

Quantum fluctuations and degeneracies of two-dimensional magnetic skyrmions

Patrick van Dieten

Utrecht University

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Supervisor:

Dr. R. A. Duine

Institute for Theoretical Physics

Utrecht University

Abstract

In this thesis we use Holstein-Primakoff and Bogoliubov transformations to find the zero-point quantum fluctuations of two-dimensional magnetic skyrmion configurations found by R. Keesman *et al.* (arXiv:1506.00271). We show that skyrmions are promoted by quantum fluctuations as they lower the groundstate energy and increase the domains in which skyrmions were expected classically. More specifically, we show that quantum fluctuations shift the parameter values (spin coupling, Dzyaloshinskii-Moriya interaction, external magnetic field) at which degenerate skyrmion configurations occur, as classically degenerate skyrmion configurations generally have different zero-point energies. Our calculations show that these effects are large enough to be measurable.

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Introduction

A magnetic skyrmion is a topological shape of spin-orientations in magnetic materials. They arise as lowest energy spin configurations for certain regimes of temperature and external magnetic field strengths, mainly as a consequence of Dzyaloshinskii-Moriya interactions. The skyrmion as a topological defect was originally introduced in particle physics by T.H.R. Skyrme in 1962 [1]. His abstract concept was also applicable to other systems and became important in the field of solid state physics. Magnetic skyrmions were predicted but only recently discovered experimentally [2][3]. Because of their topological stability and easy manipulation with very low electrical currents [4][5], skyrmions are an interesting candidate for data storage. Spintronics is one of the fields of physics investigating potential applications of magnetic skyrmions.

Two-dimensional skyrmions occur when a thin film of magnetic material is under the influence of forces that break the inversion symmetry. For example, this occurs when the magnetic material is placed between two layers of non-magnetic material, such that the difference in material at the interfaces causes Dzyaloshinskii-Moriya interactions, which prefers spins not aligned, while the ferromagnetic Heisenberg spin coupling wants to align the spins. These two forces find a compromise in the skyrmion configuration. Two common types of magnetic skyrmions exist: a spiral/vortex configuration (figure 1a) or a hedgehog configuration (figure 1b). Which type is preferred by a system depends on the asymmetric forces like the Dzyaloshinskii-Moriya interactions.

Because magnetic skyrmions come in a large variety of sizes, they can be described in both a classical and a quantum mechanical manner. Ref. [12] shows that quantum fluctuations promote skyrmion configurations through zero-point energies. In this paper we investigate how this effects the classically degenerate configurations found in ref. [9]. This paper is organized as follows: in chapter 1 we look at the classical skyrmion in a continuous medium while in chapter 2 we introduce our semi-classical Hamiltonian for spins on a square lattice, approach it quantum mechanically by introducing spin operators and diagonalize it using a Bogoliubov transformation to find the spinwave modes and zero-point energies. In chapter 3 we show the results of our calculations and in chapter 4 we present our conclusions and suggestions for future research.



(a) A two-dimensional spiral skyrmion. (b) A two-dimensional hedgehog skyrmion.

Figure 1: Two types of skyrmion configuration. [5]

Chapter 1

Single classical skyrmion in thin film at zero temperature

In this chapter, we look at a single two-dimensional classical continuous skyrmion in an infinite plane. We find the typical size of skyrmions and what parameters mainly influence them.

When a thin film of magnetic solid material is placed between two non-magnetic solids, the system (and skyrmion) becomes approximately two-dimensional. We take this film to be in the x,y -plane and the external magnetic field \mathbf{H} in the \hat{z} -direction. Let $\boldsymbol{\Omega}(\mathbf{x})$ be the unit magnetization vector, then we find an expression for the energy of such a system [6]

$$E[\boldsymbol{\Omega}(\mathbf{x})] = \int \left\{ -\frac{J}{2}\boldsymbol{\Omega} \cdot \nabla^2 \boldsymbol{\Omega} + \frac{D}{2} \left(\hat{y} \cdot \left(\boldsymbol{\Omega} \times \frac{\partial \boldsymbol{\Omega}}{\partial x} \right) - \hat{x} \cdot \left(\boldsymbol{\Omega} \times \frac{\partial \boldsymbol{\Omega}}{\partial y} \right) \right) + K(1 - \Omega_z^2) + \mu_0 H M (1 - \Omega_z) - \mu_0 M \boldsymbol{\Omega} \cdot \mathbf{H}_d \right\} d\mathbf{x},$$

with J the spin stiffness, D the Dzyaloshinskii-Moriya interaction constant, M is the magnetisation constant such that $\mathbf{M}(\mathbf{x}) = M\boldsymbol{\Omega}(\mathbf{x})$, K the anisotropy constant, μ_0 the permeability of vacuum, and \mathbf{H}_d is the demagnetization field. To keep the model simple, we ignore the effects of anisotropy and the induced demagnetization field, as these effects have minor impact on the behavior of the system while making the mathematics a lot more complicated, so we use

$$E[\boldsymbol{\Omega}(\mathbf{x})] = \int \left\{ -\frac{J}{2}\boldsymbol{\Omega} \cdot \nabla^2 \boldsymbol{\Omega} + \frac{D}{2} \left(\hat{y} \cdot \left(\boldsymbol{\Omega} \times \frac{\partial \boldsymbol{\Omega}}{\partial x} \right) - \hat{x} \cdot \left(\boldsymbol{\Omega} \times \frac{\partial \boldsymbol{\Omega}}{\partial y} \right) \right) + \mu_0 H M (1 - \Omega_z) \right\} d\mathbf{x}. \quad (1.1)$$

Following the same methods as in ref. [7] we assume translational symmetry along and rotational symmetry around the \hat{z} -axis. Using cylindrical coordinates $\mathbf{x} = (\rho, \varphi, z)$ we parametrize

$$\boldsymbol{\Omega}(\mathbf{x}) = \sin(\theta)\cos(\phi_0)\hat{\rho} + \sin(\theta)\sin(\phi_0)\hat{\varphi} + \cos(\theta)\hat{z}. \quad (1.2)$$

Note that ϕ_0 determines the twist of skyrmion. For $\phi_0 = 0$ we have a hedgehog skyrmion and $\phi_0 = \frac{1}{2}\pi$ gives a vortex skyrmion.

Suppose the film has a thickness t . We substitute (1.2) into (1.1) and integrate over z and φ using the symmetries, resulting in

$$\begin{aligned} \mathbb{E}[\theta(\rho)] = 2\pi t \int \left\{ \frac{J}{2} \left(\left(\frac{d\theta}{d\rho} \right)^2 + \frac{\sin^2(\theta)}{\rho^2} \right) \right. \\ \left. + \frac{D}{2} \cos(\phi_0) \left(\frac{d\theta}{d\rho} + \frac{\sin(\theta)\cos(\theta)}{\rho} \right) + \mu_0 HM(1 - \cos(\theta)) \right\} \rho d\rho. \end{aligned}$$

Thus we can formulate the energy density

$$\begin{aligned} \epsilon[\theta(\rho)] = \frac{\mathbb{E}[\theta(\rho)]}{2\pi t} = \int \left\{ \frac{J}{2} \left(\left(\frac{d\theta}{d\rho} \right)^2 + \frac{\sin^2(\theta)}{\rho^2} \right) \right. \\ \left. + \frac{D}{2} \cos(\phi_0) \left(\frac{d\theta}{d\rho} + \frac{\sin(\theta)\cos(\theta)}{\rho} \right) + \mu_0 HM(1 - \cos(\theta)) \right\} \rho d\rho. \end{aligned}$$

To minimize this energy density we need $\cos(\phi_0) = \pm 1$ depending on the sign of $\frac{D}{2} \left(\frac{d\theta}{d\rho} + \frac{\sin(\theta)\cos(\theta)}{\rho} \right)$. This is the case for $\phi_0 = 0$ or $\phi_0 = \pi$. Both are the configuration of a hedgehog skyrmion. The energy density can now be written as seen in ref. [6]

$$\begin{aligned} \epsilon[\theta(\rho)] = \frac{\mathbb{E}[\theta(\rho)]}{2\pi t} = \int \left\{ \frac{J}{2} \left(\left(\frac{d\theta}{d\rho} \right)^2 + \frac{\sin^2(\theta)}{\rho^2} \right) \right. \\ \left. + \frac{D}{2} \left(\frac{d\theta}{d\rho} + \frac{\sin(\theta)\cos(\theta)}{\rho} \right) + \mu_0 HM(1 - \cos(\theta)) \right\} \rho d\rho, \end{aligned} \quad (1.3)$$

which gives rise to the following Euler equation

$$J \left(\frac{d^2\theta}{d\rho^2} + \frac{1}{\rho} \frac{d\theta}{d\rho} - \frac{\sin(\theta)\cos(\theta)}{\rho^2} \right) + D \frac{\sin^2(\theta)}{\rho} - \mu_0 HM \sin(\theta) = 0. \quad (1.4)$$

Now substitute $\tilde{\rho} = \frac{D}{J}\rho$ into (1.4) and multiply with $\frac{J}{D^2}$ to get a dimensionless Euler equation

$$\frac{d^2\theta}{d\tilde{\rho}^2} + \frac{1}{\tilde{\rho}} \frac{d\theta}{d\tilde{\rho}} - \frac{\sin(\theta)\cos(\theta)}{\tilde{\rho}^2} + \frac{\sin^2(\theta)}{\tilde{\rho}} - \frac{h}{2} \sin(\theta) = 0, \quad (1.5)$$

with dimensionless constant $h = \frac{2\mu_0 JHM}{D^2}$, often in the order of 1, typically 0.72 [8]. One can numerically solve (1.5) with boundary conditions $\theta(0) = \pi$ and $\theta(\rho \rightarrow \infty) = 0$ (figure 1.1). We see that absence of an external magnetic field ($h = 0$) yields an 'infinitely large skyrmion' i.e. no skyrmion at all. A skyrmion seems to have a typical dimensionless diameter of 20, which translates to a typical diameter $20 \frac{J}{D}$. Note that in the continuous case as h gets very large, the skyrmion simply gets very small. A model with individual spins obviously has restrictions for the smallest skyrmion sizes.

