Master's thesis

NTNU
Norwegian University of Science and Technology

Andreas Götestam Fossheim

Exploring signatures of magnetic order in entanglement properties of finite-size two-dimensional quantum XXZ antiferromagnets at zero temperature

- asymptotic behaviour and crossover phenomena

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Supervisor: John Ove Fjærestad
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Norwegian University of
Science and Technology

Abstract

In this thesis, the entanglement entropy and its generalization, the Rényi entropy, of the magnetically ordered ground state of two-dimensional finite-size antiferromagnets is studied by means of modified linear spin wave theory. An extension of the framework developed in Ref. 1 to an XXZ-model was attempted. In the easy plane-case, the first subleading term was for a particular choice of subsystem analytically demonstrated to be universal with a prefactor $N_G/2$ in accordance with the prediction of Ref. 2, where N_G is the number of Goldstone modes. Furthermore, a scaling function was found showing how the system crosses over from effectively having two or three Goldstone modes near the pure Heisenberg model, to having only one as the anisotropy parameter is increased. In the easy axis-case, the modification of the spin wave theory fails for collinear types of order as they will have no broken continuous symmetries. For non-collinear order the procedure may still work, but its description will no longer fit into the framework developed here.

Sammendrag

I denne oppgaven ble entanglement-entropien, og dens generalisering Rényi-entropien, til den magnetisk ordnede grunntilstanden i to-dimensjonale endelige antiferromagneter studert ved hjelp av modifisert lineær spin-bølge-teori. En utvidelse av rammeverket utviklet i Ref. 1 til en XXZ-model ble forsøkt. I easy plane-tilfellet ble det demonstrert analytisk for et gitt subsystem at det første subdominante leddet var universelt med en prefaktor $N_G/2$ i samsvar med predikasjonen i Ref. 2, hvor N_G er antallet Goldstone-moder. En scaleringsfunskjon som viser hvordan systemet effektivt går fra å ha tre Goldstone-moder i Heisenberg-modellen til å ha kun én når anisotropien økte ble også funnet. I easy axis-tilfellet mislyktes modifiseringen av spin-bølge-teorien for modeller med kollineær orden ettersom de ikke ville bryte noen kontinuerlige symmetrier. For ikke-kollineær orden kan prosedyren fortsatt fungere, men dens beskrivelse vil ikke bli dekket av rammeverket utviklet her.

Preface & Aknowledgements

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Lastly I will direct a personal thank you to my supervisor John Ove Fjærestad; were it not for his guidance, this thesis would have never come into existence.

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Chapter 1

Introduction

Several of the most studied problems in condensed matter physics, both present and past, involve interacting magnetic moments, or spins. These systems are of great importance in fundamental research giving rise to novel physics and mathematics, as well as for technological advancements with the electron being a strongly correlated spinful particle. If we concern ourselves only with spins at some fixed locations in space as is often done in statistical mechanics with the Ising model and the Heisenberg model being prominent examples, there are a number of questions one could seek to answer. For instance: What is the ground state, and is it ordered? Are there phase transitions, and if so, how can they be quantified? How well does the model describe real physical systems, and what does the description lose when assumptions are made? One could also ask more general questions about the equations themselves, not worrying about the numerical value of any parameter, but trying instead to make comparisons between different models.

In this thesis, a rather general Heisenberg type model will serve as the starting point of the discussion. This is of course a highly complex many-body system, and even at the classical level, questions of solubility quickly arise.[3] However, with the free energy as a generating functional for thermodynamic properties, it is still possible to say a lot about a system without having to solve it exactly. In particular, the discussion here will revolve around a quantity called the entanglement entropy.

1.1 Entanglement entropy

Entanglement as described in quantum information theory is in a sense a measure of connectedness between the quantum states on different subspaces of a total state on their parent space. It means that some information about one region can be encoded in a different region, and entanglement is thus an alternative way to describe correlations. The prime example of an entangled state is the spin singlet; if you know the polarity of one spin, you also know the polarity of the other spin without having to measure it, regardless

of the physical distance between the two. If we split our Hilbert space into two, it seems plausible that one might learn something about the total state by looking at the entropy in either of the partitions. This has turned out particularly useful when characterizing states of strongly correlated many-body systems.[4;5]

For a system divided into two subsystems $\mathcal{A}$ and $\mathcal{B}$, one defines the reduced density operator in one region by "tracing out" the degrees of freedom in the other:

$$\rho_{\mathcal{A}} = \mathrm{tr}_{\mathcal{B}}\, \rho, \tag{1.1}$$

where $\mathrm{tr}_{\mathcal{B}}$ denotes a partial trace over the degrees of freedom in $\mathcal{B}$. A few useful facts about density operators and the partial trace is provided in appendix A. The density operator of the ground state, which is what we wish to study, is $|\Psi_{Gs}\rangle \langle \Psi_{Gs}|$. Finally, the entanglement entropy is defined as the von Neumann entropy of the reduced density operator:

$$S_{vN} = -\,\mathrm{tr}(\rho_{\mathcal{A}} \ln \rho_{\mathcal{A}}). \tag{1.2}$$

The more general Rényi entropy is defined as:

$$S_n = -\frac{1}{n-1} \ln \mathrm{tr}_{\mathcal{A}}(\rho_{\mathcal{A}}^n), \tag{1.3}$$

which in the limit $n \to 1$ reduces to the von Neumann entropy, as is proven in A.3. We will parameterize $\rho_{\mathcal{A}}$ as $e^{H_E} / \mathrm{tr}\left(e^{H_E}\right)$, where H_E is the so called entanglement Hamiltonian. The entanglement entropy can then be found in terms of the spectrum of the entanglement Hamiltonian.

It is known that for many types of systems, the entanglement entropy obeys a so called area law.[6;7] The leading term will usually be proportional to the size of the boundary between the subsystems, so if it has a characteristic linear dimension ℓ, the leading term in d dimension would be $\propto a_n \ell^{d-1}$, where a_n is a strictly non-universal prefactor. The area law can naively be attributed to short range interactions across the boundary, like for instance singlets and triplets.

There are however also corrections to this leading term, and the presence of a surprisingly large first correction was first observed numerically for a Heisenberg antiferromagnet.[8;9] It was hypothesised that this subleading term arose as a consequence of the broken symmetry ground state of the model, and the so called Tower of States (ToS) present in a finite geometry.[10] Ref. 2 then demonstrated analytically for certain models on certain subsystems that this subleading term in fact was universal. It is this universal property we are interested in. To study it, we will use spin wave theory that has been modified to describe finite-size lattices. To get a better grasp on how the central questions of the thesis are posed and to give a bit more motivation, an introduction to a few concepts is beneficial.

1.2 Broken symmetries, Phase transitions and Renormalization

We will in this section go on to introduce a number of concepts by merely scratching their surface. For a more comprehensive view into these subject matters see Refs. 11 and 12.

As we know, symmetry holds a special place in physics, and the theory of phase transitions is no different. Many types of phases can be described in terms of broken symmetries.[11] A spontaneous symmetry breaking occurs whenever the Hamiltonian has a higher degree of symmetry than the state the system is in. To exemplify, let us use the ferromagnet: In a ferromagnet, the lowest energy configurations are found when aligning all the spins along a given axis. At high temperatures, thermal fluctuations will make the system appear disordered with all spins pointing equally much in every direction. When decreasing the temperature and the fluctuations become small however, the spins will predominantly align in one direction and the system acquires a net magnetization. In the absence of an external field, no particular direction of the magnetization is energetically favorable over any other direction, that is to say the Hamiltonian is invariant w.r.t. global spin rotations, but in the ordered phase, the magnetization will necessarily have to point in some direction. Thus, the state is less symmetric than its Hamiltonian, and the order is said to have spontaneously broken the symmetry. A natural choice for an order parameter is then often the quantity that spontaneously broke the symmetry. This is a local observable that is zero in the symmetric phase and finite in the symmetry-broken phase.

Upon some further thought, there is no apparent reason as to why spontaneous symmetry breaking should occur. How can the order parameter ”decide” on a direction to point in? This is a rather fine point mathematically speaking, and can be traced back to the breakdown of the ergodic hypothesis on which the taking of any average value in statistical mechanics relies. Again, see Ref. 12 for details on this. Importantly, the symmetries do break, and whenever a continuous symmetry is spontaneously broken, Goldtsones theorem states that there will come into existence a massless boson in the theory.[11] These Goldstone modes will be of great importance in this thesis.

The transition just described was an example of a thermal phase transition. In this thesis however, we will look at systems in the ground state, i.e. at zero temperature. At zero temperature, there are no thermal fluctuations. However, it is still possible to get phase transitions through quantum fluctuations. It is then termed a quantum phase transition.[3] It is not always obvious what to choose as the order parameter, so a perhaps more useful insight might be that phase transitions only occur at points of non-analyticity in the free energy.[12]

Sticking with the example of the ferromagnet, the natural order parameter can be obtained through differentiation of the free energy w.r.t. external magnetic field. Since the order parameter changes continuously from being zero to being finite, the non-analyticity in the free energy cannot be fully understood by looking solely at the first derivative. Higher order derivatives, like specific heat and magnetic susceptibility will also have to play an important role.

A different way to measure order that we already touched upon is through correlation

functions. One could naively expect that in a disordered phase, correlations at distances greater than the range of interactions should be small, while the presence of long range order could imply that the correlations could be large even at a great distance. Thus, the behaviour of correlations may also change during a phase transition.

The combined behaviour of the different derivatives of the free energy and the correlation functions in the vicinity of and at the critical points determine the nature of the phase transition. It turns out in the case of the ferromagnet that six so called critical exponents, of which only two are really independent, fully describes the critical behaviour. Moreover, the values of the critical exponents turn out to only depend on the dimensionality, the symmetries of the problem, and whether or not the interactions are long ranged.[12] All models that have the same critical behaviour is said to be in the same universality class. This can all best be appreciated in the framework of the Renormalization Group (RG), which also serves as an underpinning of both field theory and statistical mechanics, strengthening the bridge between the two.

The basic idea of the RG is to iteratively probe the system at larger and larger scales. In doing so one will often converge upon a fixed point of the iteration where the resulting model only depends on a few so called relevant variables. The number of relevant variables can be though of as the number of parameters that must be tuned in order to place the system at criticality. The resulting model will also be scale invariant, which leads to the different scaling laws between the critical exponents.[12] This is also the reason for why many apparently different physical systems are in the same universality class. There are simply not that many ways for a theory to be scale invariant when constrained by dimensionality and symmetry. It is by virtue of this that universal properties can be said to be more important than microscopic details.

As stated previously, we wish to study finite-size systems, and an important corollary of saying that a phase transition only occurs at points of non-analyticity in the free energy, is that they cannot really occur in a finite system. The free energy being a sum of some finite terms cannot be non-analytic unless the number of terms is infinite. This can be understood in the context of the renormalization group as length being a relevant variable, and criticality only occurring at $L \to \infty$, or $1/L \to 0$.[12] As a consequence, the order parameter at zero field cannot in a finite system be anything other than zero. This restoration of symmetry will give rise to a Tower of States structure,[10] which is of paramount importance for the universal property we are studying.

Two final concepts that will appear in this context when we are looking at the XXZ-model are the phenomena of data collapse and crossovers. It was realized that if an order parameter was a function of two relevant variables, it could near criticality be described by one function of a single argument combining the the two.[12] This phenomenon of data collapse is a direct consequence of the scaling laws obtained in the RG, and the single function describing the combined behaviour of the two arguments is called the scaling function. In this thesis, the relevant variables will be the size of the system, and the anisotropy parameter determining how far away from a pure Heisenberg-model we are. The order parameter will be the mode occupation number of a particular mode in the entanglement Hamiltonian. These choices are unconventional and have to our knowledge never been studied

before. Since the RG is so general, it is still somehow analogous to what is seen in a ferromagnet with magnetization as the order parameter and temperature and external magnetic field as the variables.

Lastly, a crossover is something that occurs in a scaling function when it has two different asymptotic regimes in the limits of its argument approaching 0 and ∞. At some intermediate values then, the function must necessarily cross over from the one regime to the other.

1.3 The universal term

Let us proceed by taking a look at the origins of the universal terms and some of the methods that have been used in discovering it.

When describing quantum many-body systems, it is often useful to go to the second quantization formalism. For a spin-system on a lattice, this usually means going to spin wave theory. In spin wave theory, the idea is that if the system is ordered, the order can be taken to be the same as it would have been in the classical model with the spin waves as some relatively small bosonic excitations on top. When only going to linear order in the spin wave theory the bosons are free, which is often a sufficiently good approximation.

The free boson theory was well understood to give an area law term, as well as a logarithmic correction connected to any corner in the partitioning of the subsystems.[2] It was therefore a bit surprising to see a rather large logarithmic correction even in corner-free subsystems. Not only was it a bit surprising, but it appeared that in 2D, the subleading term scaled like $b_n \ln \ell$, with $b_n \simeq 1$ more or less independent of model parameters and the Rényi-index.[8] This points in the direction of universality, and in 2015, Metlitski & Grover[2] used a non-linear sigma model (NLSM) to predict $b_n = N_G(d-1)/2$, with N_G being the number of Goldstone modes, i.e. the number of broken continuous symmetries, and d being the dimensionality of the lattice. The models studied up to that point in time were models with collinear order on a 2d lattice which breaks two continuous global spin rotation symmetries, and thus b_n should be exactly 1.

Ref. 2 gave an explanation as to why the subleading term could be universal for models that broke an O(N) symmetry down to a O(N-1) subgroup, so there was an interest in expanding upon their work applying several different methods. Common to all of these methods is that they try to find the spectrum of H_E. This can for instance be done numerically via the rather computationally demanding method of exact diagonalization. Another option is Quantum Monte Carlo methods[9;13;14;15;16] which currently are rendered useless for models with non-collinear order by the so called sign problem,[17] thus making other methods all the more important. A third numerical option is Density Matrix Renormalization Group.[18] For some particularly nice choices of subsystems it is possible to work analytically as well. The analytical methods being modified linear spin wave theory (MLSWT)[1;7;16;19] and non-linear sigma model (NLSM)[2;20]. The NLSM has the advantage of being more general than MLSWT and it does not rely on the same underlying assumptions, but it is for the same reason also more complicated. Most of these references have studied classical orders where the spins align in opposing directions on two sublattices. This is the

standard picture of the antiferromagnet, and it breaks the spin rotation symmetries in the two other directions than the ordering direction. For the Heisenberg-model, the O(3) symmetry can be fully broken if the order occurs on more than two sublattices. Rademaker[20] expanded the NLSM-prediction to a triangular lattice nearest neighbour model, where the order exists on three sublattices giving $b_n = 3/2$. Bauer & Fjærestad[1] later obtained the same prediction for orders that occurs on any number of sublattices through using a more general Fourier transform of the interactions in the MLSWT. It is their framework that will be further generalized in this thesis.

In order to understand why spin wave theory can be expected to give good results for this problem, we will have to discuss the origins of the prediction in the NLSM a little bit more. The argument is complicated, but it can be shortly summarized like this: The non-linear sigma model used is a scalar field theory where the fields live on a sphere, like classical spins of fixed length. If one were to rewrite the fields in terms of a mean field and some fluctuations, the effective Hamiltonian of the system would decouple into a slow-moving part describing the mean field, and one part describing the motion of the fluctuations. Importantly, in a finite system, this introduces two energy scales in the problem, and the Rényi entropy being dimensionless could then only depend on the ratios between these energy-scales. The slow-moving part describes a ToS with an energy gap $\sim 1/L^d$, while the fluctuations behave like spin waves and will have a gap $\sim 1/L$ if they are linearly dispersing. Ref. 2 then go on to show for a particular subsystem that the form of the entanglement Hamiltonian mirrors the form of the effective Hamiltonian which in turn is used to show that there is one contribution to the Rényi entropy which scales like $\ln\left(L^{d-1}\right)$, eventually leading to the prediction for the subleading term $b_n = N_G(d-1)/2$, while the remaining part gives a contribution like the free boson theory.

The components necessary to get the universal logarithmic correction is thus the presence of a ToS and its interplay with the lowest energy spin waves, the Goldstone modes. As explained previously, spin wave theory is essentially a mean field theory where the classical ground state is the mean field, and the spin waves constitute the fluctuations. To make it seem plausible that it can capture some of the same behaviour as the NLSM, we will demonstrate the presence of a ToS in a finite lattice. A brief introduction to the Lieb-Mattis model as described in for instance Ref. 21 is given.

A 2d-square lattice has the property that it can be divided into two sublattices consisting of every other site in the lattice. In a nearest neighbour (nn)-model then, all spins only interact with spins on the other sublattice. We can denote these by A and B, and use this fact to write the Hamiltonian in terms of the total spins on each sublattice. This will be sufficient to demonstrate the presence of a ToS.

$$H = \frac{1}{2}\sum_{i,j} J_{ij}\boldsymbol{S}_i \cdot \boldsymbol{S}_j \tag{1.4}$$

Starting from a standard Heisenberg Hamiltonian and introducing Fourier transforms

$$J_{ij} = \frac{1}{N}\sum_{\boldsymbol{k}} J_k e^{i\boldsymbol{k}\cdot(\boldsymbol{r}_i - \boldsymbol{r}_j)} \tag{1.5}$$

and

$$\boldsymbol{S}_i = \frac{1}{\sqrt{N}}\sum_{\boldsymbol{k}} \boldsymbol{S}_k e^{i\boldsymbol{k}\cdot\boldsymbol{r}_i}, \tag{1.6}$$

where $\boldsymbol{k}$ takes on the values in the first Brillouin zone (BZ): $k_x, k_y = 2\pi n/L \quad n = [-L/2+1, -L/2+2, ...L/2-1, L/2]$, we can write the Hamiltonian in k-space as:

$$H = \frac{1}{2}\sum_{\boldsymbol{k}} J(\boldsymbol{k})\boldsymbol{S}_{\boldsymbol{k}}\cdot\boldsymbol{S}_{-\boldsymbol{k}}, \tag{1.7}$$

where $J(\boldsymbol{k})$ for a nn-model is $2J(\cos k_x + \cos k_y)$. In the Lieb-Mattis model only the modes at $\boldsymbol{k} = \boldsymbol{0}$ and $\boldsymbol{k} = (\pi, \pi) \equiv \boldsymbol{Q}$ are included. Transforming back to real-space, the model is:

$$H = \frac{2J}{N}\sum_{i,j} \boldsymbol{S}_i\cdot\boldsymbol{S}_j\left(e^{-i\boldsymbol{0}\cdot(\boldsymbol{r}_i-\boldsymbol{r}_j)} - e^{-i\boldsymbol{Q}\cdot(\boldsymbol{r}_i-\boldsymbol{r}_j)}\right). \tag{1.8}$$

The exponent in the last term is 1 whenever the difference between $\boldsymbol{r}_i$ and $\boldsymbol{r}_j$ is an even number, i.e. when they are on the same sublattice. It is -1 whenever they are on different sublattices. The Hamiltonian can then be written on the form:

$$\begin{aligned} H &= \frac{4J}{N}\left(\sum_{i,j}\boldsymbol{S}_i\cdot\boldsymbol{S}_j - \sum_{i\in A, j\in A}\boldsymbol{S}_i\cdot\boldsymbol{S}_j - \sum_{i\in B, j\in B}\boldsymbol{S}_i\cdot\boldsymbol{S}_j\right) \\ &= \frac{4J}{N}\left(\boldsymbol{S}_{tot}^2 - \boldsymbol{S}_A^2 - \boldsymbol{S}_B^2\right), \end{aligned} \tag{1.9}$$

where the new spin operators are the total spins on the whole lattice and sublattice A and B respectively. These operators all commute with each other, so the eigenstates of H can be labeled by their quantum numbers. From elementary spin algebra we can see that S_A and S_B can take on the values $[0, 1, ..., NS/2]$, and S_{tot} can be in the range $[|S_A - S_B|, |S_A - S_B| + 1, ..., S_A + S_B]$.

The eigenstates labeled by these quantum numbers will then have the eigenvalues:

$$E(S_{tot}, S_A, S_B) = \frac{4J}{N}\left[S_{tot}(S_{tot}+1) - S_A(S_A+1) - S_B(S_B+1)\right]. \tag{1.10}$$

It is clear then that the ground state occurs when S_A and S_B are $NS/2$ and $S_{tot} = 0$. This state is thus a spin singlet, and the restoration of symmetry in a finite system is apparent.

The energy of the first excited state would be obtained if $S_{tot} = 1$. The difference between these two states are then $\sim 1/N = 1/L^d$ which is the ToS-gap.

The spin wave gap for a linearly dispersing mode will be $\sim 1/L$, since that is the spacing between the points in k-space.

Although this is not a proof of the existence of a ToS for a general number of sublattices, this example in combination with the results of previous works is enough reason to believe that MLSWT holds the potential for obtaining good results.

As most previous work has either been done on a Heisenberg-model or an XY-model, the main effort of this thesis will be to expand the framework laid out by Ref. 1 to an XXZ-model which we will introduce shortly. This will allow for looking at both the Heisenberg-model, XY-model, and Ising-model by taking the anisotropy parameter to some limiting values. The rest of the thesis is structured as follows: There will first be a section on solving the classical problem, as its solution forms the basis on which the spin wave theory is built. Then there is a section on the procedure of spin wave theory, and the meaning of the staggered field h in the context of modified spin wave theory. Lastly, the results which now depend on both the system size and the anisotropy parameter will be presented.

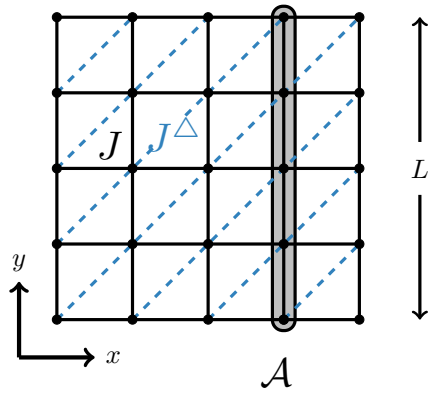

Figure 1.1: Square lattice with $N = L \times L$ sites (black dots). The black lines show the nearest neighbour interactions, J, on the square lattice. The interactions in the triangular lattice nearest neighbour model, $J^{\triangle}$, are also included on the dashed blue lines showing how the triangular lattice can be mapped onto the sqaure lattice. Periodic boundary conditions are assumed in both directions, giving the system the topology of a torus. The subsystem $\mathcal{A}$ consists of all sites inside the shaded region that wraps around the torus along the y-direction at some fixed x.

1.4 The XXZ-model

When looking at a system consisting only of interacting spins at some fixed locations, the Hamiltonian could in general be some sort of multinomial in the vector components of each spin, each term with its own coupling constant. Most of these terms would not be consistent with the symmetry of the Hamiltonian and thus have be zero. Here, we wish

to consider only Hamiltonians with second order couplings between the spins. This also implies that the external field, coupling to spins to first order, is zero. This leaves us with:

$$H = \frac{1}{2}\sum_{i,j,d} J_{ij}^d S_i^d \cdot S_j^d \tag{1.11}$$

in a d-dimensional spin-space, or

$$H = \frac{1}{2}\sum_{i,j} \left[J_{ij}^x S_i^x S_j^x + J_{ij}^y S_i^y S_j^y + J_{ij}^z S_i^z S_j^z\right] \tag{1.12}$$

in 3 dimensions. Where J_{ij} is the magnitude of the interaction between the spins at site i and j respectively. This is what is called the Heisenberg XYZ-model, and is in a sense the most general Heisenberg model.

A very natural assumption to make next is to let all spins have the same fixed length S.

So far no restrictions have been placed on the sites of the spins, so in order to make the model more mathematically tractable we would like to organize our spins on a periodic structure like a lattice since we would also like to impose translational invariance afterwards. The lattice of choice is the 2D square lattice with $N = L \times L$ sites. It has the advantage of being rather simple, and the possibility of having other lattices mapped onto it in a simple fashion. The labeling of the sites can conveniently be chosen as $\boldsymbol{r}_i = (x_i, y_i) \quad x, y \in \mathbb{N}$ setting the lattice constant to 1, which in combination with setting $\hbar = c = 1$ makes everything dimensionless. Imposing also periodic boundary conditions, i.e. $(x_i + nL, y_i + mL) = (x_i, y_i)$ for any integer n, m, will give the system a torus topology and it allows even a finite-size lattice to be fully translationally invariant.

