

Ivan Ushakov

# Phase diagram of an extended Kane-Mele-Hubbard model in strongly correlated regime

Master's thesis in Nanotechnology

Supervisor: Alireza Qaiumzadeh

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Faculty of Natural Sciences  
Department of Physics



## Abstract

The main purpose of this thesis is to consider an extended Kane-Mele-Hubbard model in strongly correlated regime from reference [1], where both anisotropic exchanges and Dzyaloshinskii-Moriya interactions (DMI) are present, and then apply Abrikosov fermion and Schwinger boson mean-field theories in order to construct phase diagrams, in a way similar to reference [2]. From Abrikosov fermion mean-field theory, we found that the DMI closes the gaps of the gapped spin liquids, turning the phase diagram into gapless spin liquid. At the same time, for intermediate DMI strength, the chiral gapped spin liquid phase, which is stable against gauge fluctuations, begins to occur for systems with strong anisotropic exchange, which is not observed when DMIs are absent. When DMI is dependent on intrinsic spin-orbit interaction and the next nearest neighbor hopping, the spin liquid gap closes completely. From Schwinger boson mean-field theory, we found that strong DMI in general introduces more order to the system, although the spin-liquid might still exist when anisotropic exchange is weak. In addition, in this thesis we present how a spin-Hamiltonian can be derived from a second quantized electron Hamiltonian, a general idea behind bosonization and fermionization, a simple example with Jordan-Wigner and Holstein-Primakoff transformations, and symmetries in quantum mechanics.

### **Acknowledgements**

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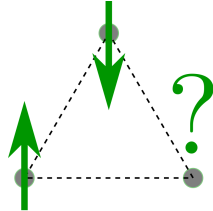
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# 1 Introduction

A development of fast and power-efficient high-capacity electronic devices is of central importance these days. The area of *spintronics* (electronics where electron spin is exploited) is a large area of research in both theoretical and experimental physics. In the end of the 80's, A. Fert and P. Grünberg independently discovered *Giant magnetoresistance* (GMR)[3][4]. In turn, GMR was used to create a variety of ferromagnetic spintronic devices, one of these being *hard disk drives* (HDD). Most of the experimentally achieved devices thus far have been ferromagnetic, despite the existence of other magnetic phases like *anti-ferromagnets* (AFM). In order to exploit potential possibilities of other phases, it might be important to construct a good theoretical description that can build a bridge between theory, experiments and eventually device engineering.



**Figure 1:** Suppose that we have a hexagonal lattice defined by triangular sections. Suppose also that the spins are of AFM nature, meaning that they "want" to point in opposite direction of each other. As seen from the figure, the geometry does not allow all the interactions to be satisfied simultaneously, and leads to magnetic frustration.

In theoretical physics, a particular interest is attributed to the so-called spin liquid phases in magnetic materials. The driving force behind these are known as *magnetic frustrations*, an effect that arises in localized electron spins, where different exchange interactions cannot be satisfied simultaneously. An example is illustrated in figure 1, where the frustration arises from geometrical and AFM nature of the material. This gives a very large degeneracy of the ground state, which in turn leads to thermal fluctuations in a correlated manner at low temperatures, giving rise to a liquid-like matter. For classical fluctuations, the spins tend to order or freeze as  $T \rightarrow 0$ . However, when quantum effects are taken into the account, we get quantum fluctuations even when  $T \rightarrow 0$ . With strong enough quantum fluctuations, the material is defined as *quantum spin liquid* (QSL), a phase with lack of order, different superpositions of spins, high quantum entanglement, fractional excitations and emerging gauge fields[5].

The QSLs have not been consistently defined experimentally, although there are some recent candidates. For instance, experiments have shown that  $\text{Ce}_2\text{Zr}_2\text{O}_7$  pyrochlore shows signs of a 3D QSL[6]. Another candidate is  $\text{EtMe}_3\text{Sb}[\text{Pd}(\text{dmit})_2]_2$ [7]. For practical reasons, we want to investigate possibility of QSLs in materials defined by a honeycomb lattice. This is a reasonable approach because honeycomb lattice materials are 2D materials that can be obtained experimentally. In particular, there have recently been obtained magnetic 2D honeycomb materials, stable even at room temperature[8]. In addition, 2D materials are more practical to work with theoretically than 3D materials, and there exists a strong theoretical knowledge related to magnetic honeycomb materials. One of the most known is the so-called *Kane-Mele-Hubbard* (KMH) model, which we are going to consider later in the text.

With this in mind, our goal for the master thesis is to investigate potential existence of QSLs in an extended strongly correlated KMH model from reference [1], and compare the result with phase diagram from reference [2]. In particular, we want to see how anisotropic exchanges and *Dzyaloshinskii-Moriya interactions* (DMI) influence the phase diagram in a such model, and what kind of phases it predicts. For Kagome lattices, it is in general known that long-range order occurs for strong DMI, whilst small DMI is subject to discussion[9][10].

The thesis is structured in following way: In chapter 2, we discuss spin-Hamiltonians, and how these can be obtained. In chapter 3, we introduce the main idea behind bosonization and fermionization, and show some examples. In chapter 4, we introduce the specific techniques that are going to be used for the derivation of the phase diagram. In chapter 5, we apply these techniques to the models from references [2][1], in order to construct phase diagrams. Finally, in chapter 6, we conclude and discuss outlook.

## 1.1 Mathematical conventions

In this thesis, the site dependent spin components are written as  $\hat{S}_i^{(\alpha)}$ , where  $i$  denotes the site, and  $\alpha$  denotes the component direction. The directions are sometimes going to be denoted as  $\{x, y, z\}$  and other times as  $\{1, 2, 3\}$ , but these notions are completely equivalent. The site independent spins are denoted as  $\hat{S}_\alpha$ . The unit-vectors in these

directions are denoted as  $\vec{e}_\alpha$  in order to avoid confusion with position operators. However, the unit vectors in an arbitrary direction are denoted as  $\hat{n}$ , and so are number operators. The specific notions should be obvious from the context. In addition, the spins are either represented by symbols or numbers, with the following correspondance:

$$\uparrow \leftrightarrow 1; \quad \downarrow \leftrightarrow 2. \tag{1.1.1}$$

That is, we have for example that:

$$\sum_{\alpha=1}^2 \hat{f}_{i\alpha}^\dagger \hat{f}_{i\alpha} = \hat{f}_{i\uparrow}^\dagger \hat{f}_{i\uparrow} + \hat{f}_{i\downarrow}^\dagger \hat{f}_{i\downarrow}. \tag{1.1.2}$$

## 2 Spin Hamiltonians

When considering classical magnetic models in branches like statistical physics, we usually deal with Hamiltonians of the form  $H(\{\vec{S}_i\})$ , where  $\vec{S}_i$  is a vector with certain magnitude pointing in certain direction. A typical example is nearest neighbor interaction Hamiltonian of a 1D chain:

$$\frac{1}{2} \sum_{\langle i,j \rangle} J \vec{S}_i \cdot \vec{S}_j = JS^2 \sum_{i=1}^N \cos \theta_{i,i+1}, \quad (2.0.1)$$

where  $J$  represents interactions,  $S$  is spin magnitude, and  $\theta_{i,i+1}$  is the angle between the spins at sites  $i$  and  $i+1$ . We see that if  $J < 0$  the Hamiltonian is minimized when all the spins point in the same direction, and we get a ferromagnetic ground state. If  $J > 0$ , the spins point in opposite directions, giving AFM. In quantum mechanics, the spin components are replaced with the corresponding spin operators, and the analysis of the ground state becomes more complicated. We will eventually return to that, but first, we will try to answer the following question: can spin-Hamiltonians like 2.0.1 be obtained from more fundamental quantum mechanical models, so that we know they represent our system in a realistic way?

### 2.1 A simple example: Antiferromagnetic Heisenberg Hamiltonian from half-filled Hubbard model in a strongly correlated regime

#### 2.1.1 The Hubbard model

The aim of this section is to show how an effective quantum mechanical spin-Hamiltonian can be derived from a second quantized electron Hamiltonian. When doing so, we will not define some general method, but rather show the idea through a simple, but important example. We follow the derivation from references [11][12]. Suppose that we have the following second quantized electron Hamiltonian:

$$\hat{H} = - \sum_{i,j} \sum_{\alpha} t_{ij} \hat{c}_{i\alpha}^{\dagger} \hat{c}_{j\alpha} + U \sum_i \hat{n}_{i\uparrow} \hat{n}_{i\downarrow}; \quad t_{ii} = 0; \quad t_{ij} = t_{ji}^*, \quad (2.1.1)$$

where  $i$  goes over all sites, and  $j = j(i)$  represents all the neighbors of the site  $i$ . This is known as the Hubbard model<sup>1</sup>, and is of central importance in condensed matter physics. The first term, known as electron hopping, corresponds to effective kinetic energy of the electrons in a periodic potential, and can be derived from the tight-binding model, where the electrons are independent from each other (electron-electron Coulomb interactions are neglected)[13]. The second term in 2.1.1 is the simplest way to introduce such electron-electron interactions. As we see, the term is non-zero only when there are two electrons (with opposite spins) on the same site. Thus, when  $U > 0$ , the electrons on the same site tend to be repulsed from each other. If  $U \gg t_{ij}; \forall i, j$ , the model is said to be *strongly correlated*. In addition, if the number of electrons is the same as number of sites, the model is said to be *half-filled*.

The main challenge with this Hamiltonian is that each  $\hat{c}_{i\alpha}^{\dagger} \hat{c}_{j\alpha}$ -term contains operators from different sites, meaning that assigning these terms to a spin-operator (which by definition has a specific site) is not possible. Instead, we want to rewrite our Hamiltonian as a function of  $\hat{c}_{i\alpha}^{\dagger} \hat{c}_{i\beta}$ -pairs. Manipulating operators is a difficult task, and appropriate approximations should usually be performed. One way is to approximate our Hamiltonian to an effective Hamiltonian which is only valid for a subset of states of interest. For the applications in this thesis, this subset corresponds to the states close to the ground state, known as *low energy subspace* (LES). The other part of the space is then known as *high energy subspace* (HES). We see that for half-filled Hubbard model in strongly correlated regime, the system eigenstates with exactly one electron per site have much lower energies than other eigenstates. We can use these two subspaces of eigenstates as definitions for LES and HES, respectively.

#### 2.1.2 Low and high energy subspace projections of a Hamiltonian

The idea of this subsection is to give an expression for an effective Hamiltonian for LES eigenstates. Let  $\{|L\rangle\}$  and  $\{|H\rangle\}$  correspond to orthonormalized sets of LES and HES energy eigenstates, respectively. The projection operators on the corresponding subspaces are then given by:

$$\hat{P} = \sum_L |L\rangle \langle L|; \quad \hat{Q} = \sum_H |H\rangle \langle H|. \quad (2.1.2)$$

<sup>1</sup>Note that  $t_{ij}$  in this model is independent of the spin. When considering spin-orbit interactions, it turns out that this amplitude is spin-dependent, meaning that the model becomes different.

Since the Hilbert space is complete, we must have that:

$$\hat{P} + \hat{Q} = \mathbb{1}. \quad (2.1.3)$$

In addition, since the eigenstates are orthonormal, we have:

$$\hat{P}^2 = \sum_{L,L'} |L\rangle \langle L|L'\rangle \langle L'| = \sum_{L,L'} |L\rangle \langle L'| \delta_{LL'} = \hat{P}. \quad (2.1.4)$$

In exactly the same manner, we can show that:

$$\hat{Q}^2 = \hat{Q} \quad (2.1.5)$$

$$\hat{P}\hat{Q} = \hat{Q}\hat{P} = 0. \quad (2.1.6)$$

By using these relations, we rewrite the time-independent Schrödinger equation (TISE) as:

$$\begin{aligned} \hat{H}|\psi\rangle = E|\psi\rangle &\implies \hat{H}(\hat{P} + \hat{Q})|\psi\rangle = E(\hat{P} + \hat{Q})|\psi\rangle \implies \\ \hat{Q}\hat{H}(\hat{P} + \hat{Q})|\psi\rangle = E\hat{Q}|\psi\rangle &\implies (\hat{Q}\hat{H}\hat{Q} - E)(\hat{Q}|\psi\rangle) = -\hat{Q}\hat{H}(\hat{P}|\psi\rangle) \implies \\ \hat{Q}|\psi\rangle &= -(\hat{Q}\hat{H}\hat{Q} - E)^{-1}\hat{Q}\hat{H}(\hat{P}|\psi\rangle). \end{aligned} \quad (2.1.7)$$

Putting 2.1.7 back into TISE, we have:

$$\begin{aligned} \hat{H}|\psi\rangle = \hat{H}(\hat{P} + \hat{Q})|\psi\rangle &= \hat{H}\hat{P}|\psi\rangle + \hat{H}\hat{Q}\hat{Q}|\psi\rangle = \\ \hat{H}\hat{P}\hat{P}|\psi\rangle - \hat{H}\hat{Q}(\hat{Q}\hat{H}\hat{Q} - E)^{-1}\hat{Q}\hat{H}\hat{P}\hat{P}|\psi\rangle &= E(\hat{P} + \hat{Q})|\psi\rangle. \end{aligned} \quad (2.1.8)$$

Multiplying both sides with  $\hat{P}$  from the left, we get:

$$\boxed{\left[ \hat{P}\hat{H}\hat{P} - \hat{P}\hat{H}\hat{Q}(\hat{Q}\hat{H}\hat{Q} - E)^{-1}\hat{Q}\hat{H}\hat{P} \right] (\hat{P}|\psi\rangle) = E(\hat{P}|\psi\rangle)}. \quad (2.1.9)$$

We see that this effectively is the TISE for LES states  $\hat{P}|\psi\rangle$ , where the effective LES Hamiltonian is given by:

$$\boxed{\hat{H}_{\text{eff}} = \hat{P}\hat{H}\hat{P} - \hat{P}\hat{H}\hat{Q}(\hat{Q}\hat{H}\hat{Q} - E)^{-1}\hat{Q}\hat{H}\hat{P}}. \quad (2.1.10)$$

### 2.1.3 Effective low energy subspace Hamiltonian of half-filled strongly correlated Hubbard model

We now try to find effective LES Hamiltonian for 2.1.1, with the assumption that the model is half-filled and strongly correlated. We divide the Hamiltonian into two terms:

$$\hat{H} = \hat{H}_K + \hat{H}_U, \quad (2.1.11)$$

where

$$\hat{H}_K := -\sum_{i,j} \sum_{\alpha} t_{ij} \hat{c}_{i\alpha}^{\dagger} \hat{c}_{j\alpha}; \quad \hat{H}_U := U \sum_i \hat{n}_{i\uparrow} \hat{n}_{i\downarrow}. \quad (2.1.12)$$

In order to make progress, we will have use for the identities in the following proposition:

**Proposition 2.1.** For the Hamiltonian 2.1.1 and the projection operators defined in terms of LES and HES for this Hamiltonian, following identities are true:

$$\hat{P}\hat{H}\hat{P} = \hat{P}\hat{H}_K\hat{P} = \hat{P}\hat{H}_U\hat{P} = 0 \quad (2.1.13)$$

$$\hat{Q}\hat{H}\hat{P} = \hat{Q}\hat{H}_K\hat{P} \quad (2.1.14)$$

$$\hat{P}\hat{H}\hat{Q} = \hat{P}\hat{H}_K\hat{Q} \quad (2.1.15)$$

*Proof.* For an arbitrary state  $|\Psi\rangle$ , we have:

$$\hat{P}\hat{H}_U\hat{P}|\Psi\rangle = \hat{P}\hat{H}_U \sum_L \langle L|\Psi\rangle |L\rangle = \hat{P}U \sum_L \langle L|\Psi\rangle \sum_i \hat{n}_{i\uparrow}\hat{n}_{i\downarrow} |L\rangle = 0, \quad (2.1.16)$$

where in the last equality, we used the fact that any  $|L\rangle$  has only singly-occupied sites. On the other hand,

$$\begin{aligned} \hat{P}\hat{H}_K\hat{P}|\Psi\rangle &= \hat{P}\hat{H}_K \sum_L \langle L|\Psi\rangle |L\rangle = -\hat{P} \sum_L \langle L|\Psi\rangle \sum_{i,j} \sum_{\alpha} t_{ij} \hat{c}_{i\alpha}^{\dagger} \hat{c}_{j\alpha} |L\rangle = \\ &= -\hat{P} \sum_L \langle L|\Psi\rangle \sum_{i,j} \sum_{\alpha} t_{ij} |H(i,j,\alpha)\rangle = 0, \end{aligned} \quad (2.1.17)$$

where in the third equality, we used the fact that an  $|L\rangle$  only has singly-occupied sites, meaning that  $\hat{c}_{i\alpha}^{\dagger} \hat{c}_{j\alpha} |L\rangle = |H(i,j,\alpha)\rangle$ , where  $|H(i,j,\alpha)\rangle$  is a HES state<sup>2</sup>. In the last equality, we used the fact that  $\hat{P}|H\rangle = 0$  for any HES state. Combining 2.1.16 and 2.1.17, the identity 2.1.13 is proved.

Next, for an arbitrary state  $|\Psi\rangle$ :

$$\hat{Q}\hat{H}_U\hat{P}|\Psi\rangle = \hat{Q}\hat{H}_U \sum_L \langle L|\Psi\rangle |L\rangle = \hat{Q}U \sum_L \langle L|\Psi\rangle \sum_i \hat{n}_{i\uparrow}\hat{n}_{i\downarrow} |L\rangle = 0, \quad (2.1.18)$$

which proves 2.1.14. Finally, since a projection operator is always Hermitian, and so is  $\hat{H}_K$  and  $\hat{H}$ , 2.1.15 is just the adjoint of 2.1.14. This completes the proof.  $\square$

By using the results in proposition 2.1, our effective Hamiltonian 2.1.10 becomes:

$$\hat{H}_{\text{eff}} = -\hat{P}\hat{H}_K\hat{Q}(\hat{Q}\hat{H}\hat{Q} - E)^{-1}\hat{Q}\hat{H}_K\hat{P}. \quad (2.1.19)$$

Our next step is to find  $(\hat{Q}\hat{H}\hat{Q} - E)^{-1}$ . At this point, we make approximations based on the fact that our system is strongly correlated ( $U \gg t_{ij}$ ). First of all, we have that the two  $\hat{H}_K$ -operators in  $\hat{H}_{\text{eff}}$  contribute with  $t_{ij}^2$ . We then set  $t_{ij} = 0$  for the  $(\hat{Q}\hat{H}\hat{Q} - E)^{-1}$ -factor in order to get lowest order approximation. In such a case, we get  $\hat{Q}\hat{H}\hat{Q} = \hat{Q}\hat{H}_U\hat{Q} \rightarrow U$ , where the limit comes from the fact that rightmost  $\hat{H}_K$  in the effective Hamiltonian creates only one doubly occupied site in a LES state. The energy for a such eigenstate is given by  $E = 0$ , and thus, we end up with following lowest order approximation:

$$(\hat{Q}\hat{H}\hat{Q} - E)^{-1} \approx \frac{1}{U}. \quad (2.1.20)$$

Inserting this into 2.1.19, we end up with:

$$\boxed{\hat{H}_{\text{eff}} \approx -\hat{P}\frac{\hat{H}_K^2}{U}\hat{P}}, \quad (2.1.21)$$

where  $\hat{Q}$  has been eliminated based on an argument similar to the one used in 2.1.17. Inserting the expression for  $\hat{H}_k$  into 2.1.21, we have:

$$\hat{H}_{\text{eff}} = -\frac{1}{U} \sum_{i,j} \sum_{\alpha} \sum_{i',j'} \sum_{\beta} t_{ij}t_{i'j'} \hat{P}\hat{c}_{i\alpha}^{\dagger} \hat{c}_{j\alpha} \hat{c}_{i'\beta}^{\dagger} \hat{c}_{j'\beta} \hat{P}. \quad (2.1.22)$$

The rightmost  $\hat{P}$  in this expression turns an arbitrary state into a linear combination of LES eigenstates. This means that for non-zero  $\hat{H}_{\text{eff}}$ -terms, we must have that  $\hat{c}_{i\alpha}^{\dagger} \hat{c}_{j\alpha} \hat{c}_{i'\beta}^{\dagger} \hat{c}_{j'\beta}$  doesn't turn all of these eigenstates to HES states (because the leftmost  $\hat{P}$  turns all HES states to 0). This means that for non-zero terms,  $\hat{c}_{i\alpha}^{\dagger} \hat{c}_{j\alpha} \hat{c}_{i'\beta}^{\dagger} \hat{c}_{j'\beta}$  cannot create a double occupancy. As we see, this operator annihilates electrons at sites  $j$  and  $j'$ , and recreates them at sites  $i$  and  $i'$ . In order to not have a double occupancy, we must either have  $i = j$  and  $i' = j'$ , or  $i = j'$  and  $j = i'$ . Since  $t_{ii} \equiv 0$ , the former case gives zero-terms, and we are left with  $i = j'$  and  $j = i'$ . We thus get:

$$\begin{aligned} \hat{H}_{\text{eff}} &= -\frac{1}{U} \sum_{i,j} \sum_{\alpha\beta} t_{ij}t_{ji} \hat{P}\hat{c}_{i\alpha}^{\dagger} \hat{c}_{j\alpha} \hat{c}_{j\beta}^{\dagger} \hat{c}_{i\beta} \hat{P} = -\frac{1}{U} \sum_{i,j} \sum_{\alpha\beta} |t_{ij}|^2 \hat{P}\hat{c}_{i\alpha}^{\dagger} \hat{c}_{j\alpha} \hat{c}_{j\beta}^{\dagger} \hat{c}_{i\beta} \hat{P} = \\ &= -\frac{1}{U} \sum_{i,j} \sum_{\alpha\beta} |t_{ij}|^2 \hat{P}\hat{c}_{i\alpha}^{\dagger} \hat{c}_{j\alpha} (\delta_{ij} - \hat{c}_{i\beta} \hat{c}_{j\beta}^{\dagger}) \hat{P} = -\frac{1}{U} \sum_{i,j} \sum_{\alpha\beta} |t_{ij}|^2 \hat{P}\hat{c}_{i\alpha}^{\dagger} \hat{c}_{i\beta} \hat{c}_{j\alpha} \hat{c}_{j\beta}^{\dagger} \hat{P} = \\ &= -\frac{1}{U} \sum_{i,j} \sum_{\alpha\beta} |t_{ij}|^2 \hat{P}\hat{c}_{i\alpha}^{\dagger} \hat{c}_{i\beta} \hat{P}\hat{c}_{j\alpha} \hat{c}_{j\beta}^{\dagger} \hat{P}, \end{aligned} \quad (2.1.23)$$

<sup>2</sup>For  $i = j$  we have  $t_{ij} = 0$ , so these situations are disregarded.

where in the last equality, we used the fact that rightmost  $\hat{P}$  creates a linear combination of LES eigenstates, whilst  $\hat{c}_{j\alpha}^\dagger \hat{c}_{j\beta}^\dagger$  creates and annihilates an electron at the same site, meaning that the state is still a linear combination of LES eigenstates. Thus, inserting a  $\hat{P}$  in the middle will not affect anything. We have now obtained a Hamiltonian, where the operators belong to the same site for each operator pair, and we are thus ready to rewrite these operator pairs in terms of spin operators.

#### 2.1.4 Rewriting second quantization operators in terms of spin operators

When achieving a fermionic Hamiltonian on the  $\hat{c}_{i\alpha}^\dagger \hat{c}_{i\beta} \hat{c}_{j\alpha} \hat{c}_{j\beta}^\dagger$ -form, the procedure for rewriting the Hamiltonian in terms of spin operators is quite standard. We know that the defining property for a spin- $\frac{1}{2}$  operators are the commutation relations:

$$[\hat{S}_i^{(a)}, \hat{S}_i^{(b)}] = i\hbar \sum_{c=1}^3 \epsilon_{abc} \hat{S}_i^{(c)}; \quad a, b \in \{1, 2, 3\}, \quad (2.1.24)$$

and the constraint:

$$\hat{S}_i^2 = \hbar^2 S(S+1) = \frac{3\hbar^2}{4}. \quad (2.1.25)$$

We want to find some function  $S_i(\{\hat{c}_{i\alpha}\}, \{\hat{c}_{i\alpha}^\dagger\})$ , where the anti-commutation relations of the fermions imply both 2.1.24 and 2.1.25. A standard process here is to use the relation<sup>3</sup>:

$$\hat{S}_i = \frac{\hbar}{2} \sum_{\alpha, \beta=1}^2 \hat{c}_{i\alpha}^\dagger \vec{\sigma}_{\alpha\beta} \hat{c}_{i\beta}. \quad (2.1.26)$$

It is straight forward to show that 2.1.26 satisfies commutation relations in 2.1.24. In addition, by using the completeness relation of Pauli matrices<sup>4</sup>, it is straight forward to show that 2.1.26 implies:

$$\hat{S}_i^2 = \frac{3\hbar^2}{4} (\hat{n}_{i\uparrow} + \hat{n}_{i\downarrow})(2 - \hat{n}_{i\uparrow} - \hat{n}_{i\downarrow}). \quad (2.1.27)$$

For the LES eigenstates in our half-filled Hubbard model,  $\hat{n}_{i\uparrow} + \hat{n}_{i\downarrow} \equiv 1$ , meaning that 2.1.25 follows directly from 2.1.27. However, this model can also be used in cases with no occupancy and double occupancy. By considering total spin at each site, both of these situations give 0 spin, which also follows from 2.1.27.

For further progress, we formulate following proposition, which can easily be proved by direct inspection:

**Proposition 2.2.** Given the operator  $\hat{S}_i$  defined in 2.1.26, following identities hold:

$$\hat{c}_{i\alpha}^\dagger \hat{c}_{i\beta} = \frac{\delta_{\alpha\beta}}{2} (\hat{n}_{i\uparrow} + \hat{n}_{i\downarrow}) + \frac{1}{\hbar} \hat{S}_i \cdot \vec{\sigma}_{\beta\alpha} \quad (2.1.28)$$

$$\hat{c}_{i\alpha} \hat{c}_{i\beta}^\dagger = \delta_{\alpha\beta} (1 - \frac{\hat{n}_{i\uparrow} + \hat{n}_{i\downarrow}}{2}) - \frac{1}{\hbar} \hat{S}_i \cdot \vec{\sigma}_{\alpha\beta}. \quad (2.1.29)$$

Based on this, we have:

$$\hat{c}_{i\alpha}^\dagger \hat{c}_{i\beta} \hat{P} = \left[ \frac{\delta_{\alpha\beta}}{2} (\hat{n}_{i\uparrow} + \hat{n}_{i\downarrow}) + \frac{1}{\hbar} \hat{S}_i \cdot \vec{\sigma}_{\beta\alpha} \right] \hat{P} = \left[ \frac{\delta_{\alpha\beta}}{2} + \frac{1}{\hbar} \hat{S}_i \cdot \vec{\sigma}_{\beta\alpha} \right] \hat{P}, \quad (2.1.30)$$

$$\hat{c}_{i\alpha} \hat{c}_{i\beta}^\dagger \hat{P} = \left[ \delta_{\alpha\beta} (1 - \frac{\hat{n}_{i\uparrow} + \hat{n}_{i\downarrow}}{2}) - \frac{1}{\hbar} \hat{S}_i \cdot \vec{\sigma}_{\alpha\beta} \right] \hat{P} = \left[ \frac{\delta_{\alpha\beta}}{2} - \frac{1}{\hbar} \hat{S}_i \cdot \vec{\sigma}_{\alpha\beta} \right] \hat{P}. \quad (2.1.31)$$

Inserting these identities into 2.1.23, and dropping the  $\hat{P}$ -operators in the middle with the same argument as earlier, we get:

$$\begin{aligned} \hat{H}_{\text{eff}} &= -\frac{1}{U} \sum_{i,j} \sum_{\alpha\beta} |t_{ij}|^2 \hat{P} \hat{c}_{i\alpha}^\dagger \hat{c}_{i\beta} \hat{P} \hat{P} \hat{c}_{j\alpha} \hat{c}_{j\beta}^\dagger \hat{P} = \\ &= -\frac{1}{U} \hat{P} \sum_{i,j} \sum_{\alpha\beta} |t_{ij}|^2 \left[ \frac{1}{4} \delta_{\alpha\beta} + \frac{1}{2\hbar} \delta_{\alpha\beta} (\hat{S}_i \cdot \vec{\sigma}_{\beta\alpha} - \hat{S}_j \cdot \vec{\sigma}_{\alpha\beta}) - \frac{1}{\hbar^2} (\hat{S}_i \cdot \vec{\sigma}_{\beta\alpha}) (\hat{S}_j \cdot \vec{\sigma}_{\alpha\beta}) \right] \hat{P}. \end{aligned} \quad (2.1.32)$$

<sup>3</sup>This relation is going to be used in a reversed manner when applying Abrikosov fermionization in chapter 5. There is however a significant difference between electron operators and Abrikosov fermion operators. Whilst the former by definition act in physical particle Fock space, the latter act in quasi-particle Fock space, which corresponds to the Hilbert space of a system with constant number of electrons.

<sup>4</sup>See A.0.3 in appendix A

For the first term, we have:

$$\sum_{i,j} \sum_{\alpha\beta} |t_{ij}|^2 \frac{\delta_{\alpha\beta}}{4} = \sum_{i,j} \frac{|t_{ij}|^2}{2}. \quad (2.1.33)$$

For the second term:

$$\sum_{i,j} \sum_{\alpha\beta} |t_{ij}|^2 \delta_{\alpha\beta} (\hat{S}_i \cdot \vec{\sigma}_{\beta\alpha} - \hat{S}_j \cdot \vec{\sigma}_{\alpha\beta}) = \sum_{i,j} \sum_{\alpha} |t_{ij}|^2 (\hat{S}_i - \hat{S}_j) \cdot \vec{\sigma}_{\alpha\alpha} = 0, \quad (2.1.34)$$

where in the last equality, we used the fact that for each  $|t_{ij}|^2 (\hat{S}_i - \hat{S}_j)$ -term, there also exists a  $|t_{ji}|^2 (\hat{S}_j - \hat{S}_i) = -|t_{ji}|^2 (\hat{S}_i - \hat{S}_j)$ -term in the sum. For the last term, we have:

$$\begin{aligned} \sum_{\alpha\beta} (\hat{S}_i \cdot \vec{\sigma}_{\beta\alpha}) (\hat{S}_j \cdot \vec{\sigma}_{\alpha\beta}) &= \sum_{a,b=1}^3 \sum_{\alpha\beta} \hat{S}_i^{(a)} \sigma_{\beta\alpha}^{(a)} \sigma_{\alpha\beta}^{(b)} \hat{S}_j^{(b)} = \\ \sum_{a,b=1}^3 \hat{S}_i^{(a)} \text{Tr}(\sigma^{(a)} \sigma^{(b)}) \hat{S}_j^{(b)} &= 2 \sum_{a=1}^3 \hat{S}_i^{(a)} \hat{S}_j^{(a)} = 2 \hat{S}_i \cdot \hat{S}_j, \end{aligned} \quad (2.1.35)$$

where we used the fact that  $\text{Tr}(\sigma^{(a)} \sigma^{(b)}) = 2\delta_{ab}$ . Putting all these expressions back into 2.1.32, we get:

$$\hat{H}_{\text{eff}} = \hat{P} \sum_{i,j} J_{ij} \left[ \hat{S}_i \cdot \hat{S}_j - \frac{\hbar^2}{4} \right] \hat{P}, \quad (2.1.36)$$

where we defined:

$$J_{ij} := \frac{2|t_{ij}|^2}{U\hbar^2} > 0. \quad (2.1.37)$$

Dropping the  $\hat{P}$ -operators by assuming that we are only interested in LES states, we arrive at an AFM spin-Hamiltonian. We emphasize once again that the derivation was based on lowest order  $t/U$ -expansion, and higher order expansions are possible (see reference [14] for a rigorous derivation). In addition, it should be said that the projection method is not the only approach. For instance, exactly the same results could have been obtained by using the time-independent perturbation theory, with  $\hat{H}_K$  as perturbation[13].

### 3 Concept of bosonization and fermionization

Working analytically with spin-Hamiltonians like the one derived in previous section is difficult. The main challenge arises from the fact that commutation relations of spin operator components give another spin component (see 2.1.24). Our goal in this thesis is to extract ground state information from a spin-Hamiltonian, which is obtained by solving the TISE  $\hat{H}|\Psi\rangle = E|\Psi\rangle$  for the lowest eigenvalues  $E$ .

The idea to solve this equation near the ground state is following: suppose that we can define a set of some quasiparticles in a such way, that different excitations of these quasiparticles represent different energy eigenstates of the system. More specifically, the higher degree of excitation gives higher energy eigenvalue. The ground state is then given by no excitation, and the lowest excitations are given by single quasiparticle excitations. Based on the theory of second quantization, a perfect choice for such quasiparticles would be fermions or bosons. First of all, a number operator is defined for fermions and bosons, from which the degree of excitation is directly obtained. This number defines the Fock space of the quasiparticles, which can be set to correspond to the Hilbert space of our system. Secondly, the commutation relations for bosons and anti-commutation relations for fermions give numbers, rather than operators, meaning that this simplifies analytical work drastically. Thirdly, spin operators can be written as lowering and rising operators, which in some sense have properties in common with creation and annihilation operators. These facts can be exploited to construct fermionic or bosonic quasiparticles from spin-operators, and this is known as fermionization and bosonization, respectively.

#### 3.1 General approach

Our initial goal is to find a set of functions  $\{f_i^{(\alpha)}\}$ , so that

$$f_i^{(\alpha)}(\{\hat{a}_n\}, \{\hat{a}_n^\dagger\}) = \hat{S}_i^{(\alpha)}; \quad \alpha \in \{1, 2, 3\}, \quad (3.1.1)$$

for a set  $\{\hat{a}_n\}$  of fermionic or bosonic operators. Such transformations can be directly inserted into spin-Hamiltonians. At this point, it should be said that in some cases, the fermionic or bosonic operators represent some physically existing quasiparticles or particles, whilst in other cases, they represent a purely mathematical abstraction, without physical motivation, constructed to solve specific problems[15]. If the functions  $f_i^{(\alpha)}$  are polynomial, and so is the spin-Hamiltonian  $H(\{\hat{S}_i^{(\alpha)}\})$ , then the Hamiltonian becomes polynomial in fermionic or bosonic operators. The task then is to find some canonical transformations<sup>5</sup>, so that the Hamiltonian can be written in terms of number operators only, with the ground state usually corresponding to no quasiparticles<sup>6</sup>. This process is known as diagonalization. In the following, we will show a general approach for diagonalizing quadratic Hamiltonians, which are of central importance. Then, we will show some simple examples of fermionization and bosonization.

#### 3.2 Quadratic Hamiltonians: a general diagonalization approach with Bogoliubov transformations

In this section, we will present a general approach to diagonalization of quadratic Hermitian Hamiltonians. In addition, we will present some specific examples of diagonalization that will be used later in the thesis. Starting with some mathematical conventions, we have that the mathematical difference between fermions and bosons essentially is the sign in the commutator, and a lot of expressions related to fermions and bosons will only have a difference in sign. Therefore, it is customary to define following quantity:

$$\zeta := \begin{cases} -1 & \text{for fermions} \\ +1 & \text{for bosons} \end{cases} \quad (3.2.1)$$

With this definition, we can combine fermionic anti-commutator and bosonic commutator into one relation, given by

$$[\hat{A}, \hat{B}]_\zeta := \hat{A}\hat{B} - \zeta\hat{B}\hat{A} = \begin{cases} \{\hat{A}, \hat{B}\} & \text{for fermions} \\ [\hat{A}, \hat{B}] & \text{for bosons.} \end{cases} \quad (3.2.2)$$

<sup>5</sup>Canonical transformation of fermionic or bosonic operators means that the corresponding anti-commutation or commutation relations are preserved.

<sup>6</sup>This is not always the case. In section 5.3, we will consider Abrikosov fermions at half-filling, meaning that number of quasiparticles is conserved. In a such case, the ground state is given by all quasiparticles occupying lower energy bands, whilst excitations happen to higher bands.



Next, for a lattice with  $N$  sites, a general quadratic Hamiltonian can be written on the form:

$$\hat{H} = \sum_{j,j'=1}^N \left[ C_{jj'} \hat{a}_j^\dagger \hat{a}_{j'} + D_{jj'} \hat{a}_j \hat{a}_{j'}^\dagger + E_{jj'} \hat{a}_j \hat{a}_{j'} + F_{jj'} \hat{a}_j^\dagger \hat{a}_{j'}^\dagger \right] + G, \quad (3.2.3)$$

where  $C_{jj'}$ ,  $D_{jj'}$ ,  $E_{jj'}$ ,  $F_{jj'}$  and  $G$  are constant coefficients, and  $\{\hat{a}_j\}$  are either fermionic or bosonic operators. The idea is to organize this Hamiltonian into a matrix defined by the coefficients. By using the definition in 3.2.2, we must have:

$$[\hat{a}_j, \hat{a}_{j'}^\dagger]_\zeta = \delta_{jj'} \quad (3.2.4)$$

$$[\hat{a}_j, \hat{a}_{j'}]_\zeta = 0 \quad (3.2.5)$$

$$[\hat{a}_j^\dagger, \hat{a}_{j'}^\dagger]_\zeta = 0. \quad (3.2.6)$$

By applying these  $\zeta$ -commutations, we can rewrite our Hamiltonian to:

$$\hat{H} = \sum_{j,j'=1}^N \left[ (C_{jj'} + \zeta D_{j'j}) \hat{a}_j^\dagger \hat{a}_{j'} + E_{jj'} \hat{a}_j \hat{a}_{j'} + F_{jj'} \hat{a}_j^\dagger \hat{a}_{j'}^\dagger \right] + G + \text{Tr}(\mathbf{D}), \quad (3.2.7)$$

where  $\mathbf{D}$  is an  $N \times N$  matrix defined by coefficients  $D_{jj'}$ .