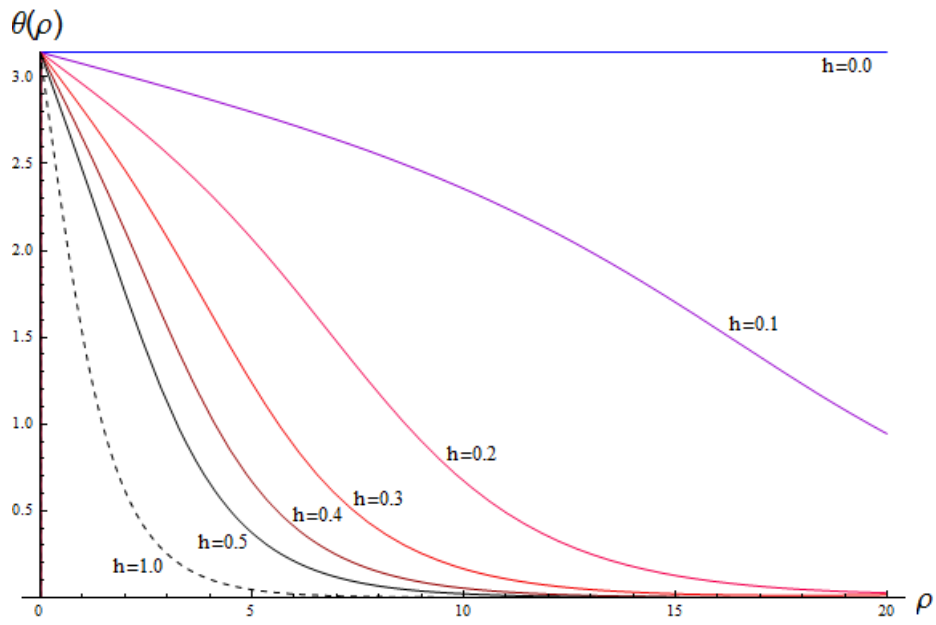


Figure 1.1: Solutions of (1.5) for different values of h .

Chapter 2

Diagonalization of the semi-classical spinwave Hamiltonian on a square lattice

In this chapter we define the Hamiltonian we use for our investigation and the techniques to diagonalize it. We show how the zero-point energies and spinwave modes can be found by means Holstein-Primakoff and Bogoliubov transformations. The Holstein-Primakoff transformation is shown entirely in this chapter, while most of the explicit algebra and motivation for the Bogoliubov transformation is located in the appendix.

We use the Hamiltonian from ref. [9] which contains the Heisenberg spin coupling, Dzyaloshinskii-Moriya interaction, an anisotropy term and a term for the external magnetic field

$$H = -\frac{1}{2} \sum_{i \neq j} J_{ij} \mathbf{S}_i \cdot \mathbf{S}_j + \frac{1}{2} \sum_{i \neq j} \mathbf{D}_{ij} \cdot (\mathbf{S}_i \times \mathbf{S}_j) + K \sum_i S_{iz}^2 - B \sum_i S_{iz}, \quad (2.1)$$

with $J_{ij} = J$ when i, j are direct neighbors (each site has two, three or four, depending on the symmetries of the system) and $J_{ij} = 0$ otherwise. Similarly $\mathbf{D}_{ij} = 0$ for all indirect neighbors, but the explicit form is a little more complicated for its direct neighbors, namely

$$\begin{aligned} \mathbf{D}_{ij} &= (0, D, 0) && \text{when } j \text{ is the neighbor to the left,} \\ \mathbf{D}_{ij} &= (0, -D, 0) && \text{when } j \text{ is the neighbor to the right,} \\ \mathbf{D}_{ij} &= (D, 0, 0) && \text{when } j \text{ is the neighbor straight above,} \\ \mathbf{D}_{ij} &= (-D, 0, 0) && \text{when } j \text{ is the neighbor straight below.} \end{aligned} \quad (2.2)$$

Notice $\mathbf{D}_{ji} = -\mathbf{D}_{ij}$, which is to counter the anti-commutivity of $(\mathbf{S}_i \times \mathbf{S}_j)$. The indices i, j refer simply to the spinvector at site i or j . If the lattice is $n \times m$, then 1 is in the bottom left corner (has the smallest (x,y)-coordinates) and mn is in the upper right corner. We count the cells in the positive x-direction on each row, such that the first row counts up to n , the second up to $2n$ and so on.

	\vdots	\vdots		\vdots
$y \uparrow$	$2n+1$	$2n+2$	\cdots	$3n$
	$n+1$	$n+2$	\cdots	$2n$
	1	2	\cdots	n
				$x \rightarrow$

Since spinwaves are described as small deviations of the spinvector \mathbf{S} from its groundstate, we can look at each spinvector \mathbf{S}_i in its own reference frame. In this local frame, the z -axis is parallel to $\mathbf{\Omega}_i$ the spin direction of the classical magnetic groundstate on site i . To accomplish this we rotate each spin \mathbf{S}_i with a unitary rotation matrix U_i [10] such that $\bar{\mathbf{S}}_i = U_i \mathbf{S}_i$. In cartesian coordinates we get

$$\mathbf{\Omega}_i = \begin{bmatrix} \sin(\theta_i) \cos(\psi_i) \\ \sin(\theta_i) \sin(\psi_i) \\ \cos(\theta_i) \end{bmatrix}, \quad U_i = \begin{bmatrix} \cos(\theta_i) \cos(\psi_i) & \cos(\theta_i) \sin(\psi_i) & -\sin(\theta_i) \\ -\sin(\psi_i) & \cos(\psi_i) & 0 \\ \sin(\theta_i) \cos(\psi_i) & \sin(\theta_i) \sin(\psi_i) & \cos(\theta_i) \end{bmatrix}.$$

We define also for future calculations

$$U_i U_j^{-1} = \begin{bmatrix} F_{ij}^{xx} & F_{ij}^{xy} & F_{ij}^{xz} \\ F_{ij}^{yx} & F_{ij}^{yy} & F_{ij}^{yz} \\ F_{ij}^{zx} & F_{ij}^{zy} & F_{ij}^{zz} \end{bmatrix}, \quad U_i^{-1} = \begin{bmatrix} G_i^{xx} & G_i^{xy} & G_i^{xz} \\ G_i^{yx} & G_i^{yy} & G_i^{yz} \\ G_i^{zx} & G_i^{zy} & G_i^{zz} \end{bmatrix}. \quad (2.3)$$

The Hamiltonian can now be written with local frame transformations

$$H = -\frac{1}{2} \sum_{i \neq j} J_{ij} \bar{\mathbf{S}}_i \cdot U_i U_j^{-1} \bar{\mathbf{S}}_j + \frac{1}{2} \sum_{i \neq j} D_{ij} \cdot ((U_i^{-1} \bar{\mathbf{S}}_i) \times (U_j^{-1} \bar{\mathbf{S}}_j)) \\ + K \sum_i (U_i^{-1} \bar{\mathbf{S}}_i)_z^2 - B \sum_i (U_i^{-1} \bar{\mathbf{S}}_i)_z. \quad (2.4)$$

Note that there is only one type of operator in this Hamiltonian [13]

$$\bar{\mathbf{S}}_i = \begin{bmatrix} \bar{S}_{ix} \\ \bar{S}_{iy} \\ \bar{S}_{iz} \end{bmatrix}, \quad \text{with} \quad \begin{aligned} [\bar{S}_{ix}, \bar{S}_{jy}] &= i \bar{S}_{iz} \delta_{ij}, \\ [\bar{S}_{iy}, \bar{S}_{iz}] &= i \bar{S}_{ix} \delta_{ij}, \\ [\bar{S}_{iz}, \bar{S}_{ix}] &= i \bar{S}_{iy} \delta_{ij}, \end{aligned}$$

where $[A, B] = AB - BA$ is the ordinary bosonic commutation relation. Since we look at small deviations from \mathbf{S}_i we introduce spin raising and lowering operators

$$\begin{aligned} \bar{S}_i^+ &= \bar{S}_{ix} + i \bar{S}_{iy}, & [\bar{S}_i^+, \bar{S}_j^-] &= 2 \bar{S}_{iz} \delta_{ij}, \\ \bar{S}_i^- &= \bar{S}_{ix} - i \bar{S}_{iy}, & [\bar{S}_{iz}, \bar{S}_j^+] &= \bar{S}_i^+ \delta_{ij}, \\ & & [\bar{S}_{iz}, \bar{S}_j^-] &= -\bar{S}_i^- \delta_{ij}. \end{aligned}$$