Translational invariance in the interactions means that $J(\boldsymbol{r}_i - \boldsymbol{r}_j) \equiv J_{ij} = J_{ji}$. This makes J in matrix form real and symmetric, and so hermiticity of the Hamiltonian becomes apparent. Note also that translational invariance is less strict than rotational invariance, i.e. $J(|\boldsymbol{r}_i - \boldsymbol{r}_j|) \equiv J_{ij}$, which leaves an opportunity for mapping for instance a triangular lattice onto the square lattice. This can be seen in figure 1.1

In this thesis the special case called the XXZ-model will be studied. This means $J_{ij}^x = J_{ij}^y \equiv J_{ij}^\perp \neq J_{ij}^z$. Assuming that $J_{ij}^\perp$ and J_{ij}^z have the same functional dependence on $\boldsymbol{r}_i$ and $\boldsymbol{r}_j$, the Hamiltonian can be written as:

$$H = \frac{1}{2}\sum_{i,j} J_{ij}[S_i^x S_j^x + S_i^y S_j^y + \Delta S_i^z S_j^z], \tag{1.13}$$

where J_{ij} is the same as $J_{ij}^\perp$ having simply omitted the superscript, and $\Delta \equiv J_{ij}^z / J_{ij}^\perp$ which under the previous assumption is just a constant which we will assume to be non-negative in the following. This Hamiltonian is of particular interest to due to the three limiting cases $\Delta \to 1$, $\Delta \to 0$ and $\Delta \to \infty$ being equivalent to the Heisenberg-, XY- and Ising- models respectively, or n-vector models of rank 3,2 and 1. These are three of

the most important models for spin systems, and a lot is known about each of them both classically and quantum mechanically. Crucially for the treatment here, the Heisenberg-model has an O(3) or SU(2) symmetry, i.e. continuous spin rotation symmetry about all axes, while the XY- and Ising- models have continuous spin rotation symmetry about the z-axis giving an O(2) or U(1) symmetry. The way to check this is to take commutator of the generators of the spin rotation groups with the Hamiltonian, as is done in appendix B.

For the purposes of this thesis, the description will often be split up into the three different cases: $\Delta = 1$, $\Delta < 1$ and $\Delta > 1$. These will be referred to as the xxx-, easy plane- and easy axis-cases respectively. The two latter will sometimes be referred to under the umbrella term xxz-case which is distinguished from the XXZ-model at the pure Heisenberg point being referred to as the xxx-case or XXX-model. Furthermore, the parameter Δ will be split up into $1-\epsilon$ and $1+\epsilon$ in the easy plane- and easy axis-cases respectively. This will allow for an easier understanding of which contributions come from the pure Heisenberg model, and which come from the anisotropy parameter ϵ.

Chapter 2

The classical problem

Since we have conceded that we will not attempt to solve the model exactly and instead use linear spin wave theory, we will first need to find the classical ground state. To find the ground state of the classical models means optimizing a configuration of N spins with 3 components each. This is not an easy task. One could think to start by pulling out a factor S^2 and writing the rest of the Hamiltonian in terms of the $2N$ angles (θ_i, ϕ_i). This is then a minimization problem w.r.t. $2N$ numbers, which for a macroscopically large N still is far too much. However, there are simplifying assumptions to be made, at least in some cases.

2.1 xxx-case - the Lagrange multiplier method

Showing some results first for the Heisenberg model will allow for easier arguments in what follows. An initial constraint is obtained by demanding that the length of the spin at every site is S or $\boldsymbol{S}_i \cdot \boldsymbol{S}_i = S^2$. A somewhat weaker, but sufficient, constraint is obtained by summing the previous constraints over all N sites:

$$\sum_i \boldsymbol{S}_i \cdot \boldsymbol{S}_i = NS^2. \tag{2.1}$$

The Hamiltonian with a single Lagrange multiplier then becomes:

$$\mathcal{H} = \frac{1}{2}\sum_{i,j} J_{ij}\boldsymbol{S}_i \cdot \boldsymbol{S}_j - \lambda(\sum_i \boldsymbol{S}_i \cdot \boldsymbol{S}_i - NS^2). \tag{2.2}$$

Going to k-space using the Fourier transforms (1.5) and (1.6), we get:

$$\mathcal{H} = \frac{1}{2}\sum_{\boldsymbol{k}} J_{\boldsymbol{k}} \boldsymbol{S}_{\boldsymbol{k}} \cdot \boldsymbol{S}_{-\boldsymbol{k}} - \lambda(\sum_{k} \boldsymbol{S}_{\boldsymbol{k}} \cdot \boldsymbol{S}_{-\boldsymbol{k}} - NS^2). \tag{2.3}$$

The extrema are found where the gradient w.r.t. all $\boldsymbol{S}_{\boldsymbol{m}}$ and λ vanishes. Noting that $\frac{\partial \boldsymbol{S}_{\boldsymbol{k}}}{\partial \boldsymbol{S}_{\boldsymbol{m}}} = \delta_{k,m}$, we get the $N+1$ equations:

$$\begin{aligned} \frac{\partial \mathcal{H}}{\partial S_{\boldsymbol{m}}} &= \frac{1}{2}(J_{-\boldsymbol{m}} + J_{\boldsymbol{m}})\boldsymbol{S}_{-\boldsymbol{m}} - 2\lambda \boldsymbol{S}_{-\boldsymbol{m}} = 0 \\ \frac{\partial \mathcal{H}}{\partial \lambda} &= \sum_{k} \boldsymbol{S}_{\boldsymbol{k}} \cdot \boldsymbol{S}_{-\boldsymbol{k}} - NS^2 = 0. \end{aligned} \tag{2.4}$$

An important fact about these equations is that $J_{\boldsymbol{m}} = J_{-\boldsymbol{m}}$ due to the translational invariance, so setting $\lambda = J_{\boldsymbol{m}}/2$ for any $\boldsymbol{m}$ would leave a non-zero contribution for all the equations where $J_{\boldsymbol{k}} \neq J_{\boldsymbol{m}}$ unless these $S_{-\boldsymbol{k}}$ are zero. The constraint then implies that the sum of the remaining spins where $J_{\boldsymbol{k}} = J_{\boldsymbol{m}}$ is equal to NS^2, so the value of the Hamiltonian becomes $\frac{1}{2}J_{\boldsymbol{m}}NS^2$. The global minimum is then at the value $\frac{1}{2}J_{\boldsymbol{Q}}NS^2$ if $J_{\boldsymbol{Q}}$ is a global minimum of J. This vector $\boldsymbol{Q}$ is called the ordering vector of the model. Another consequence of the translational invariance is that the global minimum exists at both $\pm\boldsymbol{Q}$, and unless $\boldsymbol{Q} = (0 \vee \pi, 0 \vee \pi)$, these two vectors are inequivalent in the BZ. It is also possible that there are multiple such pairs of global minima, but we will restrict ourselves to look at models with only one pair of minima at $\pm\boldsymbol{Q}$ and simply write $\boldsymbol{Q} = (q_x, q_y)$ throughout keeping in mind that there is also a minimum at $-\boldsymbol{Q}$.

We will also only consider models that are antiferromagnetic. What this means is that the nearest neighbour interaction has a positive sign, and the further away the points i and j are from each other, the smaller the interaction will get. This is not really a necessary assumption for the arguments that follow; all we really need is that the dispersion is linear. In principle, we could allow almost arbitrary interactions. However, in the real world, the interactions will depend on some microscopic physics, so not all possible models are physically sane. Usually, the interactions will decay with the distance, so we will just assume that to be the case here as well.

As a side note, we can also show that $J(\boldsymbol{Q})$ is less than zero. This can be seen by realizing that due to the translational invariance of J_{ij}, $J(\boldsymbol{k})$ will just be a sum of cosines. This means that the integral over the first BZ of $J(\boldsymbol{k})$ is zero, and it will thus have to have both positive and negative values unless it is identically zero. Therefore, $J(\boldsymbol{Q})$ being the global minimum, is negative. This quantity will appear with a negative sign under a square root multiple times, but we now know that we need not worry about that.

Under the restriction of having only one minimum (or one pair of minima), we can show that the order in real-space will be confined to a plane:

Let $\boldsymbol{S}_{\boldsymbol{Q}}$ be on the most general possible form: $\hat{n}_1 \operatorname{Re}\{\boldsymbol{S}_{\boldsymbol{Q}}\} + i\hat{n}_2 \operatorname{Im}\{\boldsymbol{S}_{\boldsymbol{Q}}\}$, where $\hat{n}_{1,2}$ are two arbitrary unit vectors. The reality condition is that $\boldsymbol{S}_{-\boldsymbol{Q}} = S^*_{\boldsymbol{Q}}$, and all other $\boldsymbol{S}_{\boldsymbol{k}}$ are zero, so transforming to real-space yields:

$$\begin{aligned}\boldsymbol{S}_i &= \frac{1}{\sqrt{N}}\left[e^{i\boldsymbol{Q}\cdot\boldsymbol{r}_i}(\hat{n}_1\,\mathrm{Re}\{\boldsymbol{S}_{\boldsymbol{Q}}\} + i\hat{n}_2\,\mathrm{Im}\{\boldsymbol{S}_{\boldsymbol{Q}}\}) + e^{-i\boldsymbol{Q}\cdot\boldsymbol{r}_i}(\hat{n}_1\,\mathrm{Re}\{\boldsymbol{S}_{\boldsymbol{Q}}\} - i\hat{n}_2\,\mathrm{Im}\{\boldsymbol{S}_{\boldsymbol{Q}}\})\right] \\ &= \frac{2}{\sqrt{N}}\left[\hat{n}_1\cos(\theta_i)\,\mathrm{Re}\{\boldsymbol{S}_{\boldsymbol{Q}}\} + \hat{n}_2\sin(\theta_i)\,\mathrm{Im}\{\boldsymbol{S}_{\boldsymbol{Q}}\}\right],\end{aligned} \tag{2.5}$$

where $\theta_i \equiv \boldsymbol{Q}\cdot\boldsymbol{r}_i$. Squaring this relation, and demanding that it holds true for all i will be sufficient.

$$\begin{aligned}\frac{NS^2}{4} &= \cos^2\theta_i\,\mathrm{Re}\{\boldsymbol{S}_{\boldsymbol{Q}}\}^2 + \sin^2(\theta_i)\,\mathrm{Im}\{\boldsymbol{S}_{\boldsymbol{Q}}\}^2 \\ &\quad + 2\hat{n}_1\cdot\hat{n}_2\cos\theta_i\sin\theta_i\,\mathrm{Re}\{\boldsymbol{S}_{\boldsymbol{Q}}\}\,\mathrm{Im}\{\boldsymbol{S}_{\boldsymbol{Q}}\}.\end{aligned} \tag{2.6}$$

The only way to satisfy this for all i is to have $\hat{n}_1\cdot\hat{n}_2 = 0$, i.e. being orthogonal to each other, and $\mathrm{Re}\{\boldsymbol{S}_{\boldsymbol{Q}}\}^2 = \mathrm{Im}\{\boldsymbol{S}_{\boldsymbol{Q}}\}^2 = NS^2/4$. The order in real-space then becomes:

$$S[\hat{n}_1\cos(\theta_i) + \hat{n}_2\sin(\theta_i)], \tag{2.7}$$

where $\hat{n}_{1,2}$ are now two arbitrary orthonormal unit vectors. The fact that we can choose these vectors arbitrarily is a manifestation of the symmetry of the problem. We can also note that the special case of collinear order occurs at exactly the vectors which had the property that the positive and the negative $\boldsymbol{Q}$ were equivalent in the Brillouin zone. These models will only have two Goldstone modes: One at $\boldsymbol{0}$ and the other at $\boldsymbol{Q}$. In the non-collinear case, there will be Goldstone modes at $\boldsymbol{0}$, $\boldsymbol{Q}$ and $-\boldsymbol{Q}$. This set of vectors will be denoted as G, and the number of vectors in this set as N_G.

Furthermore, for a given value of $\boldsymbol{Q} = (2\pi s_x/t_x, 2\pi s_y/t_y)$, with $s_{x,y}$ and $t_{x,y}$ coprime, the lattice will be split up into t sublattices in which all spins have the same alignment if t is the greatest common divisor of t_x and t_y (if $q_{x,y} = 0$, we take $t_{x,y} = 1$). We will assume that L is divisible by t such that the order is commensurate, i.e. that the sites $(x_i + nL, y_i + mL)$ are in the same sublattice for all integers m, n. This hinders the order from being geometrically frustrated by the lattice itself.

2.2 xxz-case

If we try to use the Lagrange multiplier method for a general XYZ-model, the Hamiltonian would have to be split up into its vector components, so in the XXZ-model:

$$\mathcal{H} = \frac{1}{2}\sum_{\boldsymbol{k}} J_{\boldsymbol{k}}\left[S^x_{\boldsymbol{k}}S^x_{-\boldsymbol{k}} + S^y_{\boldsymbol{k}}S^y_{-\boldsymbol{k}} + \Delta S^z_{\boldsymbol{k}}S^z_{-\boldsymbol{k}}\right] - \lambda(\sum_k \boldsymbol{S}_{\boldsymbol{k}}\cdot\boldsymbol{S}_{-\boldsymbol{k}} - NS^2). \tag{2.8}$$

If $\Delta < 1$, one could try to set all $S^z_{\boldsymbol{k}} = 0$. This gives the same solution as in the xxx-case, but with the order confined to the xy-plane. There is still a rotational symmetry in

choosing the ordering direction within this plane, implying that there is only spin rotation symmetry about the z-axis.

If $\Delta > 1$, the minimum occurs where all $S^x_{\boldsymbol{k}}, S^y_{\boldsymbol{k}} = 0$ and $\lambda = J_{\boldsymbol{Q}}\Delta/2$. When transforming back to real-space, this state does not necessarily satisfy the stronger constraint that all spins must be of length S. What we have really done is optimized for only the z-component, and for an order that occurs in a plane, some of the total spin will be in e.g. the x-direction, so the length of the spin is no longer S. The exception to this of course being collinear order in which no spins have any other components than the z-component.

This leaves us with the problem of trying to find the minimum of a state that orders non-collinearly in the easy axis-case. One could try to impose the stronger constraint directly. In k-space this constraint is a double sum over the wavevectors: $\boldsymbol{S}_i \cdot \boldsymbol{S}_i = 1/N \sum_{\boldsymbol{k}\boldsymbol{k'}} \boldsymbol{S}(\boldsymbol{k}) \cdot \boldsymbol{S}(\boldsymbol{k'}) e^{i\boldsymbol{k}\cdot\boldsymbol{r}_i} e^{i\boldsymbol{k'}\cdot\boldsymbol{r}_i}$, so trying to impose all of these with Lagrange multipliers will not be any easier than direct minimization of H in terms of the angles (θ_i, ϕ_i).

This is a daunting task, so instead let us start by looking at the nearest neighbour model on a triangular lattice which is the simplest model that orders non-collinearly. It seems likely that any model that orders coplanarly in the XXX-model also will do so in an XYZ-model, in the plane between the two largest components. This is consistent with ordering in the xy-plane in the easy plane-case, and any plane containing the z-direction in the easy axis-case. Keep in mind that this is all done in zero external field. If there was an external field, we could easily get order that was not coplanar. We take the ordering plane here to be the xz-plane, and let the polar angles instead run from 0 to 2π in this plane.

The model then has the solution $\boldsymbol{Q} = (2\pi/3, 2\pi/3)$ in the XXX-model splitting the lattice up into three sublattices on which all spins have the same alignment. We can denote the angles on each sublattice as $\theta_{A,B,C}$. One possible choice is then $\theta_A = 0$ and $\theta_B = -\theta_C = 2\pi/3$. In the pure Ising case, the order will again be divided into three sublattices where $\theta_A = 0$ and $\theta_B = -\theta_C = \pi$. It may be reasonable then to assume that for any XXZ-model in between we will also have some sort of coplanar order on three sublattices that changes continuously between the two orders just described. Attempting to find a solution on the form $\theta_A = 0$ and $\theta_B = -\theta_C = q$ and minimizing w.r.t. q allows us to quickly find a solution:

$$\begin{aligned} H &\propto \Delta(2\cos q + \cos^2 q - \sin^2 q) \implies \\ \frac{\partial H}{\partial q} &= -\Delta \sin q(2 + 2\cos q) - 2\cos q \sin q = 0 \\ \implies \cos q &= -\frac{\Delta}{1+\Delta}. \end{aligned} \tag{2.9}$$

In principle this does not have to be the global minimum, since if we assume that the model will split up into three sublattices in a plane we will really need to minimize w.r.t. three angles. In the XXX-case, there is then a solution for any choice of θ_A with $\theta_B = \theta_A + 2\pi/3$ and $\theta_C = \theta_A - 2\pi/3$. This is what rotational symmetry means. There is also such a continuous degeneracy of the ground state in the XXZ-model.[23] To show this let us start from the Hamiltonian in terms of the polar angles:

$$
\begin{aligned}
H &= \frac{S^2}{2}\sum_{i,j} J_{i,j}\left[\sin\theta_i \sin\theta_j + \Delta\cos\theta_i\cos\theta_j\right] \\
&\implies \\
H^{'} &= \left(\sin\theta_A\sin\theta_B + \Delta\cos\theta_A\cos\theta_B\right) + \left(\sin\theta_B\sin\theta_C + \Delta\cos\theta_B\cos\theta_C\right) \\
&\quad + \left(\sin\theta_C\sin\theta_A + \Delta\cos\theta_C\cos\theta_A\right),
\end{aligned}
\tag{2.10}
$$

where H' now is H/JS^2N. Differentiating now w.r.t. the angles and setting equal to zero we get the three equations:

$$\cos\theta_A(\sin\theta_B + \sin\theta_C) - \Delta\sin\theta_A(\cos\theta_C + \cos\theta_B) = 0 \tag{2.11a}$$
$$\cos\theta_B(\sin\theta_C + \sin\theta_A) - \Delta\sin\theta_B(\cos\theta_A + \cos\theta_C) = 0 \tag{2.11b}$$
$$\cos\theta_C(\sin\theta_A + \sin\theta_B) - \Delta\sin\theta_C(\cos\theta_B + \cos\theta_A) = 0. \tag{2.11c}$$

A high symmetry solution to these equations can be found by letting $\theta_A = 0$. Then, from the first equation, $\sin\theta_B = -\sin\theta$. Then, $\cos\theta_B = \pm\cos\theta_C$. Inserting into the second equation gives: $-\cos\theta_B\sin\theta_B - \Delta\sin\theta_B(1 \pm \cos\theta_B) \implies \cos\theta_B = -\Delta/(1 \pm \Delta)$. From the third equation we can deduce that we must choose the positive sign. Defining q as $\cos^{-1}(-\Delta/(1+\Delta))$, we recover the solution already found. The value of H' in this solution is $\Delta(2\cos q + \cos^2 q) - \sin^2 q = (-2\Delta^2(1+\Delta) + (1+\Delta)\Delta^2 - (1+\Delta)^2)/(1+\Delta)^2 = -(\Delta^2+\Delta+1)/(\Delta+1)$.

The symmetry of the problem will also allow us to only need to check for angles $\theta_A \in [0, \pi - q]$, where $\pi - q = \cos^{-1}(\Delta/(1+\Delta))$. This can be done because all other possible angles can be reached through either a relabeling of the sublattices, a spin flip about the x-axis, or a combination of the two.

To proceed in finding the other solutions, let us follow Ref. 24 in letting $\theta_B = \epsilon - \delta$ and $\theta_C = \epsilon + \delta$. Inserting into equation 2.11a gives:

$$
\begin{aligned}
&\cos\theta_A(\sin\epsilon\cos\delta - \cos\epsilon\sin\delta + \sin\epsilon\cos\delta + \cos\epsilon\sin\delta) \\
&= \Delta\sin\theta_A(\cos\epsilon\cos\delta + \sin\epsilon\sin\delta + \cos\epsilon\cos\delta - \sin\epsilon\sin\delta) \\
&\implies \cos\theta_A 2\sin\epsilon\cos\delta = \Delta\sin\theta_A 2\cos\epsilon\cos\delta \\
&\implies \tan\epsilon = \Delta\tan\theta_A.
\end{aligned}
\tag{2.12}
$$

Knowing that $\cos^2(a) + \sin^2(a) = 1 \implies \cos^2(a) = 1/(1+\tan^2(a))$, we can also find $\cos\epsilon$:

$$\begin{aligned}\cos\epsilon &= \frac{1}{\sqrt{1+\tan^2\epsilon}} = \frac{1}{\sqrt{1+\Delta^2\tan^2\theta_A}} \\ &= \frac{1}{\sqrt{1+\Delta^2(\frac{1}{\cos^2\theta_A}-1)}} = \frac{\cos\theta_A}{\sqrt{\cos^2\theta_A(1-\Delta^2)+\Delta^2}}.\end{aligned} \tag{2.13}$$

To find an expression for δ in terms of θ_A we must instead add together (2.11b) and (2.11c) and use some substitutions:

$$\begin{aligned}& \cos\theta_B(\sin\theta_C+\sin\theta_A)+\cos\theta_C(\sin\theta_A+\sin\theta_B) \\ = \quad & \Delta\big[\sin\theta_A(\cos\theta_C+\cos\theta_B)+\sin\theta_C(\cos\theta_B+\cos\theta_A)\big] \\ \Longrightarrow \quad & \\ & \sin\theta_A(\cos\theta_B+\cos\theta_C)+\cos\theta_B\sin\theta_C+\sin\theta_B\cos\theta_C \\ = \quad & \Delta\big[\cos\theta_A(\sin\theta_B+\sin\theta_C)+\cos\theta_B\sin\theta_C+\sin\theta_B\cos\theta_C\big].\end{aligned} \tag{2.14}$$

We know that $\cos\theta_B\sin\theta_C+\sin\theta_B\cos\theta_C = \sin(\theta_B+\theta_C) = \sin(2\epsilon) = 2\sin\epsilon\cos\epsilon$, and from (2.11a), we can substitute $\sin\theta_A(\cos\theta_B+\cos\theta_C) = 1/\Delta\cos\theta_A(\sin\theta_B+\sin\theta_C)$. Lastly, we know that $\sin\theta_B+\sin\theta_C = 2\sin\epsilon\cos\delta$, so inserting yields:

$$\begin{aligned}& \frac{1}{\Delta}\cos\theta_A(2\sin\epsilon\cos\delta)+2\sin\epsilon\cos\epsilon = \Delta\cos\theta_A(2\sin\epsilon\cos\delta)+\Delta 2\sin\epsilon\cos\epsilon \\ \Longrightarrow \quad & (\Delta-\frac{1}{\Delta})\cos\theta_A\cos\delta = (\Delta-1)\cos\epsilon \\ \Longrightarrow \quad & \cos\delta = \frac{1-\Delta}{\Delta-\frac{1}{\Delta}}\frac{\cos\epsilon}{\cos\theta_A} = \frac{-\Delta}{(\Delta+1)\sqrt{\cos^2\theta_A(1-\Delta^2)+\Delta^2}}.\end{aligned} \tag{2.15}$$

The differences in the expressions from here to [24] can be traced back to differences in the definition of the problem. They are looking at solutions in the region corresponding to $\Delta\in[-1,-\infty]$. As a sanity check, we can see whether this gives the expected results in a couple of limiting cases. Letting $\Delta\to 1$ gives $\cos\epsilon = \cos\theta_A$, and $\cos\delta = -1/2$. This angle is $2\pi/3$, so the order is thus identified by the angles $\theta_A, \theta_A-2\pi/3, \theta_A+2\pi/3$ as it should be when reverting to XXX-model.

The other sanity check would be to let $\Delta\to\infty$ instead, effectively taking us to the Ising-case. Then: $\cos\epsilon = 1$, corresponding to an angle 0, while $\cos\delta = -1$, corresponding to an angle π. The order is then identified by the angles $0, -\pi, \pi$ which is again what we would have expected in the Ising model.

To check that these solutions all give back the same value for H' we should differentiate it w.r.t. θ_A. H' contains terms that are products of either two cosines or two sines. Differentiating one of them, we see that:

$$\frac{\partial}{\partial\theta_A}\cos\theta_i\cos\theta_j = \frac{\partial\cos\theta_i}{\partial\theta_i}\frac{\partial\theta_i}{\partial\theta_A}\cos\theta_j + \frac{\partial\cos\theta_j}{\partial\theta_j}\frac{\partial\theta_j}{\partial\theta_A}\cos\theta_i. \tag{2.16}$$

Thus $\partial H'/\partial\theta_A$ will become the sum of each equation in (2.11a) multiplied with $\partial\theta_i/\partial\theta_A$, where θ_i was the coordinate one would have differentiated w.r.t. to obtain the equation in the first place. Since all these equations separately are zero, $\partial H'/\partial\theta_A$ is as well, and the states are degenerate.

A degeneracy of this type usually reflects some underlying symmetry of the problem, like spin rotational symmetry in the XXX-model. This degeneracy however, does not stem from any obvious symmetry, but it may be possible still to uncover a "hidden" symmetry. The first step in this direction would be to realize that in the limit $\Delta \to 1$, we get back the regular spin rotation symmetry. Perhaps the argument can be made that there could be a sort of "elliptic" spin rotation symmetry in the XXZ-model, since the contribution to the energy from two coupled spins will lie on an ellipse. This idea is appealing, since it may allow for continuously mapping solutions of the XXX-model onto the XXZ-model.