Next, we must have that our Hamiltonian is Hermitian, meaning that  $\hat{H} = \hat{H}^\dagger$ . We have that:

$$\hat{H}^\dagger = \sum_{j,j'=1}^N \left[ (C_{j'j}^* + \zeta D_{jj'}^*) \hat{a}_j^\dagger \hat{a}_{j'} + E_{j'j}^* \hat{a}_j^\dagger \hat{a}_{j'}^\dagger + F_{j'j}^* \hat{a}_j \hat{a}_{j'} \right] + G^* + \text{Tr}(\mathbf{D}^*). \quad (3.2.8)$$

Defining:

$$2A_{jj'} := C_{jj'} + \zeta D_{j'j}, \quad (3.2.9)$$

and setting 3.2.7 equal to 3.2.8, we must have that:

$$A_{jj'} = A_{j'j}^*; \quad F_{jj'} = E_{j'j}^*. \quad (3.2.10)$$

In addition, we have:

$$\sum_{j,j'=1}^N \left[ E_{jj'} \hat{a}_j \hat{a}_{j'} + F_{jj'} \hat{a}_j^\dagger \hat{a}_{j'}^\dagger \right] = \sum_{j,j'=1}^N \left[ \zeta E_{jj'} \hat{a}_j \hat{a}_{j'} + \zeta F_{jj'} \hat{a}_j^\dagger \hat{a}_{j'}^\dagger \right] = \sum_{j,j'=1}^N \left[ \zeta E_{j'j} \hat{a}_j \hat{a}_{j'} + \zeta F_{j'j} \hat{a}_j^\dagger \hat{a}_{j'}^\dagger \right], \quad (3.2.11)$$

meaning that:

$$E_{jj'} = \zeta E_{j'j}; \quad F_{jj'} = \zeta F_{j'j}. \quad (3.2.12)$$

The terms  $G$  and  $\text{Tr}(\mathbf{D})$  are constants, and can be dropped in the initial Hamiltonian. Defining  $B_{jj'} := F_{jj'}$ , we summarize these results in the following proposition:

**Proposition 3.1.** A Hermitian Hamiltonian which is quadratic in either fermionic or bosonic creation and annihilation operators can always be written on the form:

$$\hat{H} = \sum_{j=1}^N \sum_{j'=1}^N \left[ 2A_{jj'} \hat{a}_j^\dagger \hat{a}_{j'} + B_{jj'} \hat{a}_j^\dagger \hat{a}_{j'}^\dagger + B_{jj'}^* \hat{a}_j \hat{a}_{j'} \right], \quad (3.2.13)$$

where  $A_{jj'} = A_{j'j}^*$ ;  $B_{jj'} = \zeta B_{j'j}$

This Hamiltonian can be organized into a matrix by following proposition, which is easily proved by direct inspection:

**Proposition 3.2.** The Hamiltonian in Proposition 3.1 can be written on the form:

$$\hat{H} = \begin{bmatrix} \hat{\mathbf{a}}^\dagger & \hat{\mathbf{a}} \end{bmatrix} \begin{bmatrix} \mathbf{A} & \mathbf{B} \\ \zeta \mathbf{B}^* & \zeta \mathbf{A}^* \end{bmatrix} \begin{bmatrix} \hat{\mathbf{a}} \\ \hat{\mathbf{a}}^\dagger \end{bmatrix} - \zeta \text{Tr}(\mathbf{A}). \quad (3.2.14)$$

Here,  $\mathbf{A}$  and  $\mathbf{B}$  are  $N \times N$  matrices defined by coefficients  $[A_{jj'}]$  and  $[B_{jj'}]$ , respectively, and the operator vectors are defined as

$\begin{bmatrix} \hat{\mathbf{a}}^\dagger & \hat{\mathbf{a}} \end{bmatrix} = [\hat{a}_1^\dagger \quad \dots \quad \hat{a}_N^\dagger \quad \hat{a}_1 \quad \dots \quad \hat{a}_N]$  and  $\begin{bmatrix} \hat{\mathbf{a}} \\ \hat{\mathbf{a}}^\dagger \end{bmatrix} = [\hat{a}_1 \quad \hat{a}_1^\dagger \quad \dots \quad \hat{a}_N \quad \hat{a}_N^\dagger]^\dagger$ . The matrices have following properties:  $\mathbf{A} =$

$$\mathbf{A}^\dagger; \quad \mathbf{B} = \zeta \mathbf{B}^T.$$

Given a Hamiltonian written on the same form as in Proposition 3.1, we can easily rewrite it into a matrix form in proposition 3.2. The idea then is pretty simple - we want to find an invertible matrix  $\mathbb{T}$ , so that when having the Hamiltonian<sup>7</sup>:

$$\hat{H} = \begin{bmatrix} \hat{\mathbf{a}}^\dagger & \hat{\mathbf{a}} \end{bmatrix} \mathbb{H} \begin{bmatrix} \hat{\mathbf{a}} \\ \hat{\mathbf{a}}^\dagger \end{bmatrix} = \underbrace{\begin{bmatrix} \hat{\mathbf{a}}^\dagger & \hat{\mathbf{a}} \end{bmatrix}}_{\begin{bmatrix} \hat{\mathbf{c}}^\dagger & \hat{\mathbf{c}} \end{bmatrix}} \underbrace{(\mathbb{T}^\dagger)^{-1} (\mathbb{T}^\dagger \mathbb{H} \mathbb{T}) \mathbb{T}^{-1}}_{\mathbb{D}} \underbrace{\begin{bmatrix} \hat{\mathbf{a}} \\ \hat{\mathbf{a}}^\dagger \end{bmatrix}}_{\begin{bmatrix} \hat{\mathbf{c}} \\ \hat{\mathbf{c}}^\dagger \end{bmatrix}}, \quad (3.2.15)$$

the matrix  $\mathbb{D} := \mathbb{T}^\dagger \mathbb{H} \mathbb{T}$  becomes diagonal, and, at the same time, the operator transformation

$$\begin{bmatrix} \hat{\mathbf{c}} \\ \hat{\mathbf{c}}^\dagger \end{bmatrix} = \begin{bmatrix} \hat{c}_1 & \dots & \hat{c}_N & \hat{c}_1^\dagger & \dots & \hat{c}_N^\dagger \end{bmatrix}^T = \mathbb{T}^{-1} \begin{bmatrix} \hat{\mathbf{a}} \\ \hat{\mathbf{a}}^\dagger \end{bmatrix} \quad (3.2.16)$$

is canonical. Such transformation is in general known as Bogoliubov transformation. If such  $\mathbb{T}$  is found, the Hamiltonian becomes diagonal in the  $\hat{c}$ -operators:

$$\begin{aligned} \hat{H} &= \begin{bmatrix} \hat{\mathbf{c}}^\dagger & \hat{\mathbf{c}} \end{bmatrix} \mathbb{D} \begin{bmatrix} \hat{\mathbf{c}} \\ \hat{\mathbf{c}}^\dagger \end{bmatrix} = \begin{bmatrix} \hat{\mathbf{c}}^\dagger & \hat{\mathbf{c}} \end{bmatrix} \begin{bmatrix} D_1 & 0 & \dots & 0 \\ 0 & D_2 & \dots & 0 \\ \vdots & \vdots & \ddots & \vdots \\ 0 & 0 & \dots & D_{2N} \end{bmatrix} \begin{bmatrix} \hat{\mathbf{c}} \\ \hat{\mathbf{c}}^\dagger \end{bmatrix} = \\ & \sum_{i=1}^N [D_i \hat{c}_i^\dagger \hat{c}_i + D_{i+N} \hat{c}_i \hat{c}_i^\dagger] = \sum_{i=1}^N [(D_i + \zeta D_{i+N}) \hat{c}_i^\dagger \hat{c}_i + D_{i+N}]. \end{aligned} \quad (3.2.17)$$

Defining the operator  $\mathbb{J}$  in  $\mathbb{C}^{2N}$  by the transformation:

$$\mathbb{J} \begin{bmatrix} \mathbf{u} \\ \mathbf{v} \end{bmatrix} = \begin{bmatrix} \mathbf{v}^* \\ \mathbf{u}^* \end{bmatrix}; \quad \mathbf{u}, \mathbf{v} \in \mathbb{C}^N, \quad (3.2.18)$$

we summarize following general quadratic diagonalization theorem:

**Theorem 3.1.** Given a Hamiltonian on the form

$$\hat{H} = \begin{bmatrix} \hat{\mathbf{a}}^\dagger & \hat{\mathbf{a}} \end{bmatrix} \mathbb{H}_\zeta \begin{bmatrix} \hat{\mathbf{a}} \\ \hat{\mathbf{a}}^\dagger \end{bmatrix} - \zeta \text{Tr}(\mathbf{A}); \quad \mathbb{H}_\zeta = \begin{bmatrix} \mathbf{A} & \mathbf{B} \\ \zeta \mathbf{B}^* & \zeta \mathbf{A}^* \end{bmatrix}, \quad (3.2.19)$$

suppose that we can find an orthonormal set of  $N$  eigenvectors  $\{\mathbf{x}_1, \dots, \mathbf{x}_N\}$  of the matrix

$$\mathbb{M} = \begin{bmatrix} \mathbf{A} & \mathbf{B} \\ -\mathbf{B}^* & -\mathbf{A}^* \end{bmatrix}, \quad (3.2.20)$$

with eigenvalues  $\epsilon_i \geq 0$ . Then, the set  $\{\mathbb{J}\mathbf{x}_1, \dots, \mathbb{J}\mathbf{x}_N\}$  is also a set of orthonormal eigenvectors with eigenvalues  $\epsilon'_i = -\epsilon_i$ . If

$\{\mathbf{x}_1, \dots, \mathbf{x}_N, \mathbb{J}\mathbf{x}_1, \dots, \mathbb{J}\mathbf{x}_N\}$  is orthonormal, and hence spans  $\mathbb{C}^{2N}$ , then we can rewrite our Hamiltonian as

$$\hat{H} = \sum_{i=1}^N \left[ 2\epsilon_i \hat{c}_i^\dagger \hat{c}_i + \zeta \epsilon_i \right] - \zeta \text{Tr}(\mathbf{A}), \quad (3.2.21)$$

where  $\hat{c}$ -operators are of same type (fermionic or bosonic) as  $\hat{a}$ -operators, and are defined by the transformation

$$\begin{bmatrix} \hat{\mathbf{c}} \\ \hat{\mathbf{c}}^\dagger \end{bmatrix} = \mathbb{T}^{-1} \begin{bmatrix} \hat{\mathbf{a}} \\ \hat{\mathbf{a}}^\dagger \end{bmatrix}; \quad \mathbb{T} = \begin{bmatrix} \mathbf{x}_1 & \dots & \mathbf{x}_N & \mathbb{J}\mathbf{x}_1 & \dots & \mathbb{J}\mathbf{x}_N \end{bmatrix}. \quad (3.2.22)$$

<sup>7</sup>Note that the matrix  $\mathbb{T}$  is not necessarily unitary. In fact, this matrix turns out to be unitary for fermions, but pseudo-unitary for bosons.

A proof of this theorem, as well as the conditions for existence of the necessary eigenvectors, can be found in reference [16]. In particular, fermionic matrices are diagonalizable this way when Hermitian, and bosonic matrices are diagonalizable this way when positive definite (all eigenvalues positive). We now have a very general diagonalization method that allows us in theory to approach any kind of quadratic Hamiltonians, and in subsection 3.3.2, we will show how theorem 3.1 can be used directly. It should however be said that for most applications, the Hamiltonian matrices become unpractically large, and finding all the eigenvalues might be a challenge. In many cases, the matrix can be decoupled into smaller blocks - in particular, for a periodic lattice, we can use Fourier transform to achieve this. The smaller blocks can then be solved by using theorem 3.1. However, even the resulting blocks might be larger than necessary, and therefore, we will present some modified versions of theorem 3.1 in subsections 3.4.1 and 3.4.2. These involve smaller matrices, and are constructed specifically to solve diagonalization problems that will arise in sections 5.3 and 5.4.

### 3.3 Example: Bogoliubov transformation of a relevant special case

In this section, we will consider a Hamiltonian which is relevant if one wants to derive the results that will be presented in Holstein-Primakoff example in 3.5.2. The Hamiltonian is given by:

$$\begin{aligned} \hat{H} &= \gamma(\hat{a}_1^\dagger \hat{a}_1 + \hat{a}_2^\dagger \hat{a}_2) + \lambda \hat{a}_1^\dagger \hat{a}_2^\dagger + \lambda \hat{a}_2 \hat{a}_1 = \\ & \gamma(\hat{a}_1^\dagger \hat{a}_1 + \hat{a}_2^\dagger \hat{a}_2) + \frac{\lambda}{2}(\hat{a}_1^\dagger \hat{a}_2^\dagger + \zeta \hat{a}_2^\dagger \hat{a}_1^\dagger) + \frac{\lambda}{2}(\hat{a}_2 \hat{a}_1 + \zeta \hat{a}_1 \hat{a}_2); \quad \gamma, \lambda \in \mathbb{R}. \end{aligned} \quad (3.3.1)$$

We see that in this model, we have two non-diagonal terms with either two creation or two annihilation operators. It is also easy to verify that the Hamiltonian is Hermitian. We will now diagonalize this Hamiltonian by doing the Bogoliubov transformation directly, and then perform the same diagonalization by using theorem 3.1.

#### 3.3.1 Diagonalization by doing Bogoliubov transformation directly

In this subsection, we closely follow the approach from reference [17]. We start with defining following Bogoliubov transformation:

$$\hat{a}_1^\dagger = u \hat{c}_1^\dagger + v \hat{c}_2 \quad (3.3.2)$$

$$\hat{a}_2^\dagger = u \hat{c}_2^\dagger + \zeta v \hat{c}_1 \quad (3.3.3)$$

We want this transformation to be canonical, meaning that we require:

$$[\hat{c}_i, \hat{c}_j^\dagger]_\zeta = \delta_{ij} \quad (3.3.4)$$

$$[\hat{c}_i, \hat{c}_j]_\zeta = 0 \quad (3.3.5)$$

$$[\hat{c}_i^\dagger, \hat{c}_j^\dagger]_\zeta = 0; \quad i, j \in \{1, 2\}. \quad (3.3.6)$$

Assuming that these relations are true, we then have:

$$[\hat{a}_1, \hat{a}_2^\dagger]_\zeta = -\zeta [\hat{a}_2^\dagger, \hat{a}_1]_\zeta = [u^* \hat{c}_1 + v^* \hat{c}_2^\dagger, u \hat{c}_2^\dagger + \zeta v \hat{c}_1]_\zeta = 0 = [\hat{a}_2, \hat{a}_1^\dagger]_\zeta \quad (3.3.7)$$

$$[\hat{a}_1, \hat{a}_1^\dagger]_\zeta = [u^* \hat{c}_1 + v^* \hat{c}_2^\dagger, u \hat{c}_1^\dagger + v \hat{c}_2]_\zeta = |u|^2 [\hat{c}_1, \hat{c}_1^\dagger]_\zeta + |v|^2 [\hat{c}_2^\dagger, \hat{c}_2]_\zeta = |u|^2 [\hat{c}_1, \hat{c}_1^\dagger]_\zeta - \zeta |v|^2 [\hat{c}_2, \hat{c}_2^\dagger]_\zeta = |u|^2 - \zeta |v|^2 \quad (3.3.8)$$

$$[\hat{a}_2, \hat{a}_2^\dagger]_\zeta = [u^* \hat{c}_2 + \zeta v^* \hat{c}_1^\dagger, u \hat{c}_2^\dagger + \zeta v \hat{c}_1]_\zeta = |u|^2 - \zeta |v|^2 \quad (3.3.9)$$

$$[\hat{a}_1^\dagger, \hat{a}_2^\dagger]_\zeta = [u \hat{c}_1^\dagger + v \hat{c}_2, u \hat{c}_2^\dagger + \zeta v \hat{c}_1]_\zeta = \zeta uv [\hat{c}_1^\dagger, \hat{c}_1]_\zeta + vu [\hat{c}_2, \hat{c}_2^\dagger]_\zeta = vu - uv = 0 = [\hat{a}_2, \hat{a}_1]_\zeta. \quad (3.3.10)$$

Thus, in order to not get any contradictions, we must have:

$$\boxed{|u|^2 - \zeta |v|^2 = 1.} \quad (3.3.11)$$

Next, based on proposition 3.1, we see that:

$$2A_{11} = \gamma; \quad 2A_{22} = \gamma; \quad B_{12} = \frac{\lambda}{2}; \quad B_{21} = \zeta \frac{\lambda}{2}; \quad 0 \text{ otherwise.} \quad (3.3.12)$$

According to proposition 3.2, we then have:

$$\begin{aligned}
\hat{H} &= \frac{1}{2} \begin{bmatrix} \hat{a}_1^\dagger & \hat{a}_2^\dagger & \hat{a}_1 & \hat{a}_2 \end{bmatrix} \begin{bmatrix} \gamma & 0 & 0 & \lambda \\ 0 & \gamma & \zeta\lambda & 0 \\ 0 & \zeta\lambda & \zeta\gamma & 0 \\ \lambda & 0 & 0 & \zeta\gamma \end{bmatrix} \begin{bmatrix} \hat{a}_1 \\ \hat{a}_2 \\ \hat{a}_1^\dagger \\ \hat{a}_2^\dagger \end{bmatrix} - \zeta\gamma = \\
&\frac{1}{2} \begin{bmatrix} \hat{a}_1^\dagger & \hat{a}_2 & \hat{a}_2^\dagger & \hat{a}_1 \end{bmatrix} \begin{bmatrix} \gamma & \lambda & 0 & 0 \\ \lambda & \zeta\gamma & 0 & 0 \\ 0 & 0 & \gamma & \zeta\lambda \\ 0 & 0 & \zeta\lambda & \zeta\gamma \end{bmatrix} \begin{bmatrix} \hat{a}_1 \\ \hat{a}_2 \\ \hat{a}_1^\dagger \\ \hat{a}_2^\dagger \end{bmatrix} - \zeta\gamma = \\
&\frac{1}{2} \left[ \begin{bmatrix} \hat{a}_1^\dagger & \hat{a}_2 \end{bmatrix} \begin{bmatrix} \gamma & \lambda \\ \lambda & \zeta\gamma \end{bmatrix} \begin{bmatrix} \hat{a}_1 \\ \hat{a}_2^\dagger \end{bmatrix} + \begin{bmatrix} \hat{a}_2^\dagger & \hat{a}_1 \end{bmatrix} \begin{bmatrix} \gamma & \zeta\lambda \\ \zeta\lambda & \zeta\gamma \end{bmatrix} \begin{bmatrix} \hat{a}_2 \\ \hat{a}_1^\dagger \end{bmatrix} \right] - \zeta\gamma.
\end{aligned} \tag{3.3.13}$$

We have thus reduced the Hamiltonian matrix into two smaller blocks. This will simplify the further process. Next, since we are working with real parameters, it is reasonable to assume that the Bogoliubov coefficients in 3.3.2 and 3.3.3,  $u$  and  $v$  are real. Writing this transformation on the matrix form, we then have:

$$\begin{bmatrix} \hat{a}_1 \\ \hat{a}_2^\dagger \end{bmatrix} = \begin{bmatrix} u & v \\ \zeta v & u \end{bmatrix} \begin{bmatrix} \hat{c}_1 \\ \hat{c}_2^\dagger \end{bmatrix} \implies \begin{bmatrix} \hat{a}_1^\dagger & \hat{a}_2 \end{bmatrix} = \begin{bmatrix} \hat{c}_1^\dagger & \hat{c}_2 \end{bmatrix} \begin{bmatrix} u & \zeta v \\ v & u \end{bmatrix} \tag{3.3.14}$$

$$\begin{bmatrix} \hat{a}_2 \\ \hat{a}_1^\dagger \end{bmatrix} = \begin{bmatrix} u & \zeta v \\ v & u \end{bmatrix} \begin{bmatrix} \hat{c}_2 \\ \hat{c}_1^\dagger \end{bmatrix} \implies \begin{bmatrix} \hat{a}_2^\dagger & \hat{a}_1 \end{bmatrix} = \begin{bmatrix} \hat{c}_2^\dagger & \hat{c}_1 \end{bmatrix} \begin{bmatrix} u & v \\ \zeta v & u \end{bmatrix} \tag{3.3.15}$$

From this, we see that

$$\begin{aligned}
\hat{H} &= \frac{1}{2} \left[ \begin{bmatrix} \hat{c}_1^\dagger & \hat{c}_2 \end{bmatrix} \begin{bmatrix} u & \zeta v \\ v & u \end{bmatrix} \begin{bmatrix} \gamma & \lambda \\ \lambda & \zeta\gamma \end{bmatrix} \begin{bmatrix} u & v \\ \zeta v & u \end{bmatrix} \begin{bmatrix} \hat{c}_1 \\ \hat{c}_2^\dagger \end{bmatrix} + \right. \\
&\left. \begin{bmatrix} \hat{c}_2^\dagger & \hat{c}_1 \end{bmatrix} \begin{bmatrix} u & v \\ \zeta v & u \end{bmatrix} \begin{bmatrix} \gamma & \zeta\lambda \\ \zeta\lambda & \zeta\gamma \end{bmatrix} \begin{bmatrix} u & \zeta v \\ v & u \end{bmatrix} \begin{bmatrix} \hat{c}_2 \\ \hat{c}_1^\dagger \end{bmatrix} \right] - \zeta\gamma,
\end{aligned} \tag{3.3.16}$$

so that we want

$$\begin{bmatrix} u & \zeta v \\ v & u \end{bmatrix} \begin{bmatrix} \gamma & \lambda \\ \lambda & \zeta\gamma \end{bmatrix} \begin{bmatrix} u & v \\ \zeta v & u \end{bmatrix} = \begin{bmatrix} \gamma(u^2 + \zeta v^2) + 2\zeta\lambda uv & \lambda(u^2 + \zeta v^2) + 2\gamma uv \\ \lambda(u^2 + \zeta v^2) + 2\gamma uv & \zeta\gamma(u^2 + \zeta v^2) + 2\lambda uv \end{bmatrix} \tag{3.3.17}$$

and

$$\begin{bmatrix} u & v \\ \zeta v & u \end{bmatrix} \begin{bmatrix} \gamma & \zeta\lambda \\ \zeta\lambda & \zeta\gamma \end{bmatrix} \begin{bmatrix} u & \zeta v \\ v & u \end{bmatrix} = \begin{bmatrix} \gamma(u^2 + \zeta v^2) + 2\zeta\lambda uv & \zeta\lambda(u^2 + \zeta v^2) + 2\zeta\gamma uv \\ \zeta\lambda(u^2 + \zeta v^2) + 2\zeta\gamma uv & \zeta\gamma(u^2 + \zeta v^2) + 2\lambda uv \end{bmatrix}, \tag{3.3.18}$$

to be diagonal. We see that this is achieved when:

$$\lambda(u^2 + \zeta v^2) + 2\gamma uv = 0 \tag{3.3.19}$$

From 3.3.11, we also have the constraint:

$$u^2 - \zeta v^2 = 1. \tag{3.3.20}$$

This constraint can be satisfied by writing:

$$u = \cos(\eta_\zeta \theta); \quad v = -\zeta \eta_\zeta \sin(\eta_\zeta \theta); \quad \theta \in \mathbb{R}, \tag{3.3.21}$$

where we defined:

$$\eta_\zeta := \frac{(1 - \zeta) + i(1 + \zeta)}{2} = \begin{cases} 1 & \zeta = -1 \\ i & \zeta = +1 \end{cases}. \tag{3.3.22}$$

We thus have:

$$\begin{aligned}
\lambda(u^2 + \zeta v^2) + 2\gamma uv &= \lambda[\cos^2(\eta_\zeta \theta) + \zeta \eta_\zeta^2 \sin^2(\eta_\zeta \theta)] - 2\zeta \eta_\zeta \gamma \cos(\eta_\zeta \theta) \sin(\eta_\zeta \theta) = \\
&\lambda \cos(2\eta_\zeta \theta) - \zeta \eta_\zeta \gamma \sin(2\eta_\zeta \theta) = 0 \implies \\
&\tan(2\eta_\zeta \theta) = \frac{\lambda}{\zeta \eta_\zeta \gamma} \implies \\
\theta &= \frac{1}{2\eta_\zeta} \left[ \arctan\left(\frac{\lambda}{\zeta \eta_\zeta \gamma}\right) + n\pi \right]; \quad n \in \mathbb{Z}.
\end{aligned} \tag{3.3.23}$$

We have now found an expression for  $u$  and  $v$  which makes 3.3.17 and 3.3.18 diagonal. Finally, we want to find the diagonal values. We have:

$$\begin{bmatrix} u & v \\ \zeta v & u \end{bmatrix} \begin{bmatrix} \gamma & \zeta\lambda \\ \zeta\lambda & \zeta\gamma \end{bmatrix} \begin{bmatrix} u & \zeta v \\ v & u \end{bmatrix} = \begin{bmatrix} u & v \\ \zeta v & u \end{bmatrix} \begin{bmatrix} \gamma & \zeta\lambda \\ \zeta\lambda & \zeta\gamma \end{bmatrix} \begin{bmatrix} u & \zeta v \\ v & u \end{bmatrix} = \begin{bmatrix} \tilde{\epsilon} & 0 \\ 0 & \zeta\tilde{\epsilon} \end{bmatrix}, \quad (3.3.24)$$

where we defined:

$$\tilde{\epsilon} := \gamma(u^2 + \zeta v^2) + 2\zeta\lambda uv \quad (3.3.25)$$

Inserting 3.3.21 and  $\theta$  from 3.3.23 into 3.3.25, we have

$$\begin{aligned} \tilde{\epsilon} &= \gamma \cos\left(\arctan\left(\frac{\lambda}{\zeta\eta\zeta\gamma}\right) + n\pi\right) - \eta\zeta\lambda \sin\left(\arctan\left(\frac{\lambda}{\zeta\eta\zeta\gamma}\right) + n\pi\right) = \\ &\begin{cases} \frac{\gamma}{\sqrt{1-\zeta\frac{\lambda^2}{\gamma^2}}} - \zeta\frac{\lambda^2}{\gamma} \frac{1}{\sqrt{1-\zeta\frac{\lambda^2}{\gamma^2}}} & \text{when } n \text{ is even} \\ -\frac{\gamma}{\sqrt{1-\zeta\frac{\lambda^2}{\gamma^2}}} + \zeta\frac{\lambda^2}{\gamma} \frac{1}{\sqrt{1-\zeta\frac{\lambda^2}{\gamma^2}}} & \text{when } n \text{ is odd.} \end{cases} \end{aligned} \quad (3.3.26)$$

For the sake of second quantization stability, we want  $\tilde{\epsilon} \geq 0$ . This is because we want no quasiparticle excitation to correspond to the groundstate. This is not possible when some excitations have negative energies. Thus, we choose  $n$  to be even when  $\gamma \geq 0$  and odd when  $\gamma < 0$ . We then get that:

$$\boxed{\tilde{\epsilon} = \frac{\gamma^2}{\sqrt{\gamma^2 - \zeta\lambda^2}} - \zeta \frac{\lambda^2}{\sqrt{\gamma^2 - \zeta\lambda^2}} = \sqrt{\gamma^2 - \zeta\lambda^2}} \quad (3.3.27)$$

Inserting 3.3.27 and 3.3.24 into 3.3.16, we finally get:

$$\boxed{\hat{H} = \sqrt{\gamma^2 - \zeta\lambda^2}(\hat{c}_1^\dagger \hat{c}_1 + \hat{c}_2^\dagger \hat{c}_2) + \zeta(\sqrt{\gamma^2 - \zeta\lambda^2} - \gamma)} \quad (3.3.28)$$

and the diagonalization process is completed.

### 3.3.2 Diagonalization with theorem 3.1

The direct Bogoliubov transformation process presented in previous subsection is quite standard. However, we see that the process is lengthy, cumbersome and limiting, and instead of doing all the transformations, we can find eigenvalues of appropriate matrices, and then use theorem 3.1. Taking a look at this theorem and returning to the first equality in 3.3.13, we have that:

$$\mathbf{A} = \frac{1}{2} \begin{bmatrix} \gamma & 0 \\ 0 & \gamma \end{bmatrix}; \quad \mathbf{B} = \frac{1}{2} \begin{bmatrix} 0 & \lambda \\ \zeta\lambda & 0 \end{bmatrix}. \quad (3.3.29)$$

The  $\mathbb{M}$ -matrix is then given by:

$$\mathbb{M} = \frac{1}{2} \begin{bmatrix} \gamma & 0 & 0 & \lambda \\ 0 & \gamma & \zeta\lambda & 0 \\ 0 & -\lambda & -\gamma & 0 \\ -\zeta\lambda & 0 & 0 & -\gamma \end{bmatrix}. \quad (3.3.30)$$

Finding the eigenvalues of this matrix is not a very difficult task, and we obtain:

$$m_1, m_2 = \frac{1}{2} \sqrt{\gamma^2 - \zeta\lambda^2} \quad (3.3.31)$$

$$m_3, m_4 = -\frac{1}{2} \sqrt{\gamma^2 - \zeta\lambda^2}. \quad (3.3.32)$$

We see that the eigenvalues have a structure which is expected from the theorem. From 3.2.21, we then get:

$$\hat{H} = \sqrt{\gamma^2 - \zeta\lambda^2}(\hat{c}_1^\dagger \hat{c}_1 + \hat{c}_2^\dagger \hat{c}_2) + \zeta(\sqrt{\gamma^2 - \zeta\lambda^2} - \gamma), \quad (3.3.33)$$

which is exactly the same result. This shows the strength of theorem 3.1.

### 3.4 Some modified diagonalization theorems

As we see in theorem 3.1, the vector  $[\hat{\mathbf{a}}^\dagger \ \hat{\mathbf{a}}]$  contains the subvector  $\hat{\mathbf{a}}$  twice. Because of that, the Hamiltonian matrix  $\mathbb{H}_\zeta$  is twice as large as necessary. As we will see in sections 5.3 and 5.4, it is often possible to organize the Hamiltonians into smaller matrices, where the entries in the vectors correspond to different operators only. For that reason, we are going to present two alternative diagonalization theorems.

#### 3.4.1 A modified fermionic diagonalization approach

Suppose that we have a Hermitian  $m \times m$  matrix  $\mathbb{H}$ , and that our Hamiltonian, up to constant near, is given by:

$$\hat{H} = \hat{\mathbf{a}}^\dagger \mathbb{H} \hat{\mathbf{a}}; \quad \hat{\mathbf{a}} = [\hat{\alpha}_1 \ \dots \ \hat{\alpha}_m]^T, \quad (3.4.1)$$

where  $\hat{\mathbf{a}}$  is  $m$ -sized vector with fermionic operators as entries. As we see, the vector entries have unique operators. We then define an  $m \times m$  transformation matrix  $\mathbb{T}$  in a such way, that

$$\mathbb{T} \hat{\mathbf{a}} = \hat{\mathbf{c}} = [\hat{\gamma}_1 \ \dots \ \hat{\gamma}_m]^T, \quad (3.4.2)$$

$$(\mathbb{T} \hat{\mathbf{a}})^\dagger = \hat{\mathbf{a}}^\dagger \mathbb{T}^\dagger = \hat{\mathbf{c}}^\dagger = [\hat{\gamma}_1^\dagger \ \dots \ \hat{\gamma}_m^\dagger] \quad (3.4.3)$$

become canonical transformations. At the same time, having:

$$\hat{H} = \hat{\mathbf{a}}^\dagger \mathbb{H} \hat{\mathbf{a}} = \hat{\mathbf{a}}^\dagger \mathbb{T}^\dagger (\mathbb{T}^\dagger)^{-1} \mathbb{H} \mathbb{T}^{-1} \mathbb{T} \hat{\mathbf{a}} = \hat{\mathbf{c}}^\dagger \mathbb{D} \hat{\mathbf{c}}, \quad (3.4.4)$$

where we defined  $\mathbb{D} := (\mathbb{T}^\dagger)^{-1} \mathbb{H} \mathbb{T}^{-1}$ , we want  $\mathbb{D}$  to be diagonal, meaning that we can write it on the form:

$$\mathbb{D} = \text{diag}(\lambda_1, \dots, \lambda_m). \quad (3.4.5)$$

At this point, we want to determine whether a such transformation matrix can exist. For fermionic operators in  $\hat{\mathbf{a}}$ , we have that:

$$\{\hat{\mathbf{a}}_{p'}, \hat{\mathbf{a}}_p^\dagger\} = I_{p'p}, \quad (3.4.6)$$

where  $I$  is the identity matrix. In order to have a canonical transformation, the same relation must hold for  $\hat{\mathbf{c}}$ -vector:

$$\begin{aligned} I_{p'p} = \{\hat{\mathbf{c}}_{p'}, \hat{\mathbf{c}}_p^\dagger\} &= \{(\mathbb{T} \hat{\mathbf{a}})_{p'}, (\mathbb{T} \hat{\mathbf{a}})_p^\dagger\} = \left\{ \sum_{p''=1}^m \mathbb{T}_{p'p''} \hat{\mathbf{a}}_{p''}, \sum_{p'''=1}^m \mathbb{T}_{pp''}^* \hat{\mathbf{a}}_{p''}^\dagger \right\} = \sum_{p'', p'''=1}^m \left[ \mathbb{T}_{p'p''} (\mathbb{T}^\dagger)_{p'''p} \{\hat{\mathbf{a}}_{p''}, \hat{\mathbf{a}}_{p''}^\dagger\} \right] = \\ &= \sum_{p'', p'''=1}^m \mathbb{T}_{p'p''} I_{p''p''} (\mathbb{T}^\dagger)_{p'''p} = (\mathbb{T} \mathbb{T}^\dagger)_{p'p} = (\mathbb{T} \mathbb{T}^\dagger)_{p'p}. \end{aligned} \quad (3.4.7)$$

Thus, we have following property:

**Proposition 3.3.** A transformation matrix  $\mathbb{T}$  for fermions is canonical if and only if it is unitary.

If the transformation is canonical for fermions, we then have:

$$\mathbb{D} = (\mathbb{T}^\dagger)^{-1} \mathbb{H} \mathbb{T}^{-1} = \mathbb{T} \mathbb{H} \mathbb{T}^\dagger, \quad (3.4.8)$$

which means that  $\mathbb{H}$  should be unitary diagonalizable. From the spectral theorem in linear algebra, we know that  $\mathbb{H}$  is diagonalizable by a unitary matrix if and only if  $\mathbb{H}$  is normal. Having that all Hermitian matrices are normal, we have thus proved that diagonalization is possible.

The next step is then to find the diagonal elements in a such diagonalization. Suppose that:

$$\mathbb{D} = \mathbb{T} \mathbb{H} \mathbb{T}^\dagger = \text{diag}(\lambda_1, \dots, \lambda_m). \quad (3.4.9)$$

Writing the matrix  $\mathbb{T}^\dagger$  more explicitly on the form:

$$\mathbb{T}^\dagger = [\vec{w}_1 \ \dots \ \vec{w}_m], \quad (3.4.10)$$

we have:

$$\mathbb{H} [\vec{w}_1 \ \dots \ \vec{w}_m] = [\vec{w}_1 \ \dots \ \vec{w}_m] \text{diag}(\lambda_1, \dots, \lambda_m) = [\lambda_1 \vec{w}_1 \ \dots \ \lambda_m \vec{w}_m], \quad (3.4.11)$$

which means that:

$$\mathbb{H} \vec{w}_p = \lambda_p \vec{w}_p; \quad p \in \{1, 2, \dots, m\}. \quad (3.4.12)$$

Thus, we get following proposition:

**Proposition 3.4.** A Hermitian matrix  $\mathbb{H}$  in a Hamiltonian of the form 3.4.1 can be canonically diagonalized with a unitary matrix  $\mathbb{T}$ , so that:

$$\mathbb{D} = \mathbb{T}\mathbb{H}\mathbb{T}^\dagger = \text{diag}(\lambda_1, \dots, \lambda_m), \quad (3.4.13)$$

where  $\{\lambda_p\}$  are eigenvalues of  $\mathbb{H}$ .

Returning back to 3.4.4, we summarize the results in following theorem:

**Theorem 3.2.** Given a Hermitian  $m \times m$  matrix  $\mathbb{H}$  and a Hamiltonian:

$$\hat{H} = \hat{\mathbf{a}}^\dagger \mathbb{H} \hat{\mathbf{a}}; \quad \hat{\mathbf{a}} = [\hat{\alpha}_1 \quad \dots \quad \hat{\alpha}_m]^T, \quad (3.4.14)$$

where  $\{\hat{\alpha}_i\}$  are fermionic operators, the Hamiltonian can be canonically diagonalized into:

$$\hat{H} = \hat{\mathbf{c}}^\dagger \text{diag}(\lambda_1, \dots, \lambda_m) \hat{\mathbf{c}} = \sum_{p=1}^m \lambda_p \hat{\gamma}_p^\dagger \hat{\gamma}_p, \quad (3.4.15)$$

where  $\{\hat{\gamma}_p\}$  are fermionic operators and  $\{\lambda_p\}$  are eigenvalues of  $\mathbb{H}$ .

### 3.4.2 A modified bosonic diagonalization approach

In previous subsection, we had that all entries in operator vector  $\hat{\mathbf{a}}$  were fermionic annihilation operators. As we see from equation 3.4.6, the exactly same approach would not work for bosonic operators. However, we can reorganize the entries in the operator vector, and define a slightly modified unit matrix. In such a case, we should have the same amount of creation and annihilation operators in the operator vectors, and for that reason, we rewrite dimensions of our matrices and vectors to  $2m$ . Suppose than we now have a  $2m \times 2m$  Hamiltonian matrix:

$$\mathbb{H} = \begin{bmatrix} \mathbf{M}_1 & \mathbf{M}_2 \\ \mathbf{M}_3 & \mathbf{M}_4 \end{bmatrix}, \quad (3.4.16)$$

where  $\mathbf{M}_i$  are  $m \times m$  square matrices, and suppose next that our Hamiltonian is given by:

$$\hat{H} = \hat{\mathbf{a}}^\dagger \mathbb{H} \hat{\mathbf{a}}; \quad \hat{\mathbf{a}} = [\hat{\alpha}_1 \quad \dots \quad \hat{\alpha}_m \quad \hat{\alpha}_{m+1}^\dagger \quad \dots \quad \hat{\alpha}_{2m}^\dagger]^T, \quad (3.4.17)$$

where  $\hat{\mathbf{a}}$  is  $2m$ -sized vector with bosonic operators. Unlike the fermionic case, half of the vector entries are written as annihilation operators, and another half as creation operators.

In the same manner as for fermionic case, we define a  $2m \times 2m$  transformation matrix  $\mathbb{T}$ :

$$\mathbb{T} \hat{\mathbf{a}} = \hat{\mathbf{c}} = [\hat{\gamma}_1 \quad \dots \quad \hat{\gamma}_m \quad \hat{\gamma}_{m+1}^\dagger \quad \dots \quad \hat{\gamma}_{2m}^\dagger]^T, \quad (3.4.18)$$

$$(\mathbb{T} \hat{\mathbf{a}})^\dagger = \hat{\mathbf{a}}^\dagger \mathbb{T}^\dagger = [\hat{\gamma}_1^\dagger \quad \dots \quad \hat{\gamma}_m^\dagger \quad \hat{\gamma}_{m+1} \quad \dots \quad \hat{\gamma}_{2m}], \quad (3.4.19)$$

which we want to be canonical. Again, we write:

$$\hat{H} = \hat{\mathbf{a}}^\dagger \mathbb{H} \hat{\mathbf{a}} = \hat{\mathbf{a}}^\dagger \mathbb{T}^\dagger (\mathbb{T}^\dagger)^{-1} \mathbb{H} \mathbb{T}^{-1} \mathbb{T} \hat{\mathbf{a}} = \hat{\mathbf{c}}^\dagger \mathbb{D} \hat{\mathbf{c}}, \quad (3.4.20)$$

where  $\mathbb{D} = (\mathbb{T}^\dagger)^{-1} \mathbb{H} \mathbb{T}^{-1}$ . Also here, we want  $\mathbb{D}$  to be diagonal. However, this time, we write diagonal entries on slightly different form:

$$\mathbb{D} = \text{diag}(\lambda_1, \dots, \lambda_m, -\lambda_{m+1}, \dots, -\lambda_{2m}). \quad (3.4.21)$$

Next, we introduce a slightly modified  $2m \times 2m$  unit matrix, known as para unit matrix  $\tilde{I}$ , with entries defined by:

$$\tilde{I}_{p'p} := \begin{cases} 1 & \text{if } p' = p \text{ and } p \in \{1, 2, \dots, m\} \\ -1 & \text{if } p' = p \text{ and } p \in \{m+1, m+2, \dots, 2m\} \\ 1 & \text{if } p' \neq p \end{cases}. \quad (3.4.22)$$

We then have that:

$$[\hat{\mathbf{a}}_{p'}, \hat{\mathbf{a}}_p^\dagger] = \tilde{I}_{p'p}, \quad (3.4.23)$$

which is analogous to 3.4.6. In order to have a canonical transformation, the same relation must hold for the  $\hat{\mathbf{c}}$ -vector:

$$\begin{aligned} \tilde{I}_{p'p} = [\hat{\mathbf{c}}_{p'}, \hat{\mathbf{c}}_p^\dagger] &= [(\mathbb{T}\hat{\mathbf{a}})_{p'}, (\mathbb{T}\hat{\mathbf{a}})_p^\dagger] = \left[ \sum_{p''=1}^{2m} \mathbb{T}_{p'p''} \hat{\mathbf{a}}_{p''}, \sum_{p'''=1}^{2m} \mathbb{T}_{pp'''}^* \hat{\mathbf{a}}_{p'''}^\dagger \right] = \sum_{p'', p'''=1}^{2m} \left[ \mathbb{T}_{p'p''} (\mathbb{T}^\dagger)_{p'''p} [\hat{\mathbf{a}}_{p''}, \hat{\mathbf{a}}_{p'''}^\dagger] \right] = \\ & \sum_{p'', p'''=1}^{2m} \mathbb{T}_{p'p''} \tilde{I}_{p''p'''} (\mathbb{T}^\dagger)_{p'''p} = (\mathbb{T}\tilde{I}\mathbb{T}^\dagger)_{p'p}. \end{aligned} \quad (3.4.24)$$

Thus, we have a following property:

**Proposition 3.5.** A transformation matrix  $\mathbb{T}$  for bosons is canonical if and only if following holds:

$$\mathbb{T}\tilde{I}\mathbb{T}^\dagger = \tilde{I} \iff \mathbb{T}^\dagger\tilde{I}\mathbb{T} = \tilde{I}, \quad (3.4.25)$$

where  $\tilde{I}$  is a para unit matrix. A such matrix  $\mathbb{T}$  is known as pseudo-unitary matrix.

Next, we want to find the condition for  $\mathbb{D}$  to be diagonal. Suppose this is the case, so that

$$\mathbb{D} = (\mathbb{T}^\dagger)^{-1} \mathbb{H} \mathbb{T}^{-1} = \text{diag}(\lambda_1, \dots, \lambda_m, -\lambda_{m+1}, \dots, -\lambda_{2m}) = \tilde{I} \mathbb{L}, \quad (3.4.26)$$

where we defined:

$$\mathbb{L} := \text{diag}(\lambda_1, \dots, \lambda_m, \lambda_{m+1}, \dots, \lambda_{2m}). \quad (3.4.27)$$

We then have:

$$\mathbb{H} \mathbb{T}^{-1} = \tilde{I} \mathbb{T}^{-1} \mathbb{L}, \quad (3.4.28)$$

where we have assumed that  $\mathbb{T}$  is pseudo-unitary. We write  $\mathbb{T}^{-1}$  more explicitly as:

$$\mathbb{T}^{-1} = \begin{bmatrix} \vec{w}_1 & \dots & \vec{w}_{2m} \end{bmatrix} = \begin{bmatrix} \vec{u}_1 & \dots & \vec{u}_{2m} \\ \vec{v}_1 & \dots & \vec{v}_{2m} \end{bmatrix}, \quad (3.4.29)$$

where  $\vec{u}_i$  and  $\vec{v}_i$  are vectors of same size. We then have,

$$\mathbb{H} \begin{bmatrix} \vec{u}_1 & \dots & \vec{u}_{2m} \\ \vec{v}_1 & \dots & \vec{v}_{2m} \end{bmatrix} = \tilde{I} \begin{bmatrix} \vec{u}_1 & \dots & \vec{u}_{2m} \\ \vec{v}_1 & \dots & \vec{v}_{2m} \end{bmatrix} \text{diag}(\lambda_1, \dots, \lambda_{2m}) = \tilde{I} \begin{bmatrix} \lambda_1 \vec{u}_1 & \dots & \lambda_{2m} \vec{u}_{2m} \\ \lambda_1 \vec{v}_1 & \dots & \lambda_{2m} \vec{v}_{2m} \end{bmatrix}, \quad (3.4.30)$$

meaning that

$$\mathbb{H} \vec{w}_p = \lambda_p \tilde{I} \vec{w}_p \iff \tilde{I} \mathbb{H} \vec{w}_p = \lambda_p \vec{w}_p, \quad (3.4.31)$$

where we have used the fact that  $\tilde{I}^2 = I$ . We thus end up with following proposition:

**Proposition 3.6.** If a matrix  $\mathbb{H}$  is diagonalizable by a pseudo-unitary matrix  $\mathbb{T}$ , such that

$$(\mathbb{T}^\dagger)^{-1} \mathbb{H} \mathbb{T}^{-1} = \text{diag}(\lambda_1, \dots, \lambda_m, -\lambda_{m+1}, \dots, -\lambda_{2m}), \quad (3.4.32)$$

then the values  $\{\lambda_p\}$  are eigenvalues of the matrix  $\tilde{I} \mathbb{H}$ .

The central question then is when such diagonalization is possible. Fortunately, following theorem (which we cite word by word) is proved in reference [18]:

**Theorem 3.3.** A  $2m$ -square Hermitian matrix  $\mathbb{H}$  can be pseudo-unitary diagonalized into a matrix with all diagonal elements positive if and only if  $\mathbb{H}$  is positive definite.

A Hermitian matrix is positive definite if and only if all of its eigenvalues are positive. Thus, when diagonalizing bosonic matrices, we should find eigenvalues of  $\mathbb{H}$  to ensure that the matrix is diagonalizable, and then find eigenvalues of  $\tilde{I} \mathbb{H}$  to find diagonal elements. The fact that all diagonal elements are positive also ensures stability of the second quantization.

Returning back to 3.4.20, we end up with following theorem:

**Theorem 3.4.** Given a Hermitian  $2m \times 2m$  matrix  $\mathbb{H}$  and a Hamiltonian:

$$\hat{H} = \hat{\mathbf{a}}^\dagger \mathbb{H} \hat{\mathbf{a}}; \quad \hat{\mathbf{a}} = [\hat{\alpha}_1 \quad \dots \quad \hat{\alpha}_m \quad \hat{\alpha}_{m+1}^\dagger \quad \dots \quad \hat{\alpha}_{2m}^\dagger]^T, \quad (3.4.33)$$



where  $\{\hat{\alpha}_i\}$  are bosonic operators, the Hamiltonian can be canonically diagonalized into:

$$\hat{H} = \hat{\mathbf{c}}^\dagger \text{diag}(\lambda_1, \dots, \lambda_m, -\lambda_{m+1}, \dots, -\lambda_{2m}) \hat{\mathbf{c}} = \sum_{p=1}^m \lambda_p \hat{\gamma}_p^\dagger \hat{\gamma}_p - \sum_{p=m+1}^{2m} \lambda_p \hat{\gamma}_p^\dagger \hat{\gamma}_p - \sum_{p=m+1}^{2m} \lambda_p, \quad (3.4.34)$$

if and only if  $\mathbb{H}$  has all of its eigenvalues positive. Here,  $\{\hat{\gamma}_i\}$  are bosonic operators and  $\{\lambda_p\}$  are eigenvalues of  $\tilde{T}\mathbb{H}$ .  $\{\lambda_p\}$  are positive for  $p \in \{1, 2, \dots, m\}$  and negative for  $p \in \{m+1, m+2, \dots, 2m\}$ , so that all the terms in 3.4.34 have positive coefficients.

It should be said that a theorem similar to theorem 3.4 can also be derived for fermions. In such a case, we use fermionic anti-commutation relation and unit matrix in 3.4.23, and then follow the same derivation approach, as we did for theorem 3.2. A such fermionic diagonalization theorem can then be used to diagonalize a Hamiltonian that would arise if one derives the results that we are going to present in subsection 3.5.1.