We now introduce operators a_i, a_i^\dagger that behave like boson creation and annihilation operators by applying a Holstein Primakoff (HP) transformation [13]

$$\bar{S}_{iz} = S_i - a_i^\dagger a_i, \quad (2.5)$$

$$\bar{S}_i^+ = \sqrt{2S_i - n_i} a_i, \quad (2.6)$$

$$\bar{S}_i^- = a_i^\dagger \sqrt{2S_i - n_i}, \quad (2.7)$$

with $n_i = a_i^\dagger a_i$ with $[a_i, a_j^\dagger] = \delta_{ij}$ and $[n_i, n_j] = 0$. Expanding these operators in powers of $1/\sqrt{S_i}$ we get

$$\bar{S}_i^+ = \sqrt{2S_i} \sqrt{1 - \frac{n_i}{2S_i}} a_i = \sqrt{2S_i} a_i - \frac{n_i a_i}{2\sqrt{2S_i}} + O(a^5), \quad (2.8)$$

$$\bar{S}_i^- = a_i^\dagger \sqrt{2S_i} \sqrt{1 - \frac{n_i}{2S_i}} = \sqrt{2S_i} a_i^\dagger - \frac{a_i^\dagger n_i}{2\sqrt{2S_i}} + O(a^5). \quad (2.9)$$

Note that together with $\bar{S}_{ix} = \frac{1}{2}(\bar{S}_i^+ + \bar{S}_i^-)$ and $\bar{S}_{iy} = \frac{1}{2i}(\bar{S}_i^+ - \bar{S}_i^-)$ the third order terms of equations (2.8) and (2.9) are only going to produce third order or higher terms in the Hamiltonian (2.4). When assuming that the spin fluctuations are small relative to the total spin i.e. $S_i \gg 1$, we can approximate the spin operators in equations (2.8) and (2.9) up to quadratic order. This way we only have non-interacting spinwaves, which is what we wanted to keep the model simple, so we simplify equations (2.6) and (2.7) as seen in ref. [10]

$$\bar{S}_{iz} = S_i - a_i^\dagger a_i, \quad (2.10)$$

$$\bar{S}_i^+ = \sqrt{2S_i} a_i, \quad (2.11)$$

$$\bar{S}_i^- = \sqrt{2S_i} a_i^\dagger, \quad (2.12)$$

$$\bar{S}_{ix} = \frac{1}{\sqrt{2}} \sqrt{S_i} (a_i + a_i^\dagger), \quad (2.13)$$

$$\bar{S}_{iy} = \frac{1}{i\sqrt{2}} \sqrt{S_i} (a_i - a_i^\dagger), \quad (2.14)$$

$$\bar{S}_{iz} = S_i - a_i^\dagger a_i. \quad (2.15)$$

With this result we can write H entirely in terms of operators a_i, a_i^\dagger , but first we combine (2.4) and (2.3) such that

$$\begin{aligned} H = & -\frac{1}{2} \sum_{i \neq j} J_{ij} F_{ij}^{\alpha\beta} \bar{S}_{i\alpha} \bar{S}_{j\beta} + \frac{1}{2} \sum_{i \neq j} D_{ij}^{\alpha\beta} G_{ij}^{\gamma\alpha\beta} \bar{S}_{i\alpha} \bar{S}_{j\beta} \\ & + K \sum_i G_i^{z\alpha} G_i^{z\beta} \bar{S}_{i\alpha} \bar{S}_{i\beta} - B \sum_i G_i^{z\alpha} \bar{S}_{i\alpha}. \end{aligned} \quad (2.16)$$

We used Einstein notation (Greek indices only) within each of the four summations and a reduced notation

$$\begin{aligned} G_{ij}^{x\alpha\beta} &= G_i^{y\alpha} G_j^{z\beta} - G_i^{z\alpha} G_j^{y\beta}, \\ G_{ij}^{y\alpha\beta} &= G_i^{z\alpha} G_j^{x\beta} - G_i^{x\alpha} G_j^{z\beta}, \\ G_{ij}^{z\alpha\beta} &= G_i^{x\alpha} G_j^{y\beta} - G_i^{y\alpha} G_j^{x\beta}, \end{aligned} \quad D_{ij} = \begin{bmatrix} D_{ij}^x \\ D_{ij}^y \\ D_{ij}^z \end{bmatrix}.$$

The idea is to replace all \bar{S}_i 's by a_i terms, using the relations on the first page of the appendix, and separating the Hamiltonian in a zero, first and second order part

$$H = H_0 + H_1 + H_2 + O(a^3). \quad (2.17)$$

The explicit forms of these three Hamiltonian parts can be found in the Appendix. H_0 contains the classical energy of the (semi-classical) groundstate. H_1 (see equation 4.5) is zero by definition [10], for if the Hamiltonian contains any first order terms, then the Hamiltonian actively raises or lowers (a_i or a_i^\dagger) the energy of the system. If this is the case, the system is clearly not in its lowest

energy configuration, which we assumed to be the case. H_2 contains the second order terms which produce the spin fluctuations. This is what causes the famous spinwaves and is called the spinwave Hamiltonian. Higher order terms contain the more complex effects like spinwave interactions. We will look only at terms up to quadratic order. Following the long calculation in the Appendix, we can write the Hamiltonian in a reduced elegant form

$$\begin{aligned}
H &= E_{cl} + H_{SW} \\
&= \sum_{i \neq j} c_{ij} + \sum_i b_i - \frac{1}{2} \sum_i \lambda_i \\
&\quad + \sum_{i \neq j} (t_{ij} a_i^\dagger a_j + t_{ij}^* a_i a_j^\dagger + \tau_{ij}^* a_i a_j + \tau_{ij} a_i^\dagger a_j^\dagger) \\
&\quad + \sum_i (m_i a_i^\dagger a_i + m_i^* a_i a_i^\dagger + \mu_i^* a_i a_i + \mu_i a_i^\dagger a_i^\dagger).
\end{aligned} \tag{2.18}$$

Let the lattice consist of N spins, then the last two summations can be rewritten into matrixform. Use (4.8) to define

$$\begin{aligned}
A_{ij} &= t_{ij}, & B_{ij} &= \tau_{ij}, & \forall i \neq j \\
A_{ii} &= m_i, & B_{ii} &= \mu_i, & \forall i
\end{aligned}$$

such that

$$H = E_{cl} + E_0 + (\mathbf{a}^\dagger \quad \mathbf{a}) \mathbf{H} \begin{pmatrix} \mathbf{a} \\ \mathbf{a}^\dagger \end{pmatrix}, \tag{2.19}$$

$$\begin{aligned}
\text{with } (\mathbf{a}^\dagger \quad \mathbf{a}) &= (a_1^\dagger \quad \dots \quad a_N^\dagger \quad a_1 \quad \dots \quad a_N), \\
\mathbf{H} &= \begin{pmatrix} \mathbf{A} & \mathbf{B} \\ \mathbf{B}^* & \mathbf{A}^* \end{pmatrix}.
\end{aligned}$$

This matrix should be positive-definite, for negative eigenvalues would suggest modes/magnons with negative energy, which are physically excluded. We can now diagonalize it using a Bogoliubov approach [15], which means we can find a para-unitary $2N \times 2N$ -matrix $\mathbf{\Gamma}^{-1}$ (see Appendix) such that

$$\mathbf{H}_{diag} \equiv (\mathbf{\Gamma}^\dagger)^{-1} \mathbf{H} \mathbf{\Gamma}^{-1} = \frac{1}{2} \hbar \text{diag}(\omega_1, \omega_2, \dots, \omega_N, \omega_1, \omega_2, \dots, \omega_N), \tag{2.20}$$

with all ω_i positive. We deviate from the usual diagonalization of the form $\mathbf{\Gamma} \mathbf{H} \mathbf{\Gamma}^{-1}$ because we look for a new basis of operators $\gamma_i, \gamma_i^\dagger$, defined by

$$\begin{pmatrix} \gamma \\ \gamma^\dagger \end{pmatrix} = \mathbf{\Gamma} \begin{pmatrix} \mathbf{a} \\ \mathbf{a}^\dagger \end{pmatrix}, \quad \text{thus } (\gamma^\dagger \quad \gamma) = (\mathbf{a}^\dagger \quad \mathbf{a}) \mathbf{\Gamma}^\dagger, \tag{2.21}$$

such that

$$\begin{aligned}
(\mathbf{a}^\dagger \quad \mathbf{a}) \mathbf{H} \begin{pmatrix} \mathbf{a} \\ \mathbf{a}^\dagger \end{pmatrix} &= (\mathbf{a}^\dagger \quad \mathbf{a}) \mathbf{\Gamma}^\dagger (\mathbf{\Gamma}^\dagger)^{-1} \mathbf{H} \mathbf{\Gamma}^{-1} \mathbf{\Gamma} \begin{pmatrix} \mathbf{a} \\ \mathbf{a}^\dagger \end{pmatrix} \\
&= (\gamma^\dagger \quad \gamma) \mathbf{H}_{diag} \begin{pmatrix} \gamma \\ \gamma^\dagger \end{pmatrix}.
\end{aligned}$$