However, when going to the quantum case, the degeneracy is lifted by the spin wave correction to the ground state energy[24]. This means that if generators of "elliptical" spin rotations are found, they do not commute with the QM-model even though their classical counterparts might do so in the Poisson Bracket sense. No more effort will be put into this as the ground state indeed is the one found through the simplest argument in this subsection.

Chapter 3

Spin wave theory

3.1 Diagonalization of H

$$H = \frac{1}{2}\sum_{i,j} J_{i,j}[S_i^x S_j^x + S_i^y S_j^y + \Delta S_i^z S_j^z] \tag{3.1}$$

Starting from this Hamiltonian we will try to develop the procedure from Ref. 1 to be valid for $\Delta \neq 1$. Knowing that the classical ordering will be different for the different cases, they will be treated separately with the Heisenberg-case treated first to serve as a reference case. That will allow for an easier calculation in the two other cases.

3.1.1 xxx-case

Given a classical ordering vector and choosing the ordering to be in the xz-plane we can first go to a rotated coordinate system such that the spins point in the local z-direction:

$$\begin{aligned} S_i^z &= S_i^{\tilde{z}}\cos(\theta_i) - S_i^{\tilde{x}}\sin(\theta_i) \\ S_i^x &= S_i^{\tilde{z}}\sin(\theta_i) + S_i^{\tilde{x}}\cos(\theta_i) \\ S_i^y &= S_i^{\tilde{y}}. \end{aligned} \tag{3.2}$$

This now constitutes a particular choice for the ground state, and thus the symmetry is spontaneously broken by construction. Inserting the rotated coordinates we get:

$$
\begin{aligned}
H &= \frac{1}{2}\sum_{i,j} J_{i,j}\Big[\big(S_i^{\tilde{z}}\cos(\theta_i) - S_i^{\tilde{x}}\sin(\theta_i)\big)\big(S_j^{\tilde{z}}\cos(\theta_j) - S_j^{\tilde{x}}\sin(\theta_j)\big) + S_i^{\tilde{y}}S_j^{\tilde{y}} \\
&+ \big(S_i^{\tilde{z}}\sin(\theta_i) + S_i^{\tilde{x}}\cos(\theta_i)\big)\big(S_j^{\tilde{z}}\sin(\theta_j) + S_j^{\tilde{x}}\cos(\theta_j)\big)\Big]. \qquad (3.3)
\end{aligned}
$$

Multiplying parenthesis and using the trigonometric identities
$\cos(a \pm b) = \cos(a)\cos(b) \mp \sin(a)\sin(b)$ and
$\sin(a \pm b) = \sin(a)\cos(b) \pm \cos(a)\sin(b)$, we arrive at:

$$
\begin{aligned}
H &= \frac{1}{2}\sum_{i,j} J_{i,j}\big[\cos(\theta_i - \theta_j)(S_i^{\tilde{z}}S_j^{\tilde{z}} + S_i^{\tilde{x}}S_j^{\tilde{x}}) + \sin(\theta_i - \theta_j)(S_i^{\tilde{z}}S_j^{\tilde{x}} - S_i^{\tilde{x}}S_j^{\tilde{z}}) \\
&+ S_i^{\tilde{y}}S_j^{\tilde{y}}\big] - h\sum_i S_i^{\tilde{z}}, \qquad (3.4)
\end{aligned}
$$

where we have introduced a fictitious local magnetic field in the ordering direction for later use when looking at modified spin wave theory. This step will be discussed at length in section 3.3.

From here we switch to the Holstein-Primakoff (HP)-representation for spins ordered along the z-axis:

$$
\begin{aligned}
S_i^{\tilde{z}} &= S - n_i \\
S_i^{+} &= \sqrt{2S - n_i}\, b_i \\
S_i^{-} &= b_i^{\dagger}\sqrt{2S - n_i},
\end{aligned} \qquad (3.5)
$$

also keeping in mind that we have $S^{\pm} = S^{\tilde{x}} \pm iS^{\tilde{y}}$, so:

$$
\begin{aligned}
S_i^{\tilde{x}} &= \frac{1}{2}(S_i^{+} + S_i^{-}) = \frac{1}{2}(\sqrt{2S - n_i}\, b_i + b_i^{\dagger}\sqrt{2S - n_i}) \\
S_i^{\tilde{y}} &= \frac{1}{2i}(S_i^{+} - S_i^{-}) = \frac{1}{2i}(\sqrt{2S - n_i}\, b_i - b_i^{\dagger}\sqrt{2S - n_i}).
\end{aligned} \qquad (3.6)
$$

The bosonization of the spin-operators is in itself an interesting procedure, and it is really the crucial step in spin wave theory. What it does is define the classical ground state as a vacuum for its bosons, and then the ladder operators raise and lower the spin projection along the $\tilde{z}$-direction. A quick check that they reproduce the correct commutation relations are provided in appendix B.2. For the system to be ordered, we would naively want it to largely coincide with the mean field, keeping fluctuations small. This is the assumption one makes when justifying only going to linear order in the spin wave theory. Formally however, we make a semi-classical expansion in $1/S$ and let $S \to \infty$. This does then in general become an asymptotic series, and it may seem a bit hard to justify using it when

looking at systems where $S = 1/2$. It does indeed occur that one gets inconsistencies when lowering S, and one has to conclude that the spin wave theory does not give a stable order. If we on the other hand get consistent results, i.e. that the correction to the magnetization in the thermodynamic limit is small, we will use that as a justification without thinking anymore of it.

Before inserting this into the Hamiltonian, we will rid ourselves of some terms that are either constants, of too high order in HP-bosons, or disappear under the summation.

The square root can be expanded as $\sqrt{2S - n_i} \simeq \sqrt{2S}(1 - n_i/4S)$, and since we only care about terms of order less than 2 in HP-bosons, we can immediately replace $S_i^{\tilde{x}} \to \frac{\sqrt{2S}}{2}(b_i + b_i^\dagger)$ and $S_i^{\tilde{y}} \to \frac{\sqrt{2S}}{2i}(b_i - b_i^\dagger)$. Then, the terms with only $S^{\tilde{x}}$'s and $S^{\tilde{y}}$'s become quadratic.

The first term in H is: $(S_i^{\tilde{z}} S_j^{\tilde{z}}) = S^2 - S(n_i + n_j) + n_i n_j$, so here we only keep $-S(n_i + n_j)$. In the term with the staggered field, we obviously only keep the part proportional to n_i since S is constant.

The mixed terms between $S^{\tilde{x}}$ and $S^{\tilde{z}}$ are the remaining problem. They will have contributions proportional to one and three bosons. Removing the higher order terms leaves us with this sum of first order terms:

$$H_1 = \frac{S}{2} \sum_{i,j} J_{i,j} \sin(\theta_i - \theta_j)(b_j + b_j^\dagger - b_i - b_i^\dagger). \tag{3.7}$$

Looking at the sum with b_i, we can show that it cancels, and the three remaining sums necessarily also cancel via the same argument. Letting $j = i + \delta$ in the sum, where δ runs over the whole lattice, we get:

$$\sum_{i,\delta} J_{i,i+\delta} \sin(\theta_i - \theta_{i+\delta}) b_i = \sum_i b_i \sum_\delta J(\boldsymbol{r}_\delta) \sin(-\boldsymbol{Q} \cdot \boldsymbol{r}_\delta) = 0, \tag{3.8}$$

where we in the second step have used the definitions of J and θ_i to explicitly see that we sum over an odd function multiplied with an even function, so the inner sum is zero for all i, and the entire first order term disappears. If the first order term had not disappeared, it would have been a good indication that we were not in the ground state to begin with.

After all of this we can now get back to the original Hamiltonian:

$$\begin{aligned} H &= \frac{S}{2} \sum_{i,j} J_{i,j} \Big[\frac{1}{2} \cos(\theta_i - \theta_j)(b_i b_j + b_i b_j^\dagger + b_i^\dagger b_j + b_i^\dagger b_j^\dagger) \\ &+ \frac{1}{2}(b_i b_j - b_i b_j^\dagger - b_i^\dagger b_j + b_i^\dagger b_j^\dagger) - \cos(\theta_i - \theta_j)(n_i + n_j) \Big] + h \sum_i n_i \end{aligned} \tag{3.9}$$

which after some reorganization becomes:

$$\begin{aligned} H &= \frac{S}{2}\sum_{i,j} J_{i,j}\Big[\frac{1}{2}[\cos(\theta_i-\theta_j)+1](b_i b_j^\dagger + b_i^\dagger b_j) + \frac{1}{2}[\cos(\theta_i-\theta_j)-1](b_i b_j + b_i^\dagger b_j^\dagger) \\ &- \cos(\theta_i-\theta_j)(b_i^\dagger b_i + b_j^\dagger b_j)\Big] + h\sum_i b_i^\dagger b_i. \end{aligned} \tag{3.10}$$

Having it on this form, we are ready to perform the Fourier transform. We will use the transforms:

$$b_i = \frac{1}{\sqrt{N}}\sum_{\boldsymbol{k}} b_{\boldsymbol{k}} e^{i\boldsymbol{k}\cdot\boldsymbol{r}_i} \quad \Longrightarrow \quad b_i^\dagger = \frac{1}{\sqrt{N}}\sum_{\boldsymbol{k}} b_{\boldsymbol{k}}^\dagger e^{-i\boldsymbol{k}\cdot\boldsymbol{r}_i} \tag{3.11}$$

for the HP-bosons as well as the ones introduced in equations (1.5) and (1.6). A quick check that the Fourier transformed operators still satisfy the correct commutation relations is provided in B.3. Inserting this into H and writing the cosines in exponential form will give a whole lot of terms, but several of them have a similar form, so we need only evaluate a few of them.

$$\begin{aligned} H = &\frac{S}{2}\sum_{i,j}\frac{1}{N}\sum_{\boldsymbol{k}''} J(\boldsymbol{k}'')e^{i\boldsymbol{k}''\cdot(\boldsymbol{r}_i-\boldsymbol{r}_j)}\frac{1}{N}\sum_{\boldsymbol{k},\boldsymbol{k}'} \\ &\Bigg\{\frac{1}{2}\left[\frac{e^{i\boldsymbol{Q}\cdot(\boldsymbol{r}_i-\boldsymbol{r}_j)}}{2}+\frac{e^{-i\boldsymbol{Q}\cdot(\boldsymbol{r}_i-\boldsymbol{r}_j)}}{2}+1\right]\left[b_{\boldsymbol{k}}b_{\boldsymbol{k}'}^\dagger e^{i(\boldsymbol{k}\cdot\boldsymbol{r}_i-\boldsymbol{k}'\cdot\boldsymbol{r}_j)} + b_{\boldsymbol{k}}^\dagger b_{\boldsymbol{k}'} e^{i(-\boldsymbol{k}\cdot\boldsymbol{r}_i+\boldsymbol{k}'\cdot\boldsymbol{r}_j)}\right] \\ &+\frac{1}{2}\left[\frac{e^{i\boldsymbol{Q}\cdot(\boldsymbol{r}_i-\boldsymbol{r}_j)}}{2}+\frac{e^{-i\boldsymbol{Q}\cdot(\boldsymbol{r}_i-\boldsymbol{r}_j)}}{2}-1\right]\left[b_{\boldsymbol{k}}b_{\boldsymbol{k}'} e^{i(\boldsymbol{k}\cdot\boldsymbol{r}_i+\boldsymbol{k}'\cdot\boldsymbol{r}_j)} + b_{\boldsymbol{k}}^\dagger b_{\boldsymbol{k}'}^\dagger e^{i(-\boldsymbol{k}\cdot\boldsymbol{r}_i-\boldsymbol{k}'\cdot\boldsymbol{r}_j)}\right] \\ &-\left[\frac{e^{i\boldsymbol{Q}\cdot(\boldsymbol{r}_i-\boldsymbol{r}_j)}}{2}+\frac{e^{-i\boldsymbol{Q}\cdot(\boldsymbol{r}_i-\boldsymbol{r}_j)}}{2}\right]\left[b_{\boldsymbol{k}}^\dagger b_{\boldsymbol{k}'} e^{i(\boldsymbol{k}\cdot\boldsymbol{r}_i-\boldsymbol{k}'\cdot\boldsymbol{r}_i)+i(\boldsymbol{k}\cdot\boldsymbol{r}_j-\boldsymbol{k}'\cdot\boldsymbol{r}_j)}\right]\Bigg\} \\ &+h\sum_i\frac{1}{N}\sum_{\boldsymbol{k},\boldsymbol{k}'}\left[b_{\boldsymbol{k}}^\dagger b_{\boldsymbol{k}'} e^{i(\boldsymbol{k}\cdot\boldsymbol{r}_i-\boldsymbol{k}'\cdot\boldsymbol{r}_i)}\right]. \end{aligned} \tag{3.12}$$

After reorganizing terms and letting the sum run over negative wavevectors in the appropriate places this can be rewritten:

$$
\begin{aligned}
H = \frac{S}{2}\sum_{i,j}\frac{1}{N^2}\sum_{\boldsymbol{k''},\boldsymbol{k'},\boldsymbol{k}} J(\boldsymbol{k''})e^{i\boldsymbol{k''}\cdot(\boldsymbol{r}_i-\boldsymbol{r}_j)}e^{-i(\boldsymbol{k}\cdot\boldsymbol{r}_i-\boldsymbol{k'}\cdot\boldsymbol{r}_j)} \\
\left\{\frac{1}{2}\left[\frac{e^{i\boldsymbol{Q}\cdot(\boldsymbol{r}_i-\boldsymbol{r}_j)}}{2}+\frac{e^{-i\boldsymbol{Q}\cdot(\boldsymbol{r}_i-\boldsymbol{r}_j)}}{2}+1\right]\left(b^\dagger_{\boldsymbol{k}}b_{\boldsymbol{k'}}+b_{-\boldsymbol{k}}b^\dagger_{-\boldsymbol{k'}}\right)\right. \\
\left.+\frac{1}{2}\left[\frac{e^{i\boldsymbol{Q}\cdot(\boldsymbol{r}_i-\boldsymbol{r}_j)}}{2}+\frac{e^{-i\boldsymbol{Q}\cdot(\boldsymbol{r}_i-\boldsymbol{r}_j)}}{2}-1\right]\left(b_{-\boldsymbol{k}}b_{\boldsymbol{k'}}+b^\dagger_{\boldsymbol{k}}b^\dagger_{-\boldsymbol{k'}}\right)\right\} \\
-\frac{S}{2}\sum_{i,j}\frac{1}{N^2}\sum_{\boldsymbol{k''},\boldsymbol{k'},\boldsymbol{k}} J(\boldsymbol{k''})e^{i\boldsymbol{k''}\cdot(\boldsymbol{r}_i-\boldsymbol{r}_j)}\left[\frac{e^{i\boldsymbol{Q}\cdot(\boldsymbol{r}_i-\boldsymbol{r}_j)}}{2}+\frac{e^{-i\boldsymbol{Q}\cdot(\boldsymbol{r}_i-\boldsymbol{r}_j)}}{2}\right] \\
\left[b^\dagger_{\boldsymbol{k}}b_{\boldsymbol{k'}}e^{i(\boldsymbol{k}\cdot\boldsymbol{r}_i-\boldsymbol{k'}\cdot\boldsymbol{r}_i)}+b^\dagger_{-\boldsymbol{k}}b_{-\boldsymbol{k'}}e^{-i(\boldsymbol{k}\cdot\boldsymbol{r}_j-\boldsymbol{k'}\cdot\boldsymbol{r}_j)}\right] \\
+\frac{h}{2}\sum_i\frac{1}{N}\sum_{\boldsymbol{k},\boldsymbol{k'}}\left[b^\dagger_{\boldsymbol{k}}b_{\boldsymbol{k'}}e^{i(\boldsymbol{k}\cdot\boldsymbol{r}_i-\boldsymbol{k'}\cdot\boldsymbol{r}_i)}+b^\dagger_{-\boldsymbol{k}}b_{-\boldsymbol{k'}}e^{-i(\boldsymbol{k}\cdot\boldsymbol{r}_i-\boldsymbol{k'}\cdot\boldsymbol{r}_i)}\right].
\end{aligned}
\tag{3.13}
$$

Switching the order of the sums, we can see that we are probably going to end up with a lot of deltafunctions.

The first type of sum is:

$$
\begin{aligned}
&\frac{1}{N^2}\sum_{i,j}e^{i\boldsymbol{k''}\cdot(\boldsymbol{r}_i-\boldsymbol{r}_j)}e^{-i(\boldsymbol{k}\cdot\boldsymbol{r}_i-\boldsymbol{k'}\cdot\boldsymbol{r}_j)}e^{i\boldsymbol{C}\cdot(\boldsymbol{r}_i-\boldsymbol{r}_j)} \\
&=\frac{1}{N}\sum_i e^{-i\boldsymbol{r}_i\cdot(\boldsymbol{k}-(\boldsymbol{k''}+\boldsymbol{C}))}\frac{1}{N}\sum_j e^{i\boldsymbol{r}_j\cdot(\boldsymbol{k'}-(\boldsymbol{k''}+\boldsymbol{C}))} \\
&=\delta_{\boldsymbol{k},\boldsymbol{k''}+\boldsymbol{C}}\delta_{\boldsymbol{k'},\boldsymbol{k''}+\boldsymbol{C}}=\delta_{\boldsymbol{k},\boldsymbol{k'}}\delta_{\boldsymbol{k'}-\boldsymbol{C},\boldsymbol{k''}},
\end{aligned}
\tag{3.14}
$$

where $\boldsymbol{C}$ is now either $\pm\boldsymbol{Q}$ or $\boldsymbol{0}$. The other type of sum is:

$$
\begin{aligned}
&\frac{1}{N^2}\sum_{i,j}e^{i\boldsymbol{k''}\cdot(\boldsymbol{r}_i-\boldsymbol{r}_j)}e^{-i(\boldsymbol{k}\cdot\boldsymbol{r}_i-\boldsymbol{k'}\cdot\boldsymbol{r}_i)}e^{i\boldsymbol{C}\cdot(\boldsymbol{r}_i-\boldsymbol{r}_j)} \\
&=\frac{1}{N}\sum_i e^{-i\boldsymbol{r}_i\cdot(\boldsymbol{k}-(\boldsymbol{k'}+\boldsymbol{k''}+\boldsymbol{C}))}\frac{1}{N}\sum_j e^{i\boldsymbol{r}_j\cdot(\boldsymbol{k''}-(-\boldsymbol{C}))} \\
&=\delta_{\boldsymbol{k},\boldsymbol{k'}+\boldsymbol{k''}+\boldsymbol{C}}\delta_{\boldsymbol{k''},-\boldsymbol{C}}=\delta_{\boldsymbol{k},\boldsymbol{k'}}\delta_{\boldsymbol{k''},-\boldsymbol{C}}.
\end{aligned}
\tag{3.15}
$$

The last sum in H is already on deltafunction-form, and will simply give $\delta_{\boldsymbol{k},\boldsymbol{k'}}$, so finally inserting all of this back into H will give:

$$H = \frac{S}{4}\sum_{\boldsymbol{k}'',\boldsymbol{k}',\boldsymbol{k}} J(\boldsymbol{k}'')\delta_{\boldsymbol{k},\boldsymbol{k}'}\Bigg\{\left[\frac{\delta_{\boldsymbol{k}'-\boldsymbol{Q},\boldsymbol{k}''}}{2}+\frac{\delta_{\boldsymbol{k}'+\boldsymbol{Q},\boldsymbol{k}''}}{2}+\delta_{\boldsymbol{k}',\boldsymbol{k}''}\right]\left(b^\dagger_{\boldsymbol{k}}b_{\boldsymbol{k}'}+b_{-\boldsymbol{k}}b^\dagger_{-\boldsymbol{k}'}\right)$$
$$\left[\frac{\delta_{\boldsymbol{k}'-\boldsymbol{Q},\boldsymbol{k}''}}{2}+\frac{\delta_{\boldsymbol{k}'+\boldsymbol{Q},\boldsymbol{k}''}}{2}-\delta_{\boldsymbol{k}',\boldsymbol{k}''}\right]\left(b_{-\boldsymbol{k}}b_{\boldsymbol{k}'}+b^\dagger_{\boldsymbol{k}}b^\dagger_{-\boldsymbol{k}'}\right)$$
$$\left[\delta_{\boldsymbol{k}'-\boldsymbol{Q},\boldsymbol{k}''}+\delta_{\boldsymbol{k}'+\boldsymbol{Q},\boldsymbol{k}''}\right]\left(b^\dagger_{\boldsymbol{k}}b_{\boldsymbol{k}'}+b^\dagger_{-\boldsymbol{k}}b_{-\boldsymbol{k}'}\right)\Bigg\}$$
$$+\frac{h}{2}\sum_{\boldsymbol{k},\boldsymbol{k}'}\delta_{\boldsymbol{k},\boldsymbol{k}'}\left(b^\dagger_{\boldsymbol{k}}b_{\boldsymbol{k}'}+b^\dagger_{-\boldsymbol{k}}b_{-\boldsymbol{k}'}\right). \tag{3.16}$$

Since the operators are bosonic, their commutator is simply a constant and since we neglect all constants in H, we can safely switch the order of the last term in the last bracket in the two bottom lines to make them on the same form as the bracket on the first line. Summing over $\boldsymbol{k}'$ and $\boldsymbol{k}''$ we get:

$$H = \sum_k\Bigg\{\left[\frac{S}{4}\left(\frac{1}{2}[J(\boldsymbol{k}-\boldsymbol{Q})+J(\boldsymbol{k}+\boldsymbol{Q})]+J(\boldsymbol{k})-2J(\boldsymbol{Q})\right)+\frac{h}{2}\right]\left(b^\dagger_{\boldsymbol{k}}b_{\boldsymbol{k}}+b_{-\boldsymbol{k}}b^\dagger_{-\boldsymbol{k}}\right)$$
$$+\left[\frac{S}{4}\left(\frac{1}{2}[J(\boldsymbol{k}-\boldsymbol{Q})+J(\boldsymbol{k}+\boldsymbol{Q})]-J(\boldsymbol{k})\right)\right]\left(b^\dagger_{\boldsymbol{k}}b_{\boldsymbol{k}'}+b_{-\boldsymbol{k}}b^\dagger_{-\boldsymbol{k}'}\right)\Bigg\} \tag{3.17}$$

since $J(\boldsymbol{Q}) = J(-\boldsymbol{Q})$. Naming the square bracket in the first term $A_{\boldsymbol{k}}$, and in the second term $B_{\boldsymbol{k}}$, we can write Hamiltonian in this form:

$$H = \sum_{\boldsymbol{k}}\Psi_{\boldsymbol{k}}\begin{pmatrix}A_{\boldsymbol{k}} & B_{\boldsymbol{k}}\\ B_{\boldsymbol{k}} & A_{\boldsymbol{k}}\end{pmatrix}\Psi^\dagger_{\boldsymbol{k}}, \tag{3.18}$$

with $\Psi_{\boldsymbol{k}} = \begin{pmatrix}b_{-\boldsymbol{k}} & b^\dagger_{\boldsymbol{k}}\end{pmatrix}$. This is readily diagonalized by a Bogoliubov transform, and the matrix that works can be parameterized like this:

$$P_{\boldsymbol{k}} = \begin{pmatrix}\cosh\zeta_{\boldsymbol{k}} & -\sinh\zeta_{\boldsymbol{k}}\\ -\sinh\zeta_{\boldsymbol{k}} & \cosh\zeta_{\boldsymbol{k}}\end{pmatrix}. \tag{3.19}$$

Then, the we can rewrite H and find the conditions that diagonalizes it:

$$H = \sum_{\boldsymbol{k}}\Psi_{\boldsymbol{k}}P^{-1}_{\boldsymbol{k}}P_{\boldsymbol{k}}\begin{pmatrix}A_{\boldsymbol{k}} & B_{\boldsymbol{k}}\\ B_{\boldsymbol{k}} & A_{\boldsymbol{k}}\end{pmatrix}P^\dagger_{\boldsymbol{k}}(P^\dagger_{\boldsymbol{k}})^{-1}\Psi^\dagger_{\boldsymbol{k}} = \sum_{\boldsymbol{k}}\Psi'_{\boldsymbol{k}}D\Psi'^\dagger_{\boldsymbol{k}}, \tag{3.20}$$

where we have defined some new bosons in $\Psi'_{\boldsymbol{k}}$:

$$\alpha_{\boldsymbol{k}} = \cosh\zeta_{\boldsymbol{k}} b_{\boldsymbol{k}} + \sinh\zeta_{\boldsymbol{k}} b^{\dagger}_{-\boldsymbol{k}} \quad \Longrightarrow \quad b_{\boldsymbol{k}} = \cosh\zeta_{\boldsymbol{k}}\alpha_{\boldsymbol{k}} - \sinh\zeta_{\boldsymbol{k}}\alpha^{\dagger}_{-\boldsymbol{k}}. \tag{3.21}$$