### 3.5 Examples of fermionization and bosonization: XY-chain in transverse magnetic field

We will now finish this chapter by presenting a simple model, and summarize some results when the model is treated with a fermionization technique known as *Jordan-Wigner transformation* (JWT), and a bosonization technique known as *Holstein-Primakoff transformation* (HPT). Suppose that our system is described by the Hamiltonian:

$$\hat{H} = - \sum_{j=1}^N \left[ J^{(x)} \hat{S}_j^{(x)} \hat{S}_{j+1}^{(x)} + J^{(y)} \hat{S}_j^{(y)} \hat{S}_{j+1}^{(y)} + 2SB \hat{S}_j^{(z)} \right]; \quad \hat{S}_{N+1}^{(\alpha)} = \hat{S}_1^{(\alpha)}, \quad \forall \alpha \in \{x, y, z\}, \quad (3.5.1)$$

where the lattice is a 1D evenly spaced chain and  $S = \frac{1}{2}$  is the electron spin number. Physically, we see that this model represents a chain being closed in a ring (periodic boundary condition), where the spins interact with nearest neighbors anisotropically in the xy-plane (represented by  $J^{(x)}$  and  $J^{(y)}$ ), and also with an external transverse magnetic field (represented by  $B$ ) in the z-direction.

This model can be exactly fermionized by using the JWT. Close to the ground state (or when  $S \rightarrow \infty$ ), the model might be effectively bosonized by HPT. In the next two subsections, we will introduce these transformations and summarize the results when these transformations are applied to the model.

#### 3.5.1 Fermionization with Jordan-Wigner transformation

The JWT is defined as:

$$\begin{aligned} \hat{S}_j^{(x)} &= \frac{\hbar}{2} e^{i\pi \sum_{j'=1}^{j-1} \hat{n}_{j'}} \hat{f}_j + \text{H.c.} \\ \hat{S}_j^{(y)} &= i \frac{\hbar}{2} e^{i\pi \sum_{j'=1}^{j-1} \hat{n}_{j'}} \hat{f}_j + \text{H.c.} \\ \hat{S}_j^{(z)} &= \hbar \left( \hat{n}_j - \frac{1}{2} \right), \end{aligned} \quad (3.5.2)$$

where  $\{\hat{f}_j\}$  are fermionic operators, and  $\hat{n}_j = \hat{f}_j^\dagger \hat{f}_j$  is the number operator. By direct inspection, it is straight forward to show that this transformation is true for  $\frac{1}{2}$ -spins. However, we see that the sum within the exponent requires linear ordering of lattice sites. Even if we define some spiral-like linear ordering in 2D or 3D lattices, the realistic neighbor interactions would be virtually impossible to implement. Therefore, JWT is only suited for 1D lattices, although there exists a modified version of JWT that works in 2D[19]. In addition, the total number of fermionic particles in JWT is not conserved, and the JW fermions do not represent physical particles, but are rather convenient mathematical objects, known as auxiliary quasiparticles[15].

By inserting 3.5.2 into 3.5.1, doing Fourier transformation of the fermionic operators, and then diagonalizing the resulting Hamiltonian, we end up with following Hamiltonian[20]:

$$\hat{H} = \sum_k \epsilon_k^{(\text{JW})} (\hat{f}_k^\dagger \hat{f}_k + \hat{f}_{-k}^\dagger \hat{f}_{-k} - 1), \quad (3.5.3)$$

where

$$\epsilon_k^{(\text{JW})} = \frac{\hbar^2 J}{2} \left[ \left( \cos(ka) - \frac{2B}{\hbar J} \right)^2 + \gamma^2 \sin^2(ka) \right]^{\frac{1}{2}}. \quad (3.5.4)$$

Here,  $J$  and  $\gamma$  are defined by the relations:

$$J^{(x)} = J \frac{1+\gamma}{2}; \quad J^{(y)} = J \frac{1-\gamma}{2}, \quad (3.5.5)$$

$a$  is lattice constant, and  $k$  represents the 1D Brillouin zone in the reciprocal space of the chain. A plot of 3.5.4 can be seen in figure 2a.

### 3.5.2 Bosonization with Holstein-Primakoff transformation

The HPT relative to the  $z$ -axis is defined as:

$$\begin{cases} \hat{S}_j^{(+)} = \hbar(\sqrt{2S - \hat{a}_j^\dagger \hat{a}_j} \hat{a}_j) \\ \hat{S}_j^{(-)} = \hbar \hat{a}_j^\dagger \sqrt{2S - \hat{a}_j^\dagger \hat{a}_j} \\ \hat{S}_j^{(z)} = 2\hbar(S - \hat{a}_j^\dagger \hat{a}_j), \end{cases} \quad (3.5.6)$$

where  $\hat{S}_j^{(\pm)} := \hat{S}_j^{(y)} \pm i\hat{S}_j^{(x)}$ , and  $\{\hat{a}_j\}$  are bosonic operators. In fact, these bosonic operators represent real physical quasiparticles known as magnons[15]. By assuming that the ground state is highly ordered along the  $z$ -direction (or that spins behave classically with  $S \rightarrow \infty$ ), the square-roots can be expanded to the lowest order. The excitations of magnons then represent small fluctuations around the  $z$ -direction.

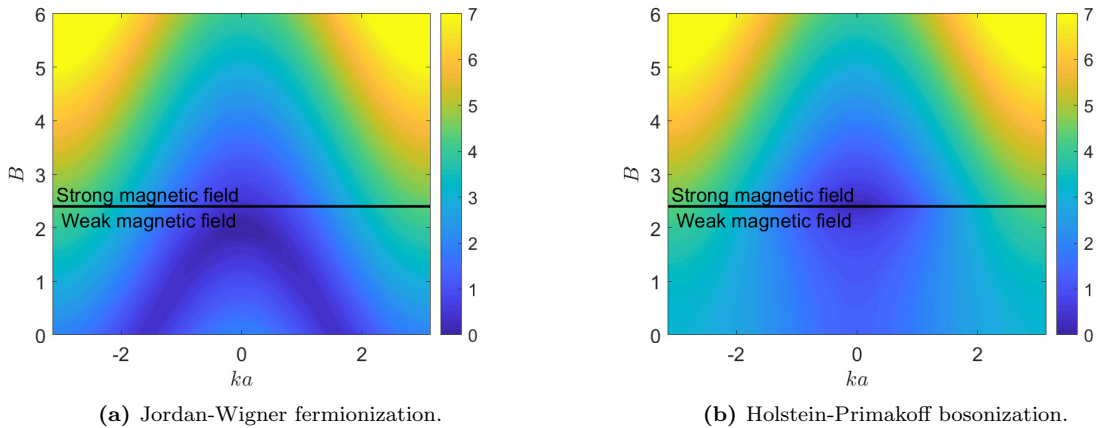
In order to insert 3.5.6 into 3.5.1, we should first define the ordered direction. For strong magnetic field, we would expect this direction to be parallel to the field. However, for weak fields, the situation becomes more complicated. To overcome this, we can use a semiclassical approach: we replace the spin operators in 3.5.1 with vector values, and then minimize the Hamiltonian as function of these vector values. Assuming that all spins point in the same direction, we can then find the assumed ordering direction of the ground state. Assuming without loss of generality that  $J^{(x)} > |J^{(y)}|$  and  $B \geq 0$ , we can then perform Fourier transform and diagonalization to get following Hamiltonian[21]:

$$\hat{H} = \sum_k \epsilon_k^{(\text{HP})} (\hat{a}_k^\dagger \hat{a}_k + \hat{a}_{-k}^\dagger \hat{a}_{-k} + 1), \quad (3.5.7)$$

where  $\{\hat{a}_k\}$  are bosonic operators, and

$$\epsilon_k^{(\text{HP})} = \begin{cases} \hbar B \left[ \left(1 - \frac{\hbar J^{(x)}}{B} \cos(ka)\right) \left(1 - \frac{\hbar J^{(y)}}{B} \cos(ka)\right) \right]^{\frac{1}{2}} & J^{(x)} \leq B \\ \hbar^2 J^{(x)} \left[ \left(1 - \frac{B^2}{(\hbar J^{(x)})^2} \cos(ka)\right) \left(1 - \frac{J^{(y)}}{J^{(x)}} \cos(ka)\right) \right]^{\frac{1}{2}} & J^{(x)} > B. \end{cases} \quad (3.5.8)$$

A plot of 3.5.8 can be seen in figure 2b.



**Figure 2:** Contour plots of  $\epsilon_k$  as function of magnetic field  $B$  and reciprocal space coordinate  $ka$  with  $\hbar = 1$ ,  $J = 4$  and  $\gamma = 0.2$ . This gives  $J^{(x)} = 2.4$ .

We are not going to analyze the results in detail. However, it should be noted that although the dispersions in figure 2 have some similarities, the models are physically very different, and a careful physical analysis should be done in order to make any comparisons and conclusions.

## 4 Symmetric bosonization and fermionization

We have previously treated Holstein-Primakoff transformation as a bosonization technique. For practical reasons, however, due to its square-root nature, we had to assume that the states near the ground state are highly ordered along some direction  $z$ . This then allowed low order expansion approximations of the square-roots. However, if we are to consider disordered states like QSLs, this technique is obviously out of question. In this chapter, we want to introduce a technique that is more of an isotropic nature, and where rotational invariance can be manifested. When doing so, we also introduce some concepts from group theory which are strongly related to many physical concepts discussed in this thesis.

### 4.1 Group theory

Mathematically, a set  $\mathcal{G}$  is called a group if there exists a certain operation "·" between all its elements, and when following axioms are satisfied:

$$\begin{aligned}
 \forall a, b \in \mathcal{G} : \quad (a \cdot b) \in \mathcal{G} & \quad \text{(closure property)} \\
 \forall a, b, c \in \mathcal{G} : \quad (a \cdot b) \cdot c = a \cdot (b \cdot c) & \quad \text{(associative property)} \\
 \exists e \in \mathcal{G} : \quad e \cdot a = a \cdot e = a, \quad \forall a \in \mathcal{G} & \quad \text{(existence of identity element)} \\
 \forall a \in \mathcal{G}, \exists a^{-1} \in \mathcal{G} : \quad a \cdot a^{-1} = a^{-1} \cdot a = e & \quad \text{(existence of inverse element)}.
 \end{aligned} \tag{4.1.1}$$

Physically, many groups that we are going to consider are related to spatial rotations (mostly in  $\mathbb{R}^3$ ) about some origin point. For instance, the  $\mathcal{G}$  can be thought as a set of all possible rotations in 3D space about some fixed point, with each element representing a specific rotation. The group operation is then to combine two subsequent rotations into one single rotation<sup>8</sup>.

If a group in addition is a continuous set, it is said to be a *Lie group*. For instance, the group of all rotations is a Lie group because we are able to perform all kind of infinitesimal rotations.

### 4.2 Matrix groups

From classical mechanics, we know that a spatial rotation can be represented by an orthogonal matrix, whilst many quantum mechanical transformations are based on unitary matrices<sup>9</sup>. It is therefore instructive to classify some types of matrix groups. The most general ones are groups of all real or complex invertible matrices of dimension  $n$ , known as general linear groups of degree  $n$ , and usually denoted as  $\text{GL}(n, \mathbb{R})$  and  $\text{GL}(n, \mathbb{C})$ , respectively. Using matrix multiplication as group operation, we obviously see that all group axioms are satisfied. However, as we will see, we are interested in more specific matrix groups. We now define following sets:

**Definition 4.1.**

- A set of all orthogonal matrices of dimension  $n$  is denoted as  $\text{O}(n)$
- A set of all unitary matrices with dimension  $n$  is denoted as  $\text{U}(n)$
- A set of all orthogonal matrices with dimension  $n$  and determinant 1 is denoted as  $\text{SO}(n)$
- A set of all unitary matrices with dimension  $n$  and determinant 1 is denoted as  $\text{SU}(n)$

**Proposition 4.1.** All the sets defined in definition 4.1 are groups.

*Proof.* The second axiom is obviously satisfied due to associative property of any matrix multiplication. The third axiom is satisfied because an identity matrix is orthogonal, unitary and has a determinant equal to 1. The inverse matrices do by definition exist for both orthogonal and unitary matrices, and due to a fundamental property of determinants  $\det(A^{-1}) = \det(A)^{-1}$ , if a matrix has determinant equal to 1, then so does its inverse matrix. Thus, we are left with only showing that first axiom is satisfied.

Suppose that  $O_1$  and  $O_2$  are arbitrary orthogonal matrices, and let their matrix product be  $O_3 := O_1 O_2$ . Then,

$$O_3^T O_3 = (O_1 O_2)^T (O_1 O_2) = O_2^T O_1^T O_1 O_2 = I \tag{4.2.1}$$

$$O_3 O_3^T = O_1 O_2 (O_1 O_2)^T = O_1 O_2 O_2^T O_1^T = I. \tag{4.2.2}$$

<sup>8</sup>If the rotation elements are represented as matrices, the operation is just matrix multiplication.

<sup>9</sup>A matrix  $O$  is orthogonal if:  $OO^T = O^T O = I$ . A matrix  $U$  is unitary if:  $UU^\dagger = U^\dagger U = I$

Thus, a product of two orthogonal matrices is itself an orthogonal matrix. Same argument holds for unitary matrices. Next, suppose that  $O_1$  and  $O_2$  both have determinant equal to 1. Then, having that  $\det(AB) = \det(A)\det(B)$ ,  $O_3$  has determinant equal to 1 as well. Same holds for unitary matrices.  $\square$

With these definitions in mind, we point out the most important matrix groups in this thesis are  $U(1)$  and  $SU(2)$ . However, due to its intuition friendly nature, the  $SO(3)$  group is going to be heavily discussed for the sake of concept understanding.

### 4.3 Homomorphism between some matrix groups

As we already have mentioned, our physical applications of groups will mostly be related to spatial rotations. However, the spatial rotations can be represented with different groups, as we now will show:

#### 4.3.1 $SO(2)$ and $U(1)$ isomorphism

Suppose that we are performing a counterclockwise rotation of some point  $(x, y)$  in 2D space by an angle  $\theta$ . The rotated point  $(x', y')$  might then be expressed by following matrix notation:

$$\begin{bmatrix} x' \\ y' \end{bmatrix} = \begin{bmatrix} \cos \theta & -\sin \theta \\ \sin \theta & \cos \theta \end{bmatrix} \begin{bmatrix} x \\ y \end{bmatrix}. \quad (4.3.1)$$

For any real  $\theta$ , we see that our rotation matrix is from the  $SO(2)$  group, and in fact, the set of all such rotation matrices is a complete  $SO(2)$  group.

However, there is another way of representing such rotations. Suppose instead that we write our point in a complex plane as  $x + iy$ . Next, suppose that we multiply this complex number by  $e^{i\theta}$ , where  $\theta \in \mathbb{R}$ . We get:

$$e^{i\theta}(x + iy) = (\cos \theta + i \sin \theta)(x + iy) = (x \cos \theta - y \sin \theta) + i(x \sin \theta + y \cos \theta) = x' + iy'. \quad (4.3.2)$$

Thus,  $e^{i\theta}$  performs a counterclockwise rotation of a complex number by an angle  $\theta$ , just like our  $SO(2)$  matrix did on a vector in  $\mathbb{R}^2$ . A complex number of the form  $e^{i\theta}$  ( $\theta \in \mathbb{R}$ ) has a norm of 1, and thus forms the  $U(1)$  group.

We thus see that we can represent the same physical phenomena with different groups. Such groups are mathematically said to be homomorphic. In addition, if there is a one-to-one correspondance between group elements, the groups are said to be isomorphic, and as we see, this is in fact the case for  $SO(2)$  and  $U(1)$ .

#### 4.3.2 $SO(3)$ and $SU(2)$ 1:2 homomorphism

The concept of 2D rotations and complex numbers can be extended to 3D. We give a brief sketch of the process, but omit mathematical details<sup>10</sup>. First of all, we can show that a 3D rotation can be represented by an  $SO(3)$  matrix, but also by a unit quaternion<sup>11</sup>. Secondly, it turns out that unit quaternions are isomorphic to  $SU(2)$ . Finally, for each 3D rotation, there exist two different unit quaternions that represent the same process. Thus, we say that there is a 1:2 homomorphism between  $SO(3)$  and  $SU(2)$ . As we will later see, in quantum mechanics, the  $SO(3)$  group is related to the rotations of spin-1 operators, whilst the  $SU(2)$  group is related to the rotations of spin- $\frac{1}{2}$  operators.

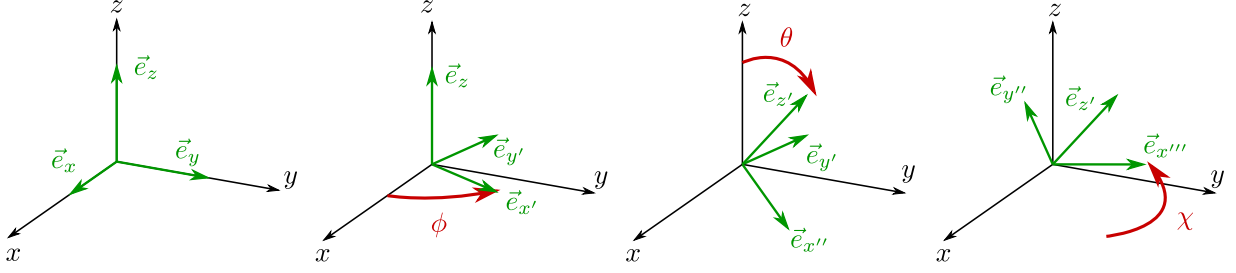
### 4.4 $SO(3)$ , $SU(2)$ , and rotations in $\mathbb{R}^3$ space

In this subsection, we provide more details related to rotations in 3D space and the corresponding groups. In particular, we want to rewrite the group elements in terms of generators, which will play a fundamental role when connecting group theory with quantum mechanics.

<sup>10</sup>More information can be found in [22]

<sup>11</sup>Quaternions are an extension of complex numbers, with one real unit and three different imaginary units.

#### 4.4.1 Euler angles



**Figure 3:** An Euler rotation is defined by three angles. In z-y'-z' convention, the first rotation is performed around the z-axis, the second around resulting y'-axis, and the last around resulting z'-axis.

The idea of Euler angles is to define a set of angles relative to some origin and some coordinate system in order to describe any 3D rotation. For convenience, we use a so-called z-y'-z' convention of Euler angles due to their close relation to polar angles (see figure 3). Suppose that we start with some orthonormal coordinate system  $\{\vec{e}_x, \vec{e}_y, \vec{e}_z\}$ , which we rotate counterclockwise by an angle  $\phi$  in the xy-plane. This gives a rotated coordinate system  $\{\vec{e}_{x'}, \vec{e}_{y'}, \vec{e}_z\}$ . Next, suppose that we rotate the resulting coordinate system counterclockwise by an angle  $\theta$  in the zx'-plane. This then gives a new coordinate system  $\{\vec{e}_{x''}, \vec{e}_{y'}, \vec{e}_{z'}\}$ . Finally, we rotate the resulting coordinate system counterclockwise by an angle  $\chi$  in the x''y'-plane, and obtain final coordinate system  $\{\vec{e}_{x'''}, \vec{e}_{y''}, \vec{e}_{z'}\}$ . The total process is depicted in figure 3, and can be described as follows:

$$\{\vec{e}_x, \vec{e}_y, \vec{e}_z\} \xrightarrow{\phi} \{\vec{e}_{x'}, \vec{e}_{y'}, \vec{e}_z\} \xrightarrow{\theta} \{\vec{e}_{x''}, \vec{e}_{y'}, \vec{e}_{z'}\} \xrightarrow{\chi} \{\vec{e}_{x'''}, \vec{e}_{y''}, \vec{e}_{z'}\}. \quad (4.4.1)$$

This defines a set of Euler angles  $\{\phi, \theta, \chi\}$  that give us a way to perform a general rotation in 3D. However, this method seems to be complicated due to the fact that rotations are intrinsic (the coordinate system is changing). For practical reasons, we want to describe a general rotation by extrinsic rotations (rotations relative to some fixed coordinate system), and fortunately, this can easily be done by using following theorem:

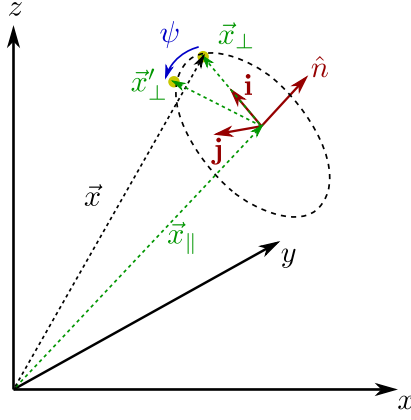
**Theorem 4.1.** Suppose that  $\mathcal{R}(\alpha, \hat{n})$  denotes a right-hand rotation by an angle  $\alpha$  about some axis defined by the unit vector  $\hat{n}$ . Then, for the Euler rotations defined above, we have

$$\mathcal{R}(\chi, \vec{e}_{z'})\mathcal{R}(\theta, \vec{e}_{y'})\mathcal{R}(\phi, \vec{e}_z) = \mathcal{R}(\phi, \vec{e}_z)\mathcal{R}(\theta, \vec{e}_y)\mathcal{R}(\chi, \vec{e}_z) \quad (4.4.2)$$

In other words, the same Euler rotation can be described by z-y-z rotations around the initial fixed coordinate system, but with angles arranged in opposite order. In addition, it turns out that any kind of rotation in 3D can be described by a such decomposition. We will later use Euler angles to describe rotations of Schwinger bosons and Abrikosov fermions, but at this point, we introduce another technique that allows rotations in 3D.

#### 4.4.2 Rodrigues' rotation formula

It turns out that instead of describing a general 3D rotation by a coordinate system and three angles, we can equally well describe it as a single rotation about some axis. Suppose that this axis is defined by a unit vector  $\hat{n}$ , and that the angle of rotation is  $\psi$ . The rotation is then described by  $\mathcal{R}(\psi, \hat{n})$ . Given an arbitrary point  $\vec{x} \in \mathbb{R}^3$ , we want to find an expression for  $\vec{x}' := \mathcal{R}(\psi, \hat{n})\vec{x}$ .



**Figure 4:** The concept of a Rodrigues' rotation. A point  $\vec{x} = \vec{x}_\perp + \vec{x}_\parallel$  is rotated by an angle  $\psi$  around an axis defined by a unit vector  $\hat{n}$ . The resulting point is given as  $\vec{x}' = \vec{x}'_\perp + \vec{x}_\parallel$ . The unit vectors  $\mathbf{i}$  and  $\mathbf{j}$  define the coordinate system in the plane of rotation.

We follow the idea depicted in figure 4. Suppose first that we decompose our  $\vec{x}$  into a part normal to  $\hat{n}$  and a part orthogonal to it:

$$\vec{x} = \vec{x}_\parallel + \vec{x}_\perp, \quad (4.4.3)$$

where

$$\vec{x}_\parallel = (\vec{x} \cdot \hat{n})\hat{n}, \quad (4.4.4)$$

$$\vec{x}_\perp = \vec{x} - (\vec{x} \cdot \hat{n})\hat{n}. \quad (4.4.5)$$

Based on the figure 4, we see that  $\vec{x}_\parallel$  is invariant during the rotation, whilst  $\vec{x}_\perp$  changes direction on the rotation circle. Thus, we see that the perpendicular component changes to

$$\vec{x}'_\perp = |\vec{x}_\perp|(\mathbf{i} \cos \psi + \mathbf{j} \sin \psi) = \vec{x}_\perp \cos \psi + \mathbf{j}|\vec{x}_\perp| \sin \psi, \quad (4.4.6)$$

where  $\mathbf{i}$  and  $\mathbf{j}$  are unit vectors in the rotation circle (see figure 4). The unit vectors are defined in a such way that  $\{\mathbf{i}, \mathbf{j}, \hat{n}\}$  form an orthonormal right-hand coordinate system, and  $\mathbf{i} = \vec{x}_\perp/|\vec{x}_\perp|$ . Based on that, we have

$$\mathbf{j} = \frac{\hat{n} \times \vec{x}_\perp}{|\hat{n} \times \vec{x}_\perp|} = \frac{\hat{n} \times \vec{x}_\perp}{|\vec{x}_\perp|} = \frac{\hat{n} \times \vec{x}}{|\vec{x}_\perp|} \quad (4.4.7)$$

Inserting 4.4.7 and 4.4.5 into 4.4.6, we get

$$\vec{x}'_\perp = [\vec{x} - (\vec{x} \cdot \hat{n})\hat{n}] \cos \psi + (\hat{n} \times \vec{x}) \sin \psi \quad (4.4.8)$$

Finally, since  $\vec{x}_\parallel$  is invariant during the rotation, we just add 4.4.4 to 4.4.8, and obtain Rodrigues' formula:

**Theorem 4.2** (Rodrigues' formula).

$$\mathcal{R}(\psi, \hat{n})\vec{x} = (\cos \psi)\vec{x} + (1 - \cos \psi)(\hat{n} \cdot \vec{x})\hat{n} + (\sin \psi)(\hat{n} \times \vec{x}); \quad \forall \vec{x} \in \mathbb{R}^3. \quad (4.4.9)$$

### 4.4.3 Generators of SO(3) group

In this subsection, we will derive the so-called generators of the SO(3) group by using the Rodrigues' formula. As briefly discussed in section 4.1, a Lie group is based on continuous transformations (in our case continuous rotations). The idea is that the neighborhood of a group element can be expanded in terms of generators, and that each group element then can be written as an exponential of these generators<sup>12</sup>.

We start off by Taylor-expanding Rodrigues' formula into an infinitesimal angle  $\Delta\psi$ :

$$\mathcal{R}(\Delta\psi, \hat{n})\vec{x} = \vec{x} + \Delta\psi(\hat{n} \times \vec{x}) + O((\Delta\psi)^2). \quad (4.4.10)$$

<sup>12</sup>In this classical approach, the generators will turn out to be matrices. However, when moving to quantum mechanics, the generators happen to be well-known operators.

Next, suppose that for each choice of  $\vec{n}$ , there exists a  $3 \times 3$  matrix  $J(\vec{n})$ , so that

$$(\vec{n} \times \vec{x}) = -iJ(\hat{n})\vec{x}; \quad \forall \vec{x} \in \mathbb{R}^3. \quad (4.4.11)$$

If a such matrix exists, our rotation becomes

$$\mathcal{R}(\Delta\psi, \hat{n}) = I - i\Delta\psi J(\hat{n}) + O((\Delta\psi)^2), \quad (4.4.12)$$

where  $I$  is identity matrix. Finally, by using a fundamental mathematical property of exponential function

$$e^x = \lim_{N \rightarrow \infty} \left( I + \frac{x}{N} \right)^N, \quad (4.4.13)$$

we get

$$\begin{aligned} \mathcal{R}(\psi, \hat{n}) &= \lim_{N \rightarrow \infty} \mathcal{R}\left(\frac{\psi}{N}N, \hat{n}\right) = \lim_{N \rightarrow \infty} \mathcal{R}(\Delta\psi N, \hat{n}) = \lim_{N \rightarrow \infty} \left( \mathcal{R}(\Delta\psi, \hat{n}) \right)^N = \\ &= \lim_{N \rightarrow \infty} \left( I - i\Delta\psi J(\hat{n}) \right)^N = \lim_{N \rightarrow \infty} \left( I - i\frac{\psi}{N} J(\hat{n}) \right)^N = e^{-i\psi J(\hat{n})} \end{aligned} \quad (4.4.14)$$

Thus, we have expressed our rotation in terms of an exponential. We now try to find an expression for generator matrices with the following idea: we find three generators that represent rotations about our three coordinate axes, and then try to use these as a basis for an arbitrary generator  $J(\hat{n})$ <sup>13</sup>. Suppose that our coordinate system is defined by the orthonormal right-hand basis  $\{\vec{e}_1, \vec{e}_2, \vec{e}_3\}$ . Then, our task is to solve:

$$(\vec{e}_k \times \vec{x}) = -iJ_k\vec{x}; \quad k \in \{1, 2, 3\}. \quad (4.4.15)$$

By using the fundamental mathematical property of cross products:

$$\vec{a} \times \vec{b} = \sum_{i=1}^3 \sum_{j=1}^3 \sum_{k=1}^3 a_i b_j \epsilon_{ijk} \vec{e}_k, \quad (4.4.16)$$

where  $\epsilon_{ijk}$  is Levi-Civita symbol, we have:

$$(\vec{e}_k \times \vec{x})_i = \sum_{k'=1}^3 \sum_{j=1}^3 \delta_{kk'} x_j \epsilon_{k'ji} = - \sum_{j=1}^3 \epsilon_{ijk} x_j \quad (4.4.17)$$

At the same time,

$$(-iJ_k\vec{x})_i = -i \sum_{j=1}^3 (J_k)_{ij} x_j. \quad (4.4.18)$$

Since those two equations are true  $\forall \vec{x} \in \mathbb{R}^3$ , we must have that:

$$(J_k)_{ij} = -i\epsilon_{ijk}. \quad (4.4.19)$$

This defines our basis generator matrices, so the final question is how those are related to arbitrary generators. Applying 4.4.16 to 4.4.11, we have:

$$(\hat{n} \times \vec{x})_i = - \sum_{j=1}^3 \sum_{k=1}^3 \epsilon_{ijk} n_k x_j = [-iJ(\hat{n})\vec{x}]_i = -i \sum_{j=1}^3 [J(\hat{n})]_{ij} x_j. \quad (4.4.20)$$

Again, being true  $\forall \vec{x} \in \mathbb{R}^3$ , we must have that:

$$[J(\hat{n})]_{ij} = -i \sum_{k=1}^3 \epsilon_{ijk} n_k. \quad (4.4.21)$$

Inserting 4.4.19 into 4.4.21, we finally get:

$$[J(\hat{n})]_{ij} = \sum_{k=1}^3 n_k (J_k)_{ij} \implies J(\hat{n}) = n_1 J_1 + n_2 J_2 + n_3 J_3. \quad (4.4.22)$$

Inserting this result into 4.4.14, we end up with the following theorem:

<sup>13</sup>Mathematically, we say that a such basis spans the Lie algebra of  $\text{SO}(3)$ . The Lie algebra of  $\text{SO}(3)$  is known as  $\mathfrak{so}(3)$ , whilst the Lie algebra of  $\text{SU}(2)$  is known as  $\mathfrak{su}(2)$ .



**Theorem 4.3.**

$$\mathcal{R}(\psi, \hat{n}) = e^{-i\psi(n_1 J_1 + n_2 J_2 + n_3 J_3)}, \quad (4.4.23)$$

where  $(J_k)_{ij} = -i\epsilon_{ijk}$  and  $i, j, k \in \{1, 2, 3\}$ .

Based on theorem 4.1 and 4.3, we now see that an Euler rotation is given by:

$$\mathcal{R}(\phi, \vec{e}_3)\mathcal{R}(\theta, \vec{e}_2)\mathcal{R}(\chi, \vec{e}_3) = e^{-i\phi J_3} e^{-i\theta J_2} e^{-i\chi J_3}. \quad (4.4.24)$$

**4.4.4 Relation between SO(3) generators and spin-1 operators**

An important point should be made based on the results from previous subsection. By direct inspection, we see that our generator basis obeys the commutation relations<sup>14</sup>:

$$[J_i, J_j] = i \sum_{k=1}^3 \epsilon_{ijk} J_k; \quad i, j \in \{1, 2, 3\}. \quad (4.4.25)$$

Thus, if we have written

$$e^{-i\psi(n_1 J_1 + n_2 J_2 + n_3 J_3)} = e^{-i\frac{\psi}{\hbar}(n_1 \hbar J_1 + n_2 \hbar J_2 + n_3 \hbar J_3)}, \quad (4.4.26)$$

and performed the substitution

$$\hbar J_k \mapsto J_k, \quad (4.4.27)$$

the commutation relations for SO(3) basis generators would be exactly the same as for quantum mechanical angular momentum operator. The question is then: what kind of angular momentum is this? Writing out our generator basis explicitly (in the new  $\hbar$ -formalism defined in 4.4.26 and 4.4.27), we have:

$$J_1 = \hbar \begin{bmatrix} 0 & 0 & 0 \\ 0 & 0 & -i \\ 0 & i & 0 \end{bmatrix}; \quad J_2 = \hbar \begin{bmatrix} 0 & 0 & i \\ 0 & 0 & 0 \\ -i & 0 & 0 \end{bmatrix}; \quad J_3 = \hbar \begin{bmatrix} 0 & -i & 0 \\ i & 0 & 0 \\ 0 & 0 & 0 \end{bmatrix}. \quad (4.4.28)$$

But we do also know from quantum mechanics that the spin-1 operators, when projected on  $z$ -axis eigenstates, are given by:

$$J'_1 = \frac{\hbar}{\sqrt{2}} \begin{bmatrix} 0 & 1 & 0 \\ 1 & 0 & 1 \\ 0 & 1 & 0 \end{bmatrix}; \quad J'_2 = \frac{\hbar}{\sqrt{2}} \begin{bmatrix} 0 & -i & 0 \\ i & 0 & -i \\ 0 & i & 0 \end{bmatrix}; \quad J'_3 = \hbar \begin{bmatrix} 1 & 0 & 0 \\ 0 & 0 & 0 \\ 0 & 0 & -1 \end{bmatrix}. \quad (4.4.29)$$

In the matter of fact, 4.4.28 can be obtained from 4.4.29 by a unitary transformation. Thus, we conclude that  $\{J_1, J_2, J_3\}$  are related to the spin-1 operator.

**4.4.5 Generators of SU(2) group and spin- $\frac{1}{2}$  operators**

As described in the previous subsection, the SO(3) group is related to spin-1 particles. In this thesis, however, we are interested in fermions, which are spin- $\frac{1}{2}$  particles. We are thus interested in finding a matrix group, where the generators can be proportional to the Pauli matrices. In fact, as we will now show, this is the case for SU(2) group.

We begin with finding an expression for arbitrary  $U \in \text{SU}(2)$ . Writing a general complex  $2 \times 2$  matrix:

$$U = \begin{bmatrix} a_{11} + ib_{11} & a_{12} + ib_{12} \\ a_{21} + ib_{21} & a_{22} + ib_{22} \end{bmatrix}; \quad a_{ij}, b_{ij} \in \mathbb{R}, \quad (4.4.30)$$

the inverse of this matrix is then given by

$$U^{-1} = \frac{1}{\det(U)} \begin{bmatrix} a_{22} + ib_{22} & -a_{12} - ib_{12} \\ -a_{21} - ib_{21} & a_{11} + ib_{11} \end{bmatrix}. \quad (4.4.31)$$

Since we are considering the SU(2) group, we must have that  $\det(U) = 1$  and  $U^{-1} = U^\dagger$ . Thus,

$$U^\dagger = \begin{bmatrix} a_{11} - ib_{11} & a_{21} - ib_{21} \\ a_{12} - ib_{12} & a_{22} - ib_{22} \end{bmatrix} = U^{-1} = \begin{bmatrix} a_{22} + ib_{22} & -a_{12} - ib_{12} \\ -a_{21} - ib_{21} & a_{11} + ib_{11} \end{bmatrix}. \quad (4.4.32)$$

<sup>14</sup>Since the basis generators do not commute,  $e^{-i\psi(n_1 J_1 + n_2 J_2 + n_3 J_3)} \neq e^{-i\psi n_1 J_1} e^{-i\psi n_2 J_2} e^{-i\psi n_3 J_3}$  in theorem 4.3. This reminds us about the fact that rotations in 3D do not commute.

This means that

$$a_{11} = a_{22}; \quad b_{11} = -b_{22}; \quad a_{21} = -a_{12}; \quad b_{21} = b_{12}. \quad (4.4.33)$$

Defining

$$u_0 := a_{11}; \quad u_1 := b_{12}; \quad u_2 := a_{12}; \quad u_3 := b_{11}, \quad (4.4.34)$$

we thus see that any SU(2) matrix can be written on the form

$$U = \begin{bmatrix} u_0 + iu_3 & u_2 + iu_1 \\ -u_2 + iu_1 & u_0 - iu_3 \end{bmatrix}; \quad \begin{cases} u_0, u_1, u_2, u_3 \in \mathbb{R} \\ u_0^2 + u_1^2 + u_2^2 + u_3^2 = 1 \end{cases}, \quad (4.4.35)$$

and that this matrix can be decomposed to

$$U = u_0 I + iu_1 \sigma_1 + iu_2 \sigma_2 + iu_3 \sigma_3 = u_0 I + i\vec{u} \cdot \vec{\sigma}, \quad (4.4.36)$$

where  $I$  is an identity matrix, and  $\sigma_k$ 's are Pauli matrices. This is the first foreshadowing to the fact that SU(2) is related to the spin- $\frac{1}{2}$  operators.

Next, inspired by the derivation of SO(3) generators, we want in a similar manner to express our general SU(2) matrix in terms of an exponential that depends on some unit vector  $\hat{n}$  and some angle  $\eta$ . Suppose that a such representation exists for any SU(2) matrix, and is of the same form as for SO(3):

$$U(\eta, \hat{n}) = e^{-i\eta \hat{n} \cdot \vec{\sigma}}. \quad (4.4.37)$$

By using Taylor expansion, we can then rewrite this as

$$e^{-i\eta \hat{n} \cdot \vec{\sigma}} = \sum_{m=0}^{\infty} \frac{(-i\eta \hat{n} \cdot \vec{\sigma})^m}{m!} = \sum_{m=0}^{\infty} (-i)^{2m} \eta^{2m} \frac{(\hat{n} \cdot \vec{\sigma})^{2m}}{(2m)!} + \sum_{m=0}^{\infty} (-i)^{2m+1} \eta^{2m+1} \frac{(\hat{n} \cdot \vec{\sigma})^{2m+1}}{(2m+1)!}. \quad (4.4.38)$$

By using the relation<sup>15</sup>  $(\vec{v} \cdot \vec{\sigma})^2 = I|\vec{v}|^2$  for all  $\vec{v} \in \mathbb{R}^3$ , and the Taylor expansions of sine and cosine functions, we have

$$e^{-i\eta \hat{n} \cdot \vec{\sigma}} = I \sum_{m=0}^{\infty} (-1)^m \frac{\eta^{2m}}{(2m)!} - i(\hat{n} \cdot \vec{\sigma}) \sum_{m=0}^{\infty} (-1)^m \frac{\eta^{2m+1}}{(2m+1)!} = I \cos \eta - i(\hat{n} \cdot \vec{\sigma}) \sin \eta. \quad (4.4.39)$$

Comparing 4.4.39 with 4.4.36, we realize that the expressions are the same when

$$u_0 = \cos \eta; \quad \vec{u} = -(\sin \eta) \hat{n}. \quad (4.4.40)$$

From 4.4.35, we see that the constraint  $u_0^2 + u_1^2 + u_2^2 + u_3^2 = 1$  is automatically satisfied with this transformation. The question is then whether this transformation covers all the elements in the SU(2) group. The constraint implies that  $-1 \leq u_0 \leq 1$  and  $|\vec{u}|^2 \leq 1$ . If  $\eta \in [0, \pi]$ , then we see that all the possible values of  $u_0$  are covered by  $\cos \eta$ . On the other hand,  $-\hat{n}$  can represent any direction in  $\mathbb{R}^3$ , whilst  $\sin \eta$  represents all vector lengths from 0 to 1, which means that all possible vectors  $\vec{u}$  are covered, and there is also a one-to-one correspondence.

These results imply that any SU(2) matrix is uniquely determined by some unit vector  $\hat{n}$  and an angle  $\eta \in [0, \pi]$ , with the relation given in 4.4.37. However, as we remember from section 4.4, all 3D rotations can uniquely be determined by a unit vector and an rotation angle in the interval  $[0, 2\pi]$ . Thus, we conclude that our  $\eta$  corresponds to the half of the rotation angle  $\psi$ , so that  $\psi = 2\eta$ . We end up with the following theorem:

**Theorem 4.4.** Any matrix  $U \in \text{SU}(2)$  is uniquely given by

$$U(\psi, \hat{n}) = e^{-i\psi \hat{n} \cdot \frac{\vec{\sigma}}{2}}, \quad (4.4.41)$$

where  $\hat{n} \in \mathbb{R}^3$  is a unit vector,  $\psi \in [0, 2\pi]$  and  $\vec{\sigma}$  are Pauli matrices.

Rewriting

$$e^{-i\psi \hat{n} \cdot \frac{\vec{\sigma}}{2}} = e^{-i\frac{\psi}{\hbar} \hat{n} \cdot \frac{\hbar \vec{\sigma}}{2}}, \quad (4.4.42)$$

we see that the generators (in  $\hbar$ -formalism) are given by

$$S_k = \frac{\hbar}{2} \sigma_k; \quad k \in \{1, 2, 3\}, \quad (4.4.43)$$

<sup>15</sup>This relation can be proved by expanding the parenthesis, and using the fact that  $\{\sigma_i, \sigma_j\} = 2I\delta_{ij}$  for Pauli matrices.

which is the spin- $\frac{1}{2}$  operator projected on its z-axis eigenstates. An SU(2) element is then given by

$$U(\psi, \hat{n}) = e^{-i\frac{\psi}{\hbar}\hat{n}\cdot\vec{S}}, \quad (4.4.44)$$

and we have therefore shown that SU(2) is related to spin- $\frac{1}{2}$  operators in the same way as SO(3) is related to spin-1 operators<sup>16</sup>.

## 4.5 Connection with quantum mechanics

### 4.5.1 Quantum mechanical rotations

In the last part of previous section, we showed that SO(3) and SU(2) groups are directly related to quantum mechanical spin-1 and spin- $\frac{1}{2}$  operators, respectively, through the so-called generators. In this section, we want to extend the concept of these groups to quantum mechanical systems, and realize that these groups then represent rotations of spins or angular momentas in 3D space.