Para-unitarity of $\mathbf{\Gamma}$ ensures the new $\gamma_i, \gamma_i^\dagger$ are also bosonic creation/annihilation operators with $[\gamma_i, \gamma_j^\dagger] = \delta_{ij}$. Write the diagonalized spinwave Hamiltonian as a

summation and use the commutation relation to get the elegant final form

$$\begin{aligned}
H_{SW} &= E_{cl} + E_0 + \sum_{i=1}^N \frac{1}{2} \hbar \omega_i \gamma_i^\dagger \gamma_i + \sum_{i=1}^N \frac{1}{2} \hbar \omega_i \gamma_i \gamma_i^\dagger \\
&= E_{cl} + E_0 + \sum_{i=1}^N \hbar \omega_i \left(\gamma_i^\dagger \gamma_i + \frac{1}{2} \right).
\end{aligned} \tag{2.22}$$

The constant term or groundstate energy of the Hamiltonian is thus

$$E_{GS} = E_{cl} + E_0 + \sum_{i=1}^N \frac{1}{2} \hbar \omega_i. \tag{2.23}$$

This shift in the energy of groundstate state caused by quantum fluctuations is known the as zero-point energy [11]

$$E_{ZP} \equiv E_{GS} - E_{cl} = -\frac{1}{2} \sum_i \lambda_i + \frac{1}{2} \sum_i \hbar \omega_i = \frac{1}{2} \sum_i (\hbar \omega_i - \lambda_i). \tag{2.24}$$

Chapter 3

Calculations and results

In this chapter we will use the theory of the previous chapter to calculate the spectrum of the spinwaves and zero-point energy of single-spin wires, and the zero-point energy of skyrmion configurations on 16 spin wide strips. Throughout this chapter, the spins are of unit length $S_i = 1$, the lattice constant $a = 1$ and the anisotropy constant K is set to zero. We now only have three constants left, so we can scale out one of them: we set $J = 1$ for convenience, and control the strengths of the magnetic field and Dzyaloshinskii-Moriya interactions with the pitch length $p \in [5.15, 12.71]$ defined in equation (3.1). The pitch length p is derived from the observation that if $\mathbf{S}_i \cdot \mathbf{S}_j = \cos(\varphi)$, then $\mathbf{S}_i \times \mathbf{S}_j = \sin(\varphi)$ for some φ . The Hamiltonian (3.4) minimizes approximately when

$$\frac{D}{J} = \frac{\sin(\varphi)}{\cos(\varphi)} = \tan(\varphi)$$

and the skyrmion is about $p = \frac{2\pi}{\varphi}$ spins across. The simulations in ref. [9] are done under the restrictions

$$D = J \tan\left(\frac{2\pi}{p}\right), \quad (3.1)$$

$$B = \frac{D^2}{2J}. \quad (3.2)$$

In comparison with the classical formulation of chapter 1, the normalization $S_i = 1$ is equivalent to $M = 1$, and we have $B = \mu_0 H$. Equation (3.2) is equivalent to $h = 1.0$ in chapter 1, and the dashed line in figure 1.1 indicates that our skyrmions should thus be about 10 in dimensionless diameter, which translates with (3.2) to skyrmions $10/\tan(\frac{2\pi}{p})$ in diameter. Note that we have a lattice constant of unit length and that $1/\tan(\frac{2\pi}{p})$ grows almost linearly from 0.366 to 1.855 as $p \in [5, 12.71]$, so the skyrmions are roughly 4 to 18 spins in diameter according to the classical analysis. Looking at the configurations found in ref. [9] we find that the pitch length approximation is more accurate than the classical estimate.

3.1 (Anti-)ferromagnetic Heisenberg model

To show that the theory of chapter 2 actually works, we calculate the spin-wave spectrum in two very simple cases: one-dimensional ferromagnetic and

anti-ferromagnetic periodic chains of 100 spins. Setting $D = 0$, $B = 0$ so that (2.1) reduces to the Heisenberg model

$$H = -\frac{1}{2}J \sum_{i \neq j} \mathbf{S}_i \cdot \mathbf{S}_j. \quad (3.3)$$

From (4.3) and (4.10), one can easily see that $E_{cl} = -100$ and $E_0 = -100$. In the classical limit we expect the spectrum to be $\hbar\omega_k = 2JS(1 - \cos(ka))$ [16], where a the lattice constant and k the wave number. And indeed our calculations produce this sinusoidal shape, see figure 3.1. Note that all values appear twice except for mode #1 and mode #100. This is because each mode is associated to some wave number k , but a spinwave going in the opposite direction (wavenumber $-k$) has the same energy (due to symmetries of this model), while mode #1 has $k = 0$ and is thus singular. Because this system has 100 spins, there can only be 100 spinwave modes, so mode #100 is also singular simply because there is no room for one more. One can see directly from figure (3.1) that the total energy of this spectrum is 200, thus their contribution to the groundstate energy (2.23) is 100, resulting in $E_{ZP} = 0$ as already mentioned in ref. [12].

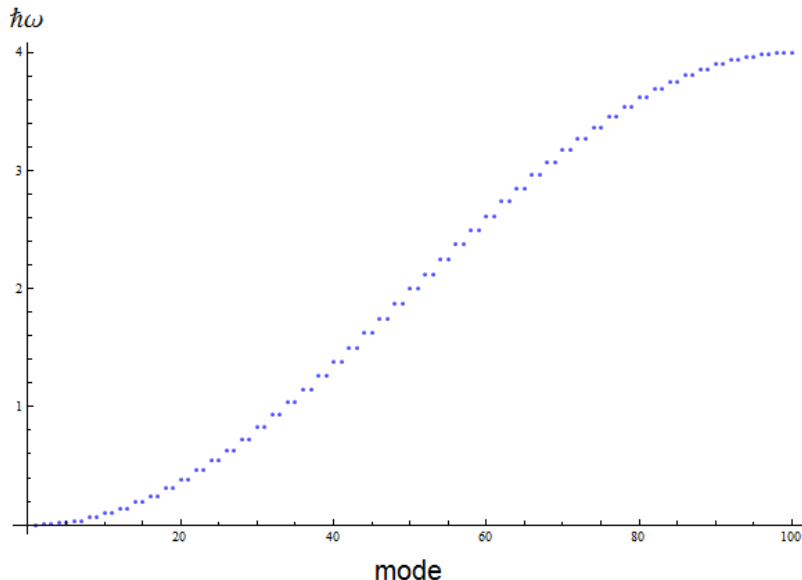


Figure 3.1: Spectrum of 100 spin periodic ferromagnetic wire, with Heisenberg model $S_i = 1$, $J = 1$.

For the anti-ferromagnetic case ($J = -1$) we once again have $E_{cl} = -100$ and $E_0 = -100$, but a different spinwave spectrum (see figure 3.2) of the form $\hbar\omega_k = 2JS|\sin(ka)|$ as predicted in ref. [14]. Note that this time each energy appears four times except the lowest and highest energy modes. This quadruple effect can best be understood as two eigenmodes competing. One consists primarily of vibrations on the spins pointing up and only minor vibrations in the spins pointing down, the other does the exact opposite. Because of the symmetries of this model, they have the exact same energy and each appears twice because of k and $-k$. This results in two zero energy modes, quadruple modes up to the highest energy mode, which is only double because there can again be only 100 modes. Note that the total energy of these modes is less than 200, resulting in $E_{ZP} = -36.36$. We thus see that the quantum fluctuations lower the groundstate energy of the anti-ferromagnetic wire.

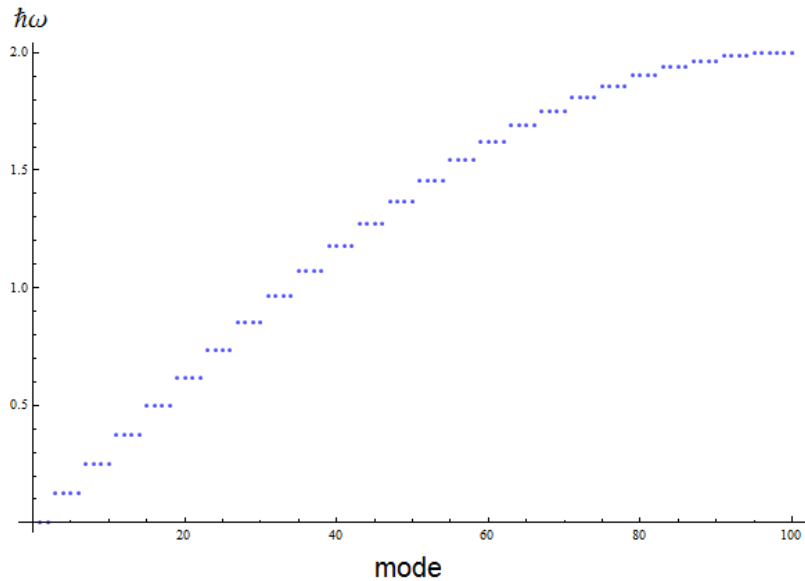


Figure 3.2: Spectrum of 100 spin periodic anti-ferromagnetic wire, with Heisenberg model $S_i = 1$, $J = -1$.