These also satisfy the correct commutation relations, as is seen in B.4. The matrix D is:

$$\begin{pmatrix} \cosh 2\zeta_{\boldsymbol{k}} A_{\boldsymbol{k}} - \sinh 2\zeta_{\boldsymbol{k}} B_{\boldsymbol{k}} & \cosh 2\zeta_{\boldsymbol{k}} B_{\boldsymbol{k}} - \sinh 2\zeta_{\boldsymbol{k}} A_{\boldsymbol{k}} \\ \cosh 2\zeta_{\boldsymbol{k}} B_{\boldsymbol{k}} - \sinh 2\zeta_{\boldsymbol{k}} A_{\boldsymbol{k}} & \cosh 2\zeta_{\boldsymbol{k}} A_{\boldsymbol{k}} - \sinh 2\zeta_{\boldsymbol{k}} B_{\boldsymbol{k}} \end{pmatrix}, \tag{3.22}$$

where the hyperbolic trigonometric identities:
$\cosh(a \pm b) = \cosh(a)\cosh(b) \pm \sinh(a)\sinh(b)$ and
$\sinh(a \pm b) = \sinh(a)\cosh(b) \pm \cosh(a)\sinh(b)$ have been used. Demanding the off-diagonals to be zero gives the condition:

$$\tanh 2\zeta_{\boldsymbol{k}} = \frac{B_{\boldsymbol{k}}}{A_{\boldsymbol{k}}}, \tag{3.23}$$

where $\zeta_{\boldsymbol{k}}$ is real and even in $\boldsymbol{k}$ since both $A_{\boldsymbol{k}}$ and $B_{\boldsymbol{k}}$ are as well. Using the identity $\cosh^2(a) - \sinh^2(a) = 1$, we can obtain an expression for the diagonal terms:

$$\Longrightarrow 1 - \tanh^2(a) = \frac{1}{\cosh^2(a)} \Longrightarrow \cosh(a) = \sqrt{\frac{1}{1-\tanh^2(a)}} \tag{3.24a}$$

$$\Longrightarrow \frac{1}{\tanh^2(a)} - 1 = \frac{1}{\sinh^2(a)} \Longrightarrow \sinh(a) = \sqrt{\frac{1}{\frac{1}{\tanh^2(a)} - 1}}. \tag{3.24b}$$

Since we know what $\tanh 2\zeta_{\boldsymbol{k}}$ is in terms of $A_{\boldsymbol{k}}$ and $B_{\boldsymbol{k}}$, we now express $\cosh 2\zeta_{\boldsymbol{k}}$ and $\sinh 2\zeta_{\boldsymbol{k}}$ in these terms as well:

$$\begin{aligned} \cosh 2\zeta_{\boldsymbol{k}} &= \sqrt{\frac{1}{1 - \frac{B_{\boldsymbol{k}}^2}{A_{\boldsymbol{k}}^2}}} = \frac{A_{\boldsymbol{k}}}{\sqrt{A_{\boldsymbol{k}}^2 - B_{\boldsymbol{k}}^2}} \\ \sinh 2\zeta_{\boldsymbol{k}} &= \sqrt{\frac{1}{\frac{A_{\boldsymbol{k}}^2}{B_{\boldsymbol{k}}^2} - 1}} = \frac{B_{\boldsymbol{k}}}{\sqrt{A_{\boldsymbol{k}}^2 - B_{\boldsymbol{k}}^2}}, \end{aligned} \tag{3.25}$$

and finally, the diagonal terms become:

$$A_{\boldsymbol{k}}\frac{A_{\boldsymbol{k}}}{\sqrt{A_{\boldsymbol{k}}^2 - B_{\boldsymbol{k}}^2}} - B_{\boldsymbol{k}}\frac{B_{\boldsymbol{k}}}{\sqrt{A_{\boldsymbol{k}}^2 - B_{\boldsymbol{k}}^2}} = \sqrt{A_{\boldsymbol{k}}^2 - B_{\boldsymbol{k}}^2} = \sqrt{[A_{\boldsymbol{k}} + B_{\boldsymbol{k}}][A_{\boldsymbol{k}} - B_{\boldsymbol{k}}]}. \tag{3.26}$$

Inserting this back into H and writing it all out leaves:

$$H = \sum_{\boldsymbol{k}} \sqrt{A_{\boldsymbol{k}}^2 - B_{\boldsymbol{k}}^2}(\alpha_{\boldsymbol{k}}^\dagger \alpha_{\boldsymbol{k}} + \alpha_{-\boldsymbol{k}} \alpha_{-\boldsymbol{k}}^\dagger). \tag{3.27}$$

After commuting the last term, generating only a constant we can neglect, and switching it to be summed over positive $\boldsymbol{k}$ we arrive at the penultimate form of the Hamiltonian:

$$H = \sum_{\boldsymbol{k}} \omega_{\boldsymbol{k}} \alpha_{\boldsymbol{k}}^\dagger \alpha_{\boldsymbol{k}}, \tag{3.28}$$

with $\omega_{\boldsymbol{k}} = 2\sqrt{(A_{\boldsymbol{k}}^2 - B_{\boldsymbol{k}}^2)}$. This now has the form of a harmonic oscillator, and the ground state is simply defined as the state with no excitations. Its eigenvalue will be the classical eigenvalue plus some quantum correction that came from terms which we dropped along the way. An important fact about the quantum correction is that it is negative, so quantum fluctuations lower the ground state energy compared to the classical value.

3.1.2 easy plane-case

As explained previously, the classical ordering vector is the same here as in the xxx-case, but the ordering now occurs in the xy-plane. Therefore we must make a few minor changes in our treatment. Starting off with the rotated coordinates where spins align along the local x-axis:

$$\begin{aligned} S_i^x &= S_i^{\tilde{x}} \cos(\theta_i) - S_i^{\tilde{y}} \sin(\theta_i) \\ S_i^{\tilde{y}} &= S_i^{\tilde{x}} \sin(\theta_i) + S_i^{\tilde{y}} \cos(\theta_i). \end{aligned} \tag{3.29}$$

Inserting into (3.1) yields the new Hamiltonian:

$$\begin{aligned} H = \frac{1}{2} \sum_{i,j} J_{i,j} [\cos(\theta_i - \theta_j)(S_i^{\tilde{x}} S_j^{\tilde{x}} + S_i^{\tilde{y}} S_j^{\tilde{y}}) \\ + \sin(\theta_i - \theta_j)(S_i^{\tilde{x}} S_j^{\tilde{y}} - S_i^{\tilde{y}} S_j^{\tilde{x}}) + \Delta S_i^{\tilde{z}} S_j^{\tilde{z}}] - h \sum_i S_i^{\tilde{x}}. \end{aligned} \tag{3.30}$$

Going to the the HP-representation for spins ordered along the x-axis:

$$\begin{aligned} S_i^{\tilde{x}} &= S - n_i \\ S_i^+ &= \sqrt{2S - n_i} b_i \\ S_i^- &= b_i^\dagger \sqrt{2S - n_i} \end{aligned} \tag{3.31}$$

and inserting again into the previous Hamiltonian, neglecting constants, keeping only terms to quadratic order one arrives at:

$$H = \frac{S}{2}\sum_{i,j} J_{i,j}\Big\{\frac{1}{2}[\cos(\theta_i-\theta_j)+\Delta](b_i b_j^\dagger + b_i^\dagger b_j) + \frac{1}{2}[\cos(\theta_i-\theta_j)-\Delta](b_i b_j + b_i^\dagger b_j^\dagger) - \cos(\theta_i-\theta_j)(n_i+n_j)\Big\} + h\sum_i n_i. \tag{3.32}$$

From this point onward, it is clear that the description in terms of HP-bosons of the xxx-case is retrieved by taking the limit $\Delta \to 1$, or as we defined: The limit $\epsilon \to 0$, where $\Delta = 1 - \epsilon$.

Retracing the steps one will finally arrive at equation (3.28) with only slight alterations to $A_{\boldsymbol{k}}$ and $B_{\boldsymbol{k}}$:

$$A_{\boldsymbol{k}} = \frac{S}{4}\Big[\frac{1}{2}[J(\boldsymbol{k}-\boldsymbol{Q}) + J(\boldsymbol{k}+\boldsymbol{Q})] + \Delta J(\boldsymbol{k}) - 2J(\boldsymbol{Q})\Big] + \frac{h}{2} \tag{3.33}$$

and

$$B_{\boldsymbol{k}} = \frac{S}{4}\Big[\frac{1}{2}[J(\boldsymbol{k}-\boldsymbol{Q}) + J(\boldsymbol{k}+\boldsymbol{Q})] - \Delta J(\boldsymbol{k})\Big]. \tag{3.34}$$

3.1.3 easy axis-case

In this case one expects ordering along the z-direction if the order is collinear, and in a plane taken to be the xz-plane when the order is coplanar. Therefore we will use the same rotated coordinates as in the xxx-case.

Inserting into equation (3.1) yields:

$$H = \frac{1}{2}\sum_{i,j} J_{i,j}\Big[\big(S_i^{\tilde{z}}\sin(\theta_i) + S_i^{\tilde{x}}\cos(\theta_i)\big)\big(S_j^{\tilde{z}}\sin(\theta_j) + S_j^{\tilde{x}}\cos(\theta_j)\big) \Delta\big(S_i^{\tilde{z}}\cos(\theta_i) - S_i^{\tilde{x}}\sin(\theta_i)\big)\big(S_j^{\tilde{z}}\cos(\theta_j) - S_j^{\tilde{x}}\sin(\theta_j)\big) + S_i^{\tilde{y}}S_j^{\tilde{y}}\Big]. \tag{3.35}$$

Writing it out gives:

$$
\begin{aligned}
H &= \frac{1}{2}\sum_{i,j} J_{i,j}\big[S_i^{\tilde{z}}S_j^{\tilde{z}}\left(\sin\theta_i\sin\theta_j + \Delta\cos\theta_i\cos\theta_j\right) \\
&+ S_i^{\tilde{x}}S_j^{\tilde{x}}\left(\cos\theta_i\cos\theta_j + \Delta\sin\theta_i\sin\theta_j\right) \\
&+ S_i^{\tilde{z}}S_j^{\tilde{x}}\left(\sin\theta_i\cos\theta_j - \Delta\cos\theta_i\sin\theta_j\right) \\
&+ S_i^{\tilde{x}}S_j^{\tilde{z}}\left(\cos\theta_i\sin\theta_j - \Delta\sin\theta_i\cos\theta_j\right) \\
&+ S_i^{\tilde{y}}S_j^{\tilde{y}}\big] - h\sum_i S_i^{\tilde{z}}.
\end{aligned} \tag{3.36}
$$

The two terms that are mixed in $S^{\tilde{x}}$ and $S^{\tilde{z}}$ do then in general not cancel under the summation, leaving some contribution linear in bosonic creation and annihilation operators signifying that there is a difference in the ground state of this model and the XXX-model. However, if the ordering vector is $(0 \vee \pi, 0 \vee \pi)$, i.e. the order is collinear, all sines cancel, and one is left with a quadratic Hamiltonian:

$$
H = \frac{1}{2}\sum_{i,j} J_{i,j}[\cos(\theta_i - \theta_j)(\Delta S_i^{\tilde{z}}S_j^{\tilde{z}} + S_i^{\tilde{x}}S_j^{\tilde{x}}) + S_i^{\tilde{y}}S_j^{\tilde{y}}] - h\sum_i S_i^{\tilde{z}}. \tag{3.37}
$$

From this point onward, the treatment is the same as in the xxx-case, and we of course retrieve it in the limit $\epsilon \to 0$, with $\Delta = 1 + \epsilon$ in this case. Finally, we arrive at the same form as equation (3.28), with:

$$
A_{\boldsymbol{k}} = \frac{S}{4}\Big[\frac{1}{2}[J(\boldsymbol{k}-\boldsymbol{Q}) + J(\boldsymbol{k}+\boldsymbol{Q})] + J(\boldsymbol{k}) - 2\Delta J(\boldsymbol{Q})\Big] + \frac{h}{2} \tag{3.38}
$$

and

$$
B_{\boldsymbol{k}} = \frac{S}{4}\Big[\frac{1}{2}[J(\boldsymbol{k}-\boldsymbol{Q}) + J(\boldsymbol{k}+\boldsymbol{Q})] - J(\boldsymbol{k})\Big]. \tag{3.39}
$$

In the non-collinear case, the treatment becomes different as we saw that the classical ground state was no longer the same as in the xxx-case. There was also a degeneracy present classically which broke down at the level of spin wave theory. Ref. 24 argues that the spin wave correction is maximal when the magnetization M_z, or equivalently S_z is extremized. This will simply be taken as a given here.

$S_z = \cos\theta_A + \cos\theta_B + \cos\theta_C = \cos\theta_A + 2\cos\epsilon\cos\delta.$

Substituting $\cos\theta_A = x$ will give $\partial S^z/\partial x\ \partial x/\partial\theta_A$. The second factor is $-\sin\theta_A$, so we immediately see that there is an extremum at $\theta_A = 0$. (There also is one at π, but as we argued before, we only need to consider θ_A in the range $[0, \cos^{-1}\Delta/(1+\Delta)]$.

There might of course also be another minimum where the remaining part is zero. Inserting the expressions from (2.13) and (2.15) and writing in terms of x, we get:

$$\frac{\partial}{\partial x} x \left(1 + C \frac{1}{ax^2 + b}\right) = 0, \tag{3.40}$$

where $a = (1 - \Delta^2)$, $b = \Delta^2$ and $C = \frac{2(\Delta - \Delta^2)}{1 - \Delta^2} = \frac{2\Delta}{1+\Delta}$, so:

$$0 = 1 + C \frac{1}{ax^2 + b} + x \left(C \frac{-2ax}{(ax^2 + b)^2}\right). \tag{3.41}$$

Defining $z = \frac{1}{ax^2+b} \implies x = \sqrt{(1/Z - b)/a}$, we get:

$$\begin{aligned} 1 + Cz - 2CZ^2(Z^-1 - b) &= 0 \\ \implies 2bCZ^2 - CZ + 1 &= 0 \\ \implies Z &= \frac{C \pm \sqrt{C^2 + 8bC}}{4bC} \\ \implies x &= \sqrt{\frac{\frac{4b}{1 \pm \sqrt{1 + 8\frac{b}{C}}} - b}{a}}. \end{aligned} \tag{3.42}$$

This will reduce nicely when inserting the expressions for a, b and C. Let us start with the inner square root: $1 + 8\Delta^2(1 + \Delta)/2\Delta = 1 + 4\Delta + 4\Delta^2 = (1 + 2\Delta)^2$. Choosing the positive branch, we get:

$$\begin{aligned} \cos\theta_A &= \sqrt{\frac{\frac{4\Delta^2}{2(1+\Delta)} - \Delta^2}{(1 - \Delta)(1 + \Delta)}} = \sqrt{\frac{2\Delta^2 - \Delta^2(1 + \Delta))}{(1 - \Delta)(1 + \Delta)^2}} \\ &= \frac{\Delta}{1 + \Delta} \sqrt{\frac{2 - (1 - \Delta)}{1 - \Delta}} = \frac{\Delta}{1 + \Delta}. \end{aligned} \tag{3.43}$$

This solution is exactly at the boundary of the regime in which we considered θ_A, so these two states are spin flips of each other.

An attempt at building a spin wave theory in the same fashion as previously is bound to fail when one realizes that the expression for θ_i no longer is the simple $\boldsymbol{Q} \cdot \boldsymbol{r}_i$. Instead it can be identified as $2q/\sqrt{3}\sin(\boldsymbol{Q} \cdot \boldsymbol{r}_i)$ which gives $0, q, -q$ on the three sublattices. It is then clear that when doing Fourier transforms, there will not be a nice reduction to deltafunctions giving simple expressions in the end. This case will therefore be exempt from the remainder of the treatment here, and an alternative approach will be discussed briefly in section 4.1.

3.2 Entanglement Hamiltonian

Having all the Hamiltonians on the same form except for when the order is non-collinear in the easy axis-case, we are ready to investigate the entanglement properties. To do so we must first choose a subsystem and then try to find the reduced density operator. Since we know that the reduced density operator is a proper density operator we can try to parameterize it on this form: $\rho_{\mathcal{A}} = e^{-H_E}/\operatorname{Tr}\big(e^{-H_E}\big)$. Where H_E is the entanglement Hamiltonian. Finding its spectrum will be exactly what is needed to calculate the entropies. To find it, we will make use of Wick's theorem.[22] Wick's theorem states that any correlation function in a Gaussian theory can be expressed in terms of two-point correlators. Gaussian here meaning that H is quadratic giving ρ the form of a Gaussian. Our expression was indeed quadratic, so Wick's theorem applies. In particular then, all correlators inside $\mathcal{A}$ can also be expressed in terms of two-point correlators. Knowing this, we can infer that $\rho_{\mathcal{A}}$, being the density operator on $\mathcal{A}$ must be Gaussian as well, and H_E quadratic. To find its explicit form, we must simply demand that it reproduces the correct correlations inside $\mathcal{A}$. This can for a general subsystem not be done analytically, but for some particularly nice choices, obtaining analytic expressions is possible. The subsystem chosen here is that of a ring on the torus as seen in figure 1.1. This system is translationally invariant in the y-direction, and we therefore expect k_y to be a good quantum number. Remembering that our sites consist of both an x- and a y-component, we can Fourier transform them in only the y-component giving:

$$b_{x,k_y} = \frac{1}{\sqrt{L}} \sum_y e^{-ik_y y} b_{x,y}. \tag{3.44}$$

The two point correlators of these operators can be found by completing the transformation to the operators in which the original Hamiltonian is diagonal:

$$\begin{aligned} \langle b^\dagger_{x,k_y} b_{x,k'_y} \rangle &= \Big\langle \frac{1}{\sqrt{L}} \sum_{k_x} e^{ik_x x} b^\dagger_{\boldsymbol{k}} \frac{1}{\sqrt{L}} \sum_{k'_x} e^{-ik'_x x} b_{\boldsymbol{k}'} \Big\rangle \\ = \frac{1}{L} \sum_{k_x,k'_x} e^{ix(k_x - \boldsymbol{k}'_x)} &\cosh\zeta_{\boldsymbol{k}} \cosh\zeta_{\boldsymbol{k}'} \langle \alpha^\dagger_{\boldsymbol{k}} \alpha_{\boldsymbol{k}'} \rangle + \sinh\zeta_{\boldsymbol{k}} \sinh\zeta_{\boldsymbol{k}'} \langle \alpha_{-\boldsymbol{k}} \alpha^\dagger_{-\boldsymbol{k}'} \rangle \\ &- \cosh\zeta_{\boldsymbol{k}} \sinh\zeta_{\boldsymbol{k}'} \langle \alpha^\dagger_{\boldsymbol{k}} \alpha^\dagger_{-\boldsymbol{k}'} \rangle - \sinh\zeta_{\boldsymbol{k}} \cosh\zeta_{\boldsymbol{k}'} \langle \alpha_{-\boldsymbol{k}} \alpha_{\boldsymbol{k}'} \rangle. \end{aligned} \tag{3.45}$$

Since we are in the ground state, what we are really looking at when evaluating expectation values is $\langle \Psi_{Gs} | \hat{O} | \Psi_{Gs} \rangle$. The ground state is identified as the state with no bosons, so acting on it to the right with an annihilation operator or to the left with a creation operator will kill it and give 0. Thus, only the second bracket can have a non-zero contribution. Moreover, having the states orthonormal, the expectation value will be one when $\boldsymbol{k} = \boldsymbol{k}'$ and zero elsewhere which is precisely what a deltafunction is used to describe. We get:

$$\langle b^\dagger_{x,k_y} b_{x,k'_y}\rangle = \frac{1}{L}\sum_{k_x,k'_x} e^{ix(k_x-\boldsymbol{k}'_x)}\sinh\zeta_{\boldsymbol{k}}\sinh\zeta_{\boldsymbol{k}'}\delta_{\boldsymbol{k},\boldsymbol{k}'} = \delta_{k_y,k'_y}\frac{1}{L}\sum_{k_x}\frac{1}{2}(\cosh(2\zeta_{\boldsymbol{k}})-1) \tag{3.46}$$

since $\sinh^2(a) = 1/2\sinh^2(a) + 1/2(\cosh^2(a)-1) = 1/2(\cosh(2a)-1)$. Defining now $\overline{f}(k_y) \equiv \frac{1}{L}\sum_{k_x} f(k_x,k_y)$, we finally obtain:

$$\langle b^\dagger_{x,k_y} b_{x,k'_y}\rangle = \frac{1}{2}\delta_{k_y,k'_y}(\overline{\cosh 2\zeta}(k_y)-1) \equiv \frac{1}{2}\delta_{k_y,k'_y}(\mathcal{C}(k_y)-1). \tag{3.47}$$

The anomalous correlations become:

$$\begin{aligned}\langle b_{x,k_y} b_{x,k'_y}\rangle &= \Big\langle \frac{1}{\sqrt{L}}\sum_{k_x} e^{-ik_x x} b_{\boldsymbol{k}} \frac{1}{\sqrt{L}}\sum_{k'_x} e^{-ik'_x x} b_{\boldsymbol{k}'}\Big\rangle \\ = \frac{1}{L}\sum_{k_x,k'_x} e^{-ix(k_x+k'_x)}&\cosh\zeta_{\boldsymbol{k}}\cosh\zeta_{\boldsymbol{k}'}\langle\alpha_{\boldsymbol{k}}\alpha_{\boldsymbol{k}'}\rangle + \sinh\zeta_{\boldsymbol{k}}\sinh\zeta_{\boldsymbol{k}'}\langle\alpha^\dagger_{-\boldsymbol{k}}\alpha^\dagger_{-\boldsymbol{k}'}\rangle \\ &- \cosh\zeta_{\boldsymbol{k}}\sinh\zeta_{\boldsymbol{k}'}\langle\alpha_{\boldsymbol{k}}\alpha^\dagger_{-\boldsymbol{k}'}\rangle - \sinh\zeta_{\boldsymbol{k}}\cosh\zeta_{\boldsymbol{k}'}\langle\alpha^\dagger_{-\boldsymbol{k}}\alpha_{\boldsymbol{k}'}\rangle.\end{aligned} \tag{3.48}$$

Here, we will only have a contribution from the third term giving a deltafunction:

$$\begin{aligned}\langle b_{x,k_y} b_{x,k'_y}\rangle &= \frac{1}{L}\sum_{k_x,k'_x} e^{-ix(k_x+k'_x)} - \cosh\zeta_{\boldsymbol{k}}\sinh\zeta_{\boldsymbol{k}'}\delta_{\boldsymbol{k},-\boldsymbol{k}'} \\ &= \delta_{k_y,-k'_y}\frac{1}{L}\sum_{k_x} -\frac{1}{2}\sinh(2\zeta_{\boldsymbol{k}}) \equiv -\frac{1}{2}\mathcal{S}(k_y)\end{aligned} \tag{3.49}$$

since $\zeta_{\boldsymbol{k}}$ is even in $\boldsymbol{k}$.

