is done by taking the density to be constant up to small fluctuations: $n = n_0 + \delta n$. The first step is to minimalize the Lagrangian in terms of n according to the substitution. Therefore we differentiate L with respect to n and substitute $n = n_0$ while maintaining that $\partial_t\theta = 0$:

$$\left.\frac{\partial\mathcal{L}}{\partial n}\right|_{n=n_0} = \mu - Kn_0 = 0 \quad\Rightarrow\quad \mu = Kn_0. \tag{70}$$

Plugging all of the above into the Lagrangian yields:

$$L[\delta n,\theta] = V\left(-(n_0+\delta n)\hbar\partial_t\theta + \mu(n_0+\delta n) - \frac{K}{2}(n_0+\delta n)^2\right) \tag{71}$$

$$\begin{aligned}&= V\left(\frac{K}{2}n_0^2 - \delta n\hbar\partial_t\theta - \frac{K}{2}(\delta n^2)\right) \\ &= \frac{VKn_0^2}{2} - V\left(\delta n\hbar\partial\theta + \frac{K}{2}(\delta n)^2\right).\end{aligned} \tag{72}$$

Here we made use of the fact that the term $-n_0\hbar\partial_t\theta$ integrates out to zero since it is an equilibruim term by definition. Furthermore, the first term in Eq.72 is a constant and could therefore in principle be shifted out. We then minimalize the Lagrangian once more, but now in terms of δn:

$$\frac{\partial\mathcal{L}}{\partial(\delta n)} = -V\hbar\partial_t\theta - VK\delta n = 0 \quad \Rightarrow \quad \delta n = -\frac{\hbar}{K}\frac{\partial\theta}{\partial t}. \tag{73}$$

Finally, what remains is the effective Lagrangian dependent only on the phase θ:

$$L_{\text{eff}}[\theta] = \frac{VKn_0^2}{2} + V\left(\frac{\hbar^2}{K}\frac{\partial^2\theta}{\partial t^2} - \frac{\hbar^2}{2K}\frac{\partial^2\theta}{\partial t^2}\right) \tag{74}$$

$$= C + \frac{V\hbar^2}{2K}\frac{\partial^2\theta}{\partial t^2}. \tag{75}$$

Where C is a constant. This effective Lagrangian describes the classical theory of our system in terms of θ. However, we now want to translate this to a quantum mechanical statement telling us something about the phase of the condensate. To do this we quantize the Lagrangian using canonical quantization of the variable θ. This ensures that the commutation relation $[\theta, p_\theta] = i\hbar$ holds. By definition we have that: $L_{\text{eff}}[\phi] = A + \frac{1}{2}m_{\text{eff}}\partial_t^2\phi$, where A can be any constant and ϕ an arbitrary scalar field operator. Therefore it is possible to immediately identify that $\frac{1}{2}m_{\text{eff}} = \frac{V\hbar^2}{2K}$. In the end, the phase must obey the Schrödinger equation according to second quantization:

$$i\hbar\frac{\partial\Psi(\theta,t)}{\partial t} = -\frac{\hbar^2}{2m_{\text{eff}}}\frac{\partial^2\Psi(\theta,t)}{\partial\theta^2} \quad \Rightarrow \quad i\hbar\frac{\partial\Psi(\theta,t)}{\partial t} = -\frac{K}{V}\frac{\partial^2\Psi(\theta,t)}{\partial\theta^2}. \tag{76}$$

This result is exactly what we expected, namely that the phase can only be well-defined if the number of magnons is not. This means that the volume must be infinitely large for the phase to be well-defined. We can easily verify this by examining Eq.76 and noticing that the right-hand side only goes to zero if $V \to \infty$. Therefore we can conclude this section by stating that the phase is ill-defined for any finite-sized system and thus that we have shown that phase diffusion indeed occurs.

6 Conclusion

We began this thesis by giving a short introduction into the prevailing concepts such as Bose-Einstein condensation, magnons, different types of phases and corresponding transitions and ultimately phase diffusion. This was followed by stating the motivation for writing about Bose-Einstein condensation of magnons and the interesting consequences that brings about, since this had not yet been done for this particular system setup.

In order to gain a better understanding of our system, we started by defining a thorough theoretical foundation yielding various Hamiltonians describing our system in different variables. This allowed us multiple approaches to describe certain situations later on. We used the Holstein-Primakoff transformation in order to map our Hamiltonian from angular momentum operators to the bosonic creation and annihilation operators. We continued by transforming our Hamiltonian using a Fourier transformation in order to let $\hat{H}$ be expressed in wave space.