3.2 Zero-point energy of skyrmion configurations

Now that we have verified that our calculations produce the right results for simple systems, we turn to the more complex skyrmion configurations. We investigate spin configurations on a 16×16 lattice that is periodic in the x-direction and has open boundaries along the sides, resulting in a two-dimensional strip that is 16 spins wide. We use the Hamiltonian (2.1) with $K = 0$,

$$H = -\frac{1}{2} \sum_{i \neq j} J_{ij} \mathbf{S}_i \cdot \mathbf{S}_j + \frac{1}{2} \sum_{i \neq j} D_{ij} \cdot (\mathbf{S}_i \times \mathbf{S}_j) - B \sum_i S_{iz}. \quad (3.4)$$

R. Keesman *et al.* have found classical groundstate configurations containing zero, one, two or four hedgehog skyrmions for hundreds of pitch lengths $p \in [5, 21.5]$ using Monte-Carlo simulations [9]. Two p values, $p = 9.336$ and $p = 7.284$, are of particular interest: at $p = 9.336$ the configurations for one skyrmion and two skyrmions yield the same classical energy and at $p = 7.284$ the classical energy of configurations with two and four skyrmions are equal, suggesting transitions of some kind. The idea is to see if the zero-point energies of classically degenerate configurations are also equal, but this turns out not to be the case.

Table 3.1: E_{ZP} at the 'phase transitions'.

p	Number of skyrmions		
	one	two	four
7.284		-1.869	-2.967
9.336	-0.702	-0.982	

Looking at the results in table 3.1, we expect the 'phase transitions' to shift, or disappear entirely, so we calculate the zero-point energies for more p values to get the bigger picture. To save time, we select only the p -values for which all four types of configuration were found, this reduces the data to a more manageable 422 p -values ranging from 5.15 to 12.71. Note that we only need to know the para-eigenvalues (see Appendix) to calculate E_{ZP} (2.24) so we exclude the calculation of the actual modes. Importing Keesman's data and calculating the zero-point energies produces figure 3.3.

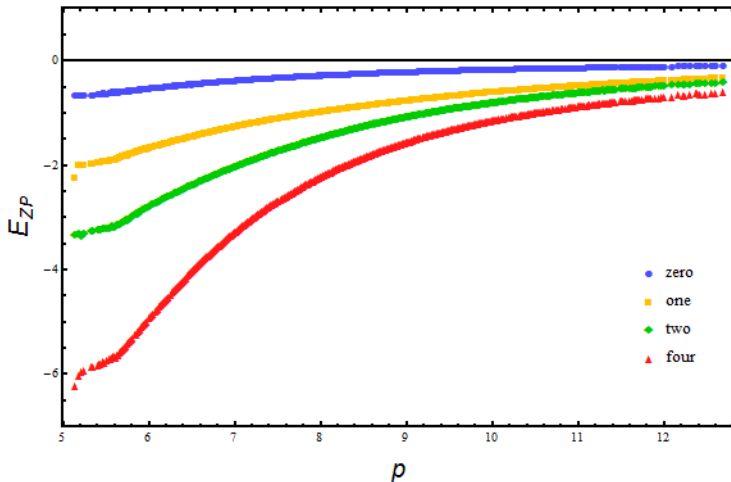


Figure 3.3: Zero-point energies for configurations with zero, one, two or four skyrmions plotted against p .

Note that all spin configurations have negative zero-point energy, even those without a skyrmion. The amount the groundstate energy gets lowered increases as p decreases or the number of skyrmions increases, so quantum fluctuations seem to prefer rapidly changing spins.

Let E_{GS}^0 be the groundstate energy of the configuration without a skyrmion and define

$$\Delta E = E_{GS} - E_{GS}^0. \quad (3.5)$$

By comparing the groundstate energies in both the classical ($E_{GS} = E_{cl}$) and quantum mechanical ($E_{GS} = E_{cl} + E_{ZP}$) case, we get figure 3.4. We now clearly see that the 'phase transitions' shift, and the domain in which skyrmions occur increases slightly as predicted in ref. [12].

Table 3.2: p value of 'phase transitions'.

Phase Transition	Classical	Quantum Mechanical
1→2	9.336	9.478
2→4	7.284	7.505

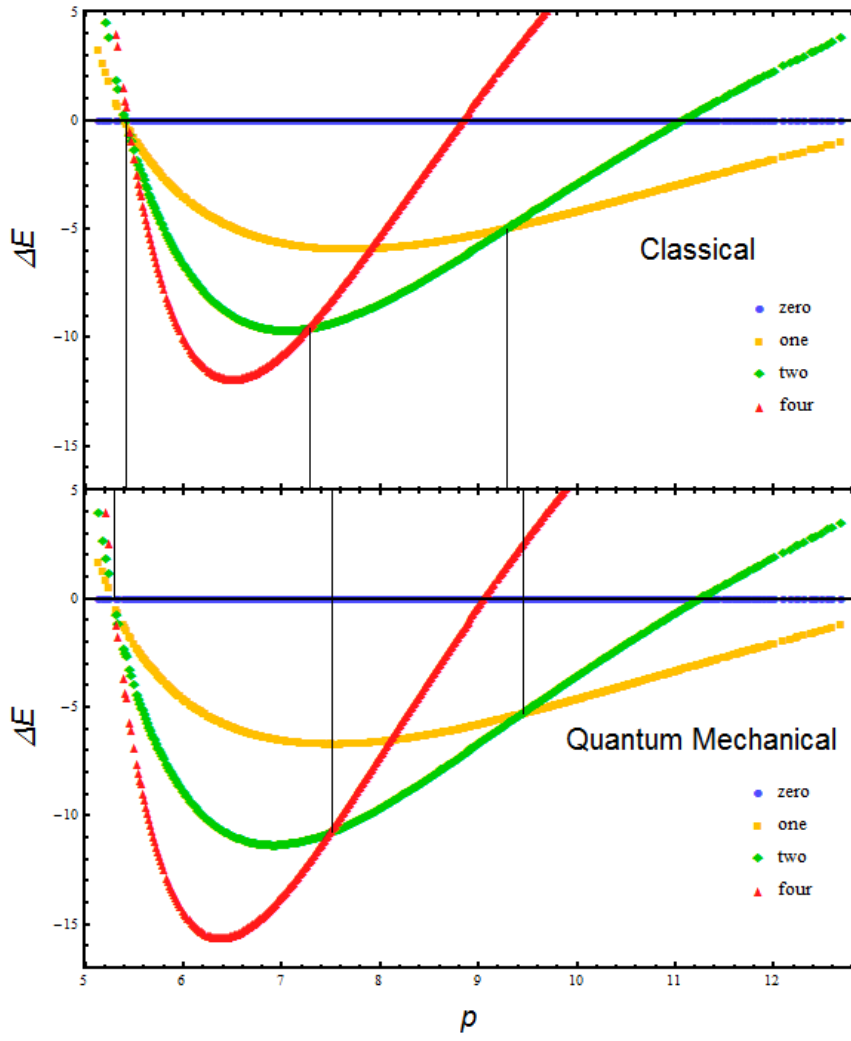


Figure 3.4: Groundstate energy differences ΔE (equation 3.5) for configurations with zero, one, two or four skyrmions plotted against p .

Chapter 4

Conclusion and suggestions

4.1 Conclusion

We used a Holstein-Primakoff transformation for the spin operators and approximated it up to quadratic order under the assumption $S \gg 1$ and that the spinwaves would only consist of small vibrations. From the spin lowering and raising operators a_i, a_i^\dagger we derived new bosonic creation and annihilation operators $\gamma_i, \gamma_i^\dagger$ through Bogoliubov diagonalization of the Hamiltonian. The new operators are linear combinations of a_i, a_i^\dagger and describe the coherent spinwave states as harmonic oscillators. These contribute to the groundstate energy and make it possible to calculate the zero-point energy of the system. We applied this technique to actual classical groundstate configurations and showed that the effects of the zero-point energies are relevant as they promote skyrmions by changing the domains where they occur and shift the parameter values at which degenerate states could be found, so much in fact that this effect could be measured.

4.2 Suggestions for future research

The classical configurations are not necessarily the correct groundstates as the zero-point energies are not taken into account. The quantum fluctuations influence the average magnetisation, which influences the spin configuration. Future research can involve finding the spin configurations that are the groundstates of the quantum mechanical system. Also the influence of spinwave-spinwave interactions could be investigated, as we ignored any higher order terms that describe such interactions.

The calculations we did can also be perfected numerically as we encountered some issues:

- 1) Eigenvalues near or equal to zero have eigenvectors, that produce large numbers when performing the Gram-Schmidt procedure.
- 2) The large numbers described in 1) are physically unrealistic, directly solving (4.14) with constraint (4.16) might find the right modes, we set those unreal modes to zero.
- 3) One might encounter configurations that do not have a positive-definite matrix \mathbf{H} , causing modes with a negative $\langle(\mathbf{u}_i, \mathbf{v}_i), (\mathbf{u}_i, \mathbf{v}_i)\rangle$ see equation (4.16). Whether any such configuration is non-physical and can be ignored, or how to deal with them is not known to us at this point.