We know that in quantum mechanics, a physical observable  $A$  corresponds to a Hermitian operator  $\hat{A}$ . Different physical states correspond to different vectors  $|\psi\rangle$  in Hilbert space, and the expectation value of this observable, that we can measure experimentally for a given physical state  $|\psi\rangle$ , is given by

$$\langle A \rangle = \langle \psi | \hat{A} | \psi \rangle. \quad (4.5.1)$$

Now, suppose that some unitary operator  $\hat{U}$  transforms any state  $|\psi\rangle$  into some other state  $|\psi'\rangle$ :

$$|\psi'\rangle = \hat{U} |\psi\rangle. \quad (4.5.2)$$

We want to see how the expectation value of some observable  $A$  changes when we perform a such state transformation. Having that  $\hat{U}^{-1} = \hat{U}^\dagger$  for a unitary transformation, we have

$$\langle \psi' | \hat{A} | \psi' \rangle = \langle \psi | \hat{U}^\dagger \hat{A} \hat{U} | \psi \rangle. \quad (4.5.3)$$

This is true for any state  $|\psi\rangle$ , meaning that instead of regarding this procedure as a state transformation, we can regard this as an operator transformation:

$$\hat{A}' = \hat{U}^\dagger \hat{A} \hat{U}. \quad (4.5.4)$$

Now, suppose that our observable is some angular momentum

$$\hat{\vec{J}} = \hat{J}_1 \vec{e}_1 + \hat{J}_2 \vec{e}_2 + \hat{J}_3 \vec{e}_3, \quad (4.5.5)$$

with defining commutations

$$[\hat{J}_i, \hat{J}_j] = i\hbar \sum_{k=1}^3 \epsilon_{ijk} \hat{J}_k; \quad i, j \in \{1, 2, 3\}. \quad (4.5.6)$$

Next, we generalize 4.4.44 to quantum mechanical operators:

$$e^{-i\frac{\psi}{\hbar}\hat{n}\cdot\vec{S}} \mapsto e^{-i\frac{\psi}{\hbar}\hat{n}\cdot\hat{\vec{J}}}, \quad (4.5.7)$$

where at this point,  $\hat{\vec{J}}$  can be any kind of angular momentum satisfying 4.5.6. Having that this is a unitary operator, we want to see what kind of transformation it does. Without loss of generality, we consider  $\hat{n} = \vec{e}_3$ . Then, based on 4.5.4, we have the transformation:

$$\hat{J}'_i = e^{i\frac{\psi}{\hbar}\hat{J}_3} \hat{J}_i e^{-i\frac{\psi}{\hbar}\hat{J}_3}; \quad i \in \{1, 2, 3\}. \quad (4.5.8)$$

Due to the exponential form of the transformation, we can use Baker-Hausdorff theorem<sup>17</sup>, along with the commutation relations, to do following:

$$\begin{aligned} \hat{J}'_1 &= e^{i\frac{\psi}{\hbar}\hat{J}_3} \hat{J}_1 e^{-i\frac{\psi}{\hbar}\hat{J}_3} = \sum_{n=0}^{\infty} \frac{1}{n!} [\hat{J}_1, -i\frac{\psi}{\hbar}\hat{J}_3]_n = \hat{J}_1 + [\hat{J}_1, -i\frac{\psi}{\hbar}\hat{J}_3] + \dots = \hat{J}_1 - \psi \hat{J}_2 + \dots = \\ &\hat{J}_1 - \psi \hat{J}_2 + \frac{1}{2!} [-\psi \hat{J}_2, -i\frac{\psi}{\hbar}\hat{J}_3] + \dots = \hat{J}_1 - \psi \hat{J}_2 - \frac{1}{2!} \psi^2 \hat{J}_1 + \dots = \hat{J}_1 - \psi \hat{J}_2 - \frac{1}{2!} \psi^2 \hat{J}_1 + \\ &\frac{1}{3!} [-\psi^2 \hat{J}_1, -i\frac{\psi}{\hbar}\hat{J}_3] + \dots = \hat{J}_1 - \psi \hat{J}_2 - \frac{1}{2!} \psi^2 \hat{J}_1 + \frac{1}{3!} \psi^3 \hat{J}_2 + \dots = \\ &\hat{J}_1 (1 - \frac{1}{2!} \psi^2 + \dots) - \hat{J}_2 (\psi - \frac{1}{3!} \psi^3 + \dots) = \hat{J}_1 \sum_{n=0}^{\infty} (-1)^n \frac{\psi^{2n}}{(2n)!} - \hat{J}_2 \sum_{n=0}^{\infty} (-1)^n \frac{\psi^{2n+1}}{(2n+1)!} = \hat{J}_1 \cos \psi - \hat{J}_2 \sin \psi. \end{aligned} \quad (4.5.9)$$

<sup>16</sup>Mathematically, since the exponential forms are the same for SO(3) and SU(2), we say that Lie algebras  $\mathfrak{so}(3)$  and  $\mathfrak{su}(2)$  are isomorphic. The 1:2 homomorphism between the groups is due to the difference in generators.

<sup>17</sup>See appendix A to recall the theorem.

In exactly the same manner, we find

$$\hat{J}'_2 = \hat{J}_1 \sin \psi + \hat{J}_2 \cos \psi, \quad (4.5.10)$$

$$\hat{J}'_3 = \hat{J}_3. \quad (4.5.11)$$

Organizing this in a matrix, we have

$$\begin{bmatrix} \hat{J}'_1 \\ \hat{J}'_2 \\ \hat{J}'_3 \end{bmatrix} = e^{i\frac{\psi}{\hbar}\hat{J}_3} \begin{bmatrix} \hat{J}_1 \\ \hat{J}_2 \\ \hat{J}_3 \end{bmatrix} e^{-i\frac{\psi}{\hbar}\hat{J}_3} = \begin{bmatrix} \cos \psi & -\sin \psi & 0 \\ \sin \psi & \cos \psi & 0 \\ 0 & 0 & 1 \end{bmatrix} \begin{bmatrix} \hat{J}_1 \\ \hat{J}_2 \\ \hat{J}_3 \end{bmatrix}. \quad (4.5.12)$$

But this is a rotation of our angular momentum operator around the  $z$ -axis by  $\psi$ . Thus, we can conclude with the following:

**Theorem 4.5.** The unitary operator

$$\hat{U}_{\hat{J}}(\psi, \hat{n}) = e^{-i\frac{\psi}{\hbar}\hat{n} \cdot \hat{J}} \quad (4.5.13)$$

produces a rotation of the corresponding angular momentum operator  $\hat{J}$  by an angle  $\psi$  about an axis defined by  $\hat{n}$ .

We want to consider this theorem more carefully from the physical point of view. In general, the total angular momentum for a physical particle is given by

$$\hat{J} = \hat{L} + \hat{S}, \quad (4.5.14)$$

where  $\hat{L}$  is orbital angular momentum related to the spatial position of the particle, and  $\hat{S}$  is intrinsic spin angular momentum related to the spin orientation of the particle. Thus, in this case,  $\hat{U}_{\hat{J}}(\psi, \hat{n})$  produces a global rotation of the particle - both in its spatial orientation and in its intrinsic spin.  $\hat{U}_{\hat{L}}(\psi, \hat{n})$  on the other hand, produces only spatial rotation of the particle, without rotating the spin, whilst  $\hat{U}_{\hat{S}}(\psi, \hat{n})$  produces only spin rotation of the particle, without changing the spatial orientation.

In this thesis, the positions of the spins are in rather fixed lattice sites, and we are thus interested in only making spin rotations. Therefore, we conclude this section with the fact that the operator  $\hat{U}_{\hat{S}}(\psi, \hat{n})$  produces rotations of the particle spin.

#### 4.5.2 Concept of symmetry breaking

We have earlier derived a unitary operator transformation, which was given by equation 4.5.4. An operator  $\hat{A}$  is then said to be invariant under a unitary transformation  $\hat{U}$  when:

$$\hat{U}^\dagger \hat{A} \hat{U} = \hat{A} \Leftrightarrow \hat{A} \hat{U} = \hat{U} \hat{A} \Leftrightarrow [\hat{A}, \hat{U}] = 0 \quad (4.5.15)$$

That is, the operator is invariant under a unitary transformation if and only if the operator commutes with the transformation. Suppose that we consider a Lie group of transformations  $\hat{U}(q)$ , where  $q$  is the amount of transformation. Then, as we have seen earlier, there exists a generator  $\hat{Q}$ , so that:

$$\hat{U}(q) = e^{-i\frac{q}{\hbar}\hat{Q}}. \quad (4.5.16)$$

If we consider an infinitesimal amount of transformation  $\Delta q$ , we can rewrite 4.5.16 as:

$$\hat{U}(\Delta q) = 1 - \frac{i}{\hbar}\hat{Q}\Delta q + \hat{O}(\Delta q^2). \quad (4.5.17)$$

Suppose that  $\hat{A}$  is invariant under this infinitesimal transformation. Then,

$$[\hat{A}, 1 - \frac{i}{\hbar}\hat{Q}\Delta q + \hat{O}(\Delta q^2)] = -\frac{i}{\hbar}[\hat{A}, \hat{Q}]\Delta q + \hat{O}(\Delta q^2) = 0. \quad (4.5.18)$$

Since  $\Delta q \rightarrow 0$ , we must have that:

$$[\hat{A}, \hat{Q}] = 0. \quad (4.5.19)$$

This means that an operator is invariant under a continuous transformation in some topological neighborhood if and only if the operator commutes with the generator of the continuous transformation.

When an operator is invariant under a discrete transformation, we say that the operator has a discrete symmetry. Analogously, when an operator is invariant under a continuous transformation, we say that the operator has a continuous symmetry. If the operator under consideration is the Hamiltonian, we say that those are the symmetries of the system. For instance, the system (Hamiltonian) might be invariant under the transformation  $z \mapsto -z$  (known as  $Z_2$  symmetry), which is a discrete symmetry. On the other hand, the Hamiltonian might be invariant under any spin- $\frac{1}{2}$  rotation transformation (SU(2) symmetry), which is a continuous symmetry.

Next, for simplicity, suppose that our Hamiltonian is given by:

$$\hat{H} = \frac{J}{2} \sum_{\langle i,j \rangle} \hat{\vec{S}}_i \cdot \hat{\vec{S}}_j; \quad J < 0. \quad (4.5.20)$$

This is a simple ferromagnetic model, meaning that for a ground state, all the spins are pointing in the same direction. Intuitively, the system (Hamiltonian) should be invariant if we perform a global spin rotation. That is, if all the spin operators in the Hamiltonian are rotated in the same manner. We can show this explicitly by using 4.5.19. Having that the total spin operator of the system is given by:

$$\hat{\vec{S}}_{tot} := \sum_i \hat{\vec{S}}_i, \quad (4.5.21)$$

the global rotation generator about a unit vector  $\hat{n}$  is given by:

$$\hat{Q} = \hat{n} \cdot \hat{\vec{S}}_{tot} = n_x \hat{S}_{tot}^{(x)} + n_y \hat{S}_{tot}^{(y)} + n_z \hat{S}_{tot}^{(z)}. \quad (4.5.22)$$

Suppose that we consider following commutation relation:

$$\begin{aligned} [\hat{\vec{S}}_i \cdot \hat{\vec{S}}_j, \hat{S}_{tot}^{(z)}] &= [\hat{S}_i^{(x)} \hat{S}_j^{(x)} + \hat{S}_i^{(y)} \hat{S}_j^{(y)} + \hat{S}_i^{(z)} \hat{S}_j^{(z)}, \hat{S}_i^{(z)} + \hat{S}_j^{(z)}] = \\ &= [\hat{S}_i^{(x)}, \hat{S}_i^{(z)}] \hat{S}_j^{(x)} + [\hat{S}_i^{(y)}, \hat{S}_i^{(z)}] \hat{S}_j^{(y)} + [\hat{S}_j^{(x)}, \hat{S}_j^{(z)}] \hat{S}_i^{(x)} + [\hat{S}_j^{(y)}, \hat{S}_j^{(z)}] \hat{S}_i^{(y)} = \\ &= -i\hbar \hat{S}_i^{(y)} \hat{S}_j^{(x)} + i\hbar \hat{S}_i^{(x)} \hat{S}_j^{(y)} - i\hbar \hat{S}_j^{(y)} \hat{S}_i^{(x)} + i\hbar \hat{S}_j^{(x)} \hat{S}_i^{(y)} = 0. \end{aligned} \quad (4.5.23)$$

Having that the Hamiltonian 4.5.20 is a sum of  $\hat{\vec{S}}_i \cdot \hat{\vec{S}}_j$ -terms, we must have that:

$$[\hat{H}, \hat{S}_{tot}^{(z)}] = 0. \quad (4.5.24)$$

In exactly the same manner, we can show a similar relation for  $\hat{S}_{tot}^{(x)}$  and  $\hat{S}_{tot}^{(y)}$ . Thus, we have:

$$[\hat{H}, \hat{n} \cdot \hat{\vec{S}}_{tot}] = 0; \quad \forall \hat{n}, \quad (4.5.25)$$

and the Hamiltonian is invariant under any kind of global spin rotation. However, as we mentioned, a ground state of this Hamiltonian does not have the same symmetry. A global rotation of a ground state would in general produce another ground state, pointing in a different direction. We say that the ground state spontaneously *breaks* the system symmetry. This concept is important, because ordered phases usually can be described in terms of broken symmetries.

## 4.6 Schwinger bosons and Abrikosov fermions

Aimed with the spin rotation theory from previous sections in this chapter, we now want to find a fermionization and bosonization technique where SU(2)-invariance is manifested. More precisely, we don't want to have one direction more special than some other. In order to find a such representation, we introduce the concept of bilinear operators.

### 4.6.1 Derivation through bilinear operators

Suppose that we can write some Hermitian operator  $\hat{A}$  on the form

$$\hat{A} = \sum_{i,j=1}^n \hat{a}_i^\dagger A_{ij} \hat{a}_j = \hat{\mathbf{a}}^\dagger \mathbf{A} \hat{\mathbf{a}}, \quad (4.6.1)$$

where  $\hat{\mathbf{a}} = [\hat{a}_1, \dots, \hat{a}_n]^T$ , the set of operators  $\{\hat{a}_i\}$  is either a set of bosonic or fermionic operators, and  $[A_{ij}]$  is some  $n \times n$  Hermitian matrix. This is known as bilinear form.

Next, suppose that two Hermitian operators  $\hat{A}$  and  $\hat{B}$  can be written on the bilinear form 4.6.1, in terms of the same set of bosonic or fermionic operators. Then, by using the bosonic commutation relations or fermionic anti-commutation relations, it is straight-forward to show that

$$[\hat{A}, \hat{B}] = [\hat{\mathbf{a}}^\dagger A \hat{\mathbf{a}}, \hat{\mathbf{a}}^\dagger B \hat{\mathbf{a}}] = \hat{\mathbf{a}}^\dagger [A, B] \hat{\mathbf{a}}, \quad (4.6.2)$$

which is true for  $\{\hat{a}_i\}$  being both bosonic and fermionic. With this relation in mind, we now turn to spin-operators. Having the defining property

$$[\hat{S}_i, \hat{S}_j] = i\hbar \sum_{k=1}^3 \epsilon_{ijk} \hat{S}_k, \quad (4.6.3)$$

suppose that each of the spin componets can be written on bilinear form in terms of the same bosonic or fermionic operators:

$$\hat{S}_i = \hat{\mathbf{a}}^\dagger S_i \hat{\mathbf{a}}; \quad i \in \{1, 2, 3\}. \quad (4.6.4)$$

At this point, we have not made any definitions of matrices  $S_i$ , other than that they are Hermitian. By combining 4.6.2 and 4.6.3, we get

$$[\hat{S}_i, \hat{S}_j] = \hat{\mathbf{a}}^\dagger [S_i, S_j] \hat{\mathbf{a}} = i\hbar \sum_{k=1}^3 \epsilon_{ijk} \hat{S}_k = i\hbar \sum_{k=1}^3 \epsilon_{ijk} \hat{\mathbf{a}}^\dagger S_k \hat{\mathbf{a}} \implies [S_i, S_j] = i\hbar \sum_{k=1}^3 \epsilon_{ijk} S_k. \quad (4.6.5)$$

Thus, such matrices should obey the same commutation relations as the spin operators. The natural choice for the matrices is then the spin operators projected on  $z$ -axis eigenstates, which for spin- $\frac{1}{2}$  are given by

$$S_i = \frac{\hbar}{2} \sigma_i; \quad i \in \{1, 2, 3\}, \quad (4.6.6)$$

where  $\{\sigma_1, \sigma_2, \sigma_3\}$  are Pauli matrices. We then get:

$$\hat{S}_i = \frac{\hbar}{2} \hat{\mathbf{a}}^\dagger \sigma_i \hat{\mathbf{a}}; \quad i \in \{1, 2, 3\}. \quad (4.6.7)$$

For this particular spin- $\frac{1}{2}$  case, such bosonic operators are known as Schwinger bosons, whilst such fermionic operators are known as Abrikosov fermions (or Schwinger fermions).

In addition, it turns out that the Fock space for Schwinger bosons and Abrikosov fermions is limited by the following constraint:

$$\hat{a}_1^\dagger \hat{a}_1 + \hat{a}_2^\dagger \hat{a}_2 = \hat{n}_{a_1} + \hat{n}_{a_2} = 1, \quad (4.6.8)$$

which basically tells us that exactly one such boson or fermion exists for a spin- $\frac{1}{2}$  particle in a given state<sup>18</sup>. For Abrikosov fermions, this constraint can be derived from the spin- $\frac{1}{2}$  constraint

$$\hat{S}^2 \equiv \hbar^2 S(S+1) = \frac{3\hbar^2}{4}, \quad (4.6.9)$$

by direct insertion of 4.6.7 into 4.6.9 and by using the completeness relation of Pauli matrices<sup>19</sup>. For Schwinger bosons, the 4.6.8 constraint can be derived by considering spin eigenstates (of  $\hat{S}^2$  and  $\hat{S}_z$ ) written in terms of second quantization (in Schwinger bosons), and applying the  $\hat{S}^2$  operator to give the constraint in 4.6.9 (see for instance equation 7.9 in reference [23]).

We now summarize these results in following definition:

**Definition 4.2** (Schwinger bosons and Abrikosov fermions). Suppose that some bosonic or fermionic operators  $\{\hat{a}_\uparrow, \hat{a}_\downarrow\}$  satisfy following equations:

$$\hat{S}_i = \frac{\hbar}{2} \begin{bmatrix} \hat{a}_\uparrow^\dagger & \hat{a}_\downarrow^\dagger \\ \hat{a}_\uparrow & \hat{a}_\downarrow \end{bmatrix} \sigma_i \begin{bmatrix} \hat{a}_\uparrow \\ \hat{a}_\downarrow \end{bmatrix}; \quad i \in \{1, 2, 3\}, \quad (4.6.10)$$

$$\hat{a}_\uparrow^\dagger \hat{a}_\uparrow + \hat{a}_\downarrow^\dagger \hat{a}_\downarrow = 1, \quad (4.6.11)$$

where  $\{\hat{S}_1, \hat{S}_2, \hat{S}_3\}$  are spin- $\frac{1}{2}$  operator components. Them, such bosonic operators are known as Schwinger bosons,

<sup>18</sup>Since there are two such bosons or fermions per spin- $\frac{1}{2}$  particle, it is common to denote such bosons or fermions as spin up and spin down. That is,  $\hat{a}_1 = \hat{a}_\uparrow$  and  $\hat{a}_2 = \hat{a}_\downarrow$ .

<sup>19</sup>See appendix A for the completeness relation of Pauli matrices.

whilst such fermionic operators are known as Abrikosov fermions.

#### 4.6.2 Rotations of Schwinger bosons and Abrikosov fermions

With this definition, unlike the approximated Holstein-Primakoff transformation, we see that Schwinger bosons and Abrikosov fermions are of a more isotropic nature. Every spin component is given on the same form, relative to a Pauli matrix in the corresponding direction. In fact, as we now will show, such operators transform like vectors in  $SU(2)$  when spin-rotated.

Considering the general bilinear operator in 4.6.1, suppose that  $\vec{v} = [v_1 \dots v_n]^T$  is an eigenvector of the matrix  $[A_{ij}]$  with eigenvalue  $v$ . We define a corresponding commutation eigenoperator  $\hat{v}^\dagger$  as

$$\hat{v}^\dagger = \sum_{i=1}^n \hat{a}_i^\dagger v_i = \hat{\mathbf{a}}^\dagger \vec{v}. \quad (4.6.12)$$

The reason for that name is that we have:

$$[\hat{A}, \hat{v}^\dagger] = \hat{\mathbf{a}}^\dagger A \vec{v} = v \hat{v}^\dagger, \quad (4.6.13)$$

which is easily obtained by direct insertion, and by using commutation or anti-commutation relations for bosons or fermions, respectively. We can then use this relation along with Baker-Hausdorff theorem to  $\hat{A}$ -rotate the commutation eigenoperator by angle  $\theta$ :

$$e^{i\frac{\theta}{\hbar}\hat{A}}\hat{v}^\dagger e^{-i\frac{\theta}{\hbar}\hat{A}} = \hat{v}^\dagger + [\hat{v}^\dagger, -i\frac{\theta}{\hbar}\hat{A}] + \dots = \hat{v}^\dagger + i\frac{\theta}{\hbar}v\hat{v}^\dagger + \dots = \hat{v}^\dagger + i\frac{\theta}{\hbar}v\hat{v}^\dagger + \frac{1}{2!}\left(i\frac{\theta}{\hbar}v\right)^2\hat{v}^\dagger + \dots = e^{i\frac{\theta}{\hbar}v}\hat{v}^\dagger. \quad (4.6.14)$$

Turning back to the spin-operators, we want to consider the spin-rotation:

$$\begin{bmatrix} (\hat{a}_1^\dagger)' \\ (\hat{a}_2^\dagger)' \end{bmatrix} = e^{i\frac{\chi}{\hbar}\hat{S}_3} e^{i\frac{\theta}{\hbar}\hat{S}_2} e^{i\frac{\phi}{\hbar}\hat{S}_3} \begin{bmatrix} \hat{a}_1^\dagger \\ \hat{a}_2^\dagger \end{bmatrix} e^{-i\frac{\phi}{\hbar}\hat{S}_3} e^{-i\frac{\theta}{\hbar}\hat{S}_2} e^{-i\frac{\chi}{\hbar}\hat{S}_3}, \quad (4.6.15)$$

which is a general Euler rotation described in theorem 4.1. Having that eigenvectors and corresponding eigenvalues for  $S_3$  are

$$\vec{v}_1 = \begin{bmatrix} 1 \\ 0 \end{bmatrix}, \quad v_1 = \frac{\hbar}{2}; \quad \vec{v}_2 = \begin{bmatrix} 0 \\ 1 \end{bmatrix}, \quad v_2 = -\frac{\hbar}{2}, \quad (4.6.16)$$

we use 4.6.12 to get

$$\hat{v}_1^\dagger = \hat{a}_1^\dagger; \quad \hat{v}_2^\dagger = \hat{a}_2^\dagger, \quad (4.6.17)$$

and then 4.6.14 to perform the first rotation:

$$e^{i\frac{\phi}{\hbar}\hat{S}_3} \begin{bmatrix} \hat{a}_1^\dagger \\ \hat{a}_2^\dagger \end{bmatrix} e^{-i\frac{\phi}{\hbar}\hat{S}_3} = \begin{bmatrix} \hat{a}_1^\dagger e^{i\frac{\phi}{2}} \\ \hat{a}_2^\dagger e^{-i\frac{\phi}{2}} \end{bmatrix} = \begin{bmatrix} e^{i\frac{\phi}{2}} & 0 \\ 0 & e^{-i\frac{\phi}{2}} \end{bmatrix} \begin{bmatrix} \hat{a}_1^\dagger \\ \hat{a}_2^\dagger \end{bmatrix}. \quad (4.6.18)$$

In similar manner, we use eigenvectors and eigenvalues of  $S_2$ :

$$\vec{v}_1 = \begin{bmatrix} 1 \\ i \end{bmatrix}, \quad v_1 = \frac{\hbar}{2}; \quad \vec{v}_2 = \begin{bmatrix} i \\ 1 \end{bmatrix}, \quad v_2 = -\frac{\hbar}{2}, \quad (4.6.19)$$

to get:

$$\begin{aligned} \hat{v}_1^\dagger = \hat{a}_1^\dagger + i\hat{a}_2^\dagger & \implies \hat{a}_1^\dagger = \frac{1}{2}(\hat{v}_1^\dagger - i\hat{v}_2^\dagger) \\ \hat{v}_2^\dagger = i\hat{a}_1^\dagger + \hat{a}_2^\dagger & \implies \hat{a}_2^\dagger = \frac{1}{2}(\hat{v}_2^\dagger - i\hat{v}_1^\dagger) \end{aligned} \quad (4.6.20)$$

We then perform the second rotation:

$$\begin{aligned} e^{i\frac{\theta}{\hbar}\hat{S}_2} \begin{bmatrix} \hat{a}_1^\dagger \\ \hat{a}_2^\dagger \end{bmatrix} e^{-i\frac{\theta}{\hbar}\hat{S}_2} &= \frac{1}{2} e^{i\frac{\theta}{\hbar}\hat{S}_2} \begin{bmatrix} \hat{v}_1^\dagger \\ \hat{v}_2^\dagger \end{bmatrix} e^{-i\frac{\theta}{\hbar}\hat{S}_2} - \frac{i}{2} e^{i\frac{\theta}{\hbar}\hat{S}_2} \begin{bmatrix} \hat{v}_2^\dagger \\ \hat{v}_1^\dagger \end{bmatrix} e^{-i\frac{\theta}{\hbar}\hat{S}_2} = \frac{1}{2} \begin{bmatrix} \hat{v}_1^\dagger e^{i\frac{\theta}{2}} - i\hat{v}_2^\dagger e^{-i\frac{\theta}{2}} \\ \hat{v}_2^\dagger e^{-i\frac{\theta}{2}} - i\hat{v}_1^\dagger e^{i\frac{\theta}{2}} \end{bmatrix} = \\ &= \begin{bmatrix} \hat{a}_1^\dagger \cos \frac{\theta}{2} - \hat{a}_2^\dagger \sin \frac{\theta}{2} \\ \hat{a}_1^\dagger \sin \frac{\theta}{2} + \hat{a}_2^\dagger \cos \frac{\theta}{2} \end{bmatrix} = \begin{bmatrix} \cos \frac{\theta}{2} & -\sin \frac{\theta}{2} \\ \sin \frac{\theta}{2} & \cos \frac{\theta}{2} \end{bmatrix} \begin{bmatrix} \hat{a}_1^\dagger \\ \hat{a}_2^\dagger \end{bmatrix}. \end{aligned} \quad (4.6.21)$$

The third rotation is the same as the first, but with angle  $\chi$ . Thus, the total rotation is given by:

$$\begin{aligned} \begin{bmatrix} (\hat{a}_1^\dagger)' \\ (\hat{a}_2^\dagger)' \end{bmatrix} &= e^{i\frac{\chi}{\hbar}\hat{S}_3} e^{i\frac{\theta}{\hbar}\hat{S}_2} e^{i\frac{\phi}{\hbar}\hat{S}_3} \begin{bmatrix} \hat{a}_1^\dagger \\ \hat{a}_2^\dagger \end{bmatrix} e^{-i\frac{\phi}{\hbar}\hat{S}_3} e^{-i\frac{\theta}{\hbar}\hat{S}_2} e^{-i\frac{\chi}{\hbar}\hat{S}_3} = \\ \begin{bmatrix} e^{i\frac{\phi}{2}} & 0 \\ 0 & e^{-i\frac{\phi}{2}} \end{bmatrix} \begin{bmatrix} \cos\frac{\theta}{2} & -\sin\frac{\theta}{2} \\ \sin\frac{\theta}{2} & \cos\frac{\theta}{2} \end{bmatrix} \begin{bmatrix} e^{i\frac{\chi}{2}} & 0 \\ 0 & e^{-i\frac{\chi}{2}} \end{bmatrix} \begin{bmatrix} \hat{a}_1^\dagger \\ \hat{a}_2^\dagger \end{bmatrix} &= \begin{bmatrix} e^{i\frac{\phi+\chi}{2}} \cos\frac{\theta}{2} & -e^{i\frac{\phi-\chi}{2}} \sin\frac{\theta}{2} \\ e^{i\frac{-\phi+\chi}{2}} \sin\frac{\theta}{2} & e^{i\frac{-\phi-\chi}{2}} \cos\frac{\theta}{2} \end{bmatrix} \begin{bmatrix} \hat{a}_1^\dagger \\ \hat{a}_2^\dagger \end{bmatrix} \end{aligned} \quad (4.6.22)$$

We realize that this is an SU(2) matrix. From that, we see that under a spin rotation, the Schwinger bosons and Abrikosov fermions transform like vectors in SU(2), and this further manifests the isotropic nature of the transformation. At this point, we leave the symmetry discussion of these operators, and rather find a way to work with them.

## 4.7 Mean-field approximation

Although Schwinger bosons and Abrikosov fermions provide a more isotropic friendly transformation, the calculations are not necessarily easier than for the techniques considered earlier. While earlier techniques and approximations allowed us to write the Hamiltonian function on quadratic form in bosonic or fermionic operators, we now see that the spin operators written on Schwinger boson or Abrikosov fermion form are given on quadratic form, meaning that a spin-Hamiltonian which is quadratic in spin-operators will be quartic in bosonic or fermionic operators. This means that we cannot directly apply diagonalization techniques introduced earlier to obtain ground state information. However, there is a standard technique known as mean-field approximation that allows us to approximate quadratic form to quadratic form.

The general idea is following: when bosonic or fermionic operators are given on quartic form, we have a certain "interaction" between these particles (unlike the quadratic case, where the particles are free). The idea then is to approximate all these interactions into a certain constant "average" interaction field. That is, the effect from other bosons or fermions comes as a certain mean-field on otherwise independent particles.

### 4.7.1 General approach

Starting very generally, suppose that our Hamiltonian is given by:

$$\hat{H} = \hat{O}_1 \hat{O}_2, \quad (4.7.1)$$

where  $\hat{O}_1$  and  $\hat{O}_2$  are some operators. Suppose that we are considering our system in the states close to the ground state<sup>20</sup>, so that the difference:

$$\Delta \hat{O}_i := \hat{O}_i - \langle \hat{O}_i \rangle; \quad i \in \{1, 2\}, \quad (4.7.2)$$

becomes very small when our Hamiltonian is projected down on the subspace of such states. Here,  $\langle O_i \rangle = \langle G | \hat{O}_i | G \rangle$ , where  $|G\rangle$  is the system ground state. We can then write:

$$\begin{aligned} \hat{H} &= (\Delta \hat{O}_1 + \langle \hat{O}_1 \rangle) (\Delta \hat{O}_2 + \langle \hat{O}_2 \rangle) = \Delta \hat{O}_1 \langle \hat{O}_2 \rangle + \Delta \hat{O}_2 \langle \hat{O}_1 \rangle + \langle \hat{O}_1 \rangle \langle \hat{O}_2 \rangle + \Delta \hat{O}_1 \Delta \hat{O}_2 = \\ &\quad \hat{O}_1 \langle \hat{O}_2 \rangle + \hat{O}_2 \langle \hat{O}_1 \rangle - \langle \hat{O}_1 \rangle \langle \hat{O}_2 \rangle + \Delta \hat{O}_1 \Delta \hat{O}_2. \end{aligned} \quad (4.7.3)$$

If the relevant states are sufficiently close to the ground state, we can neglect the last term  $\Delta \hat{O}_1 \Delta \hat{O}_2$ . This is the mean-field approximation. Now, to be more specific, suppose that the operators  $\hat{O}_i$  are linear combinations of quadratic fermionic or bosonic operators  $\{\hat{a}_{i,k}\}$ , so that:

$$\hat{O}_i = \sum_{k,l} C_{kl}^{(i)} \hat{a}_{i,k}^\dagger \hat{a}_{i,l}. \quad (4.7.4)$$

Our initial Hamiltonian is then quartic in these operators. However, writing the Hamiltonian as in 4.7.3, we get:

$$\hat{H} = \sum_{k,l} \left[ \langle \hat{O}_2 \rangle C_{kl}^{(1)} + \langle \hat{O}_1 \rangle C_{kl}^{(2)} \right] \hat{a}_{i,k}^\dagger \hat{a}_{i,l} - \langle \hat{O}_1 \rangle \langle \hat{O}_2 \rangle + \Delta \hat{O}_1 \Delta \hat{O}_2. \quad (4.7.5)$$

By neglecting  $\Delta \hat{O}_1 \Delta \hat{O}_2$ , we thus end up with a quadratic Hamiltonian. We summarize the results:

<sup>20</sup>In general, any relevant state can be chosen here. Or, we can even take thermodynamical average. However, for the applications in this thesis, we are considering the ground state.



**Definition 4.3.** Given two operators  $\hat{O}_1$  and  $\hat{O}_2$ , the mean-field approximation of their product is defined as:

$$\hat{O}_1 \hat{O}_2 \mapsto \hat{O}_1 \langle \hat{O}_2 \rangle + \hat{O}_2 \langle \hat{O}_1 \rangle - \langle \hat{O}_1 \rangle \langle \hat{O}_2 \rangle. \quad (4.7.6)$$

The task then is to find the numbers  $\langle \hat{O}_1 \rangle$  and  $\langle \hat{O}_2 \rangle$ . Usually, we need to make some physical and symmetrical assumptions to make this task solvable. One way is to assume some values, insert these values into the mean-field Hamiltonian, and see if we get any contradictions. If we do, we apply some numerical algorithm to adjust that number until the Hamiltonian becomes consistent. This is one way of finding mean-field constants self-consistently. Another way is to solve self-consistency equations which we now will present.

#### 4.7.2 Self-consistency equations

Suppose that the Hamiltonian is approximated to:

$$\hat{H} = \hat{O}_1 \langle \hat{O}_2 \rangle + \hat{O}_2 \langle \hat{O}_1 \rangle - \langle \hat{O}_1 \rangle \langle \hat{O}_2 \rangle, \quad (4.7.7)$$

The ground state energy is given by:

$$E_0 = \langle \hat{H} \rangle. \quad (4.7.8)$$

Differentiation of ground state energy with respect to one of the mean-field constants gives:

$$\frac{\partial}{\partial \langle \hat{O}_1 \rangle} E_0 = \left\langle \frac{\partial}{\partial \langle \hat{O}_1 \rangle} \hat{H} \right\rangle = \langle \hat{O}_2 - \langle \hat{O}_2 \rangle \rangle = \langle \hat{O}_2 \rangle - \langle \hat{O}_2 \rangle = 0, \quad (4.7.9)$$

and similar for differentiation with respect to  $\langle \hat{O}_2 \rangle$ . These equations are known as self-consistency equations, and they should always be satisfied when we arrive at a ground state as function of mean-field parameters. Since we are interested in the ground state, we can thus determine mean-field parameters by minimizing total energy with respect to these parameters.

As a final remark in this chapter, it should be said that mean-field approximations in reality are very crude, and one should be careful when making conclusions in models where such approximations are involved, as they at best are qualitative[24]. For that reason, different mean-field approaches are usually applied to the same model of interest, and a conclusion is made based on results from different approaches. In the next chapter, we will apply two different mean-field theories - Abrikosov fermion mean-field theory and Schwinger boson mean-field zero-flux theory.

## 5 Application to Kane-Mele-Hubbard model

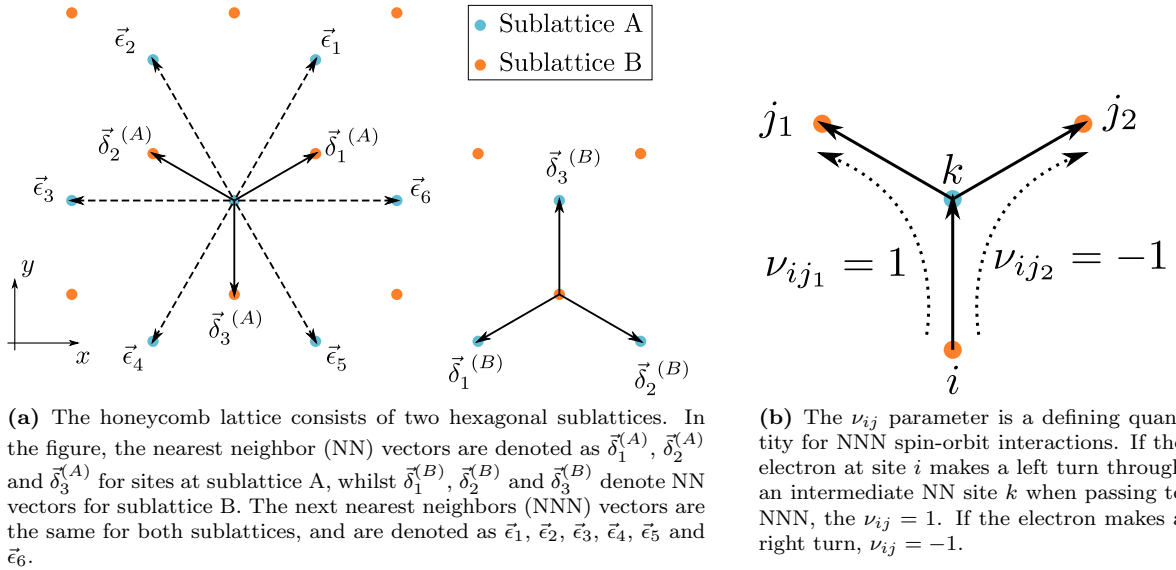
In this chapter, we will introduce an extended KMH model, to which we will apply Abrikosov fermion and Schwinger boson mean-field theories. Given different interaction parameters in the KMH model, the mean-field theories might give different sets of mean-field parameters, which might represent different physical phases. Since mean-field approximations at best are qualitative, the aim of this chapter is to give a qualitative description of predicted physical phases in extended KMH model, and in particular to find conditions for potential quantum spin liquids. In order to define and understand the KMH model, we need to define some central properties of the honeycomb lattice, for which this model is defined. In the following section, we define the lattice, and some of its properties.

### 5.1 The honeycomb lattice

#### 5.1.1 Direct lattice

The honeycomb lattice is depicted in figure 5a. As we see, this lattice is not a Bravais lattice, but rather two hexagonal (triangular) Bravais lattices symmetrically superimposed on each other<sup>21</sup>. This figure also defines the nearest neighbor (NN) and next nearest neighbor (NNN) vectors in a honeycomb lattice. A set of all the sites  $i$  (on both sublattices) with all the corresponding NNs for each site  $j = j(i)$  is denoted as  $\langle i, j \rangle$ . Analogously, a such set for NNNs is denoted as  $\langle\langle i, j \rangle\rangle$ . In this thesis, we do not go beyond the NNNs.

In addition, we want to define a quantity related to NNN hopping through an intermediate NN site. We consider the situation depicted in figure 5b. Suppose that we have an electron at a site  $i$ , which "moves" through an intermediate NN site  $k$ . If the electron then lands on the NNN site  $j_1$ , we see that the overall process is represented by a left turn, whilst for  $j_2$ , the process is represented by a right turn. In order to differentiate between these two situations, we associate them with numbers 1 and  $-1$ , respectively.



**Figure 5:** Some defining properties in this paper related to the honeycomb lattice.

Suppose that the vector pointing from site  $i$  to  $k$  in figure 5b is denoted as  $\vec{d}_{ik}$ . Next, suppose that the vector pointing from  $k$  to  $j$  (where  $j \in \{j_1, j_2\}$ ) is denoted as  $\vec{d}_{kj}$ . We then define the vector  $\vec{\nu}_{ij}$  as:

$$\vec{\nu}_{ij} := \frac{\vec{d}_{ik} \times \vec{d}_{kj}}{|\vec{d}_{ik} \times \vec{d}_{kj}|}. \quad (5.1.1)$$

From this definition, we see that the turn quantity  $\nu_{ij}$  is given by

$$\nu_{ij} = \vec{\nu}_{ij} \cdot \vec{e}_3, \quad (5.1.2)$$

<sup>21</sup>In other words, a honeycomb lattice can be described by a hexagonal Bravais lattice, with each site having a two-atomic basis separated with one of the NN vectors.

where  $\vec{e}_3$  is the unit vector pointing in z-axis direction (out of paper in figure 5).

We have that each site is associated with either sublattice  $A$  or sublattice  $B$ . Each NNN for a site is associated with one of the  $\vec{e}_i$  vectors and a value  $\nu_{ij} = \nu_l^{(X)}$ , where  $X$  is the sublattice, and  $l$  is the index of associated NNN vector. We summarize quantitative properties of the NNN vectors in table 1, where  $a$  is distance between two NNs.

**Table 1:** Properties of the NNN vectors from figure 5a. Here,  $a$  is lattice constant, defined as distance between two NNs.

Vector	Formula	Associated $\nu_{ij}$ on sublattice A	Associated $\nu_{ij}$ on sublattice B
$\vec{e}_1$	$\frac{a}{2}[\sqrt{3}\vec{e}_1 + 3\vec{e}_2]$	$\nu_1^{(A)} = 1$	$\nu_1^{(B)} = -1$
$\vec{e}_2$	$\frac{a}{2}[-\sqrt{3}\vec{e}_1 + 3\vec{e}_2]$	$\nu_2^{(A)} = -1$	$\nu_2^{(B)} = 1$
$\vec{e}_3$	$-a\sqrt{3}\vec{e}_1$	$\nu_3^{(A)} = 1$	$\nu_3^{(B)} = -1$
$\vec{e}_4$	$\frac{a}{2}[-\sqrt{3}\vec{e}_1 - 3\vec{e}_2]$	$\nu_4^{(A)} = -1$	$\nu_4^{(B)} = 1$
$\vec{e}_5$	$\frac{a}{2}[\sqrt{3}\vec{e}_1 - 3\vec{e}_2]$	$\nu_5^{(A)} = 1$	$\nu_5^{(B)} = -1$
$\vec{e}_6$	$a\sqrt{3}\vec{e}_1$	$\nu_6^{(A)} = -1$	$\nu_6^{(B)} = 1$

We also derive NN vectors from figure 5a:

$$\vec{\delta}_1^{(A)} = \frac{a}{2}(\sqrt{3}\vec{e}_1 + \vec{e}_2); \quad \vec{\delta}_2^{(A)} = \frac{a}{2}(-\sqrt{3}\vec{e}_1 + \vec{e}_2); \quad \vec{\delta}_3^{(A)} = -a\vec{e}_2, \quad (5.1.3)$$

and  $\vec{\delta}_i^{(B)} = -\vec{\delta}_i^{(A)}$ .

### 5.1.2 Reciprocal lattice

In order to do a decoupling of periodic interactions in a large lattice, it is often necessary to do Fourier expansions. Therefore, it is useful to define the reciprocal space of honeycomb lattice as well. In order to define the reciprocal lattice, we should define two non-parallel primitive translation vectors  $\{\vec{a}_1, \vec{a}_2\}$  for our direct lattice. We define:

$$\vec{a}_1 = \vec{e}_1; \quad \vec{a}_2 = \vec{e}_2. \quad (5.1.4)$$

The reciprocal lattice primitive vectors  $\{\vec{b}_1, \vec{b}_2\}$  are found from the equation[25]:

$$\vec{b}_i \cdot \vec{a}_j = 2\pi\delta_{ij}; \quad i, j \in \{1, 2\}, \quad (5.1.5)$$

which gives:

$$\vec{b}_1 = \frac{2\pi}{a\sqrt{3}}[\vec{e}_1 + \frac{1}{\sqrt{3}}\vec{e}_2]; \quad \vec{b}_2 = \frac{2\pi}{a\sqrt{3}}[-\vec{e}_1 + \frac{1}{\sqrt{3}}\vec{e}_2], \quad (5.1.6)$$

which gives a hexagonal reciprocal lattice. Next, given that interactions have the same periodicity as direct lattice, the properties of reciprocal space are periodic by Wigner-Seitz cell, known as the first Brillouin zone, denoted here by  $\mathfrak{B}_1$ . Because of this periodicity, the area spanned by  $\mathfrak{B}_1$  is equivalent to area spanned by  $\vec{b}_1$  and  $\vec{b}_2$ . This fact will make summations over  $\mathfrak{B}_1$  way more convenient in some following sections.