The delta-functions imply that almost all correlations are already zero. Organizing the rest of them in a correlation matrix we can hope to diagonalize the entanglement Hamiltonian, since if the correlation matrix is diagonal in terms of some bosons, the entanglement Hamiltonian is necessarily diagonal in those bosons as well. The correlation matrix is defined as:

$$M_{x,k_y} = \left\langle \begin{pmatrix} b_{x,k_y} \\ b^\dagger_{x,-k_y}\end{pmatrix}\begin{pmatrix} b^\dagger_{x,k_y} & b_{x,-k_y}\end{pmatrix}\right\rangle = \frac{1}{2}\begin{pmatrix}\mathcal{C}(k_y)+1 & -\mathcal{S}(k_y) \\ -\mathcal{S}(k_y) & \mathcal{C}(k_y)-1\end{pmatrix} \tag{3.50}$$

To diagonalize, we try a secondary Bogoliubov transformation:

$$P_{k_y} = \begin{pmatrix} \cosh\eta_{k_y} & -\sinh\eta_{k_y} \\ -\sinh\eta_{k_y} & \cosh\eta_{k_y} \end{pmatrix}. \tag{3.51}$$

The new correlation matrix in terms of the Bogoliubov bosons is then:

$$M'_{x,k_y} = (P^{\dagger}_{k_y})^{-1} M_{x,k_y} P^{-1}_{k_y} = \begin{pmatrix} \langle \beta_{x,k_y} \beta^{\dagger}_{x,k_y} \rangle & \langle \beta_{x,k_y} \beta_{x,-k_y} \rangle \\ \langle \beta^{\dagger}_{x,-k_y} \beta^{\dagger}_{x,k_y} \rangle & \langle \beta^{\dagger}_{x,-k_y} \beta_{x,-k_y} \rangle \end{pmatrix}. \tag{3.52}$$

Having taken the factor $1/2$ to the outside, the off-diagonal terms of the matrix are:

$$\begin{aligned} &\cosh\eta_{k_y}\sinh\eta_{k_y}(\mathcal{C}(k_y)+1) - \cosh^2\eta_{k_y}\mathcal{S}(k_y) \\ &-\sinh^2\eta_{k_y}\mathcal{S}(k_y) + \cosh\eta_{k_y}\sinh\eta_{k_y}(\mathcal{C}(k_y)-1) \end{aligned} \tag{3.53}$$

The $+1$ in the first term and the -1 in the last term cancel, so what is left is completely similar to equation (3.22). Then the condition that diagonalizes becomes:

$$\tanh 2\eta_{k_y} = \frac{\mathcal{S}(k_y)}{\mathcal{C}(k_y)}. \tag{3.54}$$

The diagonal terms are:

$$\begin{aligned} \cosh^2\eta_{k_y}(\mathcal{C}(k_y)\pm 1) + \sinh^2\eta_{k_y}(\mathcal{C}(k_y)\mp 1) - 2\cosh\eta_{k_y}\sinh\eta_{k_y}\mathcal{S}(k_y) \\ = \cosh 2\eta_{k_y}\mathcal{C}(k_y) - \sinh 2\eta_{k_y}\mathcal{S}(k_y) \pm 1, \end{aligned} \tag{3.55}$$

where the upper and lower sign refers to the first and second term on the diagonal respectively. This is again really similar to (3.22), so we can see that the diagonal terms are: $\sqrt{\mathcal{C}(k_y)^2 - \mathcal{S}(k_y)^2} \pm 1$. Defining now $\langle \beta^{\dagger}_{x,k_y} \beta_{x,k_y} \rangle \equiv \lambda_{k_y}$, the correlation matrix becomes:

$$\begin{pmatrix} \lambda_{k_y}+1 & 0 \\ 0 & \lambda_{-k_y} \end{pmatrix}, \tag{3.56}$$

and since it is diagonal, we can deduce that the form of the entanglement Hamiltonian is:

$$H_E = \sum_{k_y} \varepsilon_{k_y} \beta^{\dagger}_{k_y} \beta_{k_y}. \tag{3.57}$$

where ε_{k_y} is related to λ_{k_y}, the mode occupation number, via the standard Bose-Einstein statistics:

$$\lambda_{k_y} = \frac{1}{e^{\varepsilon_{k_y}} - 1}. \tag{3.58}$$

Let us express λ_{k_y} in terms of known quantities:

$$\lambda_{k_y} = \frac{1}{2}\left[\sqrt{\mathcal{C}(k_y)^2 - \mathcal{S}(k_y)^2} - 1\right] = \sqrt{\left(\frac{1}{L}\sum_{k_x}\frac{A_{\boldsymbol{k}}}{\omega_{\boldsymbol{k}}}\right)^2 - \left(\frac{1}{L}\sum_{k_x}\frac{B_{\boldsymbol{k}}}{\omega_{\boldsymbol{k}}}\right)^2} - \frac{1}{2} \quad (3.59)$$

since $\cosh 2\zeta_{\boldsymbol{k}} = 2A_{\boldsymbol{k}}/\omega_{\boldsymbol{k}}$ and $\sinh 2\zeta_{\boldsymbol{k}} = 2B_{\boldsymbol{k}}/\omega_{\boldsymbol{k}}$.

The Rényi entropy in terms of the occupation modes of H_e are in appendix A.4 found to be:

$$S_n = \frac{1}{n-1}\sum_{k_y}\ln\left[(1+\lambda_{k_y})^n - \lambda_{k_y}^n\right]. \quad (3.60)$$

As one might notice, the entanglement Hamiltonian is on a harmonic oscillator form, but we previously emphasized the importance of both the spin wave gap and the ToS-gap to get the scaling properties we want to demonstrate. A pressing question is then where have we "hidden" our tower of states. This is exactly the point at which the staggered field h enters the stage.

3.3 Modified Spin Wave Theory - the role of h

The one thing we have not touched on so far is the role of h, the staggered magnetization we added previously. This was a parameter that was seemingly added completely ad hoc, but the determination of its value will define a modified linear spin wave theory which can be used on finite-size lattices.[25] As explained previously, the order parameter should be zero on the finite-size lattice due to the restoration of symmetry. The order parameter we use, the staggered magnetization, is defined as follows:

$$m(N,h) \equiv \frac{1}{N}\sum_i \langle S_i^{\tilde{z}}\rangle = \frac{1}{N}\sum_i \langle S - n_i\rangle = S - \frac{1}{N}\sum_i \langle b_i^\dagger b_i\rangle. \quad (3.61)$$

To figure out what this expectation value is, we rewrite it in terms of the bosons that diagonalized H:

$$\begin{aligned}
&\frac{1}{N}\sum_i \langle b_i^\dagger b_i\rangle = \frac{1}{N}\sum_{\boldsymbol{k}}\langle b_{\boldsymbol{k}}^\dagger b_{\boldsymbol{k}}\rangle \\
&= \frac{1}{N}\sum_{\boldsymbol{k}}\langle(\cosh\zeta_{\boldsymbol{k}}\alpha_{\boldsymbol{k}}^\dagger - \sinh\zeta_{\boldsymbol{k}}\alpha_{-\boldsymbol{k}})(\cosh\zeta_{\boldsymbol{k}}\alpha_{\boldsymbol{k}} - \sinh\zeta_{\boldsymbol{k}}\alpha_{-\boldsymbol{k}}^\dagger)\rangle \\
&= \frac{1}{N}\sum_{\boldsymbol{k}}\cosh^2\zeta_{\boldsymbol{k}}\langle\alpha_{\boldsymbol{k}}^\dagger\alpha_{\boldsymbol{k}}\rangle + \sinh^2\zeta_{\boldsymbol{k}}\langle\alpha_{-\boldsymbol{k}}\alpha_{-\boldsymbol{k}}^\dagger\rangle \\
&- \cosh\zeta_{\boldsymbol{k}}\sinh\zeta_{\boldsymbol{k}}(\langle\alpha_{-\boldsymbol{k}}\alpha_{\boldsymbol{k}}\rangle + \langle\alpha_{\boldsymbol{k}}^\dagger\alpha_{-\boldsymbol{k}}^\dagger\rangle).
\end{aligned} \quad (3.62)$$

Again, only the second term can contribute leaving us with:

$$\begin{aligned} \frac{1}{N}\sum_{\boldsymbol{k}}\frac{\cosh 2\zeta_{\boldsymbol{k}}}{2}-\frac{1}{2} &= -\frac{1}{2}+\frac{1}{N}\sum_{\boldsymbol{k}}\frac{A_{\boldsymbol{k}}}{\omega_{\boldsymbol{k}}} \\ \implies m(N,h) &= S+\frac{1}{2}-\frac{1}{N}\sum_{\boldsymbol{k}}\frac{A_{\boldsymbol{k}}}{\omega_{\boldsymbol{k}}}. \end{aligned} \tag{3.63}$$

This is essentially a Riemann sum with finite-size integration element $\Delta k_x = \Delta k_y = 2\pi/L$, and so in the limit $L \to \infty$, we obtain an integral. The proper thermodynamic limit is in fact:

$$m_{AF} \equiv \lim_{h\to 0}\lim_{N\to\infty} m(N,h) = S+\frac{1}{2}-\frac{1}{(2\pi)^2}\int_{\boldsymbol{k}} d^2k\frac{A_{\boldsymbol{k}}(h=0)}{\omega_{\boldsymbol{k}}(h=0)}. \tag{3.64}$$

Let us analyze the dispersion a bit, and see what happens at $h = 0$. Due to Goldstone's theorem, and the spontaneous symmetry breaking that happened upon choosing a classical ground state, we know that there should be a massless boson in the theory. In this context that means a spin wave mode with zero dispersion. With the dispersion being in the denominator, that could be a problem.

3.3.1 xxx-case

In the xxx-case, we have:

$$\omega_{\boldsymbol{k}} = S\sqrt{\Big[\frac{1}{2}[J(\boldsymbol{k}-\boldsymbol{Q})+J(\boldsymbol{k}+\boldsymbol{Q})]-J(\boldsymbol{Q})+\frac{h}{S}\Big]\Big[J(\boldsymbol{k})-J(\boldsymbol{Q})+\frac{h}{S}\Big]}. \tag{3.65}$$

At zero field, the first bracket vanishes at $\boldsymbol{k} = \boldsymbol{0}$, and the other at $\boldsymbol{k} = \pm\boldsymbol{Q}$. This means that we have Goldstone modes at these special vectors. If the order is collinear, then the positive and negative $\boldsymbol{Q}$ are equivalent, and the number of Goldstone modes is two. Considering that a rotation about the ordering axis leaves the state unchanged, while rotations about the two other axis does not, this makes sense. When the order is not collinear, the number of Goldstone modes is three.

An important fact about the dispersion is that it is vanishes linearly as we approach these special vectors. Since the minima occurred at single points $\pm\boldsymbol{Q} \neq \boldsymbol{0}$, the model will have a Taylor expansion around those points that is $J(\boldsymbol{Q})$ plus something quadratic in the deviation, δ. Thus, at $\boldsymbol{k} = \pm\boldsymbol{Q}+\delta$, the second bracket in $\omega_{\boldsymbol{k}}$ is $\propto \delta^2$ while the other bracket is $\mathcal{O}(1)$ implying $\omega_{\pm\boldsymbol{Q}+\delta} \propto \delta$. We also know that since the model in k-space only consists of cosines, the Taylor expansion around zero will be $J(\boldsymbol{0})$ plus something quadratic in the deviation. Thus, at $\boldsymbol{k} = \boldsymbol{0}+\delta$, the first bracket is $\propto \delta^2$ while the other one is $\mathcal{O}(1)$ again implying $\omega_{\boldsymbol{0}+\delta} \propto \delta$. In the special case that $\boldsymbol{Q} = \boldsymbol{0}$ and the order is ferromagnetic. Both brackets become $\mathcal{O}(\delta)$ simultaneously implying a quadratic dispersion. This is why the Ferromagnetic case is not included in the treatment here.

Since the dispersion vanishes linearly, the integral will converge uniformly due to the integration element $d^d k \propto k^{(d-1)} d^k$ leaving a finite contribution in all dimensions greater than 1. When looking back at the finite sum, it is clear to see that the divergence is more severe and so we get an infinite magnetization on the finite-size lattice. This is a consequence of the spin wave theory itself and it needs to be remedied somehow. The answer lies in h. A nonzero field will open up a gap in the dispersion that can be used to regularize the sum. The divergent terms in the sum are: $\propto \Delta^d k/\omega_{\boldsymbol{k}\in G}$. The finite-size integration element, Δ, in d dimensions is $(2\pi/L)^d$, so in order for these terms to be finite, we could demand that the gap introduced by h is $\sim L^{-d}$. This is exactly the form of the ToS-gap, and is thus the reason we might get the desired result.

To add a field may seem paradoxical considering that we assumed to be at zero field at the start, but paraphrasing Song et. al.,[8] we will treat it as a variation on the zero-field Hamiltonian.

Rewriting the dispersion at the Goldstone modes and introducing:

$$\Upsilon_{\mathbf{0}} = \sqrt{J(\mathbf{0}) - J(\boldsymbol{Q})}, \tag{3.66a}$$

$$\Upsilon_{\boldsymbol{Q}} = \sqrt{\frac{1}{2}(J(\mathbf{0}) + J(2\boldsymbol{Q})) - J(\boldsymbol{Q})}, \tag{3.66b}$$

we get:

$$\omega_{\mathbf{0}} = S\sqrt{\left[\frac{h}{S}\right]\left[\Upsilon_{\mathbf{0}}^2 + \frac{h}{S}\right]} \tag{3.67a}$$

$$\omega_{\boldsymbol{Q}} = S\sqrt{\left[\Upsilon_{\boldsymbol{Q}}^2 + \frac{h}{S}\right]\left[\frac{h}{S}\right]}, \tag{3.67b}$$

and we can deduce that $h \sim L^{-2d}$. This is the scaling property that will give us the desired result, but the determination of the precise relationship between h and L will define for us the modified spin wave theory. The contributions to $m(N,h)$ from the "problematic" terms are now finite, but varying the ratio of h and L^{-2d} will give us different values for m. As stated before, we should have no magnetization on the finite-size lattice, so we choose our h by demanding this, and solving a set of self consistent equations numerically.

We follow Ref 19 and define the sum excluding the regularized terms as:

$$m^*(N,h) = S + \frac{1}{2} - \frac{1}{N}\sum_{\boldsymbol{k}\notin G}\frac{A_{\boldsymbol{k}}}{\omega_{\boldsymbol{k}}}. \tag{3.68}$$

Demanding $m(N,h) = 0$ gives:

$$m^*(N,h) = \frac{1}{N}\sum_{\boldsymbol{k}\in G}\frac{A_{\boldsymbol{k}}}{\omega_{\boldsymbol{k}}}. \tag{3.69}$$

This relation can be inverted to find h in terms of m^* and N, but note that m^* is still a function of h, so we must iterate the equations numerically to converge to some value for h. We have:

$$m^* = \frac{1}{N}\frac{\frac{1}{4}\Upsilon_{\mathbf{0}}^2 + \frac{h}{2S}}{\sqrt{[\frac{h}{S}][\Upsilon_{\mathbf{0}}^2 + \frac{h}{S}]}} + (N_G - 1)\frac{1}{N}\frac{\frac{1}{4}\Upsilon_{\boldsymbol{Q}}^2 + \frac{h}{2S}}{\sqrt{[\frac{h}{S}][\Upsilon_{\boldsymbol{Q}}^2 + \frac{h}{S}]}}. \tag{3.70}$$

In the collinear case, $\Upsilon_{\mathbf{0}} = \Upsilon_{\boldsymbol{Q}}$ and $N_G = 2$, so we can get an exact expression for $h(N, m^*)$:

$$\begin{aligned}
m^* &= \frac{1}{N}\frac{\frac{1}{2}\Upsilon_{\mathbf{0}}^2 + \frac{h}{S}}{\sqrt{[\frac{h}{S}][\Upsilon_{\mathbf{0}}^2 + \frac{h}{S}]}} \\
&\implies (Nm^*)^2 \frac{h}{S}\left(\Upsilon_{\mathbf{0}}^2 + \frac{h}{S}\right) = \left(\frac{1}{2}\Upsilon_{\mathbf{0}}^2 + \frac{h}{S}\right)^2 \\
&\implies \frac{h}{S}^2\left((Nm^*)^2 - 1\right) + \frac{h}{S}\left((Nm^*)^2 - 1\right)\Upsilon_{\mathbf{0}}^2 = \frac{1}{4}\Upsilon_{\mathbf{0}}^4 \\
&\overset{+\left((Nm^*)^2-1\right)\left(\frac{1}{4}\Upsilon_{\mathbf{0}}^4\right)}{\overbrace{\implies}} \left((Nm^*)^2 - 1\right)\left(\frac{h}{S} + \frac{\Upsilon_{\mathbf{0}}^2}{2}\right)^2 = (Nm^*)^2\frac{1}{4}\Upsilon_{\mathbf{0}}^4 \\
&\implies \left(\frac{h}{S} + \frac{\Upsilon_{\mathbf{0}}^2}{2}\right) = \frac{\frac{1}{2}\Upsilon_{\mathbf{0}}^2}{\sqrt{1 - \frac{1}{(Nm^*)^2}}} \\
&\implies h = \frac{S\Upsilon_{\mathbf{0}}^2}{2}\left(\frac{1}{\sqrt{1 - \frac{1}{(Nm^*)^2}}} - 1\right).
\end{aligned} \tag{3.71}$$

To illustrate why doing this is a good idea, figure 3.1 has been included. The dependence of m on h is only strong near where the dispersion vanishes, so what we have done is to separate m into a part that carries almost all the h-dependence and one that is almost constant in the region around L^{-4}. Choosing then an initial guess for h in this region, we can use equation (3.68) to get an m^* which we can then put into equation (3.71) to get a new value for h. A fixed point of this iteration is obviously at exactly the h that gives zero magnetization. Furthermore, we expect the method to converge within only a few iterations since the value of m^* at the initial guess is close to the value at the fixed point when using equation (3.68). However, each iteration contains a sum over almost the whole BZ, so the numerical cost scales quadratically with the size L

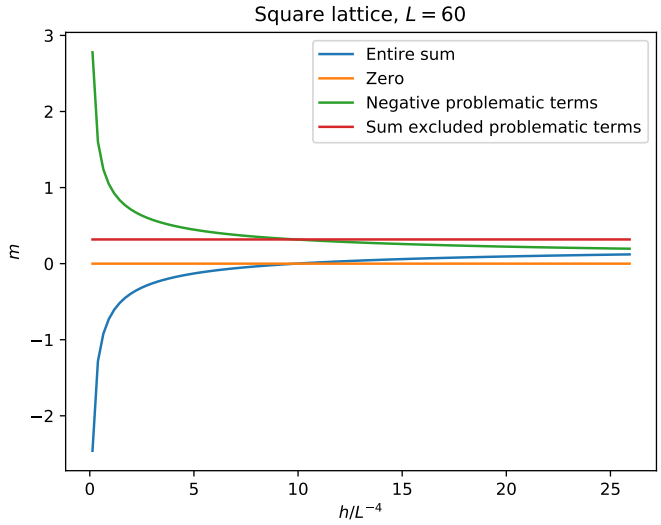

Figure 3.1: Plot of different terms in the magnetization of an nn-model on square lattice as a function of the numerical value of h/L^{-4} showing how most of the dependence on h in m stems from the problematic terms. Note also that the magnetization crosses zero at the same point as the problematic terms crosses the unproblematic terms.

For a general non-collinear case, we can only get an approximate expression:

$$m^* = \frac{1}{N}\frac{\frac{1}{4}+\frac{h}{2S\Upsilon_{\mathbf{0}}^2}}{\sqrt{[\frac{h}{S\Upsilon_{\mathbf{0}}^2}][1+\frac{h}{S\Upsilon_{\mathbf{0}}^2}]}} + (N_G-1)\frac{1}{N}\frac{\frac{1}{4}+\frac{h}{2S\Upsilon_{\mathbf{Q}}^2}}{\sqrt{[\frac{h}{S\Upsilon_{\mathbf{Q}}^2}][1+\frac{h}{S\Upsilon_{\mathbf{Q}}^2}]}}. \tag{3.72}$$

Renaming $\frac{h}{S\Upsilon_{\mathbf{0}}^2} \equiv X$ and $\frac{h}{S\Upsilon_{\mathbf{Q}}^2} \equiv Y$ and expanding the square roots using these as smallness-parameters keeping also the first correction to see the relative error, we get:

$$
\begin{aligned}
Nm^* &= \left(\frac{1}{4}+\frac{1}{2}X\right)\left(X^{-\frac{1}{2}}\left(1+X\right)^{-\frac{1}{2}}\right)+\left(N_G-1\right)\left(\frac{1}{4}+\frac{1}{2}Y\right)\left(Y^{-\frac{1}{2}}\left(1+Y\right)^{-\frac{1}{2}}\right)\\
&\simeq \left(\frac{1}{4}+\frac{1}{2}X\right)\left(X^{-\frac{1}{2}}\left(1-\frac{1}{2}X\right)\right)+\left(N_G-1\right)\left(\frac{1}{4}+\frac{1}{2}Y\right)\left(Y^{-\frac{1}{2}}\left(1-\frac{1}{2}Y\right)\right)\\
&\implies \left(Nm^*\right)^2 \simeq \left(\frac{1}{4}X^{-\frac{1}{2}}\left(1+\frac{3}{2}X\right)+\left(N_G-1\right)\frac{1}{4}Y^{-\frac{1}{2}}\left(1+\frac{3}{2}Y\right)\right)^2\\
&\simeq \frac{1}{16}\Big[X^{-1}+3+\left(N_G-1\right)^2\left(Y^{-1}+3\right)+2\left(N_G-1\right)\left(X^{-\frac{1}{2}}Y^{-\frac{1}{2}}\right)\\
&+2\left(N_G-1\right)\frac{3}{2}\left(X^{\frac{1}{2}}Y^{-\frac{1}{2}}+X^{-\frac{1}{2}}Y^{\frac{1}{2}}\right)\Big]\\
&\implies \simeq \frac{1}{16}\left[\left(\frac{h}{S\Upsilon_{\mathbf{0}}^2}^{-\frac{1}{2}}+\left(N_G-1\right)\frac{h}{S\Upsilon_{\boldsymbol{Q}}^2}^{-\frac{1}{2}}\right)^2+\overbrace{6+3\left(N_G-1\right)\left(\frac{\Upsilon_{\mathbf{0}}}{\Upsilon_{\boldsymbol{Q}}}+\frac{\Upsilon_{\boldsymbol{Q}}}{\Upsilon_{\mathbf{0}}}\right)}^{\mathrm{C}}\right]\\
&\implies \left(Nm^*\right)^2\left(1+\frac{C}{\left(Nm^*\right)^2}\right)\simeq\frac{S}{16h}\left(\Upsilon_{\mathbf{0}}+\left(N_G-1\right)\Upsilon_{\boldsymbol{Q}}\right)^2\\
&\implies h\simeq\frac{S}{16\left(Nm^*\right)^2}\left(\Upsilon_{\mathbf{0}}+\left(N_G-1\right)\Upsilon_{\boldsymbol{Q}}\right)^2\left(1+\frac{C}{\left(Nm^*\right)^2}\right)^{-1}\\
&\simeq\frac{S}{16\left(Nm^*\right)^2}\left(\Upsilon_{\mathbf{0}}+\left(N_G-1\right)\Upsilon_{\boldsymbol{Q}}\right)^2\left(1-\frac{C}{\left(Nm^*\right)^2}\right).
\end{aligned}
\tag{3.73}
$$

So $h\sim N^{-2}$ as expected, and the first correction $\sim N^{-4}$, which is rather small.

3.3.2 easy plane-case

In the easy plane case, the dispersion is:

$$
\omega_{\boldsymbol{k}}=S\sqrt{\left[\frac{1}{2}[J(\boldsymbol{k}-\boldsymbol{Q})+J(\boldsymbol{k}+\boldsymbol{Q})]-J(\boldsymbol{Q})+\frac{h}{S}\right]\left[\Delta J(\boldsymbol{k})-J(\boldsymbol{Q})+\frac{h}{S}\right]},\tag{3.74}
$$

and so at the special vectors, we can express it as:

$$
\omega_{\mathbf{0}}=S\sqrt{\left[\frac{h}{S}\right]\left[\Upsilon_{\mathbf{0}}'^2+\frac{h}{S}\right]}\tag{3.75a}
$$

$$
\omega_{\boldsymbol{Q}}=S\sqrt{\left[\Upsilon_{\boldsymbol{Q}}^2+\frac{h}{S}\right]\left[-\epsilon J(\boldsymbol{Q})+\frac{h}{S}\right]},\tag{3.75b}
$$

where $\Upsilon'_{\mathbf{0}} = \sqrt{\Delta J(\mathbf{0}) - J(\boldsymbol{Q})}$. At zero field, we see that only the zero mode vanishes completely, while the other mode is proportional to the anisotropy parameter ϵ. This naively means that there is only one Goldstone mode at $\mathbf{0}$, which in the xxz-case seems reasonable.