Appendix

A list of operator multiplications used to express the Hamiltonian (2.16) in terms of a_i, a_i^\dagger :

$$\begin{aligned}
\bar{S}_{ix}\bar{S}_{ix} &= \frac{1}{2}S_i(a_i a_i + a_i a_i^\dagger + a_i^\dagger a_i + a_i^\dagger a_i^\dagger) \\
\bar{S}_{iy}\bar{S}_{iy} &= \frac{1}{2}S_i(-a_i a_i + a_i a_i^\dagger + a_i^\dagger a_i - a_i^\dagger a_i^\dagger) \\
\bar{S}_{iz}\bar{S}_{iz} &= S_i^2 - 2S_i a_i^\dagger a_i \\
\bar{S}_{ix}\bar{S}_{iy} &= \frac{1}{2i}S_i(a_i a_i - 1 - a_i^\dagger a_i^\dagger) \\
\bar{S}_{iy}\bar{S}_{ix} &= \frac{1}{2i}S_i(a_i a_i + 1 - a_i^\dagger a_i^\dagger) \\
\bar{S}_{ix}\bar{S}_{iz} &= \frac{1}{\sqrt{2}}\sqrt{S_i^3}(a_i + a_i^\dagger) \\
\bar{S}_{iz}\bar{S}_{ix} &= \frac{1}{\sqrt{2}}\sqrt{S_i^3}(a_i + a_i^\dagger) \\
\bar{S}_{iy}\bar{S}_{iz} &= \frac{1}{i\sqrt{2}}\sqrt{S_i^3}(a_i - a_i^\dagger) \\
\bar{S}_{iz}\bar{S}_{iy} &= \frac{1}{i\sqrt{2}}\sqrt{S_i^3}(a_i - a_i^\dagger) \\
\bar{S}_{ix}\bar{S}_{jx} &= \frac{1}{2}\sqrt{S_i S_j}(a_i a_j + a_i a_j^\dagger + a_i^\dagger a_j + a_i^\dagger a_j^\dagger) \\
\bar{S}_{iy}\bar{S}_{jy} &= \frac{1}{2}\sqrt{S_i S_j}(-a_i a_j + a_i a_j^\dagger + a_i^\dagger a_j - a_i^\dagger a_j^\dagger) \\
\bar{S}_{iz}\bar{S}_{jz} &= S_i S_j - S_j a_i^\dagger a_i - S_i a_j^\dagger a_j \\
\bar{S}_{ix}\bar{S}_{jy} &= \frac{1}{2i}\sqrt{S_i S_j}(a_i a_j - a_i a_j^\dagger + a_i^\dagger a_j - a_i^\dagger a_j^\dagger) \\
\bar{S}_{iy}\bar{S}_{jx} &= \frac{1}{2i}\sqrt{S_i S_j}(a_i a_j + a_i a_j^\dagger - a_i^\dagger a_j - a_i^\dagger a_j^\dagger) \\
\bar{S}_{ix}\bar{S}_{jz} &= \frac{1}{\sqrt{2}}\sqrt{S_i S_j}(a_i + a_i^\dagger) \\
\bar{S}_{iz}\bar{S}_{jx} &= \frac{1}{\sqrt{2}}\sqrt{S_j S_i}(a_j + a_j^\dagger) \\
\bar{S}_{iy}\bar{S}_{jz} &= \frac{1}{i\sqrt{2}}\sqrt{S_i S_j}(a_i - a_i^\dagger) \\
\bar{S}_{iz}\bar{S}_{jy} &= \frac{1}{i\sqrt{2}}\sqrt{S_j S_i}(a_j - a_j^\dagger).
\end{aligned}$$

Simplification of the Hamiltonian

In this section of the appendix, we simplify the constant, first order and second order part of (2.16) after putting the relations from the previous page directly into it. We start with the resulting constant term

$$\begin{aligned}
H_0 = & -\frac{1}{2} \sum_{i \neq j} J_{ij} F_{ij}^{zz} S_i S_j + \frac{1}{2} \sum_{i \neq j} D_{\gamma}^{ij} G_{ij}^{\gamma zz} S_i S_j \\
& + K \sum_i (G_i^{zz} S_i)^2 - B \sum_i G_i^{zz} S_i,
\end{aligned} \tag{4.1}$$

which is also known as the classical energy, for it has no contributions from any commutation relations, just the classical spin configuration. Define

$$\begin{aligned}
c_{ij} = & \frac{1}{2} (D_{\gamma}^{ij} G_{ij}^{\gamma zz} - J_{ij} F_{ij}^{zz}) S_i S_j, \\
b_i = & K (G_i^{zz} S_i)^2 - B G_i^{zz} S_i,
\end{aligned} \tag{4.2}$$

such that

$$E_{cl} \equiv H_0 = \sum_{i \neq j} c_{ij} + \sum_i b_i. \tag{4.3}$$

The first order or linear terms are

$$\begin{aligned}
H_1 = & -\frac{1}{2} \sum_{i \neq j} J_{ij} \frac{1}{\sqrt{2}} \left(\sqrt{S_i} S_j \left((F_{ij}^{xz} - iF_{ij}^{yz}) a_i + (F_{ij}^{zx} + iF_{ij}^{zy}) a_i^{\dagger} \right) \right. \\
& \left. + \sqrt{S_j} S_i \left((F_{ij}^{zx} - iF_{ij}^{zy}) a_j + (F_{ij}^{xz} + iF_{ij}^{yz}) a_j^{\dagger} \right) \right) \\
& + \frac{1}{2} \sum_{i \neq j} D_{\gamma}^{ij} \frac{1}{\sqrt{2}} \left(\sqrt{S_i} S_j \left((G_{ij}^{\gamma xz} - iG_{ij}^{\gamma yz}) a_i + (G_{ij}^{\gamma xz} + iG_{ij}^{\gamma yz}) a_i^{\dagger} \right) \right. \\
& \left. + \sqrt{S_j} S_i \left((G_{ij}^{\gamma zx} - iG_{ij}^{\gamma zy}) a_j + (G_{ij}^{\gamma zx} + iG_{ij}^{\gamma zy}) a_j^{\dagger} \right) \right) \\
& + K \sum_i \frac{1}{\sqrt{2}} \sqrt{S_i^3} \left((G_i^{zx} G_i^{zz} + G_i^{zz} G_i^{zx} - iG_i^{zy} G_i^{zz} - iG_i^{zz} G_i^{zy}) a_i \right. \\
& \left. + (G_i^{zx} G_i^{zz} + G_i^{zz} G_i^{zx} + iG_i^{zy} G_i^{zz} + iG_i^{zz} G_i^{zy}) a_i^{\dagger} \right) \\
& - B \sum_i \frac{1}{\sqrt{2}} \sqrt{S_i} \left((G_i^{zx} - iG_i^{zy}) a_i + (G_i^{zx} + iG_i^{zy}) a_i^{\dagger} \right).
\end{aligned}$$

Use $J_{ij} = J_{ji}$, $D_{ij} = -D_{ji}$ and the symmetry of $\sum_{i \neq j}$ such that

$$\begin{aligned}
H_1 = & -\frac{1}{2} \sum_{i \neq j} J_{ij} \frac{1}{\sqrt{2}} \sqrt{S_i S_j} \left((F_{ij}^{xz} + F_{ji}^{zx} - iF_{ij}^{yz} - iF_{ji}^{zy}) a_i \right. \\
& \left. + (F_{ij}^{xz} + F_{ji}^{zx} + iF_{ij}^{yz} + iF_{ji}^{zy}) a_i^\dagger \right) \\
& + \frac{1}{2} \sum_{i \neq j} D_{ij} \frac{1}{\sqrt{2}} \left(\sqrt{S_i S_j} \left((G_{ij}^{\gamma xz} - G_{ji}^{\gamma zx} - iG_{ij}^{\gamma yz} + iG_{ji}^{\gamma zy}) a_i \right. \right. \\
& \left. \left. + (G_{ij}^{\gamma xz} - G_{ji}^{\gamma zx} + iG_{ij}^{\gamma yz} - iG_{ji}^{\gamma zy}) a_i^\dagger \right) \right) \\
& + K \sum_i \frac{1}{\sqrt{2}} \sqrt{S_i^3} \left((G_i^{zx} G_i^{zz} + G_i^{zz} G_i^{zx} - iG_i^{zy} G_i^{zz} - iG_i^{zz} G_i^{zy}) a_i \right. \\
& \left. + (G_i^{zx} G_i^{zz} + G_i^{zz} G_i^{zx} + iG_i^{zy} G_i^{zz} + iG_i^{zz} G_i^{zy}) a_i^\dagger \right) \\
& - B \sum_i \frac{1}{\sqrt{2}} \sqrt{S_i} \left((G_i^{zx} - iG_i^{zy}) a_i + (G_i^{zx} + iG_i^{zy}) a_i^\dagger \right).
\end{aligned}$$

Note that $G_i^{zy} = 0$ and using the symmetries $G_{ij}^{\alpha\beta} = -G_{ji}^{\beta\alpha}$, $F_{ij}^{\alpha\beta} = F_{ji}^{\beta\alpha}$ we can further simplify this expression to

$$\begin{aligned}
H_1 = & -\sum_{i \neq j} J_{ij} \frac{1}{\sqrt{2}} \sqrt{S_i S_j} \left((F_{ij}^{xz} - iF_{ij}^{yz}) a_i + (F_{ij}^{xz} + iF_{ij}^{yz}) a_i^\dagger \right) \\
& + \sum_{i \neq j} D_{ij} \frac{1}{\sqrt{2}} \left(\sqrt{S_i S_j} \left((G_{ij}^{\gamma xz} - iG_{ij}^{\gamma yz}) a_i + (G_{ij}^{\gamma xz} + iG_{ij}^{\gamma yz}) a_i^\dagger \right) \right) \\
& + K \sum_i \frac{1}{\sqrt{2}} \sqrt{S_i^3} \left(G_i^{zx} G_i^{zz} a_i + G_i^{zx} G_i^{zz} a_i^\dagger \right) \\
& - B \sum_i \frac{1}{\sqrt{2}} \sqrt{S_i} \left(G_i^{zx} a_i + G_i^{zx} a_i^\dagger \right).
\end{aligned}$$