## 5.2 The model

Having defined main properties of a honeycomb lattice, we can now present the Kane-Mele-Hubbard model, which is described by following Hamiltonian[26]:

$$\hat{H}_0^{\text{KM}} = -t_1 \sum_{\langle i,j \rangle} \sum_{\alpha} \hat{c}_{i\alpha}^{\dagger} \hat{c}_{j\alpha} + U \sum_i \hat{n}_{i\uparrow} \hat{n}_{i\downarrow} + i \frac{\lambda_R}{2} \sum_{\langle i,j \rangle} \sum_{\alpha} (\vec{\sigma} \times \hat{d}_{ij})_3 \hat{c}_{i\alpha}^{\dagger} \hat{c}_{j\alpha} + i\lambda_{SO} \sum_{\langle\langle i,j \rangle\rangle} \sum_{\alpha\beta} \nu_{ij} \sigma_{\alpha\beta}^{(3)} \hat{c}_{i\alpha}^{\dagger} \hat{c}_{j\beta}. \quad (5.2.1)$$

The first term represents NN electron hopping:  $t_1 > 0$  is the hopping amplitude, whilst  $\hat{c}_{i\alpha}^\dagger$  and  $\hat{c}_{i\alpha}$  are creation and annihilation operators, respectively, for an electron at site  $i$  with spin  $\alpha$ . The second term represents the repulsion of two electrons being at the same site:  $U \gg t_1$  is on-site repulsion amplitude and  $\hat{n}_{i\alpha} = \hat{c}_{i\alpha}^\dagger \hat{c}_{i\alpha}$  is number operator of electrons at site  $i$  with spin  $\alpha$ . The third term represents NN spin-orbit interaction, known as Rashba coupling:  $\lambda_R > 0$  is Rashba coupling amplitude,  $\vec{\sigma} = \sigma^{(1)}\vec{e}_1 + \sigma^{(2)}\vec{e}_2 + \sigma^{(3)}\vec{e}_3$  is Pauli matrix vector, and  $\hat{d}_{ij} = \vec{d}_{ij}/|\vec{d}_{ij}|$ . The last term represents intrinsic spin-orbit interaction, where  $\lambda_{SO} > 0$  is the amplitude.

From symmetry arguments, it turns out that NN Rashba coupling cancels out when the system (more precisely Hamiltonian) is invariant under the inversion  $z \mapsto -z$ [27]. This symmetry might be broken by for example applying electric field in  $z$ -direction or putting the material on a substrate. However, we assume that no such symmetry breaking is present, and neglect the term. Then, based on higher order  $t/U$  expansion similar to the one in chapter 2, it is possible to derive following effective spin-Hamiltonian from 5.2.1[2]:

$$\hat{H}_0^{\text{KMH}} = J_1 \sum_{\langle i,j \rangle} \hat{S}_i \cdot \hat{S}_j + J_2 \sum_{\langle\langle i,j \rangle\rangle} \hat{S}_i \cdot \hat{S}_j + \Gamma \sum_{\langle\langle i,j \rangle\rangle} \hat{S}_i \cdot [\text{diag}(-1, -1, 1)\hat{S}_j], \quad (5.2.2)$$

where

$$J_1 = 4\frac{t_1^2}{U} - 16\frac{t_1^4}{U^3}; \quad J_2 = 4\frac{t_1^4}{U^3}; \quad \Gamma = \frac{\lambda_{SO}^2}{U}. \quad (5.2.3)$$

We see that the first term in 5.2.2 represents isotropic scalar product interaction between NN spins, second term represents isotropic scalar product interaction between NNN spins, and the third term represents anisotropic exchange between NNN spins. Thus, spin-orbit interactions ( $\lambda_{SO}$ ) introduce an anisotropic nature to the KMH model.

The aforementioned spin-Hamiltonian has been treated with Abrikosov fermion and Schwinger boson mean-field theories in reference [2]. However, the fact that 5.2.1 considers NNN spin-orbit interactions, but not the NNN electron hopping, gives this model some limitations. By adding NNN electron hopping to the KMH model:

$$\hat{H}_{(\text{ext})}^{\text{KMH}} := \hat{H}_0^{\text{KMH}} - t_2 \sum_{\langle\langle i,j \rangle\rangle} \sum_{\alpha} \hat{c}_{i\alpha}^\dagger \hat{c}_{j\alpha}, \quad (5.2.4)$$

where  $t_2 > 0$ , following spin-Hamiltonian can be derived[1]:

$$\hat{H}_{(\text{ext})}^{\text{KMH}} = J_1 \sum_{\langle i,j \rangle} \hat{S}_i \cdot \hat{S}_j + J_2 \sum_{\langle\langle i,j \rangle\rangle} \hat{S}_i \cdot \hat{S}_j + \Gamma \sum_{\langle\langle i,j \rangle\rangle} \hat{S}_i \cdot [\text{diag}(-1, -1, 1)\hat{S}_j] + D \sum_{\langle\langle i,j \rangle\rangle} \nu_{ij}\vec{e}_3 \cdot (\hat{S}_i \times \hat{S}_j), \quad (5.2.5)$$

where

$$J_1 = \frac{2t_1^2}{U}; \quad J_2 = \frac{2t_2^2}{U}; \quad \Gamma = \frac{2\lambda_{SO}^2}{U}; \quad D = \frac{4t_2\lambda_{SO}}{U}. \quad (5.2.6)$$

We see that NNN hopping introduces a new kind of term to the spin-Hamiltonian, which in fact is DMI. Furthermore, if NNN hopping amplitude  $t_2$  is of comparable size to intrinsic spin-orbit interaction  $\lambda_{SO}$ , then the DMI is of comparable size to NNN isotropic exchange and anisotropic exchange. This motivates us to reapply the approach in reference [2] to 5.2.5, and in the rest of the thesis, we will do so. At this point, we define following operators:

$$\begin{aligned} \hat{H}_1 &:= J_1 \sum_{\langle i,j \rangle} \hat{S}_i \cdot \hat{S}_j; & \hat{H}_2 &:= J_2 \sum_{\langle\langle i,j \rangle\rangle} \hat{S}_i \cdot \hat{S}_j; & \hat{H}_\Gamma &:= \Gamma \sum_{\langle\langle i,j \rangle\rangle} \hat{S}_i \cdot [\text{diag}(-1, -1, 1)\hat{S}_j]; \\ \hat{H}_{\text{DMI}} &= D \sum_{\langle\langle i,j \rangle\rangle} \nu_{ij}\vec{e}_3 \cdot (\hat{S}_i \times \hat{S}_j). \end{aligned} \quad (5.2.7)$$

The Hamiltonian treated in reference [2] is then given by:

$$\hat{H}_0 := \hat{H}_1 + \hat{H}_2 + \hat{H}_\Gamma, \quad (5.2.8)$$

and the new Hamiltonian we want reapply the techniques to is given by:

$$\hat{H} := \hat{H}_0 + \hat{H}_{\text{DMI}}. \quad (5.2.9)$$

Further, to begin with, we will treat  $J_1, J_2, \Gamma, D$  as independent parameters, although from 5.2.6, we see that:

$$D^2 = 4J_2\Gamma. \quad (5.2.10)$$

### 5.3 Abrikosov fermion mean-field approach

In this section, we will treat 5.2.8 and 5.2.9 with Abrikosov fermion mean-field approach. For the former, we want to reproduce results from reference [2] to be sure that we are following the approach correctly. In parallel, we also apply the approach to the latter Hamiltonian. First, we will insert the Abrikosov fermions into spin-Hamiltonians, and decouple the resulting operator into appropriate mean-field operators to perform mean-field approximations. We will then use symmetry of honeycomb lattice to reduce amount of mean-field parameters. Then, we will perform Fourier transformation and diagonalization techniques in order to determine the ground state energy and the excitations. We will then present physical phases for different mean-field parameters, and finally, we will present numerical method to determine mean-field parameters for different interaction parameters and show the results through phase diagrams.

#### 5.3.1 Abrikosov fermions and decoupling

As already discussed in section 4.6, the Abrikosov fermions are given by

$$\hat{S}_i = \frac{\hbar}{2} \begin{bmatrix} \hat{f}_{i\uparrow}^\dagger & \hat{f}_{i\downarrow}^\dagger \end{bmatrix} \vec{\sigma} \begin{bmatrix} \hat{f}_{i\uparrow} \\ \hat{f}_{i\downarrow} \end{bmatrix} = \frac{\hbar}{2} \sum_{\alpha\beta} \hat{f}_{i\alpha}^\dagger \vec{\sigma}_{\alpha\beta} \hat{f}_{i\beta}, \quad (5.3.1)$$

and are constrained by

$$\hat{n}_i = \sum_{\alpha} \hat{f}_{i\alpha}^\dagger \hat{f}_{i\alpha} = \hat{f}_{i\uparrow}^\dagger \hat{f}_{i\uparrow} + \hat{f}_{i\downarrow}^\dagger \hat{f}_{i\downarrow} = 2S = 1, \quad (5.3.2)$$

where  $S = \frac{1}{2}$  is the spin of electrons in our lattice, and  $i$  denotes a honeycomb lattice site. We will now insert 5.3.1 into different spin interactions in 5.2.7. When doing so, and decoupling these into convenient mean-field operators for both Abrikosov fermions and Schwinger bosons, following relation is useful:

**Proposition 5.1.** Given a set of fermionic or bosonic operators  $\{\hat{a}_{i\alpha}\}$ , constrained by

$$\sum_{\alpha} \hat{a}_{i\alpha}^\dagger \hat{a}_{i\alpha} = 1, \quad (5.3.3)$$

following is true:

$$\sum_{\alpha\beta} \hat{a}_{j\alpha}^\dagger \hat{a}_{i\beta} \hat{a}_{i\beta}^\dagger \hat{a}_{j\alpha} = 2 + \zeta = \begin{cases} 1, & \text{fermions} \\ 3, & \text{bosons.} \end{cases} \quad (5.3.4)$$

In addition, for an arbitrary  $3 \times 3$  matrix  $A = [A_{ij}]$ , it is convenient to define:

$$g_{\alpha\beta\gamma\delta} := \vec{\sigma}_{\alpha\beta} \cdot (A \vec{\sigma}_{\gamma\delta}) = \sum_{i,j=1}^3 \sigma_{\alpha\beta}^{(i)} A_{ij} \sigma_{\gamma\delta}^{(j)}. \quad (5.3.5)$$

Then, by using the definition of Pauli matrices, we find:

$$G(A) := \begin{bmatrix} g_{1111} & g_{1112} & g_{1121} & g_{1122} \\ g_{1211} & g_{1212} & g_{1221} & g_{1222} \\ g_{2111} & g_{2112} & g_{2121} & g_{2122} \\ g_{2211} & g_{2212} & g_{2221} & g_{2222} \end{bmatrix} = \begin{bmatrix} A_{33} & A_{31} - iA_{32} & A_{31} + iA_{32} & -A_{33} \\ A_{13} - iA_{23} & A_{11} - A_{22} - i(A_{12} + A_{21}) & A_{11} + A_{22} + i(A_{12} - A_{21}) & -A_{13} + iA_{23} \\ A_{13} + iA_{23} & A_{11} + A_{22} - i(A_{12} - A_{21}) & A_{11} - A_{22} + i(A_{12} + A_{21}) & -A_{13} - iA_{23} \\ -A_{33} & -A_{31} + iA_{32} & -A_{31} - iA_{32} & A_{33} \end{bmatrix}, \quad (5.3.6)$$

which for a diagonal matrix  $D$  with two equal diagonal entries:

$$D = \begin{bmatrix} D_1 & 0 & 0 \\ 0 & D_1 & 0 \\ 0 & 0 & D_3 \end{bmatrix}, \quad (5.3.7)$$

simplifies to

$$G(D) = \begin{bmatrix} D_3 & 0 & 0 & -D_3 \\ 0 & 0 & 2D_1 & 0 \\ 0 & 2D_1 & 0 & 0 \\ -D_3 & 0 & 0 & D_3 \end{bmatrix}. \quad (5.3.8)$$

Starting with the isotropic interactions, we use 5.3.1 and 5.3.8 to write:

$$\begin{aligned}
\hat{S}_i \cdot \hat{S}_j &= \frac{\hbar^2}{4} \sum_{\alpha\beta\gamma\delta} \hat{f}_{i\alpha}^\dagger \hat{f}_{i\beta} \hat{f}_{j\gamma}^\dagger \hat{f}_{j\delta} (\vec{\sigma}_{\alpha\beta} \cdot \vec{\sigma}_{\gamma\delta}) = -\frac{\hbar^2}{4} \sum_{\alpha\beta\gamma\delta} \hat{f}_{j\gamma}^\dagger \hat{f}_{i\beta} \hat{f}_{i\alpha}^\dagger \hat{f}_{j\delta} (\vec{\sigma}_{\alpha\beta} \cdot \vec{\sigma}_{\gamma\delta}) + \frac{\hbar^2}{4} \sum_{\alpha\gamma\delta} \hat{f}_{j\gamma}^\dagger \hat{f}_{j\delta} (\vec{\sigma}_{\alpha\alpha} \cdot \vec{\sigma}_{\gamma\delta}) = \\
&= -\frac{\hbar^2}{4} [\hat{f}_{j\uparrow}^\dagger \hat{f}_{i\uparrow} \hat{f}_{i\uparrow}^\dagger \hat{f}_{j\uparrow} + \hat{f}_{j\downarrow}^\dagger \hat{f}_{i\downarrow} \hat{f}_{i\downarrow}^\dagger \hat{f}_{j\downarrow} - \hat{f}_{j\uparrow}^\dagger \hat{f}_{i\downarrow} \hat{f}_{i\downarrow}^\dagger \hat{f}_{j\uparrow} - \hat{f}_{j\downarrow}^\dagger \hat{f}_{i\uparrow} \hat{f}_{i\uparrow}^\dagger \hat{f}_{j\downarrow} + 2\hat{f}_{j\uparrow}^\dagger \hat{f}_{i\uparrow} \hat{f}_{i\downarrow}^\dagger \hat{f}_{j\downarrow} + 2\hat{f}_{j\downarrow}^\dagger \hat{f}_{i\downarrow} \hat{f}_{i\uparrow}^\dagger \hat{f}_{j\uparrow}] + \\
&= \frac{\hbar^2}{4} [\hat{f}_{j\uparrow}^\dagger \hat{f}_{j\uparrow} + \hat{f}_{j\downarrow}^\dagger \hat{f}_{j\downarrow} - \hat{f}_{j\uparrow}^\dagger \hat{f}_{j\uparrow} - \hat{f}_{j\downarrow}^\dagger \hat{f}_{j\downarrow}] = -\frac{\hbar^2}{4} [2\hat{f}_{j\uparrow}^\dagger \hat{f}_{i\uparrow} \hat{f}_{i\uparrow}^\dagger \hat{f}_{j\uparrow} + 2\hat{f}_{j\downarrow}^\dagger \hat{f}_{i\downarrow} \hat{f}_{i\downarrow}^\dagger \hat{f}_{j\downarrow} - \sum_{\alpha\beta} \hat{f}_{j\alpha}^\dagger \hat{f}_{i\beta} \hat{f}_{i\beta}^\dagger \hat{f}_{j\alpha} + \\
&= 2\hat{f}_{j\uparrow}^\dagger \hat{f}_{i\uparrow} \hat{f}_{i\downarrow}^\dagger \hat{f}_{j\downarrow} + 2\hat{f}_{j\downarrow}^\dagger \hat{f}_{i\downarrow} \hat{f}_{i\uparrow}^\dagger \hat{f}_{j\uparrow}] = -\frac{\hbar^2}{2} [\hat{f}_{j\uparrow}^\dagger \hat{f}_{i\uparrow} \hat{f}_{i\uparrow}^\dagger \hat{f}_{j\uparrow} + \hat{f}_{j\downarrow}^\dagger \hat{f}_{i\downarrow} \hat{f}_{i\downarrow}^\dagger \hat{f}_{j\downarrow} + \hat{f}_{j\uparrow}^\dagger \hat{f}_{i\uparrow} \hat{f}_{i\downarrow}^\dagger \hat{f}_{j\downarrow} + \hat{f}_{j\downarrow}^\dagger \hat{f}_{i\downarrow} \hat{f}_{i\uparrow}^\dagger \hat{f}_{j\uparrow} - \frac{1}{2}] = \\
&= -\frac{\hbar^2}{2} \sum_{\alpha\beta} \hat{f}_{j\alpha}^\dagger \hat{f}_{i\alpha} \hat{f}_{i\beta}^\dagger \hat{f}_{j\beta} + \frac{\hbar^2}{4} = -\frac{\hbar^2}{2} \sum_{\alpha\beta} \hat{A}_{i,j}^{(\alpha)} \hat{A}_{i,j}^{(\beta)} + \frac{\hbar^2}{4}
\end{aligned} \tag{5.3.9}$$

where we have defined following decoupling operator:

$$\hat{A}_{i,j}^{(\alpha)} := \hat{f}_{i\alpha}^\dagger \hat{f}_{j\alpha}. \tag{5.3.10}$$

Next, we want to decouple our anisotropic term in a similar manner:

$$\begin{aligned}
\hat{S}_i \cdot [\text{diag}(-1, -1, 1) \hat{S}_j] &= \frac{\hbar^2}{4} \sum_{\alpha\beta\gamma\delta} \hat{f}_{i\alpha}^\dagger \hat{f}_{i\beta} \hat{f}_{j\gamma}^\dagger \hat{f}_{j\delta} [\vec{\sigma}_{\alpha\beta} \cdot [\text{diag}(-1, -1, 1) \vec{\sigma}_{\gamma\delta}]] = \\
&= -\frac{\hbar^2}{4} \sum_{\alpha\beta\gamma\delta} \hat{f}_{j\gamma}^\dagger \hat{f}_{i\beta} \hat{f}_{i\alpha}^\dagger \hat{f}_{j\delta} [\vec{\sigma}_{\alpha\beta} \cdot [\text{diag}(-1, -1, 1) \vec{\sigma}_{\gamma\delta}]] + \frac{\hbar^2}{4} \sum_{\alpha\gamma\delta} \hat{f}_{j\gamma}^\dagger \hat{f}_{j\delta} [\vec{\sigma}_{\alpha\alpha} \cdot [\text{diag}(-1, -1, 1) \vec{\sigma}_{\gamma\delta}]] = \\
&= -\frac{\hbar^2}{4} [\hat{f}_{j\uparrow}^\dagger \hat{f}_{i\uparrow} \hat{f}_{i\uparrow}^\dagger \hat{f}_{j\uparrow} + \hat{f}_{j\downarrow}^\dagger \hat{f}_{i\downarrow} \hat{f}_{i\downarrow}^\dagger \hat{f}_{j\downarrow} - \hat{f}_{j\uparrow}^\dagger \hat{f}_{i\downarrow} \hat{f}_{i\downarrow}^\dagger \hat{f}_{j\uparrow} - \hat{f}_{j\downarrow}^\dagger \hat{f}_{i\uparrow} \hat{f}_{i\uparrow}^\dagger \hat{f}_{j\downarrow} - 2\hat{f}_{j\uparrow}^\dagger \hat{f}_{i\uparrow} \hat{f}_{i\downarrow}^\dagger \hat{f}_{j\downarrow} - 2\hat{f}_{j\downarrow}^\dagger \hat{f}_{i\downarrow} \hat{f}_{i\uparrow}^\dagger \hat{f}_{j\uparrow}] + \\
&= \frac{\hbar^2}{4} [\hat{f}_{j\uparrow}^\dagger \hat{f}_{j\uparrow} + \hat{f}_{j\downarrow}^\dagger \hat{f}_{j\downarrow} - \hat{f}_{j\uparrow}^\dagger \hat{f}_{j\uparrow} - \hat{f}_{j\downarrow}^\dagger \hat{f}_{j\downarrow}] = -\frac{\hbar^2}{4} [2\hat{f}_{j\uparrow}^\dagger \hat{f}_{i\uparrow} \hat{f}_{i\uparrow}^\dagger \hat{f}_{j\uparrow} + 2\hat{f}_{j\downarrow}^\dagger \hat{f}_{i\downarrow} \hat{f}_{i\downarrow}^\dagger \hat{f}_{j\downarrow} - \sum_{\alpha\beta} \hat{f}_{j\alpha}^\dagger \hat{f}_{i\beta} \hat{f}_{i\beta}^\dagger \hat{f}_{j\alpha} - \\
&= 2\hat{f}_{j\uparrow}^\dagger \hat{f}_{i\uparrow} \hat{f}_{i\downarrow}^\dagger \hat{f}_{j\downarrow} - 2\hat{f}_{j\downarrow}^\dagger \hat{f}_{i\downarrow} \hat{f}_{i\uparrow}^\dagger \hat{f}_{j\uparrow}] = -\frac{\hbar^2}{2} [\hat{f}_{j\uparrow}^\dagger \hat{f}_{i\uparrow} \hat{f}_{i\uparrow}^\dagger \hat{f}_{j\uparrow} + \hat{f}_{j\downarrow}^\dagger \hat{f}_{i\downarrow} \hat{f}_{i\downarrow}^\dagger \hat{f}_{j\downarrow} - \hat{f}_{j\uparrow}^\dagger \hat{f}_{i\uparrow} \hat{f}_{i\downarrow}^\dagger \hat{f}_{j\downarrow} - \hat{f}_{j\downarrow}^\dagger \hat{f}_{i\downarrow} \hat{f}_{i\uparrow}^\dagger \hat{f}_{j\uparrow} - \frac{1}{2}] = \\
&= -\frac{\hbar^2}{2} \sum_{\alpha\beta} (2\delta_{\alpha\beta} - 1) \hat{A}_{i,j}^{(\alpha)} \hat{A}_{i,j}^{(\beta)} + \frac{\hbar^2}{4},
\end{aligned} \tag{5.3.11}$$

Finally, we want to decouple DMI in a similar manner:

$$\begin{aligned}
\vec{e}_3 \cdot (\hat{S}_i \times \hat{S}_j) &= \hat{S}_i^x \hat{S}_j^y - \hat{S}_i^y \hat{S}_j^x = i \frac{\hbar^2}{4} (\hat{f}_{i\uparrow}^\dagger \hat{f}_{i\downarrow} + \hat{f}_{i\downarrow}^\dagger \hat{f}_{i\uparrow}) (-\hat{f}_{j\uparrow}^\dagger \hat{f}_{j\downarrow} + \hat{f}_{j\downarrow}^\dagger \hat{f}_{j\uparrow}) + \\
&= i \frac{\hbar^2}{4} (\hat{f}_{i\uparrow}^\dagger \hat{f}_{i\downarrow} - \hat{f}_{i\downarrow}^\dagger \hat{f}_{i\uparrow}) (\hat{f}_{j\uparrow}^\dagger \hat{f}_{j\downarrow} + \hat{f}_{j\downarrow}^\dagger \hat{f}_{j\uparrow}) = i \frac{\hbar^2}{2} [\hat{f}_{i\uparrow}^\dagger \hat{f}_{i\downarrow} \hat{f}_{j\downarrow}^\dagger \hat{f}_{j\uparrow} - \hat{f}_{i\downarrow}^\dagger \hat{f}_{i\uparrow} \hat{f}_{j\uparrow}^\dagger \hat{f}_{j\downarrow}] = \\
&= i \frac{\hbar^2}{2} [\hat{f}_{j\uparrow}^\dagger \hat{f}_{i\uparrow} \hat{f}_{i\downarrow}^\dagger \hat{f}_{j\downarrow} - \hat{f}_{j\downarrow}^\dagger \hat{f}_{i\downarrow} \hat{f}_{i\uparrow}^\dagger \hat{f}_{j\uparrow}] = i \frac{\hbar^2}{2} \hat{A}_{i,j}^{\uparrow(\uparrow)} \hat{A}_{i,j}^{\downarrow(\downarrow)} + \text{H.c.}
\end{aligned} \tag{5.3.12}$$

As we can see, the DMI can be decoupled into exactly the same operators as isotropic and anisotropic interactions, meaning that we can follow the same mean-field theory as presented in reference [2]. We summarize the results of this subsection with following proposition:

**Proposition 5.2.** Given a set of Abrikosov fermions  $\{\hat{f}_{i\alpha}\}$  constrained by 5.3.2, following decouplings are true:

$$\hat{S}_i \cdot \hat{S}_j = -\frac{\hbar^2}{2} \sum_{\alpha\beta} \hat{A}_{i,j}^{\uparrow(\alpha)} \hat{A}_{i,j}^{(\beta)} + \frac{\hbar^2}{4} \tag{5.3.13}$$

$$\hat{S}_i \cdot [\text{diag}(-1, -1, 1) \hat{S}_j] = -\frac{\hbar^2}{2} \sum_{\alpha\beta} (2\delta_{\alpha\beta} - 1) \hat{A}_{i,j}^{\uparrow(\alpha)} \hat{A}_{i,j}^{(\beta)} + \frac{\hbar^2}{4} \tag{5.3.14}$$

$$\vec{e}_3 \cdot (\hat{S}_i \times \hat{S}_j) = i \frac{\hbar^2}{2} \hat{A}_{i,j}^{\uparrow(\uparrow)} \hat{A}_{i,j}^{\downarrow(\downarrow)} + \text{H.c.}, \tag{5.3.15}$$

where

$$\hat{A}_{i,j}^{(\alpha)} := \hat{f}_{i\alpha}^\dagger \hat{f}_{j\alpha}. \quad (5.3.16)$$

### 5.3.2 Mean-field approximation and ansatz

Applying the mean-field approximation as described in definition 4.3, we now have that:

$$\begin{aligned} \hat{S}_i \cdot \hat{S}_j \mapsto & -\frac{\hbar^2}{2} \sum_{\alpha\beta} \left[ \langle \hat{A}_{i,j}^{(\alpha)} \rangle^* \hat{A}_{i,j}^{(\beta)} + \langle \hat{A}_{i,j}^{(\beta)} \rangle \hat{A}_{i,j}^{\dagger(\alpha)} - \langle \hat{A}_{i,j}^{(\alpha)} \rangle^* \langle \hat{A}_{i,j}^{(\beta)} \rangle \right] = \\ & -\frac{\hbar^2}{2} \sum_{\alpha\beta} \left[ \langle \hat{A}_{i,j}^{(\alpha)} \rangle^* \hat{A}_{i,j}^{(\beta)} + \text{H.c.} \right] + \frac{\hbar^2}{2} \left| \sum_{\alpha} \langle \hat{A}_{i,j}^{(\alpha)} \rangle \right|^2 \end{aligned} \quad (5.3.17)$$

$$\begin{aligned} \hat{S}_i \cdot [\text{diag}(-1, -1, 1) \hat{S}_j] \mapsto & -\frac{\hbar^2}{2} \sum_{\alpha\beta} (2\delta_{\alpha\beta} - 1) \left[ \langle \hat{A}_{i,j}^{(\alpha)} \rangle^* \hat{A}_{i,j}^{(\beta)} + \langle \hat{A}_{i,j}^{(\beta)} \rangle \hat{A}_{i,j}^{\dagger(\alpha)} - \langle \hat{A}_{i,j}^{(\alpha)} \rangle^* \langle \hat{A}_{i,j}^{(\beta)} \rangle \right] = \\ & -\frac{\hbar^2}{2} \sum_{\alpha\beta} (2\delta_{\alpha\beta} - 1) \left[ \langle \hat{A}_{i,j}^{(\alpha)} \rangle^* \hat{A}_{i,j}^{(\beta)} + \text{H.c.} \right] + \frac{\hbar^2}{2} \sum_{\alpha\beta} (2\delta_{\alpha\beta} - 1) \langle \hat{A}_{i,j}^{(\alpha)} \rangle^* \langle \hat{A}_{i,j}^{(\beta)} \rangle \end{aligned} \quad (5.3.18)$$

$$\vec{e}_3 \cdot (\hat{S}_i \times \hat{S}_j) \mapsto i \frac{\hbar^2}{2} \left[ \langle \hat{A}_{i,j}^{(\uparrow)} \rangle^* \hat{A}_{i,j}^{(\downarrow)} + \langle \hat{A}_{i,j}^{(\downarrow)} \rangle \hat{A}_{i,j}^{\dagger(\uparrow)} - \langle \hat{A}_{i,j}^{(\uparrow)} \rangle^* \langle \hat{A}_{i,j}^{(\downarrow)} \rangle \right] + \text{H.c.} \quad (5.3.19)$$

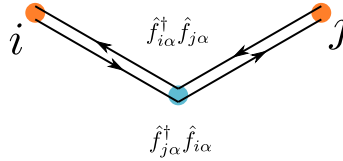
The number of mean-field constants  $\langle \hat{A}_{i,j}^{(\alpha)} \rangle$  is of the same order as number of sites in our lattice, which is assumed to approach infinity. Solving an infinite set of self-consistency equations to find these constants is obviously out of question. However, the symmetry of honeycomb lattice should allow us to reduce this number drastically. We now make several physical assumptions.

The first assumption is that  $\sum_{\alpha} \langle \hat{A}_{i,j}^{(\alpha)} \rangle$  for NN is site and neighbor independent. This is reasonable because we treat the material sheet as infinite, and because each site has a 3-fold symmetry. Thus, we write:

$$\boxed{\sum_{\alpha} \langle \hat{A}_{\langle i,j \rangle}^{(\alpha)} \rangle = \chi_1 \in \mathbb{R}}, \quad (5.3.20)$$

where this number is real because  $\sum_{\alpha} \langle \hat{A}_{\langle i,j \rangle}^{(\alpha)} \rangle = \sum_{\alpha} \langle \hat{A}_{\langle j,i \rangle}^{(\alpha)} \rangle^*$ .

The second assumption is that NNN  $\langle \hat{A}_{\langle i,j \rangle}^{(\alpha)} \rangle$  also is site independent due to same argument. However, as we see from figure 5a, the quantity is neighbor dependent. To see this, we recall that NNN spin-orbit interactions in our physical model only happen through an intermediate site. From the figure, we see that an NNN can be obtained either by a "right" turn or a "left" turn. For each site, three NNNs are obtained by a right turn, whilst three are obtained by a left turn. As seen in figure 6, if the path from  $i$  to  $j$  takes a left turn, the the same path from  $j$  to  $i$  takes a right turn.



**Figure 6:** The upper path corresponds to  $f_{i\alpha}^\dagger f_{j\alpha}$ , whilst the lower path corresponds to  $f_{j\alpha}^\dagger f_{i\alpha}$ . The paths are hermitian conjugates of each-other, and the only physical difference is that upper path takes a right turn, whilst lower path takes a left turn.

Futhermore, we have that:

$$\langle \hat{A}_{\langle i,j \rangle}^{(\alpha)} \rangle = \langle f_{i\alpha}^\dagger f_{j\alpha} \rangle = \langle \hat{A}_{\langle j,i \rangle}^{(\alpha)} \rangle^* = \langle f_{j\alpha}^\dagger f_{i\alpha} \rangle^*. \quad (5.3.21)$$

This means that  $\langle \hat{A}_{\langle i,j \rangle}^{(\alpha)} \rangle$  reduces to only two different values, which only depend on the turn, and differ by phase. We can thus write:

$$\boxed{\langle \hat{A}_{\langle i,j \rangle}^{(\alpha)} \rangle = \chi_2 e^{-i\phi_{\alpha\nu_{ij}}}; \quad \chi_2, \phi_{\alpha} \in \mathbb{R}}, \quad (5.3.22)$$

where  $\nu_{ij}$  was defined in 5.1.2.

It should be said that in the mean-field approximation, we should always ensure that the constraint 5.3.2 is satisfied. This is usually implemented with Lagrange multipliers, and we will later do that in Schwinger boson mean-field approach. However, for half-filled Abrikosov fermion case, the lagrange multipliers can all be set to 0 at mean-field level[2].

### 5.3.3 Fourier transform

We are now ready to put mean-field approximations 5.3.17, 5.3.18, and 5.3.19 with mean-field parameters 5.3.20 and 5.3.22 into our different Hamiltonian terms in 5.2.8 and 5.2.9. Due to periodicity of the lattice, the interactions can then be decoupled by using Fourier transform. Starting with the isotropic NN-interaction term, we have:

$$\hat{H}_1^{(\text{MF})} = -\frac{\hbar^2 J_1}{2} \sum_{\langle i,j \rangle} \sum_{\alpha} \left[ \chi_1 \hat{A}_{i,j}^{(\alpha)} + \text{H.c.} \right] + \sum_{\langle i,j \rangle} \frac{\hbar^2 J_1 \chi_1^2}{2}, \quad (5.3.23)$$

with:

$$\sum_{\langle i,j \rangle} \hat{A}_{i,j}^{(\alpha)} = \sum_{\langle i,j \rangle} \hat{f}_{i\alpha}^{\dagger} \hat{f}_{j\alpha} = \sum_{\vec{r}} \sum_{l=1}^3 \left[ \hat{f}_{\vec{r}\alpha}^{\dagger(A)} \hat{f}_{\vec{r}+\vec{\delta}_l^{(A)}\alpha}^{(B)} + \hat{f}_{\vec{r}\alpha}^{\dagger(B)} \hat{f}_{\vec{r}+\vec{\delta}_l^{(B)}\alpha}^{(A)} \right]. \quad (5.3.24)$$

Here,  $(X)$  in  $\hat{f}_{\vec{r}\alpha}^{(X)}$  tells us whether the operator acts on sublattice  $A$  or  $B$ . Next, each sublattice has a fixed origin site. The vector  $\vec{r}$  then points from the origin in one of the sublattices to another site in the same sublattice and is summed over all sublattice sites.

We now expand our Abrikosov fermion operators to Fourier series by writing:

$$\hat{f}_{\vec{r}\alpha}^{(X)} = \frac{1}{\sqrt{N}} \sum_{\vec{k}} e^{i\vec{k}\cdot\vec{r}} \hat{f}_{\vec{k}\alpha}^{(X)}; \quad X \in \{A, B\}. \quad (5.3.25)$$

Here,  $\vec{k} = k_x \vec{e}_1 + k_y \vec{e}_2$  is summed over the first Brillouin zone  $\mathfrak{B}_1$  of a given sublattice<sup>22</sup>, and  $N$  is number of sites on the given sublattice.

We then have:

$$\begin{aligned} \sum_{\vec{r}} \hat{f}_{\vec{r}\alpha}^{\dagger(A)} \hat{f}_{\vec{r}+\vec{\delta}_l^{(A)}\alpha}^{(B)} &= \frac{1}{N} \sum_{\vec{r}} \sum_{\vec{k}, \vec{k}'} e^{-i\vec{k}\cdot\vec{r}} e^{i\vec{k}'\cdot(\vec{r}+\vec{\delta}_l^{(A)})} \hat{f}_{\vec{k}\alpha}^{\dagger(A)} \hat{f}_{\vec{k}'\alpha}^{(B)} = \\ \frac{1}{N} \sum_{\vec{k}, \vec{k}'} e^{i\vec{k}'\cdot\vec{\delta}_l^{(A)}} \sum_{\vec{r}} e^{i(\vec{k}'-\vec{k})\cdot\vec{r}} \hat{f}_{\vec{k}\alpha}^{\dagger(A)} \hat{f}_{\vec{k}'\alpha}^{(B)} &= \sum_{\vec{k}} e^{i\vec{k}\cdot\vec{\delta}_l^{(A)}} \hat{f}_{\vec{k}\alpha}^{\dagger(A)} \hat{f}_{\vec{k}\alpha}^{(B)}, \end{aligned} \quad (5.3.26)$$

where in the last equality, we used the identity:

$$\sum_{\vec{r}} e^{i(\vec{k}'-\vec{k})\cdot\vec{r}} = N \delta_{\vec{k}\vec{k}'}. \quad (5.3.27)$$

Inserting 5.3.26 into 5.3.23, we have:

$$\begin{aligned} \hat{H}_1^{(\text{MF})} &= -\frac{\hbar^2 J_1 \chi_1}{2} \sum_{\alpha} \sum_{\vec{r}} \sum_{l=1}^3 \left[ \hat{f}_{\vec{r}\alpha}^{\dagger(A)} \hat{f}_{\vec{r}+\vec{\delta}_l^{(A)}\alpha}^{(B)} + \hat{f}_{\vec{r}\alpha}^{\dagger(B)} \hat{f}_{\vec{r}+\vec{\delta}_l^{(B)}\alpha}^{(A)} + \text{H.c.} \right] + \sum_{\vec{r}} 3\hbar^2 J_1 \chi_1^2 = \\ -\frac{\hbar^2 J_1 \chi_1}{2} \sum_{\alpha} \sum_{\vec{k}} \sum_{l=1}^3 \left[ e^{i\vec{k}\cdot\vec{\delta}_l^{(A)}} \hat{f}_{\vec{k}\alpha}^{\dagger(A)} \hat{f}_{\vec{k}\alpha}^{(B)} + e^{i\vec{k}\cdot\vec{\delta}_l^{(B)}} \hat{f}_{\vec{k}\alpha}^{\dagger(B)} \hat{f}_{\vec{k}\alpha}^{(A)} + \text{H.c.} \right] &+ \sum_{\vec{k}} 3\hbar^2 J_1 \chi_1^2 = \\ -\hbar^2 J_1 \chi_1 \sum_{\vec{k}} \sum_{\alpha} \left[ \eta_{\vec{k}} \hat{f}_{\vec{k}\alpha}^{\dagger(A)} \hat{f}_{\vec{k}\alpha}^{(B)} + \text{H.c.} \right] &+ \sum_{\vec{k}} 3\hbar^2 J_1 \chi_1^2, \end{aligned} \quad (5.3.28)$$

<sup>22</sup>The reciprocal space is actually the same for sublattice  $A$  and  $B$  because the two sublattices are just shifted relative to each other.



where for the constant term, we used the fact that there are two sublattices and three NNs for each site, and in the last equality, we used the fact that  $\vec{\delta}_l^{(A)} = -\vec{\delta}_l^{(B)}$ , and defined:

$$\begin{aligned} \eta_{\vec{k}} &:= \sum_{l=1}^3 e^{i\vec{k}\cdot\vec{\delta}_l^{(A)}} = e^{i\vec{k}\cdot\vec{\delta}_1^{(A)}} + e^{i\vec{k}\cdot\vec{\delta}_2^{(A)}} + e^{i\vec{k}\cdot\vec{\delta}_3^{(A)}} = \\ &e^{i\frac{a}{2}(k_x\sqrt{3}+k_y)} + e^{i\frac{a}{2}(-k_x\sqrt{3}+k_y)} + e^{-iak_y} = e^{-ik_y a} + 2e^{i\frac{k_y a}{2}} \cos\left(\frac{\sqrt{3}}{2}k_x a\right). \end{aligned} \quad (5.3.29)$$

Finally, we can rewrite 5.3.28 to:

$$\hat{H}_1^{(\text{MF})} = \hbar^2 \sum_{\vec{k}} \left[ -J_1 \chi_1 \sum_{\alpha} \begin{bmatrix} \hat{f}_{\vec{k}\alpha}^{\dagger(A)} & \hat{f}_{\vec{k}\alpha}^{\dagger(B)} \end{bmatrix} \begin{bmatrix} 0 & \eta_{\vec{k}} \\ \eta_{\vec{k}}^* & 0 \end{bmatrix} \begin{bmatrix} \hat{f}_{\vec{k}\alpha}^{(A)} \\ \hat{f}_{\vec{k}\alpha}^{(B)} \end{bmatrix} + 3J_1 \chi_1^2 \right]. \quad (5.3.30)$$

We note that this Hamiltonian is of the same form as the Fourier transformation of the second quantized tight-binding model for graphene. In a such model, electron-electron Coulomb interactions are neglected, meaning that the electrons are independent, and only affected by the periodic atomic potential. The electronic structure of the mobile graphene electrons in a such model gives gapless Dirac cones. This means that when only considering NN-contributions, the Abrikosov fermions are in some sense independent, and behave like electrons in graphene. Furthermore, it can be shown that this situation corresponds to the gapless QSL phase[2]. Thus, if the mean-field approximation allows  $\chi_2 = 0$ , the NNN contribution becomes 0, and we get a gapless QSL phase.