Defining m^* as the sum with the one Goldstone mode removed, the exact equation for h is then found:

$$
\begin{aligned}
m^* \quad &= \frac{1}{N}\frac{\frac{1}{4}\left(\Delta J\left(\mathbf{0}\right) - J\left(\boldsymbol{Q}\right)\right) + \frac{h}{2S}}{\sqrt{[\frac{h}{S}][\Delta J\left(\mathbf{0}\right) - J\left(\boldsymbol{Q}\right) + \frac{h}{S}]}} = \frac{1}{N}\frac{\frac{1}{4}{\Upsilon'_{\mathbf{0}}}^2 + \frac{h}{2S}}{\sqrt{\frac{h}{S}\left({\Upsilon'_{\mathbf{0}}}^2 + \frac{h}{S}\right)}} \\
\implies \quad & \left(Nm^*\right)^2 \frac{h}{S}\left({\Upsilon'_{\mathbf{0}}}^2 + \frac{h}{S}\right) = \left(\frac{1}{4}{\Upsilon'_{\mathbf{0}}}^2 + \frac{h}{2S}\right)^2 \\
\implies \quad & {\frac{h}{S}}^2\left(\left(Nm^*\right)^2 - \frac{1}{4}\right) + \frac{h}{S}\left(\left(Nm^*\right)^2 - \frac{1}{4}\right)\left({\Upsilon'_{\mathbf{0}}}^2\right) = \frac{1}{16}{\Upsilon'_{\mathbf{0}}}^4 \\
& + \left(\left(Nm^*\right)^2 - \tfrac{1}{4}\right)\left(\tfrac{1}{4}{\Upsilon'_{\mathbf{0}}}^2\right) \\
& \qquad \Uparrow \Downarrow \\
\implies \quad & \left(\left(Nm^*\right)^2 - \frac{1}{4}\right)\left(\frac{h}{S} + \frac{1}{2}{\Upsilon'_{\mathbf{0}}}^2\right)^2 = \left(Nm^*\right)^2 \frac{1}{4}{\Upsilon'_{\mathbf{0}}}^2 \\
\implies \quad & \frac{h}{S} + \frac{1}{2}{\Upsilon'_{\mathbf{0}}}^2 = \frac{1}{2}{\Upsilon'_{\mathbf{0}}}^2\left(\frac{1}{\sqrt{1 - \frac{1}{4\left(Nm^*\right)^2}}}\right) \\
\implies \quad & h = \frac{S}{2}{\Upsilon'_{\mathbf{0}}}^2\left(\frac{1}{\sqrt{1 - \frac{1}{4\left(Nm^*\right)^2}}} - 1\right).
\end{aligned}
\tag{3.76}
$$

However, when the limit $\epsilon \to 0$ is taken, we should end up in the xxx-case again. As we can see from equation (3.74), the Goldstone modes at $\boldsymbol{Q}$ are retrieved in this limit, so at some point we must cross over from having only one Goldstone mode to having two or three. The smaller ϵ gets, the stronger the dependence of m on these "almost" Goldstone modes will be. We therefore try to remove the "almost" Goldstone modes from the sum in the definition of m^* as well. This gives:

$$
m^* = \frac{1}{N}\frac{\frac{1}{4}\Upsilon_{\mathbf{0}}^2 + \frac{h}{2S} - \frac{\epsilon}{4}J(\mathbf{0})}{\sqrt{[\frac{h}{S}][\Upsilon_{\mathbf{0}}^2 + \frac{h}{S} - \epsilon J(\mathbf{0})]}} + (N_G - 1)\frac{1}{N}\frac{\frac{1}{4}\Upsilon_{\boldsymbol{Q}}^2 + \frac{h}{2S} - \frac{\epsilon}{4}J(\boldsymbol{Q})}{\sqrt{[\frac{h}{S} - \epsilon J(\boldsymbol{Q})][\Upsilon_{\boldsymbol{Q}}^2 + \frac{h}{S}]}}. \tag{3.77}
$$

Defining some new quantities:

$$
\begin{aligned}
a_{\mathbf{0}} &= \frac{h}{S} + \frac{1}{2}(\Upsilon_{\mathbf{0}}^2 - \epsilon J(\mathbf{0})) \\
b_{\mathbf{0}} &= \frac{1}{2}(\Upsilon_{\mathbf{0}}^2 - \epsilon J(\mathbf{0})) \\
a_{\boldsymbol{Q}} &= \frac{h}{S} + \frac{1}{2}(\Upsilon_{\boldsymbol{Q}}^2 - \epsilon J(\boldsymbol{Q})) \\
b_{\boldsymbol{Q}} &= \frac{1}{2}(\Upsilon_{\boldsymbol{Q}}^2 + \epsilon J(\boldsymbol{Q}))
\end{aligned} \tag{3.78}
$$

we can rewrite (3.77) as:

$$
\begin{aligned}
m^* &= \frac{1}{N}\frac{\frac{a_{\mathbf{0}}}{2}}{\sqrt{(a_{\mathbf{0}} + b_{\mathbf{0}})(a_{\mathbf{0}} - b_{\mathbf{0}})}} + (N_G - 1)\frac{1}{N}\frac{\frac{a_{\boldsymbol{Q}}}{2}}{\sqrt{(a_{\boldsymbol{Q}} + b_{\boldsymbol{Q}})(a_{\boldsymbol{Q}} - b_{\boldsymbol{Q}})}} \\
&\implies 2Nm^* = \frac{1}{\sqrt{1 - \left(\frac{b_{\mathbf{0}}}{a_{\mathbf{0}}}\right)^2}} + (N_G - 1)\frac{1}{\sqrt{1 - \left(\frac{b_{\boldsymbol{Q}}}{a_{\boldsymbol{Q}}}\right)^2}}.
\end{aligned} \tag{3.79}
$$

To proceed, we use that:

$$
\frac{b_{\mathbf{0}}}{a_{\mathbf{0}}} = \frac{\frac{1}{2}(\Upsilon_{\mathbf{0}}^2 - \epsilon J(\mathbf{0}))}{\frac{h}{S} + \frac{1}{2}(\Upsilon_{\mathbf{0}}^2 - \epsilon J(\mathbf{0}))} = \frac{1}{1 + \frac{\frac{2h}{S}}{\Upsilon_{\mathbf{0}}^2 - \epsilon J(\mathbf{0})}} \tag{3.80}
$$

$$
\frac{b_{\boldsymbol{Q}}}{a_{\boldsymbol{Q}}} = \frac{\frac{1}{2}(\Upsilon_{\boldsymbol{Q}}^2 + \epsilon J(\boldsymbol{Q}))}{\frac{h}{S} + \frac{1}{2}(\Upsilon_{\boldsymbol{Q}}^2 - \epsilon J(\boldsymbol{Q}))} = \frac{1}{1 + \frac{2(\frac{h}{S} - \epsilon J(\boldsymbol{Q}))}{\Upsilon_{\boldsymbol{Q}}^2 - \epsilon J(\boldsymbol{Q})}} \tag{3.81}
$$

and expand like a geometric series in the small quantities:

$$
\left(1 - \left(\frac{1}{1+x}\right)^2\right)^{-\frac{1}{2}} \simeq \left(1 - (1-x)\right)^2\Big)^{-\frac{1}{2}} \simeq (2x)^{-\frac{1}{2}}. \tag{3.82}
$$

This leaves us with:

$$
\begin{aligned}
2Nm^* &\simeq \left(\frac{4\frac{h}{S}}{\Upsilon_{\mathbf{0}}^2 - \epsilon J(\mathbf{0}))}\right)^{-\frac{1}{2}} + (N_G - 1)\left(\frac{4(\frac{h}{S} - \epsilon J(\boldsymbol{Q})}{\Upsilon_{\boldsymbol{Q}}^2 - \epsilon J(\boldsymbol{Q}))}\right)^{-\frac{1}{2}} \\
&\overset{\cdot(\frac{h}{S})^{\frac{1}{2}}}{\Longrightarrow} \quad 2Nm^*(\frac{h}{S})^{\frac{1}{2}} \simeq \frac{1}{2}\sqrt{\Upsilon_{\mathbf{0}}^2 - \epsilon J(\mathbf{0})} + (N_G - 1)\frac{\sqrt{\Upsilon_{\boldsymbol{Q}}^2 - \epsilon J(\boldsymbol{Q})}}{\sqrt{1+\kappa}} \\
&\Longrightarrow \quad h \simeq \frac{S}{16(Nm^*)^2}\left(\sqrt{\Upsilon_{\mathbf{0}}^2 - \epsilon J(\mathbf{0})} + (N_G - 1)\frac{\sqrt{\Upsilon_{\boldsymbol{Q}}^2 - \epsilon J(\boldsymbol{Q})}}{\sqrt{1+\kappa}}\right)^2 \quad (3.83)
\end{aligned}
$$

where $\kappa \equiv -S\epsilon J(\boldsymbol{Q})/h$. This quantity now also depends on h and must be iterated over in the same fashion as m^*. It is also from this equation seen that the "almost" Goldstone modes become more important the smaller ϵ is compared to h, and in the limit $\epsilon \to 0$ the expression reduces nicely to the leading term of equation (3.73). The first correction in this case would be different than in the previous case, but the magnitude of the order would similarly have been $\sim N^{-4}$.

3.3.3 easy axis-case

Here, the dispersion is

$$
\omega_{\boldsymbol{k}} = S\sqrt{\left[\frac{1}{2}[J(\boldsymbol{k}-\boldsymbol{Q}) + J(\boldsymbol{k}+\boldsymbol{Q})] - \Delta J(\boldsymbol{Q}) + \frac{h}{S}\right]\left[J(\boldsymbol{k}) - \Delta J(\boldsymbol{Q}) + \frac{h}{S}\right]}. \quad (3.84)
$$

Only considering collinear order and labeling $\Upsilon_{\mathbf{0}}^{\prime 2} = \sqrt{J(\mathbf{0}) - \Delta J(\boldsymbol{Q})}$, (recall that $\Delta = 1 + \epsilon$ here), we get:

$$
\omega_{\mathbf{0},\boldsymbol{Q}} = S\sqrt{\left[\Upsilon_{\mathbf{0}}^{\prime 2} + \frac{h}{S}\right]\left[-\epsilon J(\boldsymbol{Q}) + \frac{h}{S}\right]}. \quad (3.85)
$$

This is non-zero at both special vectors and it means that we have no broken continuous symmetries. The only possible symmetry to break in the XXZ-model was the spin rotational symmetry about the z-axis, and when all spins point along it, a rotation will not change the state. Thus, the symmetry is unbroken.

Taking the limit ϵ we will again retrieve all the Goldstone modes of the xxx-case. Following then immediately the same convention of defining m^* as the sum excluded the possibly problematic terms, we get the relations:

$$
\begin{aligned}
m^* &= \frac{1}{N}\frac{\frac{1}{2}\Upsilon_{\mathbf{0}}^{'2}+\frac{h}{S}-\frac{\epsilon}{2}J\left(\boldsymbol{Q}\right)}{\sqrt{\left(\frac{h}{S}-\epsilon J\left(\boldsymbol{Q}\right)\right)\left(\Upsilon_{\mathbf{0}}^{'2}+\frac{h}{S}\right)}} \\
\Longrightarrow \quad & \left(Nm^*\right)^2\left(\frac{h}{S}-\epsilon J\left(\boldsymbol{Q}\right)\right)\left(\Upsilon_{\mathbf{0}}^{'2}+\frac{h}{S}\right)=\left(\frac{1}{2}\left(\Upsilon_{\mathbf{0}}^{'2}-\epsilon J\left(\boldsymbol{Q}\right)\right)+\frac{h}{S}\right)^2 \\
\Longrightarrow \quad & \frac{h}{S}^2\left(\left(Nm^*\right)^2-1\right)+\frac{h}{S}\left(\left(Nm^*\right)^2-1\right)\left(\Upsilon_{\mathbf{0}}^{'2}-\epsilon J\left(\boldsymbol{Q}\right)\right) \\
& =\frac{1}{4}\left(\Upsilon_{\mathbf{0}}^{'2}-\epsilon J\left(\boldsymbol{Q}\right)\right)^2+\left(Nm^*\right)\Upsilon_{\mathbf{0}}^{'2}\epsilon J\left(\boldsymbol{Q}\right) \\
& \quad +\left(\left(Nm^*\right)^2-1\right)\tfrac{1}{4}\left(\Upsilon_{\mathbf{0}}^{'2}-\epsilon J\left(\boldsymbol{Q}\right)^2\right) \\
& \qquad\qquad \overbrace{\Longrightarrow} \\
\Longrightarrow \quad & \left(\left(Nm^*\right)^2-1\right)\left(\frac{h}{S}+\frac{1}{2}\left(\Upsilon_{\mathbf{0}}^{'2}-\epsilon J\left(\boldsymbol{Q}\right)\right)\right)^2 \\
& =\left(Nm^*\right)^2\underbrace{\left(\frac{1}{4}\left(\Upsilon_{\mathbf{0}}^{'2}-\epsilon J\left(\boldsymbol{Q}\right)\right)^2+\Upsilon_{\mathbf{0}}^{'2}\epsilon J\left(\boldsymbol{Q}\right)\right)}_{\frac{1}{4}\left(\Upsilon_{\mathbf{0}}^{'2}+\epsilon J\left(\boldsymbol{Q}\right)\right)^2} \\
\Longrightarrow \quad & \frac{h}{S}+\frac{1}{2}\left(\Upsilon_{\mathbf{0}}^{'2}-\epsilon J\left(\boldsymbol{Q}\right)\right)=\frac{1}{2}\left(\Upsilon_{\mathbf{0}}^{'2}+\epsilon J\left(\boldsymbol{Q}\right)\right)\left(\frac{1}{\sqrt{1-\frac{1}{\left(Nm^*\right)^2}}}\right) \\
& \qquad \overbrace{\Upsilon_{\mathbf{0}}^2=\Upsilon_{\mathbf{0}}^{'2}+\epsilon J\left(\boldsymbol{Q}\right)}^{\Longrightarrow} \\
h \quad & =\frac{S\Upsilon_{\mathbf{0}}^2}{2}\left(\frac{1}{\sqrt{1-\frac{1}{\left(Nm^*\right)^2}}}\right)+S\epsilon J\left(\boldsymbol{Q}\right). \qquad (3.86)
\end{aligned}
$$

This is now the same as in the xxx-case plus some finite part proportional to the anisotropy. This is a result that will be discussed in the next section.

Chapter 4

Results

4.1 easy axis-case

Let us first take a look at the Ising case, where we saw that h approached some finite value rather than zero. In the collinear case, it did in fact approach the rather specific value $S\epsilon J(\boldsymbol{Q})$.

As explained previously, there will only be a strong dependence on h in m if the dispersion is close to being zero. Since both the brackets in equation (3.84) were finite in the absence of a field, it makes sense that in order to manipulate the value of m by varying h, it will have to take on a finite value that cancels the bracket plus something that is small. This is however inconsistent with the assumption that h should vanish in the thermodynamic limit, so we could have just as well added a finite staggered field from the very start. Since h couples to S^z the same way S^z couples to them itself, there will be an exact cancellation. The part of $A_{\boldsymbol{k}}$ stemming from $S_i^z S_j^z$ is $-S\Delta J(\boldsymbol{Q})/2$ while the part stemming from hS_i^z is now $S\epsilon J(\boldsymbol{Q})/2 + \mathcal{O}(1/N^2)$. Recalling that $\Delta = 1 + \epsilon$, we see that the finite part of h cancels the part coming from the anisotropy parameter ϵ. This leaves us with the expression for the no field xxx-case plus something small that incidentally also was the xxx-value for h. We have by this choice of modification to our spin wave theory effectively forced ourselves back to the XXX-model, and thus the results of this procedure must be said to be nonsensical. The procedure of modified spin wave theory does not work when there are no Goldstone modes due to the dispersion not really being close to zero. This raises further questions on the validity of the approach.

When it comes to the triangular model in the easy axis-case, the ground state was correctly identified, but when trying to build a spin wave theory on top of it the description would no longer fit into the framework developed here. Even though this case was not explored for other models than the nn-model on the triangular lattice, there is reason to expect that one would run into trouble with the Fourier transforms for any other model that would

order non-collinearly. The way to proceed however, would be to split the sum up into contributions from the three sublattices inserting the appropriate value of J_{ij} and $\theta_{i,j}$ by hand. This would in turn result in three sets of spin waves defined in a magnetic Brillouin zone a third of the size of the original Brillouin zone such that the number of spin waves is the same. Considering that a non-collinear state would break the spin rotation symmetry, there should be one Goldstone mode in one of these sets. Then it is clear that these three sets of spin waves will have their own dispersions connected with them even though they exist on the same place in k-space.

Lastly, since there is a Goldstone mode present, the modification of the spin wave theory may still not be inconsistent in the same way as in the collinear case. However, since the field coupled to S^z the same way S^z coupled to itself, the converse is also true: The XXZ-Hamiltonian in the easy plane-case can be viewed as an XXX-Hamiltonian in an effective external field given by the anisotropy. It is then not clear that we could even demand zero magnetization to begin with, as that only needed to be the case in no external field. One could attempt to make the magnetization zero and relieve the need of having several sets of spin waves by averaging over each sublattice being at each site. This however, would imply choosing a different state on which to build the spin wave theory and the procedure of spin wave theory is contingent upon choosing a single ground state thus breaking the symmetry by construction.

4.2 easy plane-case

Let us now take a look at the more meaningful results. First off: In all numerical calculations the models looked at were nn-models on either the square lattice or the triangular lattice. Having mapped the triangular lattice onto the square lattice, these models are in k-space: $2J(\cos k_x + \cos k_y)$ and $2J(\cos k_x + \cos k_y + \cos(k_x + k_y)$. They will have $\boldsymbol{Q} = (\pi, \pi)$ and $(2\pi/3, 2\pi/3)$ respectively. The values for J and S were set to 1 and $1/2$. We will also denote $q \equiv q_y$ since k_x is always summed over.

Having found a way to calculate h, we are ready calculate the mode occupation numbers which we consequently will put into equation 3.60 to get the Rényi entropy. The figures 4.1 and 4.2 show λ_{k_y} plotted as a function of k_y for a few choices of ϵ. There are quite a few things to note here. Looking first only on the graph for $\epsilon = 0$, the occupation numbers at the special vectors are large. This we could have already guessed from the fact that it is at these vectors the dispersion is small. There is also a difference between the collinear and the non-collinear case in that they have different height on the peaks at $\boldsymbol{Q}$ compared to the peak at $\mathbf{0}$. This relates to the fact that for collinear order $\Upsilon_{\boldsymbol{Q}} = \Upsilon_{\mathbf{0}}$ while for non-collinear order $\Upsilon_{\boldsymbol{Q}} \neq \Upsilon_{\mathbf{0}}$. As we will see shortly, it is the modes of large occupation that give us the scaling of the subleading term, while the other modes being roughly constant will give us the area law term. The slight dependence on k_y around the special vectors is shown in Ref. 1 to fit rather well with an even smaller subleading term $\propto lnlnL$, but this will not be investigate that any further here.

Let us take a look at the asymptotic form of λ_{k_y}:

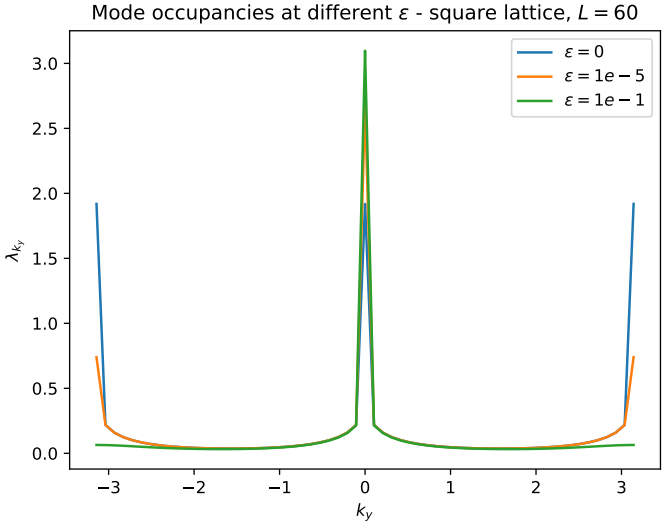

Figure 4.1: Mode occupation numbers of nn-model on a square lattice of size $L = 60$ as a function of k_y for three different values of the anisotropy parameter ϵ.

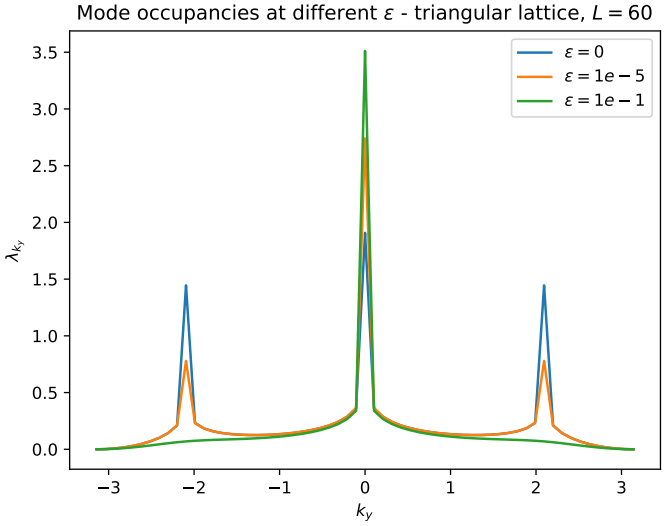

Figure 4.2: Mode occupation numbers of nn-model on a triangular lattice of size $L = 60$ as a function of k_y for three different values of the anisotropy parameter ϵ.

$$\begin{aligned}\lambda_{k_y} &= \frac{1}{2L}\sqrt{\left(\sum_{k_x}\frac{A_{\boldsymbol{k}}}{\sqrt{A_{\boldsymbol{k}}^2-B_{\boldsymbol{k}}^2}}\right)^2-\left(\sum_{k_x}\frac{B_{\boldsymbol{k}}}{\sqrt{A_{\boldsymbol{k}}^2-B_{\boldsymbol{k}}^2}}\right)^2}-\frac{1}{2} \quad \overset{a^2-b^2=(a+b)(a-b)}{\Longrightarrow} \\ &= \frac{1}{2L}\sqrt{\left(\sum_{k_x}\frac{A_{\boldsymbol{k}}-B_{\boldsymbol{k}}}{\sqrt{(A_{\boldsymbol{k}}+B_{\boldsymbol{k}})(A_{\boldsymbol{k}}-B_{\boldsymbol{k}})}}\right)\left(\sum_{k_x'}\frac{A_{\boldsymbol{k}'}+B_{\boldsymbol{k}'}}{\sqrt{(A_{\boldsymbol{k}'}+B_{\boldsymbol{k}'})(A_{\boldsymbol{k}'}-B_{\boldsymbol{k}'})}}\right)}-\frac{1}{2} \\ &= \frac{1}{2L}\sqrt{\sum_{k_x}\Theta_{k_x,k_y}\sum_{k_x'}\Theta^{-1}_{k_x',k_y}}-\frac{1}{2},\end{aligned} \tag{4.1}$$

where we define $\Theta_{k_x,k_y} \equiv \sqrt{\frac{A_{\boldsymbol{k}}-B_{\boldsymbol{k}}}{A_{\boldsymbol{k}}+B_{\boldsymbol{k}}}}$

Now we can see that everything is $\mathcal{O}(1)$ as long as $A_{\boldsymbol{k}} - B_{\boldsymbol{k}}$ and $A_{\boldsymbol{k}} + B_{\boldsymbol{k}}$ do not tend to zero. However, as we have discussed already, they will tend to zero at the Goldstone modes. The manner in which they approach zero will thus give us the asymptotic behaviour of our mode occupancy.

At $\boldsymbol{k} = 0$, we have:

$$\Theta_{\mathbf{0}} = \sqrt{\frac{\frac{S}{4}(2\Delta J(\mathbf{0}) - 2J(\boldsymbol{Q})) + \frac{h}{2}}{\frac{h}{2}}} \simeq \Upsilon'_{\mathbf{0}}\sqrt{\frac{S}{h}}, \tag{4.2}$$

and at $\boldsymbol{k} = \pm\boldsymbol{Q}$, we have:

$$\Theta^{-1}_{\boldsymbol{Q}} = \sqrt{\frac{\frac{S}{4}\big((J(\mathbf{0}) + J(2Q)) - 2J(\boldsymbol{Q})\big) + \frac{h}{2}}{\frac{S}{4}\left(-2\epsilon J(\boldsymbol{Q})\right) + \frac{h}{2}}} \simeq \Upsilon_{\boldsymbol{Q}}\sqrt{\frac{1}{1+\kappa}}\sqrt{\frac{S}{h}}. \tag{4.3}$$

In the limit of no anisotropy, this reduces to $\Upsilon_{\mathbf{0}}\sqrt{S/h}$ and $\Upsilon_{\boldsymbol{Q}}\sqrt{S/h}$.

Let us proceed by inserting our approximations for h and check how the contributions from the Goldstone modes scales with L:

In the limit of large N, we have $m^*(N,h) \to m_{\mathrm{AF}}$. This is true since G is a set of single points in which the integrand is finite, and so having them removed from the integral does not change its value.

Equation 3.83 simplifies to

$$h = \frac{S}{16(Nm_{AF})^2}C(\kappa)^2, \tag{4.4}$$

where $C(\kappa) \equiv \sqrt{\Upsilon^2_{\mathbf{0}} - \epsilon J(\mathbf{0})} + (N_G - 1)\frac{\sqrt{\Upsilon^2_{\boldsymbol{Q}} - \epsilon J(\boldsymbol{Q})}}{\sqrt{1+\kappa}}$.