Define

$$\begin{aligned}
\kappa_i = & \sum_{\substack{j=1 \\ j \neq i}}^n \frac{1}{\sqrt{2}} \sqrt{S_i S_j} \left(D_{ij} (G_{ij}^{\gamma xz} - iG_{ij}^{\gamma yz}) - J_{ij} (F_{ij}^{xz} - iF_{ij}^{yz}) \right) \\
& + K \frac{1}{\sqrt{2}} \sqrt{S_i^3} G_i^{zx} G_i^{zz} - B \frac{1}{\sqrt{2}} \sqrt{S_i} G_i^{zx},
\end{aligned} \tag{4.4}$$

then the final form is

$$\begin{aligned}
H_1 = & \sum_i (\kappa_i a_i + \kappa_i^* a_i^\dagger) \\
= & \sum_i \kappa_i a_i + \text{H.c.}
\end{aligned} \tag{4.5}$$

H.c. denotes the Hermitian conjugate of the previous terms.

We now collect all quadratic terms into one equation

$$\begin{aligned}
H_2 = & -\frac{1}{2} \sum_{i \neq j} J_{ij} \left\{ \frac{1}{2} \sqrt{S_i S_j} \left((F_{ij}^{xx} - F_{ij}^{yy} - iF_{ij}^{xy} - iF_{ij}^{yx}) a_i a_j \right. \right. \\
& + (F_{ij}^{xx} + F_{ij}^{yy} + iF_{ij}^{xy} - iF_{ij}^{yx}) a_i a_j^\dagger \\
& + (F_{ij}^{xx} + F_{ij}^{yy} - iF_{ij}^{xy} + iF_{ij}^{yx}) a_i^\dagger a_j \\
& \left. \left. + (F_{ij}^{xx} - F_{ij}^{yy} + iF_{ij}^{xy} + iF_{ij}^{yx}) a_i^\dagger a_j^\dagger \right) \right. \\
& \left. - S_j F_{ij}^{zz} a_i^\dagger a_i - S_i F_{ij}^{zz} a_j^\dagger a_j \right\} \\
& + \frac{1}{2} \sum_{i \neq j} D_\gamma^{ij} \left\{ \frac{1}{2} \sqrt{S_i S_j} \left((G_{ij}^{\gamma xx} - G_{ij}^{\gamma yy} - iG_{ij}^{\gamma xy} - iG_{ij}^{\gamma yx}) a_i a_j \right. \right. \\
& + (G_{ij}^{\gamma xx} + G_{ij}^{\gamma yy} + iG_{ij}^{\gamma xy} - iG_{ij}^{\gamma yx}) a_i a_j^\dagger \\
& + (G_{ij}^{\gamma xx} + G_{ij}^{\gamma yy} - iG_{ij}^{\gamma xy} + iG_{ij}^{\gamma yx}) a_i^\dagger a_j \\
& \left. \left. + (G_{ij}^{\gamma xx} - G_{ij}^{\gamma yy} + iG_{ij}^{\gamma xy} + iG_{ij}^{\gamma yx}) a_i^\dagger a_j^\dagger \right) \right. \\
& \left. - S_j G_{ij}^{\gamma zz} a_i^\dagger a_i - S_i G_{ij}^{\gamma zz} a_j^\dagger a_j \right\} \\
& + K \sum_i \frac{1}{2} S_i \left((G_i^{zx} G_i^{zx} - G_i^{zy} G_i^{zy} - iG_i^{zx} G_i^{zy} - iG_i^{zy} G_i^{zx}) a_i a_i \right. \\
& + (G_i^{zx} G_i^{zx} + G_i^{zy} G_i^{zy}) a_i a_i^\dagger \\
& + (G_i^{zx} G_i^{zx} + G_i^{zy} G_i^{zy} - 4G_i^{zz} G_i^{zz}) a_i^\dagger a_i \\
& \left. + (G_i^{zx} G_i^{zx} - G_i^{zy} G_i^{zy} + iG_i^{zx} G_i^{zy} + iG_i^{zy} G_i^{zx}) a_i^\dagger a_i^\dagger \right) \\
& - B \sum_i \left(-G_i^{zz} a_i^\dagger a_i \right).
\end{aligned}$$

Note that

$$\begin{aligned}
\frac{1}{2} \sum_{i \neq j} J_{ij} (S_j F_{ij}^{zz} a_i^\dagger a_i + S_i F_{ij}^{zz} a_j^\dagger a_j) &= \frac{1}{2} \sum_i \sum_k (J_{ik} S_k F_{ik}^{zz} + J_{ki} S_k F_{ki}^{zz}) a_i^\dagger a_i \\
&= \frac{1}{2} \sum_i \sum_k J_{ik} S_k (F_{ik}^{zz} + F_{ki}^{zz}) a_i^\dagger a_i \\
&= \sum_i \sum_k J_{ik} S_k F_{ik}^{zz} a_i^\dagger a_i, \\
-\frac{1}{2} \sum_{i \neq j} D_\gamma^{ij} (S_j G_{ij}^{\gamma zz} a_i^\dagger a_i + S_i G_{ij}^{\gamma zz} a_j^\dagger a_j) &= -\frac{1}{2} \sum_i \sum_k (D_\gamma^{ik} S_k G_{ik}^{\gamma zz} + D_\gamma^{ki} S_k G_{ki}^{\gamma zz}) a_i^\dagger a_i \\
&= -\frac{1}{2} \sum_i \sum_k D_\gamma^{ik} S_k (G_{ik}^{\gamma zz} - G_{ki}^{\gamma zz}) a_i^\dagger a_i \\
&= -\sum_i \sum_k D_\gamma^{ik} S_k G_{ik}^{\gamma zz} a_i^\dagger a_i,
\end{aligned}$$

where k takes the integer values of the direct neighbors of i . This way we move those terms from $\sum_{i \neq j}$ to \sum_i . Define

$$\lambda_i = \left(\sum_k J_{ik} S_k F_{ik}^{zz} \right) - \left(\sum_k D_\gamma^{ik} S_k G_{ik}^{\gamma zz} \right) - 2K G_i^{zz} G_i^{zz} + B G_i^{zz}, \quad (4.6)$$

then the second order part of the Hamiltonian takes a more elegant form

$$\begin{aligned}
H_2 = & -\frac{1}{2} \sum_{i \neq j} J_{ij} \frac{1}{2} \sqrt{S_i S_j} \left((F_{ij}^{xx} - F_{ij}^{yy} - iF_{ij}^{xy} - iF_{ij}^{yx}) a_i a_j \right. \\
& + (F_{ij}^{xx} + F_{ij}^{yy} + iF_{ij}^{xy} - iF_{ij}^{yx}) a_i a_j^\dagger \\
& + (F_{ij}^{xx} + F_{ij}^{yy} - iF_{ij}^{xy} + iF_{ij}^{yx}) a_i^\dagger a_j \\
& \left. + (F_{ij}^{xx} - F_{ij}^{yy} + iF_{ij}^{xy} + iF_{ij}^{yx}) a_i^\dagger a_j^\dagger \right) \\
& + \frac{1}{2} \sum_{i \neq j} D_\gamma^{ij} \frac{1}{2} \sqrt{S_i S_j} \left((G_{ij}^{\gamma xx} - G_{ij}^{\gamma yy} - iG_{ij}^{\gamma xy} - iG_{ij}^{\gamma yx}) a_i a_j \right. \\
& + (G_{ij}^{\gamma xx} + G_{ij}^{\gamma yy} + iG_{ij}^{\gamma xy} - iG_{ij}^{\gamma yx}) a_i a_j^\dagger \\
& + (G_{ij}^{\gamma xx} + G_{ij}^{\gamma yy} - iG_{ij}^{\gamma xy} + iG_{ij}^{\gamma yx}) a_i^\dagger a_j \\
& \left. + (G_{ij}^{\gamma xx} - G_{ij}^{\gamma yy} + iG_{ij}^{\gamma xy} + iG_{ij}^{\gamma yx}) a_i^\dagger a_j^\dagger \right) \\
& + K \sum_i \frac{1}{2} S_i \left((G_i^{zx} G_i^{zx} - G_i^{zy} G_i^{zy} - iG_i^{zx} G_i^{zy} - iG_i^{zy} G_i^{zx}) a_i a_i \right. \\
& + (G_i^{zx} G_i^{zx} + G_i^{zy} G_i^{zy}) a_i a_i^\dagger \\
& + (G_i^{zx} G_i^{zx} + G_i^{zy} G_i^{zy}) a_i^\dagger a_i \\
& \left. + (G_i^{zx} G_i^{zx} - G_i^{zy} G_i^{zy} + iG_i^{zx} G_i^{zy} + iG_i^{zy} G_i^{zx}) a_i^\dagger a_i^\dagger \right) \\
& + \sum_i \lambda_i a_i^\dagger a_i.
\end{aligned}$$