Next, we want to consider the NNN isotropic and anisotropic interactions. As we see from 5.3.17 and 5.3.18, both of these are decoupled in the same manner, except for the anisotropic factor  $(2\delta_{\alpha\beta} - 1)$ . This means that the NNN isotropic and anisotropic terms of the Hamiltonian can be combined to do a Fourier transformation instead of considering the two separately. By inserting 5.3.17 and 5.3.18 into  $\hat{H}_2 + \hat{H}_{\Gamma}$ , we have:

$$\begin{aligned} \hat{H}_2^{(\text{MF})} + \hat{H}_{\Gamma}^{(\text{MF})} &= -\frac{\hbar^2 J_2}{2} \sum_{\langle\langle i,j \rangle\rangle} \sum_{\alpha\beta} \left[ \langle \hat{A}_{i,j}^{(\alpha)} \rangle^* \hat{A}_{i,j}^{(\beta)} + \text{H.c.} \right] - \frac{\hbar^2 \Gamma}{2} \sum_{\langle\langle i,j \rangle\rangle} \sum_{\alpha\beta} (2\delta_{\alpha\beta} - 1) \left[ \langle \hat{A}_{i,j}^{(\alpha)} \rangle^* \hat{A}_{i,j}^{(\beta)} + \text{H.c.} \right] + \\ &\frac{\hbar^2 J_2}{2} \sum_{\langle\langle i,j \rangle\rangle} \left| \sum_{\alpha} \langle \hat{A}_{i,j}^{(\alpha)} \rangle \right|^2 + \frac{\hbar^2 \Gamma}{2} \sum_{\langle\langle i,j \rangle\rangle} \sum_{\alpha\beta} (2\delta_{\alpha\beta} - 1) \langle \hat{A}_{i,j}^{(\alpha)} \rangle^* \langle \hat{A}_{i,j}^{(\beta)} \rangle. \end{aligned} \quad (5.3.31)$$

We start with the operator term:

$$\begin{aligned} -\frac{\hbar^2 J_2}{2} \sum_{\langle\langle i,j \rangle\rangle} \sum_{\alpha\beta} \left[ \langle \hat{A}_{i,j}^{(\alpha)} \rangle^* \hat{A}_{i,j}^{(\beta)} + \text{H.c.} \right] - \frac{\hbar^2 \Gamma}{2} \sum_{\langle\langle i,j \rangle\rangle} \sum_{\alpha\beta} (2\delta_{\alpha\beta} - 1) \left[ \langle \hat{A}_{i,j}^{(\alpha)} \rangle^* \hat{A}_{i,j}^{(\beta)} + \text{H.c.} \right] = \\ -\frac{\hbar^2}{2} \sum_{\langle\langle i,j \rangle\rangle} \sum_{\alpha\beta} \mathfrak{J}_{\alpha\beta} \left[ \langle \hat{A}_{i,j}^{(\alpha)} \rangle^* \hat{A}_{i,j}^{(\beta)} + \text{H.c.} \right], \end{aligned} \quad (5.3.32)$$

where we defined:

$$\mathfrak{J}_{\alpha\beta} := J_2 + \Gamma(2\delta_{\alpha\beta} - 1) = J_-(1 - \delta_{\alpha\beta}) + J_+\delta_{\alpha\beta}; \quad J_{\pm} := J_2 \pm \Gamma. \quad (5.3.33)$$

By using 5.3.22, we then have:

$$\begin{aligned} -\frac{\hbar^2}{2} \sum_{\langle\langle i,j \rangle\rangle} \sum_{\alpha\beta} \mathfrak{J}_{\alpha\beta} \left[ \langle \hat{A}_{i,j}^{(\alpha)} \rangle^* \hat{A}_{i,j}^{(\beta)} + \text{H.c.} \right] &= -\frac{\hbar^2}{2} \sum_{\langle\langle i,j \rangle\rangle} \left[ J_- \left[ \langle \hat{A}_{i,j}^{(\uparrow)} \rangle^* \hat{A}_{i,j}^{(\downarrow)} + \langle \hat{A}_{i,j}^{(\downarrow)} \rangle^* \hat{A}_{i,j}^{(\uparrow)} \right] + \right. \\ J_+ \left[ \langle \hat{A}_{i,j}^{(\uparrow)} \rangle^* \hat{A}_{i,j}^{(\uparrow)} + \langle \hat{A}_{i,j}^{(\downarrow)} \rangle^* \hat{A}_{i,j}^{(\downarrow)} \right] &+ \text{H.c.} \left. \right] = -\frac{\hbar^2}{2} \sum_{\langle\langle i,j \rangle\rangle} \sum_{\alpha} \left[ \left[ J_- \langle \hat{A}_{i,j}^{(\bar{\alpha})} \rangle^* + J_+ \langle \hat{A}_{i,j}^{(\alpha)} \rangle^* \right] \hat{A}_{i,j}^{(\alpha)} + \text{H.c.} \right] = \\ -\frac{\hbar^2 \chi_2}{2} \sum_{\langle\langle i,j \rangle\rangle} \sum_{\alpha} \left[ \left[ J_- e^{i\phi_{\bar{\alpha}\nu_{ij}}} + J_+ e^{i\phi_{\alpha\nu_{ij}}} \right] \hat{f}_{i\alpha}^{\dagger} \hat{f}_{j\alpha} + \text{H.c.} \right] &= \\ -\frac{\hbar^2 \chi_2}{2} \sum_X \sum_{\vec{r}} \sum_{l=1}^6 \sum_{\alpha} \left[ \left[ J_- e^{i\phi_{\bar{\alpha}\nu_l^{(X)}}} + J_+ e^{i\phi_{\alpha\nu_l^{(X)}}} \right] \hat{f}_{\vec{r}\alpha}^{\dagger(X)} \hat{f}_{\vec{r}+\vec{e}_l\alpha}^{(X)} + \text{H.c.} \right], \end{aligned} \quad (5.3.34)$$

where  $\bar{\alpha}$  means opposite spin of  $\alpha$ ,  $X$  sums over the two sublattices  $A$  and  $B$ , and  $\nu_l^{(X)}$  was defined in table 1. The vector  $\vec{r}$  is the same as in NN case, and since we consider the same sublattices as we did for NN Fourier transformation, we can use 5.3.25 here as well. Doing following Fourier transformation:

$$\begin{aligned} \sum_{\vec{r}} \hat{f}_{\vec{r}\alpha}^\dagger \hat{f}_{\vec{r}+\vec{\epsilon}_l\alpha}^{(X)} &= \frac{1}{N} \sum_{\vec{r}} \sum_{\vec{k}\vec{k}'} e^{-i\vec{k}\cdot\vec{r}} e^{i\vec{k}'\cdot(\vec{r}+\vec{\epsilon}_l)} \hat{f}_{\vec{k}\alpha}^\dagger \hat{f}_{\vec{k}'\alpha}^{(X)} = \\ &= \frac{1}{N} \sum_{\vec{k}\vec{k}'} e^{i\vec{k}'\cdot\vec{\epsilon}_l} \sum_{\vec{r}} e^{i(\vec{k}'-\vec{k})\cdot\vec{r}} \hat{f}_{\vec{k}\alpha}^\dagger \hat{f}_{\vec{k}'\alpha}^{(X)} = \sum_{\vec{k}} e^{i\vec{k}\cdot\vec{\epsilon}_l} \hat{f}_{\vec{k}\alpha}^\dagger \hat{f}_{\vec{k}\alpha}^{(X)}, \end{aligned} \quad (5.3.35)$$

we can insert 5.3.35 into 5.3.34, which gives:

$$\begin{aligned} & -\frac{\hbar^2}{2} \sum_{\langle(i,j)\rangle} \sum_{\alpha\beta} \mathfrak{J}_{\alpha\beta} \left[ \langle \hat{A}_{i,j}^{(\alpha)} \rangle^* \hat{A}_{i,j}^{(\beta)} + \text{H.c.} \right] = \\ & -\frac{\hbar^2 \chi_2}{2} \sum_X \sum_{\vec{k}} \sum_{\alpha} \sum_{l=1}^6 \left[ [J_- e^{i\phi_{\bar{\alpha}} \nu_l^{(X)}} + J_+ e^{i\phi_{\alpha} \nu_l^{(X)}}] e^{i\vec{k}\cdot\vec{\epsilon}_l} \hat{f}_{\vec{k}\alpha}^\dagger \hat{f}_{\vec{k}\alpha}^{(X)} + \text{H.c.} \right] = \\ & -\frac{\hbar^2 \chi_2}{2} \sum_X \sum_{\vec{k}} \sum_{\alpha} \left[ S_{\vec{k}\alpha}^{(X)} \hat{f}_{\vec{k}\alpha}^\dagger \hat{f}_{\vec{k}\alpha}^{(X)} + \text{H.c.} \right], \end{aligned} \quad (5.3.36)$$

where we defined the quantity

$$S_{\vec{k}\alpha}^{(X)} := \sum_{l=1}^6 \left[ (J_- e^{i\phi_{\bar{\alpha}} \nu_l^{(X)}} + J_+ e^{i\phi_{\alpha} \nu_l^{(X)}}) e^{i\vec{k}\cdot\vec{\epsilon}_l} \right]. \quad (5.3.37)$$

We now consider this quantity for sublattice  $A$  by using table 1:

$$\begin{aligned} S_{\vec{k}\alpha}^{(A)} &= \sum_{l=1}^6 \left[ J_- e^{i\phi_{\bar{\alpha}} \nu_l^{(A)}} + J_+ e^{i\phi_{\alpha} \nu_l^{(A)}} \right] e^{i\vec{k}\cdot\vec{\epsilon}_l} = \\ & [J_- e^{i\phi_{\bar{\alpha}}} + J_+ e^{i\phi_{\alpha}}] \left[ e^{i\frac{\alpha}{2}(\sqrt{3}k_x+3k_y)} + e^{-ia\sqrt{3}k_x} + e^{i\frac{\alpha}{2}(\sqrt{3}k_x-3k_y)} \right] + \\ & [J_- e^{-i\phi_{\bar{\alpha}}} + J_+ e^{-i\phi_{\alpha}}] \left[ e^{i\frac{\alpha}{2}(-\sqrt{3}k_x+3k_y)} + e^{-i\frac{\alpha}{2}(\sqrt{3}k_x+3k_y)} + e^{ia\sqrt{3}k_x} \right]. \end{aligned} \quad (5.3.38)$$

The first parenthesis in the two terms can be split into a cosine and a sine part:

$$J_- e^{\pm i\phi_{\bar{\alpha}}} + J_+ e^{\pm i\phi_{\alpha}} = (J_- \cos \phi_{\bar{\alpha}} + J_+ \cos \phi_{\alpha}) \pm i(J_- \sin \phi_{\bar{\alpha}} + J_+ \sin \phi_{\alpha}). \quad (5.3.39)$$

The total cosine part of 5.3.38 is then given by

$$\begin{aligned} & [J_- \cos \phi_{\bar{\alpha}} + J_+ \cos \phi_{\alpha}] \left[ e^{i\frac{\alpha}{2}\sqrt{3}k_x} (e^{i\frac{\alpha}{2}3k_y} + e^{-i\frac{\alpha}{2}3k_y}) + e^{-i\frac{\alpha}{2}\sqrt{3}k_x} (e^{i\frac{\alpha}{2}3k_y} + e^{-i\frac{\alpha}{2}3k_y}) + e^{ia\sqrt{3}k_x} + e^{-ia\sqrt{3}k_x} \right] = \\ & [J_- \cos \phi_{\bar{\alpha}} + J_+ \cos \phi_{\alpha}] \left[ (e^{i\frac{\alpha}{2}\sqrt{3}k_x} + e^{-i\frac{\alpha}{2}\sqrt{3}k_x}) (e^{i\frac{\alpha}{2}3k_y} + e^{-i\frac{\alpha}{2}3k_y}) + e^{ia\sqrt{3}k_x} + e^{-ia\sqrt{3}k_x} \right] = \\ & [J_- \cos \phi_{\bar{\alpha}} + J_+ \cos \phi_{\alpha}] \left[ 4 \cos\left(\frac{\sqrt{3}}{2}k_x a\right) \cos\left(\frac{3}{2}k_y a\right) + 2 \cos(\sqrt{3}k_x a) \right] = A_{\alpha} \zeta_{\vec{k}}, \end{aligned} \quad (5.3.40)$$

where we defined:

$$A_{\alpha} := J_- \cos \phi_{\bar{\alpha}} + J_+ \cos \phi_{\alpha} \quad (5.3.41)$$

$$\zeta_{\vec{k}} := 2 \left[ 2 \cos\left(\frac{\sqrt{3}}{2}k_x a\right) \cos\left(\frac{3}{2}k_y a\right) + \cos(\sqrt{3}k_x a) \right]. \quad (5.3.42)$$

Similarly, the total sine part of 5.3.38 is given by:

$$\begin{aligned} & i [J_- \sin \phi_{\bar{\alpha}} + J_+ \sin \phi_{\alpha}] \left[ e^{i\frac{\alpha}{2}3k_y} (e^{i\frac{\alpha}{2}\sqrt{3}k_x} - e^{-i\frac{\alpha}{2}\sqrt{3}k_x}) + \right. \\ & \left. e^{-i\frac{\alpha}{2}3k_y} (e^{i\frac{\alpha}{2}\sqrt{3}k_x} - e^{-i\frac{\alpha}{2}\sqrt{3}k_x}) - (e^{ia\sqrt{3}k_x} - e^{-ia\sqrt{3}k_x}) \right] = \\ & i [J_- \sin \phi_{\bar{\alpha}} + J_+ \sin \phi_{\alpha}] \left[ (e^{i\frac{\alpha}{2}3k_y} + e^{-i\frac{\alpha}{2}3k_y}) (e^{i\frac{\alpha}{2}\sqrt{3}k_x} - e^{-i\frac{\alpha}{2}\sqrt{3}k_x}) - (e^{ia\sqrt{3}k_x} - e^{-ia\sqrt{3}k_x}) \right] = \\ & - [J_- \sin \phi_{\bar{\alpha}} + J_+ \sin \phi_{\alpha}] \left[ 4 \cos\left(\frac{3}{2}k_y a\right) \sin\left(\frac{\sqrt{3}}{2}k_x a\right) - 2 \sin(a\sqrt{3}k_x) \right] = \\ & - [J_- \sin \phi_{\bar{\alpha}} + J_+ \sin \phi_{\alpha}] 4 \sin\left(\frac{\sqrt{3}}{2}k_x a\right) \left[ \cos\left(\frac{3}{2}k_y a\right) - \cos\left(\frac{\sqrt{3}}{2}k_x a\right) \right] = -B_{\alpha} \xi_{\vec{k}}. \end{aligned} \quad (5.3.43)$$

where we defined:

$$B_\alpha := J_- \sin \phi_{\bar{\alpha}} + J_+ \sin \phi_\alpha \quad (5.3.44)$$

$$\xi_{\vec{k}} := 4 \sin \left( \frac{\sqrt{3}}{2} k_x a \right) \left[ \cos \left( \frac{3}{2} k_y a \right) - \cos \left( \frac{\sqrt{3}}{2} k_x a \right) \right]. \quad (5.3.45)$$

The quantity 5.3.38 is the sum of 5.3.40 and 5.3.43:

$$S_{\vec{k}\alpha}^{(A)} = A_\alpha \zeta_{\vec{k}} - B_\alpha \xi_{\vec{k}}. \quad (5.3.46)$$

Next, by taking a look at table 1, we see that  $\nu_l^{(A)} = -\nu_l^{(B)}$ . From 5.3.38, we see that the  $\nu$ -value only determines the sign in front of the  $\phi$ -values. Hence, sublattice B part can be obtained from sublattice A part by doing the substitutions  $\phi_{\bar{\alpha}} \mapsto -\phi_{\bar{\alpha}}$  and  $\phi_\alpha \mapsto -\phi_\alpha$ . We then have:

$$S_{\vec{k}\alpha}^{(B)} = A_\alpha \zeta_{\vec{k}} + B_\alpha \xi_{\vec{k}}, \quad (5.3.47)$$

and 5.3.36 becomes:

$$\begin{aligned} & -\frac{\hbar^2}{2} \sum_{\langle\langle i,j \rangle\rangle} \sum_{\alpha\beta} \tilde{\mathcal{J}}_{\alpha\beta} \left[ \langle \hat{A}_{i,j}^{(\alpha)} \rangle^* \hat{A}_{i,j}^{(\beta)} + \text{H.c.} \right] = -\frac{\hbar^2 \chi_2}{2} \sum_X \sum_{\vec{k}} \sum_\alpha \left[ S_{\vec{k}\alpha}^{(X)} \hat{f}_{\vec{k}\alpha}^{\dagger(X)} \hat{f}_{\vec{k}\alpha}^{(X)} + \text{H.c.} \right] = \\ & -\hbar^2 \chi_2 \sum_X \sum_{\vec{k}} \sum_\alpha S_{\vec{k}\alpha}^{(X)} \hat{f}_{\vec{k}\alpha}^{\dagger(X)} \hat{f}_{\vec{k}\alpha}^{(X)} = -\hbar^2 \chi_2 \sum_{\vec{k}} \sum_\alpha \begin{bmatrix} \hat{f}_{\vec{k}\alpha}^{\dagger(A)} & \hat{f}_{\vec{k}\alpha}^{\dagger(B)} \\ A_\alpha \zeta_{\vec{k}} - B_\alpha \xi_{\vec{k}} & 0 \\ 0 & A_\alpha \zeta_{\vec{k}} + B_\alpha \xi_{\vec{k}} \end{bmatrix} \begin{bmatrix} \hat{f}_{\vec{k}\alpha}^{(A)} \\ \hat{f}_{\vec{k}\alpha}^{(B)} \end{bmatrix}. \end{aligned} \quad (5.3.48)$$

Next, we want to consider the constant terms in 5.3.31:

$$\begin{aligned} & \frac{\hbar^2 J_2}{2} \sum_{\langle\langle i,j \rangle\rangle} \left| \sum_\alpha \langle \hat{A}_{i,j}^{(\alpha)} \rangle \right|^2 + \frac{\hbar^2 \Gamma}{2} \sum_{\langle\langle i,j \rangle\rangle} \sum_{\alpha\beta} (2\delta_{\alpha\beta} - 1) \langle \hat{A}_{i,j}^{(\alpha)} \rangle^* \langle \hat{A}_{i,j}^{(\beta)} \rangle = \frac{\hbar^2}{2} \sum_{\langle\langle i,j \rangle\rangle} \sum_{\alpha\beta} \tilde{\mathcal{J}}_{\alpha\beta} \langle \hat{A}_{i,j}^{(\alpha)} \rangle^* \langle \hat{A}_{i,j}^{(\beta)} \rangle = \\ & \frac{\hbar^2}{2} \sum_{\langle\langle i,j \rangle\rangle} \left[ J_+ (\langle \hat{A}_{i,j}^{(\uparrow)} \rangle^* \langle \hat{A}_{i,j}^{(\uparrow)} \rangle + \langle \hat{A}_{i,j}^{(\downarrow)} \rangle^* \langle \hat{A}_{i,j}^{(\downarrow)} \rangle) + J_- (\langle \hat{A}_{i,j}^{(\uparrow)} \rangle^* \langle \hat{A}_{i,j}^{(\downarrow)} \rangle + \langle \hat{A}_{i,j}^{(\downarrow)} \rangle^* \langle \hat{A}_{i,j}^{(\uparrow)} \rangle) \right] = \\ & \hbar^2 \chi_2^2 \sum_{\langle\langle i,j \rangle\rangle} \left[ J_+ + J_- \cos(\phi_\uparrow - \phi_\downarrow) \right] = 12\hbar^2 \chi_2^2 \sum_{\vec{k}} \left[ J_+ + J_- \cos(\phi_\uparrow - \phi_\downarrow) \right], \end{aligned} \quad (5.3.49)$$

where we have used 5.3.22 and the fact that there are two sublattices and six NNNs for each site. By combining 5.3.48 and 5.3.49, our Hamiltonian term in 5.3.31 becomes:

$$\begin{aligned} \hat{H}_2^{(\text{MF})} + \hat{H}_\Gamma^{(\text{MF})} = \hbar^2 \sum_{\vec{k}} \left[ -\chi_2 \sum_\alpha \begin{bmatrix} \hat{f}_{\vec{k}\alpha}^{\dagger(A)} & \hat{f}_{\vec{k}\alpha}^{\dagger(B)} \\ A_\alpha \zeta_{\vec{k}} - B_\alpha \xi_{\vec{k}} & 0 \\ 0 & A_\alpha \zeta_{\vec{k}} + B_\alpha \xi_{\vec{k}} \end{bmatrix} \begin{bmatrix} \hat{f}_{\vec{k}\alpha}^{(A)} \\ \hat{f}_{\vec{k}\alpha}^{(B)} \end{bmatrix} + \right. \\ \left. 12\chi_2^2 [J_+ + J_- \cos(\phi_\uparrow - \phi_\downarrow)] \right]. \end{aligned} \quad (5.3.50)$$

Finally, we do the same to the DMI term. By inserting 5.3.19 into  $\hat{H}_{\text{DMI}}$ , we have:

$$\begin{aligned} \hat{H}_{\text{DMI}}^{(\text{MF})} = i \frac{\hbar^2 D}{2} \sum_{\langle\langle i,j \rangle\rangle} \nu_{ij} \left[ \langle \hat{A}_{i,j}^{(\uparrow)} \rangle^* \hat{A}_{i,j}^{(\downarrow)} + \langle \hat{A}_{i,j}^{(\downarrow)} \rangle \hat{A}_{i,j}^{\dagger(\uparrow)} - \langle \hat{A}_{i,j}^{(\uparrow)} \rangle^* \langle \hat{A}_{i,j}^{(\downarrow)} \rangle \right] + \text{H.c.} = \\ \frac{\hbar^2 D \chi_2}{2} \sum_{\langle\langle i,j \rangle\rangle} \nu_{ij} \left[ i e^{i\phi_\uparrow \nu_{ij}} \hat{A}_{i,j}^{(\downarrow)} + i e^{-i\phi_\downarrow \nu_{ij}} \hat{A}_{i,j}^{\dagger(\uparrow)} + \text{H.c.} \right] - i \frac{\hbar^2 D}{2} \sum_{\langle\langle i,j \rangle\rangle} \nu_{ij} \chi_2^2 \left[ e^{i(\phi_\uparrow - \phi_\downarrow) \nu_{ij}} - e^{-i(\phi_\uparrow - \phi_\downarrow) \nu_{ij}} \right] = \\ \frac{\hbar^2 D \chi_2}{2} \sum_{\langle\langle i,j \rangle\rangle} \nu_{ij} \left[ i e^{i\phi_\uparrow \nu_{ij}} \hat{f}_{i\downarrow}^\dagger \hat{f}_{j\downarrow} - i e^{i\phi_\downarrow \nu_{ij}} \hat{f}_{i\uparrow}^\dagger \hat{f}_{j\uparrow} + \text{H.c.} \right] + \hbar^2 D \chi_2^2 \sum_{\langle\langle i,j \rangle\rangle} \sin(\phi_\uparrow - \phi_\downarrow). \end{aligned} \quad (5.3.51)$$

Inserting the Fourier transformation 5.3.35 into the first term, we get:

$$\begin{aligned}
& \frac{\hbar^2 D\chi_2}{2} \sum_{\langle(i,j)\rangle} \nu_{ij} \left[ i e^{i\phi_\uparrow \nu_{ij}} \hat{f}_{i\downarrow}^\dagger \hat{f}_{j\downarrow} - i e^{i\phi_\downarrow \nu_{ij}} \hat{f}_{i\uparrow}^\dagger \hat{f}_{j\uparrow} + \text{H.c.} \right] = \\
& \frac{\hbar^2 D\chi_2}{2} \sum_X \sum_{\vec{r}} \sum_{l=1}^6 \nu_l^{(X)} \left[ i e^{i\phi_\uparrow \nu_l^{(X)}} \hat{f}_{\vec{r}\downarrow}^\dagger \hat{f}_{\vec{r}+\vec{e}_l\downarrow} - i e^{i\phi_\downarrow \nu_l^{(X)}} \hat{f}_{\vec{r}\uparrow}^\dagger \hat{f}_{\vec{r}+\vec{e}_l\uparrow} + \text{H.c.} \right] = \\
& \frac{\hbar^2 D\chi_2}{2} \sum_X \sum_{\vec{k}} \sum_{l=1}^6 \nu_l^{(X)} \left[ i e^{i\vec{k}\cdot\vec{e}_l} e^{i\phi_\uparrow \nu_l^{(X)}} \hat{f}_{\vec{k}\downarrow}^\dagger \hat{f}_{\vec{k}\downarrow} - i e^{i\vec{k}\cdot\vec{e}_l} e^{i\phi_\downarrow \nu_l^{(X)}} \hat{f}_{\vec{k}\uparrow}^\dagger \hat{f}_{\vec{k}\uparrow} + \text{H.c.} \right] = \quad (5.3.52) \\
& \hbar^2 D\chi_2 \sum_X \sum_{\vec{k}} \sum_{l=1}^6 \nu_l^{(X)} \left[ \sin(\vec{k}\cdot\vec{e}_l + \phi_\downarrow \nu_l^{(X)}) \hat{f}_{\vec{k}\uparrow}^\dagger \hat{f}_{\vec{k}\uparrow} - \sin(\vec{k}\cdot\vec{e}_l + \phi_\uparrow \nu_l^{(X)}) \hat{f}_{\vec{k}\downarrow}^\dagger \hat{f}_{\vec{k}\downarrow} \right] = \\
& -\hbar^2 D\chi_2 \sum_X \sum_{\vec{k}} \sum_{\alpha} C_{\vec{k}\alpha}^{(X)} \hat{f}_{\vec{k}\alpha}^\dagger \hat{f}_{\vec{k}\alpha},
\end{aligned}$$

where

$$C_{\vec{k}\alpha}^{(X)} := \sigma_\alpha \sum_{l=1}^6 \sin(\phi_\alpha + \nu_l^{(X)} \vec{k}\cdot\vec{e}_l); \quad \sigma_\alpha = \begin{cases} +1, & \text{if } \alpha = \uparrow \\ -1, & \text{if } \alpha = \downarrow \end{cases}. \quad (5.3.53)$$

By using table 1, we find this quantity more explicitly for the two sublattices:

$$C_{\vec{k}\alpha}^{(A)} = 2\sigma_\alpha \left[ \sin(\phi_\alpha + \frac{\sqrt{3}}{2}k_x a + \frac{3}{2}k_y a) + \sin(\phi_\alpha + \frac{\sqrt{3}}{2}k_x a - \frac{3}{2}k_y a) + \sin(\phi_\alpha - \sqrt{3}k_x a) \right] \quad (5.3.54)$$

$$C_{\vec{k}\alpha}^{(B)} = 2\sigma_\alpha \left[ \sin(\phi_\alpha - \frac{\sqrt{3}}{2}k_x a - \frac{3}{2}k_y a) + \sin(\phi_\alpha - \frac{\sqrt{3}}{2}k_x a + \frac{3}{2}k_y a) + \sin(\phi_\alpha + \sqrt{3}k_x a) \right]. \quad (5.3.55)$$

We now summarize the results of this subsection in following proposition:

**Proposition 5.3.** The Hamiltonians  $\hat{H}_0$  and  $\hat{H} = \hat{H}_0 + \hat{H}_{\text{DMI}}$  from section 5.2, decoupled with Abrikosov fermions as in proposition 5.2 and approximated by a mean-field theory described in subsection 5.3.2, are given by:

$$\begin{aligned}
\hat{H}_0^{(\text{MF})} = \hbar^2 \sum_{\vec{k}} \left[ \sum_{\alpha} \left( \begin{bmatrix} \hat{f}_{\vec{k}\alpha}^{(A)} & \hat{f}_{\vec{k}\alpha}^{(B)} \end{bmatrix} \begin{bmatrix} -\chi_2(A_\alpha \zeta_{\vec{k}} - B_\alpha \xi_{\vec{k}}) & -J_1 \chi_1 \eta_{\vec{k}} \\ -J_1 \chi_1 \eta_{\vec{k}}^* & -\chi_2(A_\alpha \zeta_{\vec{k}} + B_\alpha \xi_{\vec{k}}) \end{bmatrix} \begin{bmatrix} \hat{f}_{\vec{k}\alpha}^{(A)} \\ \hat{f}_{\vec{k}\alpha}^{(B)} \end{bmatrix} \right) + \right. \\
\left. 3J_1 \chi_1^2 + 12\chi_2^2 [J_+ + J_- \cos(\phi_\uparrow - \phi_\downarrow)] \right], \quad (5.3.56)
\end{aligned}$$

and  $\hat{H}^{(\text{MF})} = \hat{H}_0^{(\text{MF})} + \hat{H}_{\text{DMI}}^{(\text{MF})}$ ;

$$\hat{H}_{\text{DMI}}^{(\text{MF})} = \hbar^2 \sum_{\vec{k}} \left[ \sum_{\alpha} \left( \begin{bmatrix} \hat{f}_{\vec{k}\alpha}^{(A)} & \hat{f}_{\vec{k}\alpha}^{(B)} \end{bmatrix} \begin{bmatrix} -D\chi_2 C_{\vec{k}\alpha}^{(A)} & 0 \\ 0 & -D\chi_2 C_{\vec{k}\alpha}^{(B)} \end{bmatrix} \begin{bmatrix} \hat{f}_{\vec{k}\alpha}^{(A)} \\ \hat{f}_{\vec{k}\alpha}^{(B)} \end{bmatrix} \right) + 12D\chi_2^2 \sin(\phi_\uparrow - \phi_\downarrow) \right], \quad (5.3.57)$$

where

$$\eta_{\vec{k}} = e^{-ik_y a} + 2e^{i\frac{k_y a}{2}} \cos\left(\frac{\sqrt{3}}{2}k_x a\right), \quad (5.3.58)$$

$$A_\alpha := J_- \cos \phi_{\bar{\alpha}} + J_+ \cos \phi_\alpha, \quad (5.3.59)$$

$$B_\alpha := J_- \sin \phi_{\bar{\alpha}} + J_+ \sin \phi_\alpha, \quad (5.3.60)$$

$$\zeta_{\vec{k}} := 2 \left[ 2 \cos\left(\frac{\sqrt{3}}{2}k_x a\right) \cos\left(\frac{3}{2}k_y a\right) + \cos(\sqrt{3}k_x a) \right], \quad (5.3.61)$$

$$\xi_{\vec{k}} := 4 \sin\left(\frac{\sqrt{3}}{2}k_x a\right) \left[ \cos\left(\frac{3}{2}k_y a\right) - \cos\left(\frac{\sqrt{3}}{2}k_x a\right) \right], \quad (5.3.62)$$

$$C_{\vec{k}\alpha}^{(A)} = 2\sigma_\alpha \left[ \sin(\phi_\alpha + \frac{\sqrt{3}}{2}k_x a + \frac{3}{2}k_y a) + \sin(\phi_\alpha + \frac{\sqrt{3}}{2}k_x a - \frac{3}{2}k_y a) + \sin(\phi_\alpha - \sqrt{3}k_x a) \right], \quad (5.3.63)$$

$$C_{\vec{k}\alpha}^{(B)} = 2\sigma_\alpha \left[ \sin(\phi_\alpha - \frac{\sqrt{3}}{2}k_x a - \frac{3}{2}k_y a) + \sin(\phi_\alpha - \frac{\sqrt{3}}{2}k_x a + \frac{3}{2}k_y a) + \sin(\phi_\alpha + \sqrt{3}k_x a) \right]. \quad (5.3.64)$$

Here,

$$J_\pm := J_2 \pm \Gamma; \quad \sigma_\alpha = \begin{cases} +1, & \text{if } \alpha = \uparrow \\ -1, & \text{if } \alpha = \downarrow \end{cases}, \quad (5.3.65)$$

and  $\chi_1, \chi_2, \phi_\uparrow, \phi_\downarrow \in \mathbb{R}$  are mean-field parameters.

### 5.3.4 Diagonalization, groundstate energy and excitations

Having our Hamiltonians in matrix form in proposition 5.3, we are now ready for the diagonalization. We start with the Hamiltonian without DMI. According to theorem 3.2, our aim is to find eigenvalues  $E_{\vec{k}\alpha}^{(\pm)}$  of the matrix:

$$\mathbb{H}_{\vec{k}\alpha,0}^{(\text{MF})} = \begin{bmatrix} -\chi_2(A_\alpha \zeta_{\vec{k}} - B_\alpha \xi_{\vec{k}}) & -J_1 \chi_1 \eta_{\vec{k}} \\ -J_1 \chi_1 \eta_{\vec{k}}^* & -\chi_2(A_\alpha \zeta_{\vec{k}} + B_\alpha \xi_{\vec{k}}) \end{bmatrix}, \quad (5.3.66)$$

which are found by solving following equation:

$$\begin{aligned} \det(I E_{\vec{k}\alpha}^{(\pm)} - \mathbb{H}_{\vec{k}\alpha,0}^{(\text{MF})}) &= \begin{vmatrix} E_{\vec{k}\alpha}^{(\pm)} + \chi_2(A_\alpha \zeta_{\vec{k}} - B_\alpha \xi_{\vec{k}}) & J_1 \chi_1 \eta_{\vec{k}} \\ J_1 \chi_1 \eta_{\vec{k}}^* & E_{\vec{k}\alpha}^{(\pm)} + \chi_2(A_\alpha \zeta_{\vec{k}} + B_\alpha \xi_{\vec{k}}) \end{vmatrix} = \\ &= [E_{\vec{k}\alpha}^{(\pm)} + \chi_2(A_\alpha \zeta_{\vec{k}} - B_\alpha \xi_{\vec{k}})] [E_{\vec{k}\alpha}^{(\pm)} + \chi_2(A_\alpha \zeta_{\vec{k}} + B_\alpha \xi_{\vec{k}})] - J_1^2 \chi_1^2 |\eta_{\vec{k}}|^2 = \\ &= (E_{\vec{k}\alpha}^{(\pm)})^2 + 2\chi_2 A_\alpha \zeta_{\vec{k}} E_{\vec{k}\alpha}^{(\pm)} + \chi_2^2 [(A_\alpha \zeta_{\vec{k}})^2 - (B_\alpha \xi_{\vec{k}})^2] - J_1^2 \chi_1^2 |\eta_{\vec{k}}|^2 = 0, \end{aligned} \quad (5.3.67)$$

which gives:

$$E_{\vec{k}\alpha}^{(\pm)} = -\chi_2 A_\alpha \zeta_{\vec{k}} \pm \sqrt{\chi_2^2 (B_\alpha \xi_{\vec{k}})^2 + J_1^2 \chi_1^2 |\eta_{\vec{k}}|^2}, \quad (5.3.68)$$

which effectively is exactly the same result as equation 28 in reference [2]. The diagonalized Hamiltonian is then given by:

$$\hat{H}_0^{(\text{MF})} = \hbar^2 \sum_{\vec{k}} \left[ \sum_{\alpha} [E_{\vec{k}\alpha}^{(+)} \hat{\phi}_{\vec{k}\alpha}^{(+A)} \hat{\phi}_{\vec{k}\alpha}^{(A)} + E_{\vec{k}\alpha}^{(-)} \hat{\phi}_{\vec{k}\alpha}^{(-B)} \hat{\phi}_{\vec{k}\alpha}^{(B)}] + 3J_1 \chi_1^2 + 12\chi_2^2 [J_+ + J_- \cos(\phi_\uparrow - \phi_\downarrow)] \right]. \quad (5.3.69)$$

For the ground state in half-filled fermionic case, only the lower bands are occupied, meaning that the ground state energy is given by:

$$\frac{E_{(\text{tot})}^{(\text{no DMI})}}{\hbar^2} = \sum_{\vec{k}} \left[ E_{\vec{k}\uparrow}^{(-)} + E_{\vec{k}\downarrow}^{(-)} + 3J_1 \chi_1^2 + 12\chi_2^2 [J_+ + J_- \cos(\phi_\uparrow - \phi_\downarrow)] \right], \quad (5.3.70)$$

and the excitations are described by  $E_{\vec{k}\alpha}^{(+)}$ .

Finally, we do the same procedure for the Hamiltonian with DMI. We have the following matrix:

$$\mathbb{H}_{\vec{k}\alpha}^{(\text{MF})} = \mathbb{H}_{\vec{k}\alpha,0}^{(\text{MF})} + \mathbb{H}_{\vec{k}\alpha,\text{DMI}}^{(\text{MF})} = \begin{bmatrix} -D\chi_2 C_{\vec{k}\alpha}^{(A)} - \chi_2(A_\alpha \zeta_{\vec{k}} - B_\alpha \xi_{\vec{k}}) & -J_1 \chi_1 \eta_{\vec{k}} \\ -J_1 \chi_1 \eta_{\vec{k}}^* & -D\chi_2 C_{\vec{k}\alpha}^{(B)} - \chi_2(A_\alpha \zeta_{\vec{k}} + B_\alpha \xi_{\vec{k}}) \end{bmatrix}. \quad (5.3.71)$$

We get:

$$\begin{aligned} & \begin{vmatrix} E_{\vec{k}\alpha}^{(\pm)} + D\chi_2 C_{\vec{k}\alpha}^{(A)} + \chi_2(A_\alpha \zeta_{\vec{k}} - B_\alpha \xi_{\vec{k}}) & J_1 \chi_1 \eta_{\vec{k}} \\ J_1 \chi_1 \eta_{\vec{k}}^* & E_{\vec{k}\alpha}^{(\pm)} + D\chi_2 C_{\vec{k}\alpha}^{(B)} + \chi_2(A_\alpha \zeta_{\vec{k}} + B_\alpha \xi_{\vec{k}}) \end{vmatrix} = \\ & \begin{vmatrix} E_{\vec{k}\alpha}^{(\pm)} + \Theta_A & J_1 \chi_1 \eta_{\vec{k}} \\ J_1 \chi_1 \eta_{\vec{k}}^* & E_{\vec{k}\alpha}^{(\pm)} + \Theta_B \end{vmatrix} = [E_{\vec{k}\alpha}^{(\pm)} + \Theta_A] [E_{\vec{k}\alpha}^{(\pm)} + \Theta_B] - J_1^2 \chi_1^2 |\eta_{\vec{k}}|^2 = \\ & (E_{\vec{k}\alpha}^{(\pm)})^2 + (\Theta_A + \Theta_B) E_{\vec{k}\alpha}^{(\pm)} + \Theta_A \Theta_B - J_1^2 \chi_1^2 |\eta_{\vec{k}}|^2 = 0, \end{aligned} \quad (5.3.72)$$

where we defined:

$$\Theta_A := D\chi_2 C_{\vec{k}\bar{\alpha}}^{(A)} + \chi_2(A_\alpha \zeta_{\vec{k}} - B_\alpha \xi_{\vec{k}}), \quad (5.3.73)$$

$$\Theta_B := D\chi_2 C_{\vec{k}\bar{\alpha}}^{(B)} + \chi_2(A_\alpha \zeta_{\vec{k}} + B_\alpha \xi_{\vec{k}}). \quad (5.3.74)$$

This gives:

$$E_{\vec{k}\alpha}^{(\pm)} = -\frac{\Theta_A + \Theta_B}{2} \pm \sqrt{\frac{(\Theta_A + \Theta_B)^2}{4} - \Theta_A \Theta_B + J_1^2 \chi_1^2 |\eta_{\vec{k}}|^2} = -\frac{\Theta_A + \Theta_B}{2} \pm \sqrt{\frac{(\Theta_A - \Theta_B)^2}{4} + J_1^2 \chi_1^2 |\eta_{\vec{k}}|^2} = -\chi_2 \left[ D \frac{C_{\vec{k}\bar{\alpha}}^{(A)} + C_{\vec{k}\bar{\alpha}}^{(B)}}{2} + A_\alpha \zeta_{\vec{k}} \right] \pm \sqrt{\chi_2^2 \frac{(DC_{\vec{k}\bar{\alpha}}^{(A)} - DC_{\vec{k}\bar{\alpha}}^{(B)} - 2B_\alpha \xi_{\vec{k}})^2}{4} + J_1^2 \chi_1^2 |\eta_{\vec{k}}|^2}. \quad (5.3.75)$$

We can now summarize the results of this subsection in following proposition:

**Proposition 5.4.** The ground state energies of half-filled fermionic Hamiltonians  $\hat{H}_0^{(\text{MF})}$  and  $\hat{H}^{(\text{MF})} = \hat{H}_0^{(\text{MF})} + \hat{H}_{\text{DMI}}^{(\text{MF})}$  presented in proposition 5.3 are given by:

$$\frac{E_{\text{(tot)}}}{\hbar^2} = \sum_{\vec{k}} \left[ E_{\vec{k}\uparrow}^{(-)} + E_{\vec{k}\downarrow}^{(-)} + C \right], \quad (5.3.76)$$

with  $E_{\vec{k}\alpha}^{(-)}$  being occupied bands, and  $E_{\vec{k}\alpha}^{(+)}$  representing the excitations.

Here, for  $\hat{H}_0^{(\text{MF})}$ , we have:

$$E_{\vec{k}\alpha}^{(\pm)} = -\chi_2 A_\alpha \zeta_{\vec{k}} \pm \sqrt{\chi_2^2 (B_\alpha \xi_{\vec{k}})^2 + J_1^2 \chi_1^2 |\eta_{\vec{k}}|^2}, \quad (5.3.77)$$

$$C = 3J_1 \chi_1^2 + 12\chi_2^2 [J_+ + J_- \cos(\phi_\uparrow - \phi_\downarrow)], \quad (5.3.78)$$

and for  $\hat{H}^{(\text{MF})}$ , we have:

$$E_{\vec{k}\alpha}^{(\pm)} = -\chi_2 \left[ D \frac{C_{\vec{k}\bar{\alpha}}^{(A)} + C_{\vec{k}\bar{\alpha}}^{(B)}}{2} + A_\alpha \zeta_{\vec{k}} \right] \pm \sqrt{\chi_2^2 \frac{(DC_{\vec{k}\bar{\alpha}}^{(A)} - DC_{\vec{k}\bar{\alpha}}^{(B)} - 2B_\alpha \xi_{\vec{k}})^2}{4} + J_1^2 \chi_1^2 |\eta_{\vec{k}}|^2}, \quad (5.3.79)$$

$$C = 3J_1 \chi_1^2 + 12\chi_2^2 [J_+ + J_- \cos(\phi_\uparrow - \phi_\downarrow)] + 12D\chi_2^2 \sin(\phi_\uparrow - \phi_\downarrow). \quad (5.3.80)$$

We see that  $\hat{H}^{(\text{MF})}$  reduces to  $\hat{H}_0^{(\text{MF})}$  when  $D = 0$ , just as expected, so that the general discussion at this point will involve the results with DMI included.

### 5.3.5 Physical phases

Depending on the mean-field parameters  $\chi_1, \chi_2, \phi_\uparrow, \phi_\downarrow \in \mathbb{R}$ , the form of our Hamiltonian and the dispersions will change, and some different forms will represent different physical phases. Following the approach in reference [2], we will consider three physical phases, and check which of these is most likely to exist for different interaction parameters  $J_1, J_2, \Gamma, D$ . Based on that, we can construct a phase diagram. In this subsection, we will present the three physical phases, and determine what values mean-field parameters must have for these phases.

In order to define the three phases, we first recall our mean-field approximated Hamiltonian before Fourier transfor-

mations were performed. Combining 5.3.23, 5.3.31 and 5.3.51, we have that:

$$\begin{aligned}
\hat{H}^{(\text{MF})} = & -\frac{\hbar^2 J_1 \chi_1}{2} \sum_{\langle i,j \rangle} \sum_{\alpha} \left[ \hat{f}_{i\alpha}^{\dagger} \hat{f}_{j\alpha} + \text{H.c.} \right] - \frac{\hbar^2 \chi_2}{2} \sum_{\langle\langle i,j \rangle\rangle} \sum_{\alpha} \left[ [J_- e^{i\phi_{\bar{\alpha}} \nu_{ij}} + J_+ e^{i\phi_{\alpha} \nu_{ij}}] \hat{f}_{i\alpha}^{\dagger} \hat{f}_{j\alpha} + \text{H.c.} \right] - \\
& \frac{\hbar^2 D \chi_2}{2} \sum_{\langle\langle i,j \rangle\rangle} \sum_{\alpha} \nu_{ij} \left[ i\sigma_{\alpha} e^{i\phi_{\bar{\alpha}} \nu_{ij}} \hat{f}_{i\alpha}^{\dagger} \hat{f}_{j\alpha} + \text{H.c.} \right] + \sum_{\langle i,j \rangle} \frac{\hbar^2 J_1 \chi_1^2}{2} + \\
& \hbar^2 \chi_2^2 \sum_{\langle\langle i,j \rangle\rangle} \left[ J_+ + J_- \cos(\phi_{\uparrow} - \phi_{\downarrow}) + D \sin(\phi_{\uparrow} - \phi_{\downarrow}) \right] = \\
- \frac{\hbar^2 J_1 \chi_1}{2} \sum_{\langle i,j \rangle} \sum_{\alpha} \left[ \hat{f}_{i\alpha}^{\dagger} \hat{f}_{j\alpha} + \text{H.c.} \right] - \frac{\hbar^2 \chi_2}{2} \sum_{\langle\langle i,j \rangle\rangle} \sum_{\alpha} \left[ [J_- e^{i\phi_{\bar{\alpha}} \nu_{ij}} + J_+ e^{i\phi_{\alpha} \nu_{ij}} + D\sigma_{\alpha} e^{i(\phi_{\bar{\alpha}} + \frac{\pi}{2}) \nu_{ij}}] \hat{f}_{i\alpha}^{\dagger} \hat{f}_{j\alpha} + \text{H.c.} \right] + \\
& \sum_{\langle i,j \rangle} \frac{\hbar^2 J_1 \chi_1^2}{2} + \hbar^2 \chi_2^2 \sum_{\langle\langle i,j \rangle\rangle} \left[ J_+ + J_- \cos(\phi_{\uparrow} - \phi_{\downarrow}) + D \sin(\phi_{\uparrow} - \phi_{\downarrow}) \right].
\end{aligned} \tag{5.3.81}$$

With this formula in mind, we now present Hamiltonians for the three phases: *gapless spin liquid*, *chiral spin liquid*, and *topologically gapped spin liquid*, as described in reference [2].

**Gapless spin liquid phase** The gapless spin liquid phase is effectively described by the non-interacting graphene Hamiltonian:

$$\hat{H}_{(\text{gapless})} = C \sum_{\langle i,j \rangle} \sum_{\alpha} \hat{f}_{i\alpha}^{\dagger} \hat{f}_{j\alpha} + \text{H.c.}, \tag{5.3.82}$$

where  $C \in \mathbb{R}$ . From 5.3.81, we see that this phase is obtained when  $\chi_2 = 0$ .