Inserting this into our expressions for λ_q and λ_0, we get:

$$\begin{aligned}\lambda_0 &\sim \frac{1}{2L}\sqrt{\Theta_0\sum_{k_x}\Theta^{-1}_{k_x,k_y}} - \frac{1}{2} \simeq \sqrt{\frac{1}{4L}\Upsilon'_{\mathbf{0}}\sqrt{\frac{16(Nm_{AF})^2}{C(\kappa)^2}\alpha_0} - \frac{1}{2}} \\ &\sim \sqrt{\frac{\Upsilon'_{\mathbf{0}}Lm_{AF}\alpha_0}{C(\kappa)}} \qquad (4.5a)\\ \lambda_q &\sim \frac{1}{2L}\sqrt{\Theta_q^{-1}\sum_{k_x}\Theta_{k_x,k_y}} - \frac{1}{2} \simeq \sqrt{\frac{1}{4L}\Upsilon_{\boldsymbol{Q}}\frac{1}{\sqrt{1+\kappa}}\sqrt{\frac{16(Nm_{AF})^2}{C(\kappa)^2}\alpha_q} - \frac{1}{2}} \\ &\sim \sqrt{\frac{\Upsilon_Q Lm_{AF}\alpha_q}{C(\kappa)\sqrt{1+\kappa}}}, \qquad (4.5b)\end{aligned}$$

where

$$\begin{aligned}\alpha_0 &= \frac{1}{2\pi}\int_{-\pi}^{\pi}\mathrm{d}k_x\Theta^{-1}_{k_x,0} \qquad (4.6a)\\ \alpha_q &= \frac{1}{2\pi}\int_{-\pi}^{\pi}\mathrm{d}k_x\Theta_{k_x,q}. \qquad (4.6b)\end{aligned}$$

In the Goldstone modes then, to leading order, we have in the argument of the logarithm $(1+\lambda_G)^n - \lambda_G^n \simeq \lambda_G^{n-1}$ in (3.60). Because of log-properties the exponent exactly cancels the factor in front, and we can forget about all the factors in $\lambda_{0,q}$ except $L^{1/2}$. The contribution to S_n from each of these terms will now be $\sim \ln(L)/2$, giving a universal prefactor then $b_n = N_G/2$.

The remaining $L - N_G$ values of k_y will each give some constant contribution, and since there are $\sim L$ of them, these accumulate to give the area law term.

One question that remains now is what do we do with the "almost" Goldstone modes in equation 4.5b? We know that we should only have one Goldstone mode in the XXZ-model, but the form of the equation suggests that there will be a contribution to the subleading term from each of the "almost" Goldstone modes as well. It is important then to remember how we defined κ: $\kappa \equiv -S\epsilon J(\boldsymbol{Q})/h$. In the thermodynamic limit where $h \to 0$, κ will be infinite for all nonzero values of ϵ, and zero at the Heisenberg point. Using $\lambda_q/\sqrt{L}$ as an order parameter, we then get a sharp phase transition between the XXX-model and the XXZ-model. On the finite-size lattice, the crossover will occur over some range of ϵ for a given L. It will therefore, for sufficiently small ϵ appear as if the system has two or three broken symmetries even though strictly speaking, for non-zero ϵ, there will only be one broken symmetry.

Let us now look a bit more at the dependence on ϵ in figures 4.1 and 4.2. We can see that at the peak in the modes at $\boldsymbol{Q}$ become smaller as ϵ is increased almost disappearing

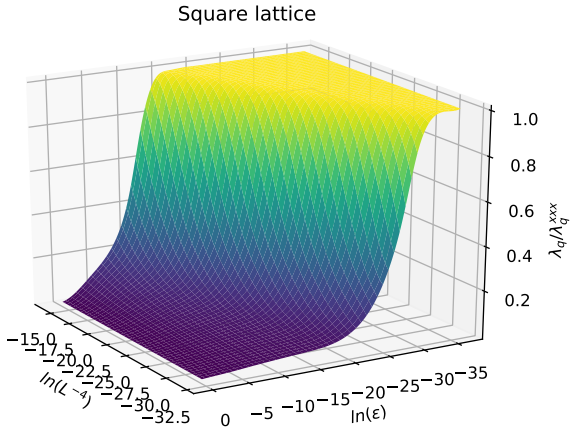

Figure 4.3: Mode occupation number of the nn-model on the square lattice at $k_y = q$ as a function of system size L and anisotropy parameter ϵ

totally at large enough values. This is precisely the behaviour we would have predicted in going from two or three Goldstone modes to one. There is also a similar effect on the zero mode, but its value increases instead. This seems a bit harder to explain, but at least it remains a clear peak consistent with having one Goldstone mode. Another question now is how this behaviour depends on L when it is finite. How big does the system have to be to appreciably notice a given change in ϵ? To try to understand this crossover better, let us plot only these modes as functions of L and ϵ. In fact, they will be plotted as a function of ϵ and L^{-4} as it initially was in the region where $\epsilon \sim h$ we expected the contribution of the "almost" Goldstone modes to become important when finding h. To make for easier comparisons between different models these have also been normalized with their value at $\epsilon = 0$ for any given L.

The results of doing so is shown in figures 4.3, 4.4, 4.5 and 4.6, and the crossover is clear as day in all of them. The first thing to note is that the plots for the different models have many similarities again perhaps pointing to some connection at a deeper level in this scaling phenomenon. The modes at q move away from 1 to some small value, and the way in which they do so seems to be similar for all L, only starting at a different value of ϵ. In the mode at 0, there appears to be two separate crossovers: One when moving from pure Heisenberg to XXZ-model and one in the region around $\epsilon = 1$. At $\epsilon = 1$, we are really in the XY-model, so this may be interpreted as a crossover from XY-model to XXZ-model. The plot is on "loglog" format, so the details of the second crossover are impossible to make out from it. The first crossover however, appears to be linear in this representation. A view of figure 4.5 from a different angle, as shown in figure 4.7, demonstrates the data collapse that occurs. By the right choice of argument, the crossover could be described

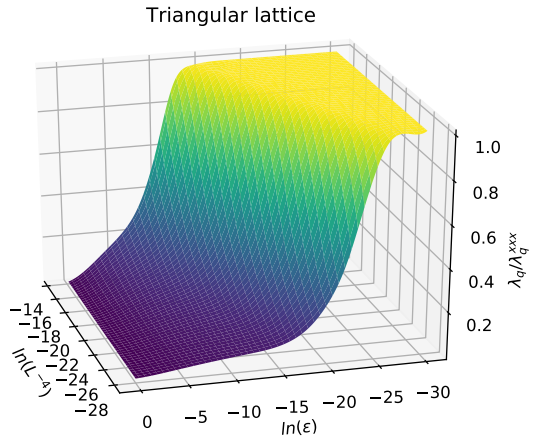

Figure 4.4: Mode occupation number of the nn-model on the triangular lattice at $k_y = q$ as a function of system size L and anisotropy parameter ϵ

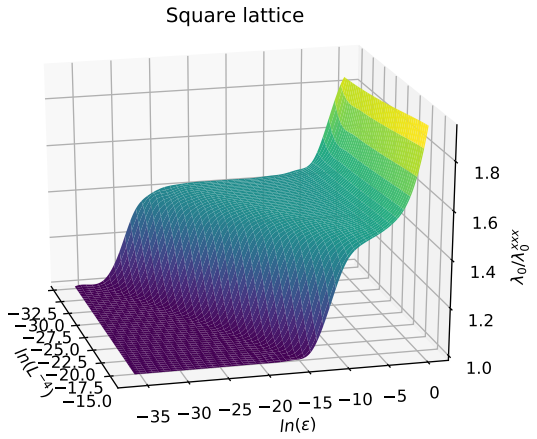

Figure 4.5: Mode occupation number of the nn-model on the square lattice at $k_y = 0$ as a function of system size L and anisotropy parameter ϵ

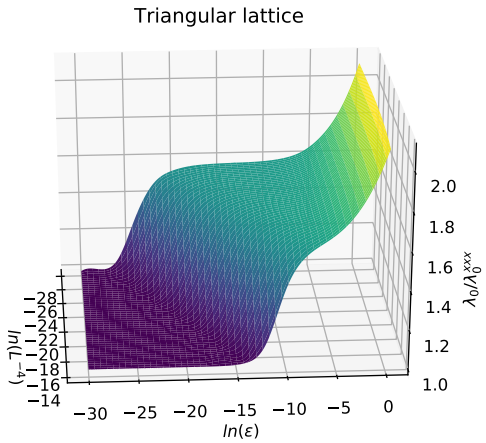

Figure 4.6: Mode occupation number of the nn-model on the triangular lattice at $k_y = 0$ as a function of system size L and anisotropy parameter ϵ

by a function of a single argument. Adopting the notation of equation 8.7 in Ref. 12, we have:

$$\lambda_{0,q} \sim L^{\beta} f_{0,q}(\epsilon/L^{\Delta}), \tag{4.7}$$

where β and Δ are some critical exponents, and f denotes the scaling functions. This is then somehow analogous to the crossover seen in ferromagnets with $\lambda_{0,q}$ taking the place of the order parameter, and L and ϵ taking the places of the relevant variables, but has never before been seen in this context.

We already saw that the limiting behaviour of the modes were to approach $\sqrt{L}$, so $\beta = 1/2$. Figure 4.8 shows $\lambda_q/\sqrt{L}$ as a function of L so we can try and see how quickly it approaches its asymptotic form. Note also that the different models approaches different values which was why we gave them the same normalization when looking at the crossover in the first place.

Since the crossover appeared linear in a "loglog"-plot, finding its slope is enough to determine the exponent Δ. Some arbitrary linear regressions gave the slope 1 to within 5%, so It will be taken to be 1 from here on out. This gives $\Delta = -4$, and the argument of the scaling function should then be ϵ/L^{-4}. The data collapse is not perfect, so there might be some differences in the scaling depending on the actual values of both parameters.

In figure 4.9 a comparison is made for the same values of the argument but keeping either L or ϵ fixed. As we can see, they do not entirely match, but the discrepancies can be

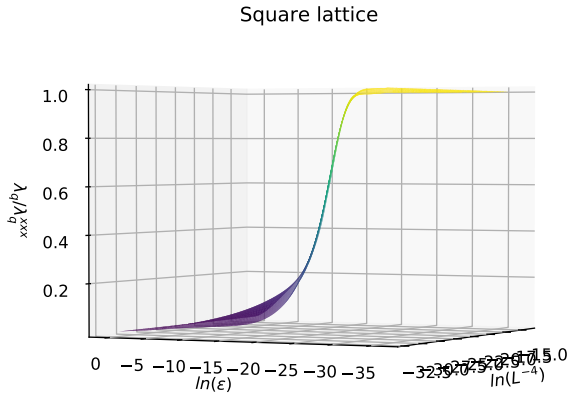

Figure 4.7: Mode occupation number of the nn-model on the square lattice at $k_y = q$ as a function of system size L and anisotropy parameter ϵ as viewed from a different angle. The axes are a bit unclear, but they are the same as in 4.5. The main point of this figure is to showcase the phenomenon of data collapse.

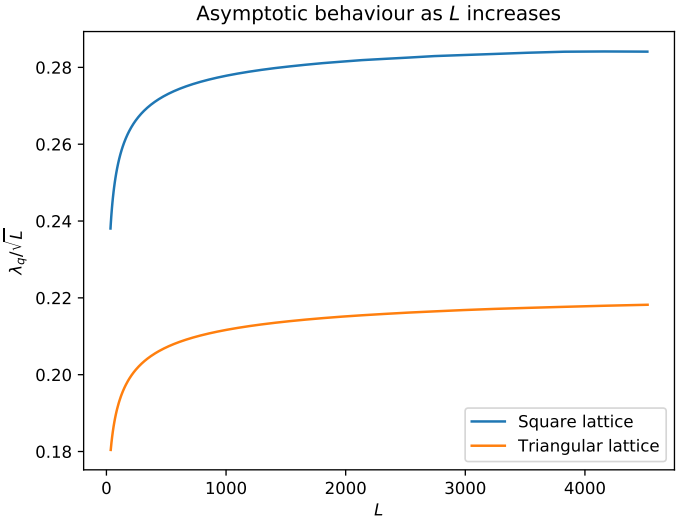

Figure 4.8: Plot showing how the mode occupation number approaches its asymptotic behaviour at $L \to \infty$ as a function of L in both nn-model on the triangular- and the square- lattice.

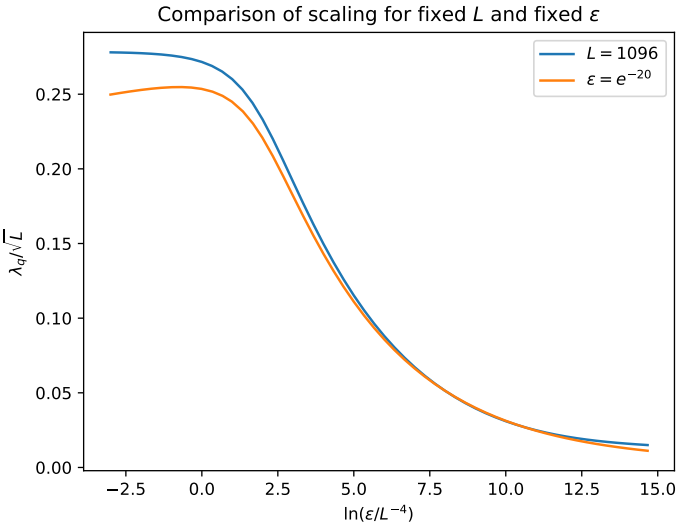

Figure 4.9: Comparison of the dependence of λ_q on ϵ at a fixed L and on L at a fixed ϵ with the same values of the ratio ϵ/L^{-4}

explained by realizing that the values of L in the constant ϵ curve are rather small. They will therefore not have attained their asymptotic $\sqrt{L}$ form yet. Another way to look at it without being very precise is that the scaling function is only well defined when both the denominator and the numerator in its argument are really small. Their ratio however could still be arbitrary.

As a matter of fact, we already have the basis for finding the scaling function in equation 3.83. This is expressed in terms of κ, which relates ϵ to $h \sim L^{-4}$. Let us also normalize it with its value at $\kappa = 0$, i.e. the xxx-value, since we already did that previously.

Since we really are in the asymptotic limit $L \gg 1$, it means that both h and ϵ will tend to zero, but κ could still be any finite number. In the chosen normalization a lot will cancel, and we will be left with:

$$f_0 = \sqrt{\frac{\Upsilon_{\mathbf{0}} + (N_G - 1)\Upsilon_{\boldsymbol{Q}}}{\left(\Upsilon_{\mathbf{0}} + (N_G - 1)\frac{\Upsilon_{\boldsymbol{Q}}}{\sqrt{1+\kappa}}\right)}} \tag{4.8a}$$

$$f_q = \sqrt{\frac{\Upsilon_{\mathbf{0}} + (N_G - 1)\Upsilon_{\boldsymbol{Q}}}{\left(\Upsilon_{\mathbf{0}}\sqrt{1+\kappa} + (N_G - 1)\Upsilon_{\boldsymbol{Q}}\right)}}. \tag{4.8b}$$

These are the scaling functions in terms of κ. However, we want them to be in terms of ϵ/L^{-4}, and since h and L^{-4} are different, the x-axis needs to be modified.

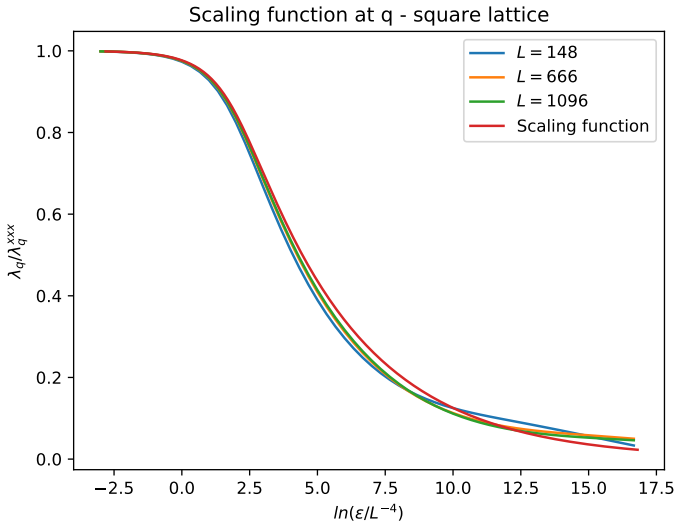

Figure 4.10: Comparison of analytic scaling function and λ_q in the nn-model on the square lattice at some fixed values of L as a function of the argument ϵ/L^{-4}

We have, for a given κ, the relation (4.4) between h and L, so

$$\frac{\epsilon}{L^{-4}} \simeq \frac{\kappa}{16 m_{AF}^2 (-J(\boldsymbol{Q})} \left(\Upsilon_{\mathbf{0}} + \frac{(N_G - 1)\Upsilon_{\boldsymbol{Q}}}{\sqrt{1+\kappa}} \right)^2 \tag{4.9}$$

m_{AF} must be computed numerically, and $J(\boldsymbol{Q})$ and $\Upsilon_{\boldsymbol{Q},\mathbf{0}}$ are model dependent, so the scaling function is not completely universal.

Using this we get the final results in figures 4.10, 4.11, 4.12 and 4.13. These show the scaling function found analytically compared to the numerically calculated values of $\lambda_{0,q}$ for some given L's. The match is mostly good for both modes on both types of lattice. We get closer to the analytic scaling function the larger L is and the smaller ϵ is. In the zero modes for the smallest values of L where the largest values of ϵ occur, we can actually see the beginnings of the second crossover. So perhaps there is some vaguely noticeable second crossover in the modes at q as well explaining why the values do not match that well in that region. Either way, we should only really look at scaling close to the XXX-model.

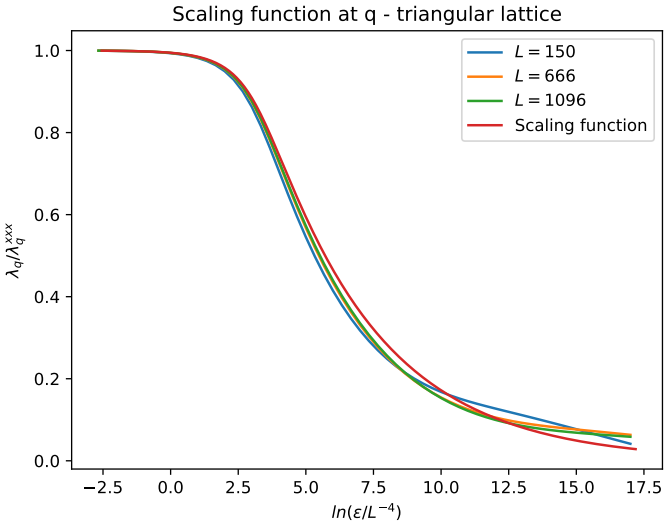

Figure 4.11: Comparison of analytic scaling function and λ_q in the nn-model on the triangular lattice at some fixed values of L as a function of the argument ϵ/L^{-4}

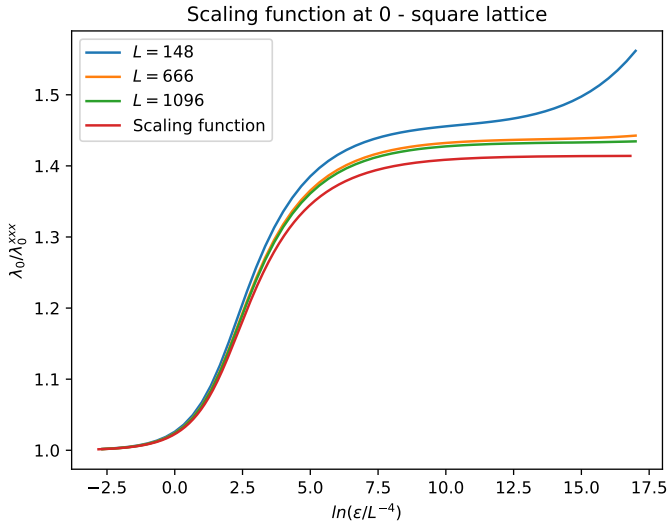

Figure 4.12: Comparison of analytic scaling function and λ_0 in the nn-model on the square lattice at some fixed values of L as a function of the argument ϵ/L^{-4}

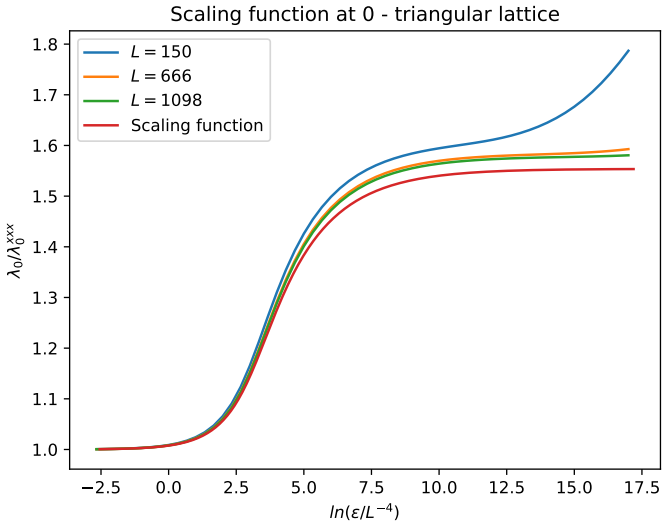

Figure 4.13: Comparison of analytic scaling function and λ_0 in the nn-model on the triangular lattice at some fixed values of L as a function of the argument ϵ/L^{-4}

Chapter 5

Conclusion

To conclude we could say that the framework was successfully expanded to apply in the easy plane sector of the XXZ-model, and although the only models studied numerically here were the nearest neighbour models on triangular and square lattice, we stress that the framework is valid for any model that has only one global minimum in $J(\boldsymbol{k})$ and linearly dispersing spin waves. We are thus able to explain analytically the scaling of both the leading term and the first subleading term in the Rényi entropy, and we demonstrated that the subleading term indeed was universal with a prefactor only dependent upon the number of broken symmetries in the system. Furthermore, a crossover was seen when going into the xxz-case from the xxx-case, and scaling functions determining its behaviour was found in both the mode at 0 and at q. To my knowledge, no work has been done on scaling functions as seen in the Rényi entropy of antiferromagnetic systems. A natural next step here would be to place this in the context of the renormalization group, and try to make sense of the critical exponents found in the scaling function.

In the easy axis sector, quite a few difficulties were encountered leaving more questions than answers. First off, we saw that the types of classical order were not necessarily the same as in the xxx-case, and thus did not immediately fit into the framework developed. The problem of solving classically for most models still remains open, but a continuous degeneracy not related to any obvious symmetry was observed in the nn-model on a triangular lattice, and so there is hope of connecting the types of order occurring in the XXX-model to the XXZ-model by uncovering the "hidden" symmetry, if present. For a model that orders collinearly, the order will be the same in both cases, but there will be no broken continuous symmetries in the easy axis-case, and as a consequence, the method of MLSWT broke down. The pressing question is then what would have happened if we had not tried to modify our spin wave theory by demanding the magnetization to be zero? There are not any problematic divergences in this case, and thus we need not introduce h to regularize, but we would like the same theory to describe this case as the other, so is there a way to include h as to give consistent results for all XXZ-models? As Ref. 7

argues, the only thing needed to get the correct scaling is that the regularizing field h is $\sim L^{-2d}$, and so we could in principle choose any value of m as a requirement to modify the theory. The only other option that appears naturally would be m_{AF}, so what would happen if that was chosen? However, a check of the assumption that there should be zero magnetization on the finite lattice in the easy axis-case should be done first.

We assumed here that we were looking at antiferromagnets, but the only mathematical requirement really was that the spin waves were linearly dispersing. This means that other models than strictly antiferromagnetic are within range. Away from the pure Heisenberg-, XY- and Ising-models, even the ferromagnet disperses linearly.

It would also be interesting to check for negative values of Δ. For values up until -1, the ordering should still be the same as in the XY-model. At $\Delta = -1$, the interactions in the z-direction being ferromagnetic now will mean that ferromagnetic ordering along the z-direction will have the same energy as antiferromagnetic ordering in the xy-plane. Decreasing Δ further will open up a whole new range of possible classical ground states. However, it should be possible to use this framework to explore the easy plane sector for both positive and negative Δ.

Other directions to take following this work may be to try and expand to orders where there are several minima in $J(\boldsymbol{k})$. Will the order still be coplanar? Averaging over several possible ground states should not be expected to give the desired results. Is it then necessary to choose one of the minima and discard the other? If one were to add some infinitesimal interaction that would pick out one minimum over the others, we would essentially be back in the framework we have laid out here. Another option would be to increase the dimensionality of the lattice going to a hypercubic lattice in d dimensions. We expect that it should be relatively straight forward for models that order collinearly, but already at the nn-model on a 3-dimensional triangular lattice, the order is no longer coplanar. It would also be possible to try and extend the framework to other lattices that cannot be mapped onto the square lattice.

After all, there are many possible ways to continue developing the theory from this paper and the thought of someone, someday picking it up is exciting

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Appendices

Appendix A

Density operators, the partial trace, and Rényi entropy

A.1 Density matrices

The definition of a density matrix in quantum statistical mechanics is $\rho = \sum_i p_i |\psi_i\rangle \langle\psi_i|$, where $\langle\psi_i|$ is some normalized basis for its Hilbert space, and p_i has the interpretation of the probability of being in state $\langle\psi_i|$. If the basis states are taken to be orthonormal, ρ in matrix form becomes diagonal, and the eigenvalues of ρ are the set of p_i. ρ is therefore positive semi-definite, and its eigenvalues sum to one. It is also Hermitian, which can be seen from its definition. Because of this it is possible to parameterize it as $e^{-H}/\operatorname{tr}\left(e^{-H}\right)$ where H is another Hermitian operator on the same Hilbert space. The prime example of this being the Boltzmann distribution, where $\rho = e^{-\beta H}/\operatorname{tr}\left(e^{-\beta H}\right)$.