The third section described the Bose-Einstein condensation of our magnon system and the phase diagrams corresponding to it. We derived an expression for the chemical potential μ and used the restrictions imposed on it, due to the fact that our system is bosonic, in order to create a phase diagram which was independent of temperature. Of course the latter can not be true, since our system must be near absolute zero for it to Bose-Einstein condensate. A more realistic diagram would have had a curved (to the left) line instead of a vertical boundary. See p.342-343 of [9] for a more detailed discussion about this particular subject. Nevertheless, the diagram gives us a good approximation of the value of $\frac{B}{K}$ for which our sytem become a BEC, since we are looking at very low values of T. After the BEC boundary had been established, we continued on to examine the behaviour of the magnons when the magnon-magnon interactions were ignored, i.e. $J = 0$. We initially researched this for a single spin at $T = 0$, deriving a phase diagram which showed discrete 'step'-behaviour. Furthermore, we also calculated the partition function and corresponding phase diagram for $T \neq 0$, this yielded the continuous counterpart of the earlier derived phase diagram as expected. We plotted this, along with the corresponding variation in magnon number, at different temperatures. The conclusion that followed was that thermal fluctuations become increasingly more important when the temperature gets higher up to the point where the system is governed by a large variance in magnon quantity.

Moreover, we devoted the next section to finding the phase diagram corresponding to the Mott insulating to superfluid phase transition. Initially we gave some information about what these phases represent and what the conditions to achieve it were. As it turns out, the boundary between the phases could be calculated analytically by applying an appropriate mean-field approximation to the Hamiltonian expressed in terms of the bosonic particle operators. We then compared our Hamiltonian to the Bose-Hubbard Hamiltonian and used a relation for the chemical potential derived in [8] to find an equation describing how $\frac{J}{K}$ is expressed in terms of $\frac{B}{K}$. The result was again plotted and we saw that the right-most slope's intersection with the $\frac{J}{K} = 0$-axis coincides with the BEC boundary determined in Fig.2.

In the final section, we relayed our focus to another interesting phenomenon occuring in the superfluid regime, namely phase diffusion. We hypothesized that, since the phase and number of magnons are conjugate variables, the system can not have a well-defined phase if the system has a finite size. This hypothesis was approached using two different methods; one involved applying Ehrenfest's theorem to the Spin-Hamiltonian, calculating the time-derivatives of each spin-component seperately. These derivates were then expressed in terms of the particle operators which in turn were subject to another mean-field approach, yielding two (conjugate) equations of motion for the field operators for a single lattice site. The other method revolved around varying a predefined action with a Hamiltonian already expressed in terms of the field operators. This also yielded two equations of motion, but these each had an extra term originating from the commutation relation between the operators and did not appear in the spin variant since we approximated the Hamiltonian in that approach. In both methods, we were allowed to use the fact that our condensate was homogeneously distributed, meaning that we could take $\phi_k = \phi$, which greatly simplified our equations.

In an effort to obtain information about the phase of the condensate, the Lagrangian had to be dependent only on the phase. To achieve this, we made an average density approximation which allowed us to integrate out the density. After minimalising the Lagrangian, in order to eliminate the small deviation in density δn, we could write our Lagrangian solely in terms of θ. Finally we translated this into the corresponding Schrödinger equation, resulting in the confirmation of the hypothesis, namely that phase diffusion indeed must occur in a finite-sized system.

To conclude this thesis, we note that phase diffusion is indeed measurable directly, because we can extract the phase from the magnetization in the x-y plane. We leave for future work the interesting features in behaviour of a low-dimensional magnon system, because the phase possibly fluctuates more than in three dimensions.

7 Acknowledgements

I hereby acknowledge Victor Dagnelie, with whom I collaborated in order to obtain the calculations needed to create the subsections 2.1, 2.2, 3.1, 3.2, 4.1 and 4.2.

References

[1] F.Bloch. *Über die quantenmechanik der elektronen in kristallgittern.* Zeits. Phys. **52**, 555-600 (1928).

[2] T.Holstein and H.Primakoff. *Field Dependence of the Intrinsic Domain Magnetization of a Ferromagnet.* Physical Review **53**, 1098 (1940).

[3] S.J. Blundell and K.M. Blundell. *Concepts in Thermal Physics.* Oxford University Press (2008).

[4] S.Sachdev. *Quantum Phase Transitions.* Cambridge University Press (2011).

[5] J.Kono. *Spintronics: Coherent terahertz control.* Nature **5**, 5-6 (2011).

[6] A.-W. de Leeuw, E.C.I. van der Wurff, R.A. Duine and H.T.C. Stoof. *Phase diffusion in a Bose-Einstein condensate of light.* arXiv:1406.1403 [cond-mat.quant-gas] (2014).

[7] M. Greiner, O. Mandel, T. Esslinger, T.W. Hänsch and I. Bloch. *Quantum phase transition from a superfluid to a Mott insulator in a gas of ultracold atoms.* Nature **415**, 39-44 (2002).

[8] D. van Oosten, P. van der Straten and H.T.C. Stoof. *Quantum phases in an optical lattice.* Physical Review A **63**, 053601 (2001).

[9] H.T.C. Stoof, K.B. Gubbels and D.B.M. Dickerscheid. *Ultracold Quantum Fields.* (Springer 2009).

[10] M.Lewenstein and L.You. *Quantum Phase Diffusion of a Bose-Einstein Condensate.* Physical Review Letters **77**, 17 3489-3493.