**Chiral gapped spin liquid** Next, we consider the chiral gapped spin liquid, which effectively is described by Haldane model on a honeycomb lattice:

$$\hat{H}_{(\text{chiral})} = C_1 \sum_{\langle i,j \rangle} \sum_{\alpha} \hat{f}_{i\alpha}^{\dagger} \hat{f}_{j\alpha} + iC_2 \sum_{\langle\langle i,j \rangle\rangle} \sum_{\alpha} \nu_{ij} \hat{f}_{i\alpha}^{\dagger} \hat{f}_{j\alpha} + \text{H.c.}, \tag{5.3.83}$$

where  $C_1, C_2 \in \mathbb{R} \setminus \{0\}$ . From 5.3.81, this means that we must have:

$$\begin{aligned}
J_- e^{i\phi_{\bar{\alpha}} \nu_{ij}} + J_+ e^{i\phi_{\alpha} \nu_{ij}} + D\sigma_{\alpha} e^{i(\phi_{\bar{\alpha}} + \frac{\pi}{2}) \nu_{ij}} = iC_2 \nu_{ij} = C_2 e^{i\frac{\pi}{2} \nu_{ij}} & \implies \\
J_+ e^{i(\phi_{\alpha} - \frac{\pi}{2}) \nu_{ij}} + (D\sigma_{\alpha} + J_- e^{-i\frac{\pi}{2} \nu_{ij}}) e^{i\phi_{\bar{\alpha}} \nu_{ij}} = C_2 \in \mathbb{R} & \implies \\
J_+ \sin(\phi_{\alpha} - \frac{\pi}{2}) + J_- \sin(\phi_{\bar{\alpha}} - \frac{\pi}{2}) + D\sigma_{\alpha} \sin \phi_{\bar{\alpha}} = & \\
D\sigma_{\alpha} \sin \phi_{\bar{\alpha}} - J_+ \cos \phi_{\alpha} - J_- \cos \phi_{\bar{\alpha}} = 0. &
\end{aligned} \tag{5.3.84}$$

At the same time,  $C_2$  should be invariant when inverting the spins, meaning that:

$$\begin{aligned}
J_+ e^{i(\phi_{\bar{\alpha}} - \frac{\pi}{2}) \nu_{ij}} + (D\sigma_{\alpha} + J_- e^{-i\frac{\pi}{2} \nu_{ij}}) e^{i\phi_{\alpha} \nu_{ij}} = J_+ e^{i(\phi_{\alpha} - \frac{\pi}{2}) \nu_{ij}} + (D\sigma_{\bar{\alpha}} + J_- e^{-i\frac{\pi}{2} \nu_{ij}}) e^{i\phi_{\alpha} \nu_{ij}} & \implies \\
2\Gamma(e^{i\phi_{\alpha}} - e^{i\phi_{\bar{\alpha}}}) + D\sigma_{\alpha} e^{i\frac{\pi}{2}} (e^{i\phi_{\alpha}} + e^{i\phi_{\bar{\alpha}}}) = 0 &
\end{aligned} \tag{5.3.85}$$

We see immediately that when  $D = 0$ , a solution is given by  $\phi_{\alpha} = \phi_{\bar{\alpha}} = \pm \frac{\pi}{2}$  and  $\chi_1, \chi_2 \neq 0$ , which agrees well with reference [2]. If  $\Gamma = 0$ , then  $\phi_{\alpha} = \phi_{\bar{\alpha}} + \pi = n\pi$  and  $\chi_1, \chi_2 \neq 0$ , where  $n$  is an integer. When both  $D$  and  $\Gamma$  are non-zero, the situation becomes more complicated, and solutions should be checked individually for different interaction parameters.

**Topologically gapped spin liquid** Finally, we consider the topologically gapped spin liquid, which effectively is described by Kane-Mele model for the topological insulator phase on honeycomb lattice:

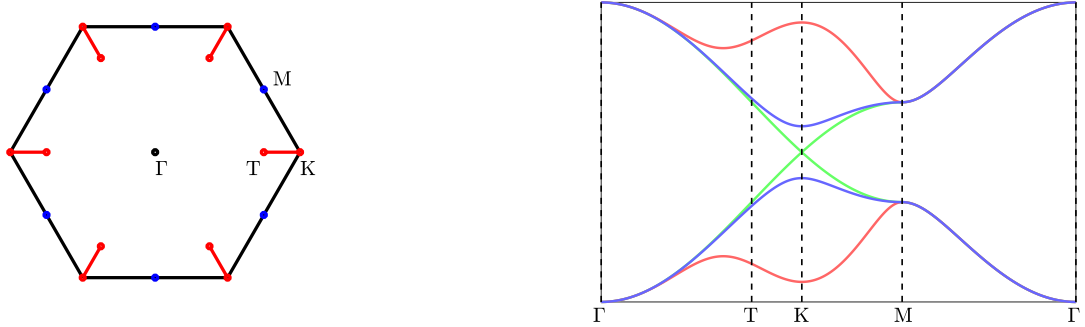
$$\hat{H}_{(\text{topological})} = C_1 \sum_{\langle i,j \rangle} \sum_{\alpha} \hat{f}_{i\alpha}^{\dagger} \hat{f}_{j\alpha} + iC_2 \sum_{\langle\langle i,j \rangle\rangle} \sum_{\alpha} \sigma_{\alpha} \nu_{ij} \hat{f}_{i\alpha}^{\dagger} \hat{f}_{j\alpha} + \text{h.c.}, \tag{5.3.86}$$

where  $C_1, C_2 \in \mathbb{R} \setminus \{0\}$ . In similar manner as for chiral gapped spin liquid phase, we get:

$$D\sigma_{\alpha} \sin \phi_{\bar{\alpha}} - J_+ \cos \phi_{\alpha} - J_- \cos \phi_{\bar{\alpha}} = 0, \tag{5.3.87}$$

$$2J_2\sigma_\alpha(e^{i\phi_\alpha} + e^{i\phi_{\bar{\alpha}}}) - De^{i\frac{\pi}{2}}(e^{i\phi_\alpha} - e^{i\phi_{\bar{\alpha}}}) = 0. \quad (5.3.88)$$

Here, when  $D = 0$ , a solution is given by  $\phi_\alpha = -\phi_{\bar{\alpha}} = \pm\sigma_\alpha\frac{\pi}{2}$  and  $\chi_1, \chi_2 \neq 0$ , which also agrees with reference [2]. If  $J_2 = 0$ , then  $\phi_\alpha = \phi_{\bar{\alpha}} = n\pi$  and  $\chi_1, \chi_2 \neq 0$ , where  $n$  is an integer. The dispersions  $E_{\vec{k}\alpha}^{(\pm)}$  for the presented phases are plotted in figure 7b.



(a) First Brillouin zone and some important points:  $\Gamma$ , T, K and M. The distance from  $\Gamma$  to T is  $\frac{3}{4}$  of distance from  $\Gamma$  to K. The  $\Gamma$ -point should not be confused with the anisotropic interaction parameter  $\Gamma$ .

(b) Dispersions  $E_{\vec{k}\alpha}^{(\pm)}$  as functions of  $\vec{k}$  for the three spin liquid phases. The points  $\Gamma$ , T, K, M are defined in figure 7a. The green plot is for gapless spin liquid, red for chiral gapped spin liquid, and blue for topologically gapped spin liquid. In half-filling case, the lower bands are occupied in the ground state, and upper bands represent excitations. The numerical parameters are  $J_1 = 1$ ,  $J_2 = 0.5$ ,  $\Gamma = 0.1$ , and  $D = 0$ . For chiral and topologically gapped spin liquids, we used  $\chi_2 = 0.5$ .

**Figure 7:** First Brillouin zone and dispersions for different quantum spin liquids in Abrikosov fermion mean-field theory.

We see that equations 5.3.84 and 5.3.87 are exactly the same. Thus, for a given set of interaction parameters  $J_2, \Gamma, D$ , we can find necessary  $\phi_\uparrow, \phi_\downarrow$  that give chiral gapped spin liquid phase by simultaneously solving 5.3.87 and 5.3.88. On the other hand, we can find necessary  $\phi_\uparrow, \phi_\downarrow$  that give topologically gapped spin liquid phase by simultaneously solving 5.3.87 and 5.3.85. We have used Levenberg–Marquardt algorithm to solve 5.3.87 numerically, and the found solutions always satisfied either 5.3.88 or 5.3.85. An initial guess close to  $\phi_\uparrow = \phi_\downarrow = \frac{\pi}{2}$  mostly returned a solution for chiral gapped spin liquid phase, whilst an initial guess close to  $\phi_\uparrow = -\phi_\downarrow = \frac{\pi}{2}$  mostly returned a solution for topologically gapped spin liquid phase.

### 5.3.6 Summing over first Brillouin zone

In subsection 5.1.2, we defined reciprocal space and first Brillouin zone  $\mathfrak{B}_1$  of honeycomb lattice. In addition, in 5.3.25, we defined a  $\vec{k}$ -sum over  $\mathfrak{B}_1$  without further specifications. In order to define this sum more precisely, we should define boundary conditions for our honeycomb lattice. In this thesis, we will consider *periodic boundary condition* along the direct lattice primitive vectors  $\{\vec{a}_1, \vec{a}_2\}$  defined in subsection 5.1.2. We start by writing  $\vec{k}$  as a linear combination of  $\vec{b}_1$  and  $\vec{b}_2$ :

$$\vec{k} = m_1\vec{b}_1 + m_2\vec{b}_2. \quad (5.3.89)$$

We now determine  $\{m_1, m_2\}$  by implementing periodic boundary condition. We had that each sublattice had  $N$  sites. Suppose that there are  $\mathcal{N}_1$  sites in  $\vec{a}_1$  direction and  $\mathcal{N}_2$  sites in  $\vec{a}_2$  direction, so that  $N = \mathcal{N}_1\mathcal{N}_2$ . Going back to Fourier transformation formula 5.3.25, we then must have that:

$$\hat{f}_{\vec{r}+\mathcal{N}_j\vec{a}_j} = \hat{f}_{\vec{r}} \implies \sum_{\vec{k} \in \mathfrak{B}_1} e^{i\vec{k}\cdot\vec{r}} \hat{f}_{\vec{k}} = \sum_{\vec{k} \in \mathfrak{B}_1} e^{i\mathcal{N}_j\vec{k}\cdot\vec{a}_j} e^{i\vec{k}\cdot\vec{r}} \hat{f}_{\vec{k}} \implies \mathcal{N}_j\vec{k}\cdot\vec{a}_j = 2\pi n_j; \quad n_j \in \mathbb{Z}. \quad (5.3.90)$$

Combining 5.3.89, 5.3.90 and 5.1.5, we have that:

$$m_i = \frac{n_i}{\mathcal{N}_i}; \quad i \in \{1, 2\}. \quad (5.3.91)$$

Finally, as discussed in subsection 5.1.2, we had that first Brillouin zone is periodic and equivalent to the area spanned by  $\vec{b}_1$  and  $\vec{b}_2$ . Inserting 5.3.91 into 5.3.89, and setting  $\mathcal{N}_1 = \mathcal{N}_2 = \mathcal{N}$ , we end up with following proposition:



**Proposition 5.5.** Given periodic boundary condition along translation vectors  $\vec{a}_1 = \vec{e}_1$  and  $\vec{a}_2 = \vec{e}_2$ , suppose that each sublattice of our honeycomb lattice has  $\mathcal{N}$  sites along each of these directions, so that  $\mathcal{N}^2 = N$ . Then, the  $\vec{k}$ -sum in 5.3.25 runs over  $\mathfrak{B}_1$ , defined by:

$$\mathfrak{B}_1 := \left\{ \vec{k} \mid k_x = \frac{2\pi}{a\mathcal{N}\sqrt{3}}(n_x - n_y); \quad k_y = \frac{2\pi}{3a\mathcal{N}}(n_x + n_y); \quad n_x, n_y \in \{1, 2, \dots, \mathcal{N}\} \right\}. \quad (5.3.92)$$

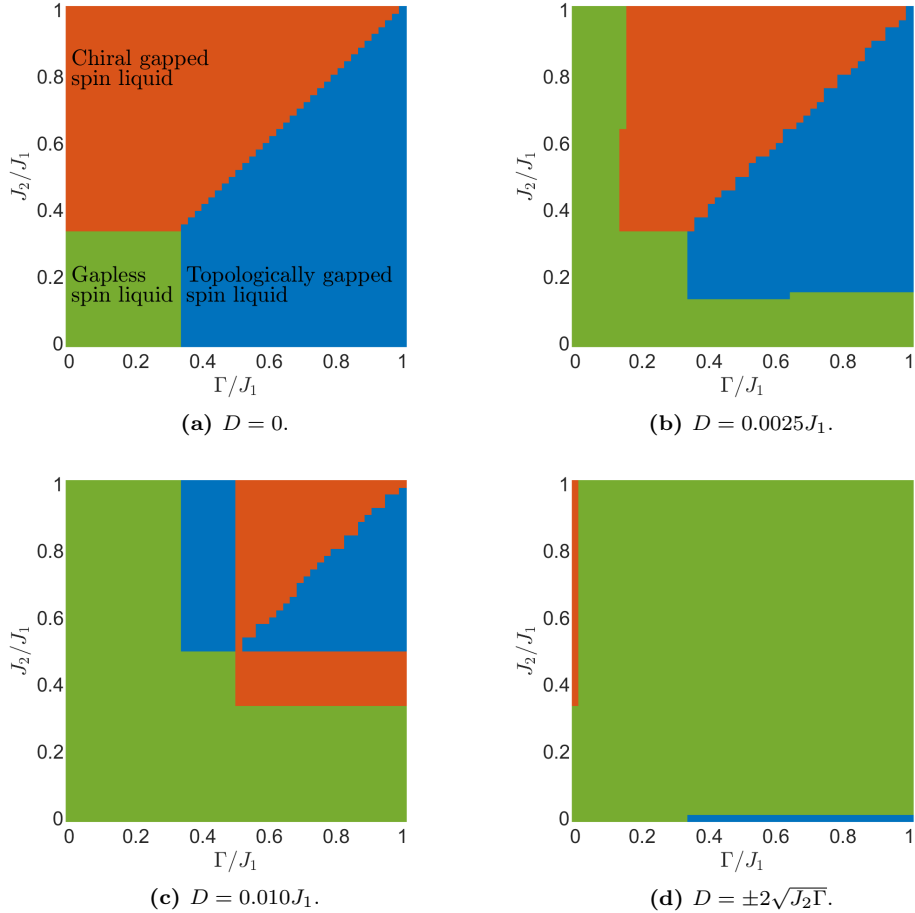
With this proposition, we can now evaluate our  $\vec{k}$ -sums numerically.

### 5.3.7 Numerical method and phase diagram

Our next step is to determine mean-field parameters  $\chi_1, \chi_2, \phi_\uparrow, \phi_\downarrow$  as functions of interaction parameters  $J_1, J_2, \Gamma, D$ . In the same manner as in 4.7.9, we can differentiate the ground state average of 5.3.81 with respect to  $\chi_1, \chi_2, \phi_\uparrow, \phi_\downarrow$ , and show that all should be equal to 0. Thus, our aim is to find minimal critical point of the total ground state energy in 5.3.76, with respect to mean-field parameters. We have used symbolic computation to do differentiation of total energy and find self-consistency equations. Then, by using the Levenberg–Marquardt algorithm, we have solved the four resulting non-linear equations numerically. For each set of interaction parameters, we used three initial guesses for the mean-field parameters, with each representing one of the three liquid phases presented in subsection 5.3.5. If solutions for several phases were found at a given point, then we kept the one with lowest total energy. Based on equation 5.3.81, we defined following quantity as transition parameter between gapless and gapped phases:

$$b_1 := \frac{|\chi_2| \left| J_- e^{i\phi_\alpha \nu_{ij}} + J_+ e^{i\phi_\alpha \nu_{ij}} + D \sigma_\alpha e^{i(\phi_\alpha + \frac{\pi}{2}) \nu_{ij}} \right|}{|J_1 \chi_1|}. \quad (5.3.93)$$

Numerically, we defined a phase as gapless, if  $b_1 < 0.0001$ , and gapped otherwise. The resulting phase diagrams can be found in figure 8.



**Figure 8:** Phase diagrams for the extended Kane-Mele-Hubbard model, obtained with Abrikosov fermion mean-field theory for different Dzyaloshinskii-Moriya interactions  $D$ . Green color corresponds to gapless spin liquid phase, red color corresponds to chiral gapped spin liquid phase, and blue color corresponds to topologically gapped spin liquid phase. For all cases, we used  $\mathcal{N} = 20$ , which gives 800 lattice sites in total. The resolution is  $50 \times 50$  points.

For  $D = 0$ , figure 8a reassembles the results from reference [2] very well. The only difference is the numerical value of transition between gapless phase and the other phases, which we see is  $J_2 \vee \Gamma \sim 0.33J_1$  in our case, and  $\sim 0.85J_1$  in the article. This difference might be due to possibly different numerical approaches. As we slightly introduce the DMI, we see from figure 8b that spin liquid gap closes for weak anisotropy with strong isotropic NNN interaction and vice versa. With increasing DMI, the gap continues to close until it reaches initial transition zone  $\sim 0.33J_1$  (we found that this happens at  $D \sim 0.0070J_1$ ). After that, a certain inversion happens between chiral gapped and topologically gapped phases, as seen in figure 8c. Thus, we see that with strong DMI, chiral gapped phase is possible even when  $\Gamma > J_2$ , and topologically gapped phase is possible even when  $\Gamma < J_2$ . Finally, we have used relation 5.2.10 in figure 8d. In this case, the gap closes completely, except for the axes, where  $D = 0$ .

## 5.4 Schwinger boson mean-field approach

As we saw in previous section, Abrikosov fermion mean-field approach is well-suited for studying potential spin liquids in detail. However, the method is at best qualitative, and an analysis with alternative method is reasonable. In this section, we are going to apply Schwinger boson mean-field approach in order to make a deeper analysis of physical phases. In particular, whilst Abrikosov fermion mean-field approach gives insight about spin liquid, Schwinger boson mean-field approach is well-suited for determining where exactly the spin liquid might be expected. This section is structured in similar manner to section 5.3, where we do insertion, decoupling, mean-field approximation, Fourier transform, and diagonalization, which gives us ground state energy and excitations. Based on that, we present physical phases and construct phase diagrams.

### 5.4.1 Schwinger bosons and decoupling

As discussed in section 4.6, the Schwinger bosons are given by

$$\hat{S}_i = \frac{\hbar}{2} \begin{bmatrix} \hat{b}_{i\uparrow}^\dagger & \hat{b}_{i\downarrow}^\dagger \end{bmatrix} \vec{\sigma} \begin{bmatrix} \hat{b}_{i\uparrow} \\ \hat{b}_{i\downarrow} \end{bmatrix} = \frac{\hbar}{2} \sum_{\alpha\beta} \hat{b}_{i\alpha}^\dagger \vec{\sigma}_{\alpha\beta} \hat{b}_{i\beta}, \quad (5.4.1)$$

and are constrained by

$$\hat{n}_i = \sum_{\alpha} \hat{b}_{i\alpha}^\dagger \hat{b}_{i\alpha} = 2S, \quad (5.4.2)$$

where  $S = \frac{1}{2}$  is the spin of electrons in our lattice.

Starting with the isotropic interaction term, we can use 5.4.1, 5.3.8, 5.4.2 and proposition 5.1 to do following decoupling, which also can be found in reference [28]:

$$\hat{S}_i \cdot \hat{S}_j = \frac{\hbar^2}{4} \left[ \hat{B}_{ij}^\dagger \hat{B}_{ij} - \hat{A}_{ij}^\dagger \hat{A}_{ij} - 1 \right], \quad (5.4.3)$$

where we have defined

$$\hat{B}_{ij} := \hat{b}_{i\uparrow}^\dagger \hat{b}_{j\uparrow} + \hat{b}_{i\downarrow}^\dagger \hat{b}_{j\downarrow}; \quad \hat{A}_{ij} := \hat{b}_{i\uparrow} \hat{b}_{j\downarrow} - \hat{b}_{i\downarrow} \hat{b}_{j\uparrow}. \quad (5.4.4)$$

In a very similar manner, we can do following decoupling for anisotropic interaction term, which also can be found in reference [2]:

$$\hat{S}_i \cdot [\text{diag}(-1, -1, 1) \hat{S}_j] = \frac{\hbar^2}{4} \left[ \hat{D}_{ij}^\dagger \hat{D}_{ij} - \hat{E}_{ij}^\dagger \hat{E}_{ij} - 1 \right], \quad (5.4.5)$$

where we have defined

$$\hat{D}_{ij} := \hat{b}_{i\uparrow}^\dagger \hat{b}_{j\uparrow} - \hat{b}_{i\downarrow}^\dagger \hat{b}_{j\downarrow}; \quad \hat{E}_{ij} := \hat{b}_{i\uparrow} \hat{b}_{j\downarrow} + \hat{b}_{i\downarrow} \hat{b}_{j\uparrow}. \quad (5.4.6)$$

Finally, for our purposes, we also want to find similar decoupling for the DMI-term. We will now derive this step in detail. Having from 5.4.1 that

$$\hat{S}^x = \frac{\hbar}{2} (\hat{b}_\uparrow^\dagger \hat{b}_\downarrow + \hat{b}_\downarrow^\dagger \hat{b}_\uparrow); \quad \hat{S}^y = i \frac{\hbar}{2} (\hat{b}_\downarrow^\dagger \hat{b}_\uparrow - \hat{b}_\uparrow^\dagger \hat{b}_\downarrow), \quad (5.4.7)$$

we have that the DMI-component becomes

$$\begin{aligned} \vec{e}_3 \cdot (\hat{S}_i \times \hat{S}_j) &= \hat{S}_i^x \hat{S}_j^y - \hat{S}_i^y \hat{S}_j^x = i \frac{\hbar^2}{4} [(\hat{b}_{i\uparrow}^\dagger \hat{b}_{i\downarrow} + \hat{b}_{i\downarrow}^\dagger \hat{b}_{i\uparrow})(\hat{b}_{j\downarrow}^\dagger \hat{b}_{j\uparrow} - \hat{b}_{j\uparrow}^\dagger \hat{b}_{j\downarrow}) - (\hat{b}_{i\downarrow}^\dagger \hat{b}_{i\uparrow} - \hat{b}_{i\uparrow}^\dagger \hat{b}_{i\downarrow})(\hat{b}_{j\uparrow}^\dagger \hat{b}_{j\downarrow} + \hat{b}_{j\downarrow}^\dagger \hat{b}_{j\uparrow})] = \\ &= i \frac{\hbar^2}{4} [2\hat{b}_{i\uparrow}^\dagger \hat{b}_{i\downarrow} \hat{b}_{j\downarrow}^\dagger \hat{b}_{j\uparrow} - 2\hat{b}_{i\downarrow}^\dagger \hat{b}_{i\uparrow} \hat{b}_{j\uparrow}^\dagger \hat{b}_{j\downarrow}] = i \frac{\hbar^2}{4} [2\hat{b}_{j\downarrow}^\dagger \hat{b}_{i\downarrow} \hat{b}_{i\uparrow}^\dagger \hat{b}_{j\uparrow} - 2\hat{b}_{j\uparrow}^\dagger \hat{b}_{i\uparrow} \hat{b}_{i\downarrow}^\dagger \hat{b}_{j\downarrow}]. \end{aligned} \quad (5.4.8)$$

This can be decoupled in terms of aforementioned mean-field operators in several ways:

$$\begin{aligned} \vec{e}_3 \cdot (\hat{S}_i \times \hat{S}_j) &= i \frac{\hbar^2}{4} [(\hat{b}_{j\uparrow}^\dagger \hat{b}_{i\uparrow} + \hat{b}_{j\downarrow}^\dagger \hat{b}_{i\downarrow})(\hat{b}_{i\uparrow}^\dagger \hat{b}_{j\uparrow} - \hat{b}_{i\downarrow}^\dagger \hat{b}_{j\downarrow}) - (\hat{b}_{j\uparrow}^\dagger \hat{b}_{i\uparrow} - \hat{b}_{j\downarrow}^\dagger \hat{b}_{i\downarrow})(\hat{b}_{i\uparrow}^\dagger \hat{b}_{j\uparrow} + \hat{b}_{i\downarrow}^\dagger \hat{b}_{j\downarrow})] = \\ &= i \frac{\hbar^2}{4} [\hat{B}_{ij}^\dagger \hat{D}_{ij} - \hat{D}_{ij}^\dagger \hat{B}_{ij}], \end{aligned} \quad (5.4.9)$$

or:

$$\begin{aligned} \vec{e}_3 \cdot (\hat{S}_i \times \hat{S}_j) &= i \frac{\hbar^2}{4} [(\hat{b}_{j\downarrow}^\dagger \hat{b}_{i\uparrow} - \hat{b}_{j\uparrow}^\dagger \hat{b}_{i\downarrow})(\hat{b}_{i\uparrow} \hat{b}_{j\downarrow} + \hat{b}_{i\downarrow} \hat{b}_{j\uparrow}) - (\hat{b}_{j\downarrow}^\dagger \hat{b}_{i\uparrow} + \hat{b}_{j\uparrow}^\dagger \hat{b}_{i\downarrow})(\hat{b}_{i\uparrow} \hat{b}_{j\downarrow} - \hat{b}_{i\downarrow} \hat{b}_{j\uparrow})] = \\ &= i \frac{\hbar^2}{4} [\hat{A}_{ij}^\dagger \hat{E}_{ij} - \hat{E}_{ij}^\dagger \hat{A}_{ij}], \end{aligned} \quad (5.4.10)$$

In references [28][2], when several decouplings were possible, an average was taken, so we do the same for the DMI:

$$\vec{e}_3 \cdot (\hat{S}_i \times \hat{S}_j) = i \frac{\hbar^2}{8} [\hat{A}_{ij}^\dagger \hat{E}_{ij} + \hat{B}_{ij}^\dagger \hat{D}_{ij}] + \text{H.c.} \quad (5.4.11)$$

We summarize all these decouplings in the following proposition:

**Proposition 5.6.** Given a set of Schwinger bosons  $\{\hat{b}_{i\alpha}\}$  constrained by 5.4.2, following decouplings are true:

$$\hat{S}_i \cdot \hat{S}_j = \frac{\hbar^2}{4} \left[ \hat{B}_{ij}^\dagger \hat{B}_{ij} - \hat{A}_{ij}^\dagger \hat{A}_{ij} - 1 \right] \quad (5.4.12)$$

$$\hat{S}_i \cdot [\text{diag}(-1, -1, 1) \hat{S}_j] = \frac{\hbar^2}{4} \left[ \hat{D}_{ij}^\dagger \hat{D}_{ij} - \hat{E}_{ij}^\dagger \hat{E}_{ij} - 1 \right] \quad (5.4.13)$$

$$\vec{e}_3 \cdot (\hat{S}_i \times \hat{S}_j) = i \frac{\hbar^2}{8} [\hat{A}_{ij}^\dagger \hat{E}_{ij} + \hat{B}_{ij}^\dagger \hat{D}_{ij}] + \text{H.c.}, \quad (5.4.14)$$

where

$$\hat{B}_{ij} := \hat{b}_{i\uparrow}^\dagger \hat{b}_{j\uparrow} + \hat{b}_{i\downarrow}^\dagger \hat{b}_{j\downarrow}; \quad \hat{A}_{ij} := \hat{b}_{i\uparrow} \hat{b}_{j\downarrow} - \hat{b}_{i\downarrow} \hat{b}_{j\uparrow}; \quad \hat{D}_{ij} := \hat{b}_{i\uparrow}^\dagger \hat{b}_{j\uparrow} - \hat{b}_{i\downarrow}^\dagger \hat{b}_{j\downarrow}; \quad \hat{E}_{ij} := \hat{b}_{i\uparrow} \hat{b}_{j\downarrow} + \hat{b}_{i\downarrow} \hat{b}_{j\uparrow}. \quad (5.4.15)$$

### 5.4.2 Mean-field approximation

In order to make our Hamiltonian quadratic, and hence diagonalizable, we now perform a mean-field approximation with respect to the decoupled operators, as described in section 4.7. We then have that (we also drop constant terms that are not dependent on mean-field parameters):

$$\hat{S}_i \cdot \hat{S}_j \mapsto \frac{\hbar^2}{4} [\langle \hat{B}_{ij} \rangle^* \hat{B}_{ij} - \langle \hat{A}_{ij} \rangle^* \hat{A}_{ij} + \text{H.c.}] + \frac{\hbar^2 |\langle \hat{A}_{ij} \rangle|^2}{4} - \frac{\hbar^2 |\langle \hat{B}_{ij} \rangle|^2}{4} \quad (5.4.16)$$

$$\hat{S}_i \cdot [\text{diag}(-1, -1, 1) \hat{S}_j] \mapsto \frac{\hbar^2}{4} [\langle \hat{D}_{ij} \rangle^* \hat{D}_{ij} - \langle \hat{E}_{ij} \rangle^* \hat{E}_{ij} + \text{H.c.}] + \frac{\hbar^2 |\langle \hat{E}_{ij} \rangle|^2}{4} - \frac{\hbar^2 |\langle \hat{D}_{ij} \rangle|^2}{4} \quad (5.4.17)$$

$$\vec{e}_3 \cdot (\hat{S}_i \times \hat{S}_j) \mapsto i \frac{\hbar^2}{8} [\langle \hat{A}_{ij} \rangle^* \hat{E}_{ij} + \langle \hat{E}_{ij} \rangle \hat{A}_{ij}^\dagger + \langle \hat{B}_{ij} \rangle^* \hat{D}_{ij} + \langle \hat{D}_{ij} \rangle \hat{B}_{ij}^\dagger - \langle \hat{A}_{ij} \rangle^* \langle \hat{E}_{ij} \rangle - \langle \hat{B}_{ij} \rangle^* \langle \hat{D}_{ij} \rangle] + \text{H.c.} \quad (5.4.18)$$

### 5.4.3 Implementing the Schwinger boson constraint: Lagrange multipliers and chemical potential

We can now insert the aforementioned mean-field approximations into the Hamiltonians  $\hat{H}_0$  and  $\hat{H} = \hat{H}_0 + \hat{H}_{\text{DMI}}$ . As mentioned before, the mean-field approximation is at best qualitative, so we have to ensure its self-consistency. First of all, the self-consistency equations should be satisfied. The task is therefore related to total energy minimization with respect to mean-field parameters. In addition, we must have that the Schwinger boson constraint 5.4.2 is true. The latter property can be implemented by introducing Lagrange multipliers, which is done by adding following term to the mean-field Hamiltonian in question:

$$\hat{H}_L = \hbar^2 \sum_i \mu_i (\hat{n}_i - \kappa). \quad (5.4.19)$$

Here,  $\mu_i$  are the Lagrange multipliers, and can physically be regarded as chemical potentials for the Schwinger bosons.  $\kappa = \langle \hat{n}_i \rangle$  is boson density at mean-field level, which is treated as a continuous parameter that represents quantum limit when  $\kappa \rightarrow 0$  and classical limit when  $\kappa \rightarrow \infty$  [24].

### 5.4.4 Mean-field ansatz: the zero-flux mean-field theory

We must have that the mean-field parameters (also known as ansatz)  $\langle \hat{A}_{ij} \rangle$ ,  $\langle \hat{B}_{ij} \rangle$ ,  $\langle \hat{E}_{ij} \rangle$ ,  $\langle \hat{D}_{ij} \rangle$  and the chemical potentials  $\mu_i$  are invariant under gauge-group and physical lattice symmetry groups. The Schwinger boson mean-field theory for a honeycomb lattice has been rigorously studied in reference [28]. It is then shown that there can be only two different Schwinger boson mean-field theories in a honeycomb lattice: zero-flux theory and  $\pi$ -flux theory. In this thesis, we're only going to consider the zero-flux theory.

Based on the zero-flux theory for honeycomb lattice in reference [28] and [2], we reduce our mean-field parameters and chemical potentials to:

**Table 2:** Mean-field parameters for a honeycomb lattice, based on Schwinger boson mean-field zero-flux theory.

Sublattice A:	$\langle \hat{A}_{\langle i,j \rangle} \rangle = -\Delta_1$	$\langle \hat{A}_{\langle\langle i,j \rangle\rangle} \rangle = +\nu_{ij} \Delta_2$	$\langle \hat{B}_{\langle i,j \rangle} \rangle = \langle \hat{B}_{\langle\langle i,j \rangle\rangle} \rangle = \langle \hat{D}_{\langle\langle i,j \rangle\rangle} \rangle = 0$	$\langle \hat{E}_{\langle\langle i,j \rangle\rangle} \rangle = \Delta_3$	$\mu_i = \mu$
Sublattice B:	$\langle \hat{A}_{\langle i,j \rangle} \rangle = +\Delta_1$	$\langle \hat{A}_{\langle\langle i,j \rangle\rangle} \rangle = -\nu_{ij} \Delta_2$	$\langle \hat{B}_{\langle i,j \rangle} \rangle = \langle \hat{B}_{\langle\langle i,j \rangle\rangle} \rangle = \langle \hat{D}_{\langle\langle i,j \rangle\rangle} \rangle = 0$	$\langle \hat{E}_{\langle\langle i,j \rangle\rangle} \rangle = \Delta_3$	$\mu_i = \mu,$

where  $\Delta_1, \Delta_2, \Delta_3, \mu \in \mathbb{R}$ .

### 5.4.5 Fourier transform

We start by taking a look at the Lagrange term:

$$\hat{H}_L = \hbar^2 \mu \sum_i (\hat{n}_i - \kappa). \quad (5.4.20)$$

We have:

$$\sum_i \hat{n}_i = \sum_i \sum_{\alpha} \hat{b}_{i\alpha}^{\dagger} \hat{b}_{i\alpha} = \sum_{\vec{r}} \sum_{\alpha} \sum_X \hat{b}_{\vec{r}\alpha}^{\dagger(X)} \hat{b}_{\vec{r}\alpha}^{(X)}, \quad (5.4.21)$$

where  $X$  runs over sublattices  $A$  and  $B$ . In the same manner as we did in 5.3.25, we define Fourier transform for bosons:

$$\hat{b}_{\vec{r}\alpha}^{(X)} = \frac{1}{\sqrt{N}} \sum_{\vec{k}} e^{i\vec{k}\cdot\vec{r}} \hat{b}_{\vec{k}\alpha}^{(X)}. \quad (5.4.22)$$

We then have:

$$\begin{aligned} \sum_i \hat{n}_i &= \sum_{\vec{r}} \sum_{\alpha} \sum_X \hat{b}_{\vec{r}\alpha}^{\dagger(X)} \hat{b}_{\vec{r}\alpha}^{(X)} = \frac{1}{N} \sum_{\vec{k}\vec{k}'} \sum_{\vec{r}} \sum_{\alpha} \sum_X e^{i(\vec{k}'-\vec{k})\cdot\vec{r}} \hat{b}_{\vec{k}\alpha}^{\dagger(X)} \hat{b}_{\vec{k}'\alpha}^{(X)} = \sum_{\vec{k}\vec{k}'} \sum_{\alpha} \sum_X \delta_{\vec{k}\vec{k}'} \hat{b}_{\vec{k}\alpha}^{\dagger(X)} \hat{b}_{\vec{k}'\alpha}^{(X)} = \\ &= \sum_{\vec{k}} \sum_{\alpha, X} \hat{b}_{\vec{k}\alpha}^{\dagger(X)} \hat{b}_{\vec{k}\alpha}^{(X)} = \sum_{\vec{k}} \sum_X \left[ \hat{b}_{\vec{k}\uparrow}^{\dagger(X)} \hat{b}_{\vec{k}\uparrow}^{(X)} + \hat{b}_{\vec{k}\downarrow}^{\dagger(X)} \hat{b}_{\vec{k}\downarrow}^{(X)} \right] = \sum_{\vec{k}} \sum_X \left[ \hat{b}_{\vec{k}\uparrow}^{\dagger(X)} \hat{b}_{\vec{k}\uparrow}^{(X)} + \hat{b}_{-\vec{k}\downarrow}^{\dagger(X)} \hat{b}_{-\vec{k}\downarrow}^{(X)} \right] = \\ &= \sum_{\vec{k}} \sum_X \left[ \hat{b}_{\vec{k}\uparrow}^{\dagger(X)} \hat{b}_{\vec{k}\uparrow}^{(X)} + \hat{b}_{-\vec{k}\downarrow}^{\dagger(X)} \hat{b}_{-\vec{k}\downarrow}^{(X)} - 1 \right] = \sum_{\vec{k}} \left[ \hat{b}_{\vec{k}\uparrow}^{\dagger(A)} \hat{b}_{\vec{k}\uparrow}^{(A)} + \hat{b}_{\vec{k}\uparrow}^{\dagger(B)} \hat{b}_{\vec{k}\uparrow}^{(B)} + \hat{b}_{-\vec{k}\downarrow}^{\dagger(A)} \hat{b}_{-\vec{k}\downarrow}^{(A)} + \hat{b}_{-\vec{k}\downarrow}^{\dagger(B)} \hat{b}_{-\vec{k}\downarrow}^{(B)} - 2 \right]. \end{aligned} \quad (5.4.23)$$

Inserting 5.4.23 into 5.4.20, we have

$$\begin{aligned} \hat{H}_L &= \hbar^2 \mu \sum_{\vec{r}} \sum_X \sum_{\alpha} \left[ \hat{b}_{\vec{r}\alpha}^{\dagger(X)} \hat{b}_{\vec{r}\alpha}^{(X)} \right] - \kappa = \hbar^2 \mu \left[ \sum_{\vec{r}} \sum_{\alpha} \sum_X \hat{b}_{\vec{r}\alpha}^{\dagger(X)} \hat{b}_{\vec{r}\alpha}^{(X)} - 2 \sum_{\vec{r}} \kappa \right] = \\ &= \hbar^2 \mu \sum_{\vec{k}} \left[ \hat{b}_{\vec{k}\uparrow}^{\dagger(A)} \hat{b}_{\vec{k}\uparrow}^{(A)} + \hat{b}_{\vec{k}\uparrow}^{\dagger(B)} \hat{b}_{\vec{k}\uparrow}^{(B)} + \hat{b}_{-\vec{k}\downarrow}^{\dagger(A)} \hat{b}_{-\vec{k}\downarrow}^{(A)} + \hat{b}_{-\vec{k}\downarrow}^{\dagger(B)} \hat{b}_{-\vec{k}\downarrow}^{(B)} - 2 - 2\kappa \right] = \\ &= \hbar^2 \sum_{\vec{k}} \left[ \begin{bmatrix} \hat{b}_{\vec{k}\uparrow}^{\dagger(A)} & \hat{b}_{\vec{k}\uparrow}^{\dagger(B)} & \hat{b}_{-\vec{k}\downarrow}^{(A)} & \hat{b}_{-\vec{k}\downarrow}^{(B)} \end{bmatrix} \begin{bmatrix} \mu & 0 & 0 & 0 \\ 0 & \mu & 0 & 0 \\ 0 & 0 & \mu & 0 \\ 0 & 0 & 0 & \mu \end{bmatrix} \begin{bmatrix} \hat{b}_{\vec{k}\uparrow}^{(A)} \\ \hat{b}_{\vec{k}\uparrow}^{(B)} \\ \hat{b}_{-\vec{k}\downarrow}^{(A)} \\ \hat{b}_{-\vec{k}\downarrow}^{(B)} \end{bmatrix} - (2 + 2\kappa)\mu \right]. \end{aligned} \quad (5.4.24)$$

We are now ready to put mean-field approximations 5.4.16, 5.4.17 and 5.4.18 into different Hamiltonian terms in  $\hat{H}_0$  and  $\hat{H} = \hat{H}_0 + \hat{H}_{\text{DMI}}$ . Starting with the isotropic NN-interaction term:

$$\hat{H}_1^{(\text{MF})} = -\frac{\hbar^2 J_1}{4} \sum_{\langle i,j \rangle} \left[ \langle \hat{A}_{ij} \rangle^* \hat{A}_{ij} + \text{H.c.} \right] + \frac{\hbar^2 J_1}{4} \sum_{\langle i,j \rangle} |\langle \hat{A}_{ij} \rangle|^2, \quad (5.4.25)$$

we have:

$$\sum_{\langle i,j \rangle} \langle \hat{A}_{ij} \rangle^* \hat{A}_{ij} = \sum_{\langle i,j \rangle} \langle \hat{A}_{ij} \rangle^* (\hat{b}_{i\uparrow} \hat{b}_{j\downarrow} - \hat{b}_{i\downarrow} \hat{b}_{j\uparrow}). \quad (5.4.26)$$

Considering the first sum on the right hand side in 5.4.26, we split the sum into the two sublattices and do the Fourier transform:

$$\begin{aligned} \sum_{\langle i,j \rangle} \langle \hat{A}_{ij} \rangle^* \hat{b}_{i\uparrow} \hat{b}_{j\downarrow} &= \sum_{\vec{r}} \sum_{l=1}^3 \left[ \langle \hat{A}_{\vec{r}, \vec{r}+\vec{\delta}_l^{(A)}} \rangle^* \hat{b}_{\vec{r}\uparrow}^{(A)} \hat{b}_{\vec{r}+\vec{\delta}_l^{(A)}\downarrow}^{(B)} + \langle \hat{A}_{\vec{r}, \vec{r}+\vec{\delta}_l^{(B)}} \rangle^* \hat{b}_{\vec{r}\uparrow}^{(B)} \hat{b}_{\vec{r}+\vec{\delta}_l^{(B)}\downarrow}^{(A)} \right] = \\ \Delta_1 \sum_{\vec{r}} \sum_{l=1}^3 \left[ \hat{b}_{\vec{r}\uparrow}^{(B)} \hat{b}_{\vec{r}+\vec{\delta}_l^{(B)}\downarrow}^{(A)} - \hat{b}_{\vec{r}\uparrow}^{(A)} \hat{b}_{\vec{r}+\vec{\delta}_l^{(A)}\downarrow}^{(B)} \right] &= \Delta_1 \sum_{\vec{k}} \sum_{l=1}^3 \left[ e^{-i\vec{k}\cdot\vec{\delta}_l^{(B)}} \hat{b}_{\vec{k}\uparrow}^{(B)} \hat{b}_{-\vec{k}\downarrow}^{(A)} - e^{-i\vec{k}\cdot\vec{\delta}_l^{(A)}} \hat{b}_{\vec{k}\uparrow}^{(A)} \hat{b}_{-\vec{k}\downarrow}^{(B)} \right]. \end{aligned} \quad (5.4.27)$$

Inserting this back into 5.4.26, we get:

$$\begin{aligned} \sum_{\langle i,j \rangle} \langle \hat{A}_{ij} \rangle^* \hat{A}_{ij} &= \Delta_1 \sum_{\vec{k}} \sum_{l=1}^3 \left[ e^{-i\vec{k}\cdot\vec{\delta}_l^{(B)}} \hat{b}_{\vec{k}\uparrow}^{(B)} \hat{b}_{-\vec{k}\downarrow}^{(A)} - e^{-i\vec{k}\cdot\vec{\delta}_l^{(A)}} \hat{b}_{\vec{k}\uparrow}^{(A)} \hat{b}_{-\vec{k}\downarrow}^{(B)} + \right. \\ &\left. e^{-i\vec{k}\cdot\vec{\delta}_l^{(B)}} \hat{b}_{-\vec{k}\downarrow}^{(B)} \hat{b}_{-\vec{k}\uparrow}^{(A)} - e^{-i\vec{k}\cdot\vec{\delta}_l^{(A)}} \hat{b}_{-\vec{k}\downarrow}^{(A)} \hat{b}_{-\vec{k}\uparrow}^{(B)} \right] = 2\Delta_1 \sum_{\vec{k}} \left[ \eta_{\vec{k}} \hat{b}_{-\vec{k}\downarrow}^{(A)} \hat{b}_{\vec{k}\uparrow}^{(B)} - \eta_{\vec{k}}^* \hat{b}_{-\vec{k}\downarrow}^{(B)} \hat{b}_{\vec{k}\uparrow}^{(A)} \right], \end{aligned} \quad (5.4.28)$$

where:

$$\eta_{\vec{k}} = \sum_{l=1}^3 e^{i\vec{k}\cdot\vec{\delta}_l^{(A)}} = e^{-ik_y a} + 2e^{i\frac{k_y a}{2}} \cos\left(\frac{\sqrt{3}}{2}k_x a\right). \quad (5.4.29)$$

Putting this into 5.4.25, we can organize our Hamiltonian term into following matrix:

$$\hat{H}_1^{(\text{MF})} = \hbar^2 \sum_{\vec{k}} \left[ \frac{J_1 \Delta_1}{2} \begin{bmatrix} \hat{b}_{\vec{k}\uparrow}^{\dagger(A)} & \hat{b}_{\vec{k}\uparrow}^{\dagger(B)} & \hat{b}_{-\vec{k}\downarrow}^{(A)} & \hat{b}_{-\vec{k}\downarrow}^{(B)} \end{bmatrix} \begin{bmatrix} 0 & 0 & 0 & \eta_{\vec{k}} \\ 0 & 0 & -\eta_{\vec{k}}^* & 0 \\ 0 & -\eta_{\vec{k}} & 0 & 0 \\ \eta_{\vec{k}}^* & 0 & 0 & 0 \end{bmatrix} \begin{bmatrix} \hat{b}_{\vec{k}\uparrow}^{(A)} \\ \hat{b}_{\vec{k}\uparrow}^{(B)} \\ \hat{b}_{-\vec{k}\downarrow}^{\dagger(A)} \\ \hat{b}_{-\vec{k}\downarrow}^{\dagger(B)} \end{bmatrix} + \frac{3}{2} J_1 |\Delta_1|^2 \right], \quad (5.4.30)$$

where for the constant term, we have used the fact that there are two sublattices and that each site has three NNs.