A.2 The partial trace and reduced density operators

We wish to look at the ground state, so we take the density operator to be $|\Psi\rangle_{Gs} \langle\Psi|_{Gs}$. This also corresponds to the Boltzmann distribution at zero temperature if the ground state is non-degenerate, since it means that we are in the ground state with probability 1.

A state defined on a composite Hilbert space $\mathcal{H} = \mathcal{H}_\mathcal{A} \otimes \mathcal{H}_\mathcal{B}$ can be expressed via the Schmidt decomposition as: $|\Psi\rangle = \sum_i c_i |\psi_i\rangle_\mathcal{A} \otimes |\psi_i\rangle_\mathcal{B}$, where $|\psi_i\rangle_{\mathcal{A},\mathcal{B}}$ constitute orthonormal bases for their respective Hilbert spaces. Then,

$$\rho = \sum_i c_i |\psi_i\rangle_{\mathcal{A}} \otimes |\psi_i\rangle_{\mathcal{B}} \sum_j c_j^* \langle\psi_j|_{\mathcal{B}} \otimes \langle\psi_j|_{\mathcal{A}} \quad \Longrightarrow$$

$$\rho_{\mathcal{A}} = \mathrm{tr}_{\mathcal{B}} \left(\sum_{i,j} c_i c_j^* |\psi_i\rangle_{\mathcal{A}} \langle\psi_j|_{\mathcal{A}} \otimes |\psi_i\rangle_{\mathcal{B}} \langle\psi_j|_{\mathcal{B}} \right).$$

The trace acts only on $|\psi_i\rangle_{\mathcal{B}}$, and it will evaluate to $\langle\psi_i|_{\mathcal{B}} |\psi_j\rangle_{\mathcal{B}} = \delta_{i,j}$. Thus, $\rho_{\mathcal{A}} = \sum_i |c_i|^2 |\psi_i\rangle_{\mathcal{A}} \langle\psi_i|_{\mathcal{A}}$, which is precisely the form we expect a density operator to have.

Furthermore, we have $\mathrm{tr}(\rho) = \mathrm{tr}_{\mathcal{A}}(\mathrm{tr}_{\mathcal{B}}(\rho)) = \mathrm{tr}_{\mathcal{A}}(\rho_{\mathcal{A}})$, so the eigenvalues are indeed non-negative and sum to one.

The same could be said for $\rho_{\mathcal{B}}$, and thus the total density operator can be expressed in terms of one density operator on each subspace of the initial Hilbert space.

A.3 Reduction of Rényi entropy to von Neumann entropy

$\mathrm{tr}_{\mathcal{A}}(\rho_{\mathcal{A}}^n)$ is simply the trace of region $\mathcal{A}$ on the density operator in $\mathcal{A}$.

We also know that we can diagonalize ρ as $D = U\rho U^\dagger$ where D now consists of the eigenvalues of ρ, that is: $D = diag(p_1, p_2, ..., p_N)$ Then, because of trace-properties we have:

$$\mathrm{tr}(\rho) = \mathrm{tr}\big(U^\dagger U\rho\big) = \mathrm{tr}\big(U\rho U^\dagger\big) = \mathrm{tr}(D) = \sum_{i=1}^{N} p_i$$

and for an exponent in the natural numbers,

$$\mathrm{tr}(\rho^q) = \mathrm{tr}\big((U^\dagger U\rho)^q\big) = \mathrm{tr}\left(\overbrace{(U\rho U^\dagger)(U\rho U^\dagger)...(U\rho U^\dagger}^{q \text{ times}}\right) = \mathrm{tr}(D^q) = \sum_{i=1}^{N} p_i^q$$

Since the trace operation also is linear, any polynomial expansion of an operator will under the trace be the polynomial expansion of the sum of its eigenvalues. That is:

$$\mathrm{tr}\left(\sum_{q=0}^{\infty} a_q \rho^q\right) = \sum_{q=0}^{\infty} a_q \,\mathrm{tr}(\rho^q) = \sum_{q=0}^{\infty} a_q (\sum_{i=1}^{N} p_i^q)$$

assuming the infinite sum is well behaved. This is sufficient to prove that $\lim_{q\to 1} S_q = S_{vN}$. We have:

$$S_q = \frac{1}{1-q} \ln \mathrm{tr}_{\mathcal{A}}(\rho_{\mathcal{A}}^q).$$

We can see that in the limit, both the numerator and the denominator approaches 0, so we attempt to find the limit via L'Hôpitals rule. $d/dq(1-q) = -1$ and:

$$\frac{d}{dq} \ln \mathrm{tr}(\rho^q) = \frac{d}{dq} \ln \sum_{i=1}^{N} p_i^q = \frac{1}{\sum_{i=1}^{N} p_i^q} \frac{d}{dq} \sum_{i=1}^{N} p_i^q = \sum_{i=1}^{N} \frac{p_i^q \ln p_i}{\sum_{i=1}^{N} p_i^q}$$

which in the limit reduces to $\sum_{i=1}^{N} p_i \ln p_i$ since the denominator becomes 1, and so:

$$\lim_{q \to 1} S_q = -\sum_{i=1}^{N} p_i \ln p_i = -\mathrm{tr}(\rho \ln \rho) = S_{vN}$$

A.4 Expressing the Rényi entropy in terms of the mode energies of H_e

Given an entanglement Hamiltonian on harmonic oscillator form $H_e = \sum_\nu \varepsilon_\nu \hat{n}_\nu$. With the number operator $\hat{n}_\nu = \beta_\nu^\dagger \beta_\nu$, and eigenvalues n_ν, the eigenvalues of $\rho = e^{-H}/Z$ are

$$(1/Z) \exp\left(-\sum_\nu \varepsilon_\nu n_\nu \right)$$

where the set $\{n_\nu\}$ are non-negative integers. Each eigenvalue of ρ is thus labeled by one such unique collection of boson occupation numbers, one number for each ν. The trace is equivalent to the sum over the eigenvalues, but now the sum $\sum_i$ over eigenvalues of ρ_A becomes $\prod_\nu \left(\sum_{n_\nu=0}^{\infty} \right) = \sum_{n_{\nu_1}} \sum_{n_{\nu_2}} \ldots$.

$$\begin{aligned}
\sum_i p_i^q &= \prod_\nu \left(\sum_{n_\nu=0}^{\infty} \right) \left[(1/Z) \exp\left(-\sum_\nu \varepsilon_\nu n_\nu \right) \right]^q \\
&= Z^{-q} \prod_\nu \left(\sum_{n_\nu} \left[\exp(-q\varepsilon_\nu) \right]^{n_\nu} \right) \\
&= Z^{-q} \prod_\nu \frac{1}{1 - \exp(-q\varepsilon_\nu)}.
\end{aligned}$$

With $q = 1$, we see that

$$Z = \prod_\nu \frac{1}{1 - \exp(-\varepsilon_\nu)}.$$

Thus the Rényi entropy is

$$\begin{aligned} S_q &= \frac{1}{1-q}\ln\left(Z^{-q}\prod_\nu \frac{1}{1-\exp(-q\varepsilon_\nu)}\right) \\ &= \frac{1}{1-q}\left(-q\ln Z - \sum_\nu \ln\left[1-\exp(-q\varepsilon_\nu)\right]\right) \\ &= \frac{1}{1-q}\sum_\nu \left(q\ln\left[1-\exp(-\varepsilon_\nu)\right] - \ln\left[1-\exp(-q\varepsilon_\nu)\right]\right). \end{aligned}$$

The relationship between the mode occupancy and the eigenvalues of such a Hamiltonian is given by the Bose-Einstein distribution function:

$$\langle \hat{n}_\nu \rangle = \frac{1}{\exp(\varepsilon_\nu)-1}.$$

denoting $\langle \hat{n}_\nu \rangle \equiv \lambda_\nu$ we get

$$\lambda_\nu = \frac{1}{\exp(\varepsilon_\nu)-1} \quad \Leftrightarrow \quad \exp(\varepsilon_\nu) = 1+\frac{1}{\lambda_\nu} \quad \Leftrightarrow \quad \exp(-\varepsilon_\nu) = (1+\frac{1}{\lambda_\nu})^{-1} = \frac{\lambda_\nu}{1+\lambda_\nu}$$

This can be used to express the Rényi entropy in terms of λ_ν:

$$\begin{aligned} S_q &= \frac{1}{1-q}\sum_\nu \left(q\ln\left[1-\frac{\lambda_\nu}{1+\lambda_\nu}\right] - \ln\left[1-\left(\frac{\lambda_\nu}{1+\lambda_\nu}\right)^q\right]\right) \\ &= \frac{1}{1-q}\sum_\nu \left(q\ln\left[\frac{1}{1+\lambda_\nu}\right] - \ln\left[\frac{(1+\lambda_\nu)^q-\lambda_\nu^q}{(1+\lambda_\nu)^q}\right]\right) \\ &= \frac{1}{q-1}\sum_\nu \ln\left[(1+\lambda_\nu)^q-\lambda_\nu^q\right]. \end{aligned}$$

Appendix B

Commutators

B.1 Commutators between generators of global spin rotations and H

The spin operator commutation relations can succinctly be written as:

$$\left[S_i^\alpha, S_j^\beta\right] = \delta_{i,j} i \sum_\gamma \epsilon_{\alpha\beta\gamma} S_i^\gamma, \quad (\alpha, \beta, \gamma = x, y, z).$$

The generators of spin rotations are the total spin operators in each of the three directions. $S^\alpha = \sum_i S_i^\alpha$. Let us first remind ourselves of the form of H, and then check the commutator of one such operator with the terms stemming from one of the components in H.

$$H = \frac{1}{2} \sum_{i,j} J_{ij} [S_i^x S_j^x + S_i^y S_j^y + \Delta S_i^z S_j^z]$$

$$\left[\sum_l S_l^\alpha, \sum_{i,j} S_i^\beta S_j^\beta\right]$$

Assuming $i \neq j$, l can only be equal to one of them at a time. The deltafunction will then give one contribution when $l = i$ and one when $l = j$ that both still need to be summed over all i, j:

$$\sum_{i,j} \left[S_i^\alpha, S_i^\beta\right] S_j^\beta + S_i^\beta \left[S_j^\alpha, S_j^\beta\right] = \sum_{i,j,\gamma} \epsilon_{\alpha\beta\gamma} (S_i^\gamma S_j^\beta + S_i^\beta S_j^\gamma)$$

The Levi-Civita symbol makes the term where $\alpha = \beta$ equal to zero. The terms coming from the two other choices of β will come with the opposite signs of each other.

In our XXZ-Hamiltonian, the prefactor Δ in the z-terms will make it so that the cancellation between these two parts does not occur unless $\Delta = 1$. Thus, the XXZ-Hamiltonian only has global spin-rotation symmetry about all axes when it is equal to the Heisenberg-model. Otherwise, it will only have global spin-rotation symmetry about the z-axis

B.2 Commutation relations in the Holstein-Primakoff representation

We will here show that the HP-representation of spin operators satisfy the correct commutation relations. The representation for spins ordered along the z-axis is:

$$\begin{aligned} S_i^z &= S - n_i \\ S_i^+ &= \sqrt{2S - n_i} b_i \\ S_i^- &= b_i^\dagger \sqrt{2S - n_i} \end{aligned}$$

where

$$S^\pm = S^x \pm iS^y$$

And thus we have:

$$\left[S^z, S^\pm\right] = \left[S^z, S^x\right] \pm i \left[S^z, S^y\right] = iS^y \pm i(-iS^x) = \pm S^\pm$$

$$\left[S^+, S^-\right] = \left[S^x, S^x\right] + i \left[S^y, S^x\right] - i \left[S^x, s^y\right] + i(-i) \left[S^y, S^y\right] = i(-iS^z) - i(iS^z) = 2S^z$$

Having bosonic commutation relations on the HP-bosons:

$$\left[b, b^\dagger\right] = 1$$

remembering that $n = b^\dagger b$, we also have:

$$\left[n, b^\dagger\right] = b^\dagger \underbrace{bb^\dagger}_{1 + b^\dagger b} - b^\dagger b^\dagger b = b^\dagger$$

and

$$[n, b] = b^\dagger bb - \underbrace{bb^\dagger}_{1 + b^\dagger b} b = -b$$

Then, the commutation relations are:

$$\begin{aligned}
\left[S^z, S^+\right] &= (S-n)\sqrt{(2S-n)}b - \sqrt{(2S-n)}b(S-n) \overbrace{=}^{bn = b + nb} \\
(S-n)\sqrt{(2S-n)}b &- \left((S-n)\sqrt{(2S-n)}b - \sqrt{(2S-n)}b\right) = S^+
\end{aligned}$$

$$\begin{aligned}
\left[S^z, S^-\right] &= (S-n)b^\dagger\sqrt{(2S-n)} - b^\dagger\sqrt{(2S-n)}(S-n) \overbrace{=}^{nb^\dagger = b^\dagger n + b^\dagger} \\
\left(b\sqrt{(2S-n)}(S-n) - b^\dagger\sqrt{(2S-n)}\right) &- b\sqrt{(2S-n)}(S-n) = -S^-
\end{aligned}$$

Where we have used that the commutator of an operator of and a polynomial expansion in that same operator is zero, i.e. $n\sqrt{2S-n} = \sqrt{2S-n}n$.

lastly we have:

$$\begin{aligned}
\left[S^+, S^-\right] = \sqrt{(2S-n)}bb^\dagger\sqrt{(2S-n)} - b^\dagger\sqrt{(2S-n)}\sqrt{(2S-n)}b &\overbrace{=}^{bb^\dagger = n+1} \\
\sqrt{(2S-n)}(n+1)\sqrt{(2S-n)} - b^\dagger(2S-n)b &\overbrace{=}^{nb = bn - b} \\
(n+1)(2S-n) - n(2S-n) - (2S+n) = 2(S-n) = 2S^z &
\end{aligned}$$

B.3 Commutation relations for Fourier transformed HP-bosons

With Fourier transformed operators as follows:

$$\begin{aligned}
b_{\boldsymbol{k}} &= \frac{1}{\sqrt{N}}\sum_j b_j e^{-i\boldsymbol{k}\cdot\boldsymbol{r}_j} \\
\implies b^\dagger_{\boldsymbol{k}} &= \frac{1}{\sqrt{N}}\sum_j b^\dagger_j e^{i\boldsymbol{k}\cdot\boldsymbol{r}_j}
\end{aligned}$$

We can immediately see that $\left[b_{\boldsymbol{k}}, b_{\boldsymbol{k}'}\right] = \left[b^\dagger_{\boldsymbol{k}}, b^\dagger_{\boldsymbol{k}'}\right] = 0$ as they should be.

$$\left[b_{\boldsymbol{k}}, b^\dagger_{\boldsymbol{k}'}\right] = \frac{1}{N}\sum_{i,j} e^{-i\boldsymbol{k}\cdot\boldsymbol{r}_i + i\boldsymbol{k}'\cdot\boldsymbol{r}_j}\overbrace{\left[b_i, b^\dagger_j\right]}^{\delta_{i,j}} = \frac{1}{N}\sum_i e^{-i\boldsymbol{r}_i\cdot(\boldsymbol{k}-\boldsymbol{k}')} = \delta_{\boldsymbol{k},\boldsymbol{k}'}$$

B.4 Commutation relations of Bogoliubov bosons

Here we give a short proof that Bogoliubov bosons satisfy the correct commutation relations:

$$\begin{aligned}\left[b_{\boldsymbol{k}}, b_{\boldsymbol{k}'}\right] = \left[b^\dagger_{\boldsymbol{k}}, b^\dagger_{\boldsymbol{k}'}\right] = 0\\ \left[b_{\boldsymbol{k}}, b^\dagger_{\boldsymbol{k}'}\right] = \delta_{\boldsymbol{k},\boldsymbol{k}'}\end{aligned}$$

Starting from their definition:

$$\begin{aligned}\alpha_{\boldsymbol{k}} &= \cosh\zeta_{\boldsymbol{k}} b_{\boldsymbol{k}} + \sinh\zeta_{\boldsymbol{k}} b^\dagger_{-\boldsymbol{k}}\\ \alpha^\dagger_{\boldsymbol{k}} &= \cosh\zeta_{\boldsymbol{k}} b^\dagger_{\boldsymbol{k}} + \sinh\zeta_{\boldsymbol{k}} b_{-\boldsymbol{k}}\end{aligned}$$

$\Longrightarrow$

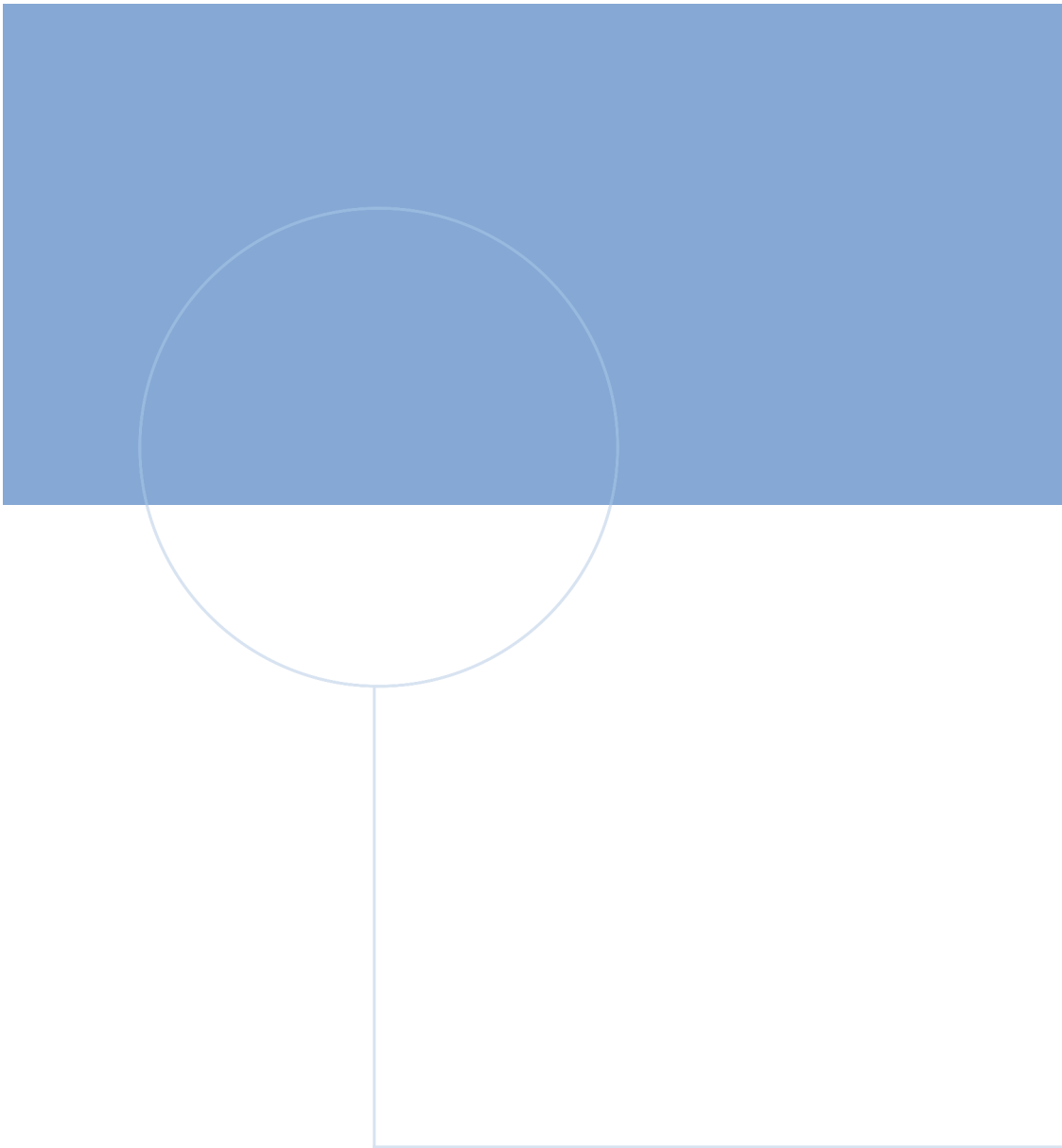
$$\begin{aligned}\left[\alpha_{\boldsymbol{k}}, \alpha_{\boldsymbol{k}'}\right] &= \cosh\zeta_{\boldsymbol{k}}\cosh\zeta_{\boldsymbol{k}'}\left[b_{\boldsymbol{k}}, b_{\boldsymbol{k}'}\right] + \sinh\zeta_{\boldsymbol{k}}\sinh\zeta_{\boldsymbol{k}'}\left[b^\dagger_{-\boldsymbol{k}}, b^\dagger_{-\boldsymbol{k}'}\right]\\ &+ \cosh\zeta_{\boldsymbol{k}}\sinh\zeta_{\boldsymbol{k}'}\left[b_{\boldsymbol{k}}, b^\dagger_{-\boldsymbol{k}'}\right] + \sinh\zeta_{\boldsymbol{k}}\cosh\zeta_{\boldsymbol{k}'}\left[b^\dagger_{-\boldsymbol{k}}, b_{\boldsymbol{k}'}\right]\\ &= -\cosh\zeta_{\boldsymbol{k}}\sinh\zeta_{\boldsymbol{k}'}\delta_{\boldsymbol{k},-\boldsymbol{k}'} + \sinh\zeta_{\boldsymbol{k}}\cosh\zeta_{\boldsymbol{k}'}\delta_{-\boldsymbol{k},\boldsymbol{k}'} = 0\end{aligned}$$

Since $\zeta_{\boldsymbol{k}}$ is even in $\boldsymbol{k}$.

$$\begin{aligned}\left[\alpha^\dagger_{\boldsymbol{k}}, \alpha^\dagger_{\boldsymbol{k}'}\right] &= \cosh\zeta_{\boldsymbol{k}}\cosh\zeta_{\boldsymbol{k}'}\left[b^\dagger_{\boldsymbol{k}}, b^\dagger_{\boldsymbol{k}'}\right] + \sinh\zeta_{\boldsymbol{k}}\sinh\zeta_{\boldsymbol{k}'}\left[b_{-\boldsymbol{k}}, b_{-\boldsymbol{k}'}\right]\\ &+ \cosh\zeta_{\boldsymbol{k}}\sinh\zeta_{\boldsymbol{k}'}\left[b^\dagger_{\boldsymbol{k}}, b_{-\boldsymbol{k}'}\right] + \sinh\zeta_{\boldsymbol{k}}\cosh\zeta_{\boldsymbol{k}'}\left[b_{-\boldsymbol{k}}, b^\dagger_{\boldsymbol{k}'}\right]\\ &= +\cosh\zeta_{\boldsymbol{k}}\sinh\zeta_{\boldsymbol{k}'}\delta_{\boldsymbol{k},-\boldsymbol{k}'} - \sinh\zeta_{\boldsymbol{k}}\cosh\zeta_{\boldsymbol{k}'}\delta_{-\boldsymbol{k},\boldsymbol{k}'} = 0\end{aligned}$$

and lastly:

$$\begin{aligned}\left[\alpha^\dagger_{\boldsymbol{k}}, \alpha_{\boldsymbol{k}'}\right] &= \cosh\zeta_{\boldsymbol{k}}\cosh\zeta_{\boldsymbol{k}'}\left[b^\dagger_{\boldsymbol{k}}, b_{\boldsymbol{k}'}\right] + \sinh\zeta_{\boldsymbol{k}}\sinh\zeta_{\boldsymbol{k}'}\left[b_{-\boldsymbol{k}}, b^\dagger_{-\boldsymbol{k}'}\right]\\ &+ \cosh\zeta_{\boldsymbol{k}}\sinh\zeta_{\boldsymbol{k}'}\left[b^\dagger_{\boldsymbol{k}}, b^\dagger_{-\boldsymbol{k}'}\right] + \sinh\zeta_{\boldsymbol{k}}\cosh\zeta_{\boldsymbol{k}'}\left[b_{-\boldsymbol{k}}, b_{\boldsymbol{k}'}\right]\\ &= \cosh\zeta_{\boldsymbol{k}}\cosh\zeta_{\boldsymbol{k}'}\delta_{\boldsymbol{k},\boldsymbol{k}'} - \sinh\zeta_{\boldsymbol{k}}\sinh\zeta_{\boldsymbol{k}'}\delta_{-\boldsymbol{k},-\boldsymbol{k}'} = (\cosh^2\zeta_{\boldsymbol{k}} - \sinh^2\zeta_{\boldsymbol{k}})\delta_{\boldsymbol{k},\boldsymbol{k}'} = \delta_{\boldsymbol{k},\boldsymbol{k}'}\end{aligned}$$



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Norwegian University of
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