Note that λ_i is a real number. Using the commutation relation $[a_i, a_i^\dagger] = 1$, which implies $a_i^\dagger a_i = a_i a_i^\dagger - 1$, we can split the summation over λ_i such that

$$\sum_i \lambda_i a_i^\dagger a_i = \frac{1}{2} \sum_i \lambda_i a_i^\dagger a_i + \frac{1}{2} \sum_i \lambda_i a_i a_i^\dagger - \frac{1}{2} \sum_i \lambda_i. \quad (4.7)$$

Define

$$\begin{aligned}
t_{ij} &= \frac{1}{4} \sqrt{S_i S_j} \left(D_\gamma^{ij} (G_{ij}^{\gamma xx} + G_{ij}^{\gamma yy} - iG_{ij}^{\gamma xy} + iG_{ij}^{\gamma yx}) - J_{ij} (F_{ij}^{xx} + F_{ij}^{yy} - iF_{ij}^{xy} + iF_{ij}^{yx}) \right) \\
\tau_{ij} &= \frac{1}{4} \sqrt{S_i S_j} \left(D_\gamma^{ij} (G_{ij}^{\gamma xx} - G_{ij}^{\gamma yy} + iG_{ij}^{\gamma xy} + iG_{ij}^{\gamma yx}) - J_{ij} (F_{ij}^{xx} - F_{ij}^{yy} + iF_{ij}^{xy} + iF_{ij}^{yx}) \right) \\
m_i &= \frac{1}{2} K S_i (G_i^{zx} G_i^{zx} + G_i^{zy} G_i^{zy}) + \frac{1}{2} \lambda_i \\
\mu_i &= \frac{1}{2} K S_i (G_i^{zx} G_i^{zx} - G_i^{zy} G_i^{zy} + iG_i^{zx} G_i^{zy} + iG_i^{zy} G_i^{zx}),
\end{aligned} \quad (4.8)$$

such that the final form of the second order part of the Hamiltonian becomes

$$\begin{aligned}
H_2 = & \sum_{i \neq j} (t_{ij} a_i^\dagger a_j + t_{ij}^* a_i a_j^\dagger + \tau_{ij}^* a_i a_j + \tau_{ij} a_i^\dagger a_j^\dagger) \\
& + \sum_i (m_i a_i^\dagger a_i + m_i^* a_i a_i^\dagger + \mu_i^* a_i a_i + \mu_i a_i^\dagger a_i^\dagger) \\
& - \frac{1}{2} \sum_i \lambda_i.
\end{aligned} \quad (4.9)$$

H_2 is also known as the (non-interacting) spinwave Hamiltonian since it contains the direct quadratic terms and any constant contributions caused by them. Often written more compactly as

$$\begin{aligned}
H_{SW} \equiv H_2 = & \sum_{i \neq j} (t_{ij} a_i^\dagger a_j + \tau_{ij} a_i^\dagger a_j^\dagger) + \text{H.c.} \\
& + \sum_i (m_i a_i^\dagger a_i + \mu_i a_i^\dagger a_i^\dagger) + \text{H.c.} \\
& + E_0.
\end{aligned} \tag{4.10}$$

H.c. denotes the Hermitian conjugate of the previous terms.

Calculation of Γ^{-1}

This section shows the Bogoliubov approach [15] explicitly and explain some aspects and requirement of this technique. We first show why Γ^{-1} has to be para-unitary. Let

$$\gamma_i = \sum_{k=1}^N (u_{ki}^* a_k - v_{ki}^* a_k^\dagger)$$

be a new mode, then its Hermitian adjoint is

$$\gamma_i^\dagger = \sum_{k=1}^N (-v_{ki} a_k + u_{ki} a_k^\dagger).$$

The commutation relation for γ, γ^\dagger operators is then

$$\begin{aligned} [\gamma_i, \gamma_j^\dagger] &= \gamma_i \gamma_j^\dagger - \gamma_j^\dagger \gamma_i = \\ &= \left(\sum_{k=1}^N (u_{ki}^* a_k - v_{ki}^* a_k^\dagger) \right) \left(\sum_{k'=1}^N (-v_{k'j} a_{k'} + u_{k'j} a_{k'}^\dagger) \right) \\ &\quad - \left(\sum_{k'=1}^N (-v_{k'j} a_{k'} + u_{k'j} a_{k'}^\dagger) \right) \left(\sum_{k=1}^N (u_{ki}^* a_k - v_{ki}^* a_k^\dagger) \right) \\ &= \sum_{k,k'=1}^N (-u_{ki}^* v_{k'j} a_k a_{k'} + u_{ki}^* u_{k'j} a_k a_{k'}^\dagger + v_{ki}^* v_{k'j} a_k^\dagger a_{k'} - v_{ki}^* u_{k'j} a_k^\dagger a_{k'}^\dagger) \\ &\quad - \sum_{k,k'=1}^N (-u_{k'i}^* v_{k'j} a_{k'} a_k + u_{k'i}^* u_{k'j} a_{k'}^\dagger a_k + v_{k'i}^* v_{k'j} a_{k'} a_k^\dagger - v_{k'i}^* u_{k'j} a_{k'}^\dagger a_k^\dagger) \\ &= \sum_{k,k'=1}^N (-u_{ki}^* v_{k'j} [a_k, a_{k'}] + u_{ki}^* u_{k'j} [a_k, a_{k'}^\dagger] + v_{ki}^* v_{k'j} [a_k^\dagger, a_{k'}] - v_{ki}^* u_{k'j} [a_k^\dagger, a_{k'}^\dagger]) \\ &= \sum_{k=1}^N (u_{ki}^* u_{kj} - v_{ki}^* v_{kj}). \end{aligned}$$

We look for a new basis of bosonic creation and annihilation operators $\gamma_i, \gamma_i^\dagger$, so we require

$$[\gamma_i, \gamma_j^\dagger] = \sum_{k=1}^N (u_{ki}^* u_{kj} - v_{ki}^* v_{kj}) = \delta_{ij}. \quad (4.11)$$

Define matrices by $U_{ij} = u_{ij}$ and $V_{ij} = v_{ij}$, then

$$\Gamma = \begin{pmatrix} \mathbf{U}^\dagger & -\mathbf{V}^\dagger \\ -\mathbf{V}^T & \mathbf{U}^T \end{pmatrix} \quad \text{and} \quad \Gamma^{-1} = \begin{pmatrix} \mathbf{U} & \mathbf{V}^* \\ \mathbf{V} & \mathbf{U}^* \end{pmatrix}, \quad (4.12)$$

which are called para-unitary matrices [15]. Define the $2N \times 2N$ para-unit matrix

$$\hat{\mathbf{I}}_{2N} = \begin{pmatrix} \mathbf{I}_N & 0 \\ 0 & -\mathbf{I}_N \end{pmatrix}$$

and note that

$$(\Gamma^\dagger)^{-1} \Gamma^{-1} = (\Gamma^{-1})^\dagger \Gamma^{-1} = \hat{\mathbf{I}}_{2N}. \quad (4.13)$$

Together with a positive-definite \mathbf{H} regular eigenvectors fail to produce (2.20), for we would end up with negative values on the diagonal. J. H. P. Colpa solves this by introducing para-eigenvectors with para-eigenvalues, which are defined as solutions of

$$\begin{pmatrix} \mathbf{A} & \mathbf{B} \\ \mathbf{B}^* & \mathbf{A}^* \end{pmatrix} \begin{pmatrix} \mathbf{u}_k \\ \mathbf{v}_k \end{pmatrix} = \frac{1}{2}\hbar\omega_k \begin{pmatrix} \mathbf{u}_k \\ -\mathbf{v}_k \end{pmatrix}. \quad (4.14)$$

Note that if $(\mathbf{u}_k, \mathbf{v}_k)$ is a solution for $\frac{1}{2}\hbar\omega_k$, then $(\mathbf{v}_k^*, \mathbf{u}_k^*)$ is a solution for $-\frac{1}{2}\hbar\omega_k^*$. These subvectors $\mathbf{u}_k, \mathbf{v}_k$ form the columns of \mathbf{U}, \mathbf{V} .

The para-eigenvalues are easily calculated by solving

$$\begin{vmatrix} \mathbf{A} - \frac{1}{2}\hbar\omega\mathbf{I}_N & \mathbf{B} \\ \mathbf{B}^* & \mathbf{A}^* + \frac{1}{2}\hbar\omega\mathbf{I}_N \end{vmatrix} = 0, \quad (4.15)$$

which produces N non-negative para-eigenvalues and N non-positive eigenvalues as expected. The para-eigenvectors associated with the non-negative para-eigenvalues can be calculated directly while taking into account that they must be para-perpendicular:

$$\langle (\mathbf{u}_i, \mathbf{v}_i), (\mathbf{u}_j, \mathbf{v}_j) \rangle = \mathbf{u}_i \mathbf{u}_j^* - \mathbf{v}_i \mathbf{v}_j^* = \delta_{ij} \quad (4.16)$$

to ensure the matrix $\mathbf{\Gamma}^{-1}$ is para-unitary. Unfortunately most build-in functions in programs produce solutions of (4.14) with regular perpendicularity and normalization. Luckily a simple Gram-Schmidt procedure can enforce (4.16).

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