Next, in similar manner, we consider the isotropic NNN-interaction sum:

$$\hat{H}_2^{(\text{MF})} = -\frac{\hbar^2 J_2}{4} \sum_{\langle\langle i,j \rangle\rangle} \left[ \langle \hat{A}_{ij} \rangle^* \hat{A}_{ij} + \text{H.c.} \right] + \frac{\hbar^2 J_2}{4} \sum_{\langle\langle i,j \rangle\rangle} |\langle \hat{A}_{ij} \rangle|^2. \quad (5.4.31)$$

We then have that the operator terms is:

$$\begin{aligned} \sum_{\langle\langle i,j \rangle\rangle} \langle \hat{A}_{ij} \rangle^* \hat{A}_{ij} &= \sum_{\langle\langle i,j \rangle\rangle} \langle \hat{A}_{ij} \rangle^* (\hat{b}_{i\uparrow} \hat{b}_{j\downarrow} - \hat{b}_{i\downarrow} \hat{b}_{j\uparrow}); \\ \sum_{\langle\langle i,j \rangle\rangle} \langle \hat{A}_{ij} \rangle^* \hat{b}_{i\uparrow} \hat{b}_{j\downarrow} &= \sum_{\vec{r}} \sum_{l=1}^6 \left[ \langle \hat{A}_{\vec{r}, \vec{r} + \vec{\epsilon}_l} \rangle^* \hat{b}_{\vec{r}\uparrow}^{(A)} \hat{b}_{\vec{r} + \vec{\epsilon}_l \downarrow}^{(A)} + \langle \hat{A}_{\vec{r}, \vec{r} + \vec{\epsilon}_l} \rangle^* \hat{b}_{\vec{r}\uparrow}^{(B)} \hat{b}_{\vec{r} + \vec{\epsilon}_l \downarrow}^{(B)} \right] = \\ &= \sum_{\vec{r}} \sum_{l=1}^6 \left[ \nu_l^{(A)} \Delta_2 \hat{b}_{\vec{r}\uparrow}^{(A)} \hat{b}_{\vec{r} + \vec{\epsilon}_l \downarrow}^{(A)} - \nu_l^{(B)} \Delta_2 \hat{b}_{\vec{r}\uparrow}^{(B)} \hat{b}_{\vec{r} + \vec{\epsilon}_l \downarrow}^{(B)} \right] = \\ &= \sum_{\vec{k}} \sum_{l=1}^6 \Delta_2 \left[ \nu_l^{(A)} e^{-i\vec{k}\cdot\vec{\epsilon}_l} \hat{b}_{\vec{k}\uparrow}^{(A)} \hat{b}_{-\vec{k}\downarrow}^{(A)} - \nu_l^{(B)} e^{-i\vec{k}\cdot\vec{\epsilon}_l} \hat{b}_{\vec{k}\uparrow}^{(B)} \hat{b}_{-\vec{k}\downarrow}^{(B)} \right] = \\ &= \sum_{\vec{k}} \sum_{l=1}^6 \Delta_2 \nu_l^{(A)} e^{-i\vec{k}\cdot\vec{\epsilon}_l} \left[ \hat{b}_{\vec{k}\uparrow}^{(A)} \hat{b}_{-\vec{k}\downarrow}^{(A)} + \hat{b}_{\vec{k}\uparrow}^{(B)} \hat{b}_{-\vec{k}\downarrow}^{(B)} \right]; \\ \sum_{\langle\langle i,j \rangle\rangle} \langle \hat{A}_{ij} \rangle^* \hat{b}_{i\downarrow} \hat{b}_{j\uparrow} &= \sum_{\vec{k}} \sum_{l=1}^6 \Delta_2 \nu_l^{(A)} e^{-i\vec{k}\cdot\vec{\epsilon}_l} \left[ \hat{b}_{\vec{k}\downarrow}^{(A)} \hat{b}_{-\vec{k}\uparrow}^{(A)} + \hat{b}_{\vec{k}\downarrow}^{(B)} \hat{b}_{-\vec{k}\uparrow}^{(B)} \right] = \\ &= \sum_{\vec{k}} \sum_{l=1}^6 \Delta_2 \nu_l^{(A)} e^{i\vec{k}\cdot\vec{\epsilon}_l} \left[ \hat{b}_{\vec{k}\uparrow}^{(A)} \hat{b}_{-\vec{k}\downarrow}^{(A)} + \hat{b}_{\vec{k}\uparrow}^{(B)} \hat{b}_{-\vec{k}\downarrow}^{(B)} \right]. \end{aligned} \quad (5.4.33)$$

$$\begin{aligned} \sum_{\langle\langle i,j \rangle\rangle} \langle \hat{A}_{ij} \rangle^* \hat{b}_{i\downarrow} \hat{b}_{j\uparrow} &= \sum_{\vec{k}} \sum_{l=1}^6 \Delta_2 \nu_l^{(A)} e^{-i\vec{k}\cdot\vec{\epsilon}_l} \left[ \hat{b}_{\vec{k}\downarrow}^{(A)} \hat{b}_{-\vec{k}\uparrow}^{(A)} + \hat{b}_{\vec{k}\downarrow}^{(B)} \hat{b}_{-\vec{k}\uparrow}^{(B)} \right] = \\ &= \sum_{\vec{k}} \sum_{l=1}^6 \Delta_2 \nu_l^{(A)} e^{i\vec{k}\cdot\vec{\epsilon}_l} \left[ \hat{b}_{\vec{k}\uparrow}^{(A)} \hat{b}_{-\vec{k}\downarrow}^{(A)} + \hat{b}_{\vec{k}\uparrow}^{(B)} \hat{b}_{-\vec{k}\downarrow}^{(B)} \right]. \end{aligned} \quad (5.4.34)$$

Inserting 5.4.34 and 5.4.33 into 5.4.32, we have:

$$\sum_{\langle\langle i,j \rangle\rangle} \langle \hat{A}_{ij} \rangle^* \hat{A}_{ij} = -i2\Delta_2 \sum_{\vec{k}} \xi_{\vec{k}} \left[ \hat{b}_{\vec{k}\uparrow}^{(A)} \hat{b}_{-\vec{k}\downarrow}^{(A)} + \hat{b}_{\vec{k}\uparrow}^{(B)} \hat{b}_{-\vec{k}\downarrow}^{(B)} \right], \quad (5.4.35)$$

where

$$\xi_{\vec{k}} = \sum_{l=1}^6 \nu_l^{(A)} \sin(\vec{k} \cdot \vec{\epsilon}_l) = 4 \sin(k_x a \frac{\sqrt{3}}{2}) \left[ \cos(k_y a \frac{3}{2}) - \cos(k_x a \frac{\sqrt{3}}{2}) \right]. \quad (5.4.36)$$

Putting 5.4.35 into 5.4.31, we get:

$$\hat{H}_2^{(\text{MF})} = \hbar^2 \sum_{\vec{k}} \left[ \frac{J_2 \Delta_2}{2} \begin{bmatrix} \hat{b}_{\vec{k}\uparrow}^{\dagger(A)} & \hat{b}_{\vec{k}\uparrow}^{\dagger(B)} & \hat{b}_{-\vec{k}\downarrow}^{(A)} & \hat{b}_{-\vec{k}\downarrow}^{(B)} \end{bmatrix} \begin{bmatrix} 0 & 0 & -i\xi_{\vec{k}} & 0 \\ 0 & 0 & 0 & -i\xi_{\vec{k}} \\ +i\xi_{\vec{k}} & 0 & 0 & 0 \\ 0 & +i\xi_{\vec{k}} & 0 & 0 \end{bmatrix} \begin{bmatrix} \hat{b}_{\vec{k}\uparrow}^{(A)} \\ \hat{b}_{\vec{k}\uparrow}^{(B)} \\ \hat{b}_{-\vec{k}\downarrow}^{\dagger(A)} \\ \hat{b}_{-\vec{k}\downarrow}^{\dagger(B)} \end{bmatrix} + 3J_2 |\Delta_2|^2 \right]. \quad (5.4.37)$$

Next, in a very similar manner, we consider the anisotropic interaction sum:

$$\hat{H}_\Gamma^{(\text{MF})} = -\frac{\hbar^2\Gamma}{4} \sum_{\langle\langle i,j \rangle\rangle} [\langle \hat{E}_{ij} \rangle^* \hat{E}_{ij} + \text{H.c.}] + \frac{\hbar^2\Gamma}{4} \sum_{\langle\langle i,j \rangle\rangle} |\langle \hat{E}_{ij} \rangle|^2. \quad (5.4.38)$$

$$\sum_{\langle\langle i,j \rangle\rangle} \langle \hat{E}_{ij} \rangle^* \hat{E}_{ij} = \sum_{\langle\langle i,j \rangle\rangle} \Delta_3 (\hat{b}_{i\uparrow} \hat{b}_{j\downarrow} + \hat{b}_{i\downarrow} \hat{b}_{j\uparrow}) = 2\Delta_3 \sum_{\vec{k}} \zeta_{\vec{k}} [\hat{b}_{\vec{k}\uparrow}^{(A)} \hat{b}_{-\vec{k}\downarrow}^{(A)} + \hat{b}_{\vec{k}\uparrow}^{(B)} \hat{b}_{-\vec{k}\downarrow}^{(B)}], \quad (5.4.39)$$

where:

$$\zeta_{\vec{k}} = \sum_{l=1}^6 \cos(\vec{k} \cdot \vec{\epsilon}_l) = 2[2 \cos(k_x a \frac{\sqrt{3}}{2}) \cos(k_y a \frac{3}{2}) + \cos(k_x a \sqrt{3})]. \quad (5.4.40)$$

We get:

$$\hat{H}_\Gamma^{(\text{MF})} = \hbar^2 \sum_{\vec{k}} \left[ \frac{\Gamma\Delta_3}{2} \begin{bmatrix} \hat{b}_{\vec{k}\uparrow}^{(A)} & \hat{b}_{\vec{k}\uparrow}^{(B)} & \hat{b}_{-\vec{k}\downarrow}^{(A)} & \hat{b}_{-\vec{k}\downarrow}^{(B)} \end{bmatrix} \begin{bmatrix} 0 & 0 & -\zeta_{\vec{k}} & 0 \\ 0 & 0 & 0 & -\zeta_{\vec{k}} \\ -\zeta_{\vec{k}} & 0 & 0 & 0 \\ 0 & -\zeta_{\vec{k}} & 0 & 0 \end{bmatrix} \begin{bmatrix} \hat{b}_{\vec{k}\uparrow}^{(A)} \\ \hat{b}_{\vec{k}\uparrow}^{(B)} \\ \hat{b}_{-\vec{k}\downarrow}^{(A)} \\ \hat{b}_{-\vec{k}\downarrow}^{(B)} \end{bmatrix} + 3\Gamma|\Delta_3|^2 \right]. \quad (5.4.41)$$

Finally, we determine the DMI-term:

$$\hat{H}_{\text{DMI}}^{(\text{MF})} = i \frac{\hbar^2 D}{8} \sum_{\langle\langle i,j \rangle\rangle} \nu_{ij} [\langle \hat{A}_{ij} \rangle^* \hat{E}_{ij} - \langle \hat{E}_{ij} \rangle^* \hat{A}_{ij} - \langle \hat{A}_{ij} \rangle^* \langle \hat{E}_{ij} \rangle] + \text{H.c.} \quad (5.4.42)$$

Considering the terms separately, we start with:

$$\sum_{\langle\langle i,j \rangle\rangle} \nu_{ij} \langle \hat{A}_{ij} \rangle^* \hat{E}_{ij} = \sum_{\langle\langle i,j \rangle\rangle} \nu_{ij} \langle \hat{A}_{ij} \rangle^* (\hat{b}_{i\uparrow} \hat{b}_{j\downarrow} + \hat{b}_{i\downarrow} \hat{b}_{j\uparrow}); \quad (5.4.43)$$

$$\begin{aligned} \sum_{\langle\langle i,j \rangle\rangle} \nu_{ij} \langle \hat{A}_{ij} \rangle^* \hat{b}_{i\uparrow} \hat{b}_{j\downarrow} &= \sum_{\vec{r}} \sum_{l=1}^6 \left[ \nu_l^{(A)} \nu_l^{(A)} \Delta_2 \hat{b}_{\vec{r}\uparrow}^{(A)} \hat{b}_{\vec{r}+\vec{\epsilon}_l\downarrow}^{(A)} - \nu_l^{(B)} \nu_l^{(B)} \Delta_2 \hat{b}_{\vec{r}\uparrow}^{(B)} \hat{b}_{\vec{r}+\vec{\epsilon}_l\downarrow}^{(B)} \right] = \\ &\Delta_2 \sum_{\vec{r}} \sum_{l=1}^6 [\hat{b}_{\vec{r}\uparrow}^{(A)} \hat{b}_{\vec{r}+\vec{\epsilon}_l\downarrow}^{(A)} - \hat{b}_{\vec{r}\uparrow}^{(B)} \hat{b}_{\vec{r}+\vec{\epsilon}_l\downarrow}^{(B)}] = \Delta_2 \sum_{\vec{k}} \sum_{l=1}^6 e^{-i\vec{k} \cdot \vec{\epsilon}_l} [\hat{b}_{-\vec{k}\downarrow}^{(A)} \hat{b}_{\vec{k}\uparrow}^{(A)} - \hat{b}_{-\vec{k}\downarrow}^{(B)} \hat{b}_{\vec{k}\uparrow}^{(B)}]; \end{aligned} \quad (5.4.44)$$

$$\sum_{\langle\langle i,j \rangle\rangle} \nu_{ij} \langle \hat{A}_{ij} \rangle^* \hat{b}_{i\downarrow} \hat{b}_{j\uparrow} = \Delta_2 \sum_{\vec{k}} \sum_{l=1}^6 e^{i\vec{k} \cdot \vec{\epsilon}_l} [\hat{b}_{-\vec{k}\downarrow}^{(A)} \hat{b}_{\vec{k}\uparrow}^{(A)} - \hat{b}_{-\vec{k}\downarrow}^{(B)} \hat{b}_{\vec{k}\uparrow}^{(B)}]. \quad (5.4.45)$$

Putting 5.4.45 and 5.4.44 into 5.4.43, we get:

$$\sum_{\langle\langle i,j \rangle\rangle} \nu_{ij} \langle \hat{A}_{ij} \rangle^* \hat{E}_{ij} = 2\Delta_2 \sum_{\vec{k}} \zeta_{\vec{k}} [\hat{b}_{-\vec{k}\downarrow}^{(A)} \hat{b}_{\vec{k}\uparrow}^{(A)} - \hat{b}_{-\vec{k}\downarrow}^{(B)} \hat{b}_{\vec{k}\uparrow}^{(B)}]. \quad (5.4.46)$$

In similar manner,

$$\sum_{\langle\langle i,j \rangle\rangle} \nu_{ij} \langle \hat{E}_{ij} \rangle^* \hat{A}_{ij} = \sum_{\langle\langle i,j \rangle\rangle} \nu_{ij} \langle \hat{E}_{ij} \rangle^* (\hat{b}_{i\uparrow} \hat{b}_{j\downarrow} - \hat{b}_{i\downarrow} \hat{b}_{j\uparrow}); \quad (5.4.47)$$

$$\begin{aligned} \sum_{\langle\langle i,j \rangle\rangle} \nu_{ij} \langle \hat{E}_{ij} \rangle^* \hat{b}_{i\uparrow} \hat{b}_{j\downarrow} &= \sum_{\vec{r}} \sum_{l=1}^6 \left[ \nu_l^{(A)} \Delta_3 \hat{b}_{\vec{r}\uparrow}^{(A)} \hat{b}_{\vec{r}+\vec{\epsilon}_l\downarrow}^{(A)} + \nu_l^{(B)} \Delta_3 \hat{b}_{\vec{r}\uparrow}^{(B)} \hat{b}_{\vec{r}+\vec{\epsilon}_l\downarrow}^{(B)} \right] = \\ &\Delta_3 \sum_{\vec{r}} \sum_{l=1}^6 \nu_l^{(A)} [\hat{b}_{\vec{r}\uparrow}^{(A)} \hat{b}_{\vec{r}+\vec{\epsilon}_l\downarrow}^{(A)} - \hat{b}_{\vec{r}\uparrow}^{(B)} \hat{b}_{\vec{r}+\vec{\epsilon}_l\downarrow}^{(B)}] = \Delta_3 \sum_{\vec{k}} \sum_{l=1}^6 \nu_l^{(A)} e^{-i\vec{k} \cdot \vec{\epsilon}_l} [\hat{b}_{-\vec{k}\downarrow}^{(A)} \hat{b}_{\vec{k}\uparrow}^{(A)} - \hat{b}_{-\vec{k}\downarrow}^{(B)} \hat{b}_{\vec{k}\uparrow}^{(B)}]; \end{aligned} \quad (5.4.48)$$

$$\sum_{\langle\langle i,j \rangle\rangle} \nu_{ij} \langle \hat{E}_{ij} \rangle^* \hat{b}_{i\downarrow} \hat{b}_{j\uparrow} = \Delta_3 \sum_{\vec{k}} \sum_{l=1}^6 \nu_l^{(A)} e^{i\vec{k} \cdot \vec{\epsilon}_l} [\hat{b}_{-\vec{k}\downarrow}^{(A)} \hat{b}_{\vec{k}\uparrow}^{(A)} - \hat{b}_{-\vec{k}\downarrow}^{(B)} \hat{b}_{\vec{k}\uparrow}^{(B)}]. \quad (5.4.49)$$

By putting 5.4.49 and 5.4.48 into 5.4.47, we get:

$$\sum_{\langle i,j \rangle} \nu_{ij} \langle \hat{E}_{ij} \rangle^* \hat{A}_{ij} = -i2\Delta_3 \sum_{\vec{k}} \xi_{\vec{k}} [\hat{b}_{-\vec{k}\downarrow}^{(A)} \hat{b}_{\vec{k}\uparrow}^{(A)} - \hat{b}_{-\vec{k}\downarrow}^{(B)} \hat{b}_{\vec{k}\uparrow}^{(B)}]. \quad (5.4.50)$$

Before putting the terms together, we also want to determine the constant term:

$$\sum_{\langle i,j \rangle} \nu_{ij} \langle \hat{A}_{ij} \rangle^* \langle \hat{E}_{ij} \rangle = \sum_{\vec{r}} \sum_{l=1}^6 [\nu_l^{(A)} \nu_l^{(A)} \Delta_2 \Delta_3 - \nu_l^{(B)} \nu_l^{(B)} \Delta_2 \Delta_3] = 0. \quad (5.4.51)$$

By putting 5.4.46, 5.4.50 and 5.4.51 into 5.4.42, then we have:

$$\begin{aligned} & i \frac{\hbar^2 D}{8} \sum_{\langle i,j \rangle} \nu_{ij} \left[ \langle \hat{A}_{ij} \rangle^* \hat{E}_{ij} - \langle \hat{E}_{ij} \rangle^* \hat{A}_{ij} - \langle \hat{A}_{ij} \rangle^* \langle \hat{E}_{ij} \rangle \right] = \\ & \hbar^2 \sum_{\vec{k}} \left[ -\frac{D\Delta_3}{4} \xi_{\vec{k}} + i \frac{D\Delta_2}{4} \zeta_{\vec{k}} \right] [\hat{b}_{-\vec{k}\downarrow}^{(A)} \hat{b}_{\vec{k}\uparrow}^{(A)} - \hat{b}_{-\vec{k}\downarrow}^{(B)} \hat{b}_{\vec{k}\uparrow}^{(B)}] = -\hbar^2 \sum_{\vec{k}} \tau_{\vec{k}}^* [\hat{b}_{-\vec{k}\downarrow}^{(A)} \hat{b}_{\vec{k}\uparrow}^{(A)} - \hat{b}_{-\vec{k}\downarrow}^{(B)} \hat{b}_{\vec{k}\uparrow}^{(B)}], \end{aligned} \quad (5.4.52)$$

where we defined:

$$\tau_{\vec{k}} := \frac{D\Delta_3}{4} \xi_{\vec{k}} + i \frac{D\Delta_2}{4} \zeta_{\vec{k}}. \quad (5.4.53)$$

We now summarize the results of the subsection in the following proposition:

**Proposition 5.7.** The Hamiltonians  $\hat{H}_0$  and  $\hat{H} = \hat{H}_0 + \hat{H}_{\text{DMI}}$  from section 5.2, decoupled with Schwinger bosons as in proposition 5.6 and approximated by the zero-flux mean-field theory summarized in table 2, are given by:

$$\begin{aligned} \hat{H}_0^{(\text{MF})} = \hbar^2 \sum_{\vec{k}} \left[ \begin{array}{cccc} \hat{b}_{\vec{k}\uparrow}^{\dagger(A)} & \hat{b}_{\vec{k}\uparrow}^{\dagger(B)} & \hat{b}_{-\vec{k}\downarrow}^{(A)} & \hat{b}_{-\vec{k}\downarrow}^{(B)} \end{array} \right] & \begin{bmatrix} \mu & 0 & -\psi_{\vec{k}} & \tilde{\eta}_{\vec{k}} \\ 0 & \mu & -\tilde{\eta}_{\vec{k}}^* & -\psi_{\vec{k}} \\ -\psi_{\vec{k}}^* & -\tilde{\eta}_{\vec{k}} & \mu & 0 \\ \tilde{\eta}_{\vec{k}}^* & -\psi_{\vec{k}}^* & 0 & \mu \end{bmatrix} \begin{bmatrix} \hat{b}_{\vec{k}\uparrow}^{(A)} \\ \hat{b}_{\vec{k}\uparrow}^{(B)} \\ \hat{b}_{-\vec{k}\downarrow}^{\dagger(A)} \\ \hat{b}_{-\vec{k}\downarrow}^{\dagger(B)} \end{bmatrix} + \\ & \left. \frac{3}{2} J_1 |\Delta_1|^2 + 3J_2 |\Delta_2|^2 + 3\Gamma |\Delta_3|^2 - (2 + 2\kappa)\mu \right], \end{aligned} \quad (5.4.54)$$

and  $\hat{H}^{(\text{MF})} = \hat{H}_0^{(\text{MF})} + \hat{H}_{\text{DMI}}^{(\text{MF})}$ ;

$$\hat{H}_{\text{DMI}}^{(\text{MF})} = \hbar^2 \sum_{\vec{k}} \left[ \begin{array}{cccc} \hat{b}_{\vec{k}\uparrow}^{\dagger(A)} & \hat{b}_{\vec{k}\uparrow}^{\dagger(B)} & \hat{b}_{-\vec{k}\downarrow}^{(A)} & \hat{b}_{-\vec{k}\downarrow}^{(B)} \end{array} \right] \begin{bmatrix} 0 & 0 & -\tau_{\vec{k}} & 0 \\ 0 & 0 & 0 & \tau_{\vec{k}} \\ -\tau_{\vec{k}}^* & 0 & 0 & 0 \\ 0 & \tau_{\vec{k}}^* & 0 & 0 \end{bmatrix} \begin{bmatrix} \hat{b}_{\vec{k}\uparrow}^{(A)} \\ \hat{b}_{\vec{k}\uparrow}^{(B)} \\ \hat{b}_{-\vec{k}\downarrow}^{\dagger(A)} \\ \hat{b}_{-\vec{k}\downarrow}^{\dagger(B)} \end{bmatrix}, \quad (5.4.55)$$

where

$$\tilde{\eta}_{\vec{k}} := \frac{J_1 \Delta_1}{2} \eta_{\vec{k}}; \quad \psi_{\vec{k}} := \frac{\Gamma \Delta_3}{2} \zeta_{\vec{k}} + i \frac{J_2 \Delta_2}{2} \xi_{\vec{k}}; \quad \tau_{\vec{k}} := \frac{D\Delta_3}{4} \xi_{\vec{k}} + i \frac{D\Delta_2}{4} \zeta_{\vec{k}}, \quad (5.4.56)$$

$$\eta_{\vec{k}} = e^{-ik_y a} + 2e^{i\frac{k_y a}{2}} \cos\left(\frac{\sqrt{3}}{2} k_x a\right), \quad (5.4.57)$$

$$\xi_{\vec{k}} = 4 \sin\left(k_x a \frac{\sqrt{3}}{2}\right) \left[ \cos\left(k_y a \frac{3}{2}\right) - \cos\left(k_x a \frac{\sqrt{3}}{2}\right) \right], \quad (5.4.58)$$

$$\zeta_{\vec{k}} = 2 \left[ 2 \cos\left(k_x a \frac{\sqrt{3}}{2}\right) \cos\left(k_y a \frac{3}{2}\right) + \cos\left(k_x a \sqrt{3}\right) \right]. \quad (5.4.59)$$

Here,  $\kappa$  is boson density, and  $\mu, \Delta_1, \Delta_2, \Delta_3 \in \mathbb{R}$  are mean-field parameters.



### 5.4.6 Diagonalization through Bogoliubov transformation

Having organized our Hamiltonians into matrices, we are now ready for the diagonalization as described in theorem 3.4. We start with the Hermitian matrix presented in 5.4.54, given by:

$$\mathbb{H}_{\vec{k},0}^{(\text{MF})} := \begin{bmatrix} \mu & 0 & -\psi_{\vec{k}} & \tilde{\eta}_{\vec{k}} \\ 0 & \mu & -\tilde{\eta}_{\vec{k}}^* & -\psi_{\vec{k}} \\ -\psi_{\vec{k}}^* & -\tilde{\eta}_{\vec{k}} & \mu & 0 \\ \tilde{\eta}_{\vec{k}}^* & -\psi_{\vec{k}}^* & 0 & \mu \end{bmatrix} \quad (5.4.60)$$

In order to use theorem 3.4, we have to be sure that the matrix is positive definite, which means that all eigenvalues are positive. By using symbolic computation, we find the four eigenvalues of this matrix to be:

$$\lambda_i = \mu(\pm)_1 \sqrt{(\pm)_2 \sqrt{-\tilde{\eta}_{\vec{k}}(\psi_{\vec{k}} - \psi_{\vec{k}}^*)^2 \tilde{\eta}_{\vec{k}}^* + |\psi_{\vec{k}}|^2 + |\tilde{\eta}_{\vec{k}}|^2}} = \mu(\pm)_1 \sqrt{(\pm)_2 2|\tilde{\eta}_{\vec{k}}| \text{Im}\{\psi_{\vec{k}}\} + |\psi_{\vec{k}}|^2 + |\tilde{\eta}_{\vec{k}}|^2}. \quad (5.4.61)$$

In order to keep these eigenvalues positive, we get following constraints:

$$|\psi_{\vec{k}}|^2 + |\tilde{\eta}_{\vec{k}}|^2 \geq 2|\tilde{\eta}_{\vec{k}}| \text{Im}\{\psi_{\vec{k}}\} \quad (5.4.62)$$

$$\mu > \sqrt{2|\tilde{\eta}_{\vec{k}}| \text{Im}\{\psi_{\vec{k}}\} + |\psi_{\vec{k}}|^2 + |\tilde{\eta}_{\vec{k}}|^2}. \quad (5.4.63)$$

The first constraint is always satisfied by definition:

$$|\psi_{\vec{k}}|^2 + |\tilde{\eta}_{\vec{k}}|^2 - 2|\tilde{\eta}_{\vec{k}}| \text{Im}\{\psi_{\vec{k}}\} = \text{Re}\{\psi_{\vec{k}}\}^2 + (|\text{Im}\{\psi_{\vec{k}}\}| - |\tilde{\eta}_{\vec{k}}|)^2 \geq 0. \quad (5.4.64)$$

The second constraint implies that chemical potential for bosons has to be positive. This fact can physically be hard to interpret, because chemical potential for bosons typically is supposed to be negative.

Next, as described in theorem 3.4, we find the energy dispersion by finding eigenvalues of  $\tilde{H}_{\vec{k},0}^{(\text{MF})}$ . By using symbolic computation, we find that the four eigenvalues are:

$$\tilde{\lambda}_i = (\pm)_1 \sqrt{\mu^2 (\pm)_2 2|\tilde{\eta}_{\vec{k}}| \text{Im}\{\psi_{\vec{k}}\} - |\psi_{\vec{k}}|^2 - |\tilde{\eta}_{\vec{k}}|^2}. \quad (5.4.65)$$

We must thus have:

$$\mu^2 > 2|\tilde{\eta}_{\vec{k}}| \text{Im}\{\psi_{\vec{k}}\} + |\psi_{\vec{k}}|^2 + |\tilde{\eta}_{\vec{k}}|^2. \quad (5.4.66)$$

We see that when this is satisfied, the positive definiteness constraint in 5.4.63 is also satisfied, as long as  $\mu > 0$ . We now define the energy dispersion as positive eigenvalues in 5.4.65. After rewriting slightly, we get:

$$E_{\vec{k}}^{\pm} = \sqrt{\mu^2 - (|\tilde{\eta}_{\vec{k}}| \pm \text{Im}\{\psi_{\vec{k}}\})^2 - \text{Re}\{\psi_{\vec{k}}\}^2}. \quad (5.4.67)$$

By using theorem 3.4, we can diagonalize our Hamiltonian 5.4.54 into:

$$\frac{\hat{H}_0^{(\text{MF})}}{\hbar^2} = \sum_{\vec{k}} \left[ E_{\vec{k}}^+ (\hat{\beta}_{\vec{k}\uparrow}^{\dagger(A)} \hat{\beta}_{\vec{k}\uparrow}^{(A)} + \hat{\beta}_{-\vec{k}\downarrow}^{\dagger(A)} \hat{\beta}_{-\vec{k}\downarrow}^{(A)}) + E_{\vec{k}}^- (\hat{\beta}_{\vec{k}\uparrow}^{\dagger(B)} \hat{\beta}_{\vec{k}\uparrow}^{(B)} + \hat{\beta}_{-\vec{k}\downarrow}^{\dagger(B)} \hat{\beta}_{-\vec{k}\downarrow}^{(B)}) + E_{\vec{k}}^+ + E_{\vec{k}}^- + \frac{3}{2} J_1 |\Delta_1|^2 + 3J_2 |\Delta_2|^2 + 3\Gamma |\Delta_3|^2 - (2 + 2\kappa)\mu \right]. \quad (5.4.68)$$

The ground state is then given by absence of  $\beta$ -bosons, which gives us following ground state energy:

$$\frac{E_{\text{(tot)}}}{\hbar^2} = \sum_{\vec{k}} \left[ E_{\vec{k}}^+ + E_{\vec{k}}^- + \frac{3}{2} J_1 |\Delta_1|^2 + 3J_2 |\Delta_2|^2 + 3\Gamma |\Delta_3|^2 - (2 + 2\kappa)\mu \right], \quad (5.4.69)$$

which agrees well with the results in reference [2]<sup>23</sup>.

<sup>23</sup>The only difference is sign and factor for the constant  $\mu$ -term. After checking other references like reference [24], we concluded that the difference is a typo.

Next, in the same manner, we want to find the ground state energy when DMI is included. Considering the matrix:

$$\mathbb{H}_{\vec{k}}^{(\text{MF})} := \mathbb{H}_{\vec{k},0}^{(\text{MF})} + \mathbb{H}_{\vec{k},\text{DMI}}^{(\text{MF})} = \begin{bmatrix} \mu & 0 & -\psi_{\vec{k}} - \tau_{\vec{k}} & \tilde{\eta}_{\vec{k}} \\ 0 & \mu & -\tilde{\eta}_{\vec{k}}^* & -\psi_{\vec{k}} + \tau_{\vec{k}} \\ -\psi_{\vec{k}}^* - \tau_{\vec{k}}^* & -\tilde{\eta}_{\vec{k}} & \mu & 0 \\ \tilde{\eta}_{\vec{k}}^* & -\psi_{\vec{k}}^* + \tau_{\vec{k}}^* & 0 & \mu \end{bmatrix}, \quad (5.4.70)$$

the symbolic computation of eigenvalues of  $\tilde{H}_{\vec{k}}^{(\text{MF})}$  gives following dispersions:

$$E_{\vec{k},\text{DMI}}^{\pm} = \sqrt{\mu^2 \pm \sqrt{\Xi_{\vec{k}} - |\psi_{\vec{k}}|^2 - |\tilde{\eta}_{\vec{k}}|^2 - |\tau_{\vec{k}}|^2}}, \quad (5.4.71)$$

where

$$\begin{aligned} \Xi_{\vec{k}} := & -\psi_{\vec{k}}^2 |\tilde{\eta}_{\vec{k}}|^2 + \psi_{\vec{k}}^2 (\tau_{\vec{k}}^*)^2 + 2|\psi_{\vec{k}}|^2 |\tilde{\eta}_{\vec{k}}|^2 - (\psi_{\vec{k}}^*)^2 |\tilde{\eta}_{\vec{k}}|^2 + \tau_{\vec{k}}^2 (\psi_{\vec{k}}^*)^2 + 2|\psi_{\vec{k}}|^2 |\tau_{\vec{k}}|^2 + \tau_{\vec{k}}^2 |\tilde{\eta}_{\vec{k}}|^2 + \\ & (\tau_{\vec{k}}^*)^2 |\tilde{\eta}_{\vec{k}}|^2 + 2|\tilde{\eta}_{\vec{k}}|^2 |\tau_{\vec{k}}|^2 = |\tilde{\eta}_{\vec{k}}|^2 [(\tau_{\vec{k}}^2 + 2|\tau_{\vec{k}}|^2 + (\tau_{\vec{k}}^*)^2) - (\psi_{\vec{k}}^2 - 2|\psi_{\vec{k}}|^2 + (\psi_{\vec{k}}^*)^2)] + \\ & [(\psi_{\vec{k}} \tau_{\vec{k}}^*)^2 + 2|\psi_{\vec{k}} \tau_{\vec{k}}|^2 + [(\psi_{\vec{k}} \tau_{\vec{k}}^*)^*]^2] = |\tilde{\eta}_{\vec{k}}|^2 [(\tau_{\vec{k}} + \tau_{\vec{k}}^*)^2 - (\psi_{\vec{k}} - \psi_{\vec{k}}^*)^2] + (\psi_{\vec{k}} \tau_{\vec{k}}^* + \psi_{\vec{k}}^* \tau_{\vec{k}})^2 = \\ & |\tilde{\eta}_{\vec{k}}|^2 [4 \operatorname{Re}\{\tau_{\vec{k}}\}^2 + 4 \operatorname{Im}\{\psi_{\vec{k}}\}^2] + 4 \operatorname{Re}\{\psi_{\vec{k}} \tau_{\vec{k}}^*\}^2. \end{aligned} \quad (5.4.72)$$

We have that:

$$\begin{aligned} \psi_{\vec{k}} \tau_{\vec{k}}^* &= (\operatorname{Re}\{\psi_{\vec{k}}\} + i \operatorname{Im}\{\psi_{\vec{k}}\})(\operatorname{Re}\{\tau_{\vec{k}}\} - i \operatorname{Im}\{\tau_{\vec{k}}\}) = \\ \operatorname{Re}\{\psi_{\vec{k}}\} \operatorname{Re}\{\tau_{\vec{k}}\} + \operatorname{Im}\{\psi_{\vec{k}}\} \operatorname{Im}\{\tau_{\vec{k}}\} + i [\operatorname{Im}\{\psi_{\vec{k}}\} \operatorname{Re}\{\tau_{\vec{k}}\} - \operatorname{Re}\{\psi_{\vec{k}}\} \operatorname{Im}\{\tau_{\vec{k}}\}] &\implies \end{aligned} \quad (5.4.73)$$

$$\operatorname{Re}\{\psi_{\vec{k}} \tau_{\vec{k}}^*\} = \operatorname{Re}\{\psi_{\vec{k}}\} \operatorname{Re}\{\tau_{\vec{k}}\} + \operatorname{Im}\{\psi_{\vec{k}}\} \operatorname{Im}\{\tau_{\vec{k}}\}. \quad (5.4.74)$$

We thus obtain:

$$\Xi_{\vec{k}} = 4|\tilde{\eta}_{\vec{k}}|^2 (\operatorname{Re}\{\tau_{\vec{k}}\}^2 + \operatorname{Im}\{\psi_{\vec{k}}\}^2) + 4(\operatorname{Re}\{\psi_{\vec{k}}\} \operatorname{Re}\{\tau_{\vec{k}}\} + \operatorname{Im}\{\psi_{\vec{k}}\} \operatorname{Im}\{\tau_{\vec{k}}\})^2. \quad (5.4.75)$$

We now summarize the results of this subsection:

**Proposition 5.8.** The ground state energies of Hamiltonians  $\hat{H}_0^{(\text{MF})}$  and  $\hat{H}^{(\text{MF})} = \hat{H}_0^{(\text{MF})} + \hat{H}_{\text{DMI}}^{(\text{MF})}$  presented in proposition 5.7 are given by:

$$\frac{E_{\text{(tot)}}}{\hbar^2} = \sum_{\vec{k}} \left[ E_{\vec{k}}^+ + E_{\vec{k}}^- + \frac{3}{2} J_1 |\Delta_1|^2 + 3J_2 |\Delta_2|^2 + 3\Gamma |\Delta_3|^2 - (2 + 2\kappa)\mu \right], \quad (5.4.76)$$

where

$$E_{\vec{k}}^{\pm} = \sqrt{\mu^2 - (|\tilde{\eta}_{\vec{k}}| \pm |\operatorname{Im}\{\psi_{\vec{k}}\}|)^2 - \operatorname{Re}\{\psi_{\vec{k}}\}^2} \quad (5.4.77)$$

for  $\hat{H}_0^{(\text{MF})}$ , and

$$E_{\vec{k}}^{\pm} = \sqrt{\mu^2 \pm \sqrt{\Xi_{\vec{k}} - |\psi_{\vec{k}}|^2 - |\tilde{\eta}_{\vec{k}}|^2 - |\tau_{\vec{k}}|^2}} \quad (5.4.78)$$

for  $\hat{H}^{(\text{MF})}$ , where

$$\Xi_{\vec{k}} = 4|\tilde{\eta}_{\vec{k}}|^2 (\operatorname{Re}\{\tau_{\vec{k}}\}^2 + \operatorname{Im}\{\psi_{\vec{k}}\}^2) + 4(\operatorname{Re}\{\psi_{\vec{k}}\} \operatorname{Re}\{\tau_{\vec{k}}\} + \operatorname{Im}\{\psi_{\vec{k}}\} \operatorname{Im}\{\tau_{\vec{k}}\})^2. \quad (5.4.79)$$

The excitation energies are described by  $E_{\vec{k}}^{\pm}$ .

With  $D = 0$ , 5.4.78 reduces to 5.4.77, as expected.

### 5.4.7 Physical phases, numerical methods and phase diagrams

In general, three different physical phases are expected to appear in Schwinger boson mean-field zero-flux theory. The phases are described by the dispersion<sup>24</sup>  $E_{\vec{k}}^-$  in 5.4.78, and depend on the mean-field parameters  $\Delta_1, \Delta_2, \Delta_3, \mu$  and

<sup>24</sup>Since  $E_{\vec{k}}^+ \geq E_{\vec{k}}^-$ , and because the phases are determined by the gap, the phase information is extracted from  $E_{\vec{k}}^-$ .

interaction parameters  $J_1, J_2, \Gamma, D$ . As discussed in references [28][2], a gapped dispersion ( $E_{\vec{k}}^- > 0; \forall \vec{k}$ ) corresponds to a phase known as *zero-flux  $Z_2$  spin liquid* ( $Z_2$ ). We see that this is obtained when  $\mu \gg \Delta_1, \Delta_2, \Delta_3$ . If the dispersion is gapless, the bosons will begin to condense, leading to an ordered phase. A condensate at the  $\Gamma$ -point corresponds to the *Néel order* (NO), whilst a condensate anywhere between T-point and K-point corresponds to the *incommensurate magnetic order* (IMO).

Just like in Abrikosov fermion mean-field approach, the mean-field parameters for a given set of interaction parameters can be determined by solving self-consistency equations, and choosing solutions that give lowest total energy (or minimizing total energy). Also here, we have used symbolic computation to find self-consistency equations by differentiating total energy 5.4.76 with respect to mean-field parameters. However, constructing relevant initial guesses is now more difficult to do. Therefore, we have used a Monte-Carlo-like method, where we defined initial guesses randomly. For our interaction parameters of interest, we found it most convenient to define  $\Delta_1, \Delta_2, \Delta_3$  as random values between 0 and 1, and  $\mu$  between 0 and 10. For each given set of interaction parameters, we typically generated a set of 60 initial guesses (although some points close to  $\Gamma = 0$  required more guesses in order to find solutions). In addition, the Levenberg–Marquardt algorithm tended to enter imaginary domain due to square-root nature of the dispersion. This difficulty was overcome by doing following transformation<sup>25</sup>:

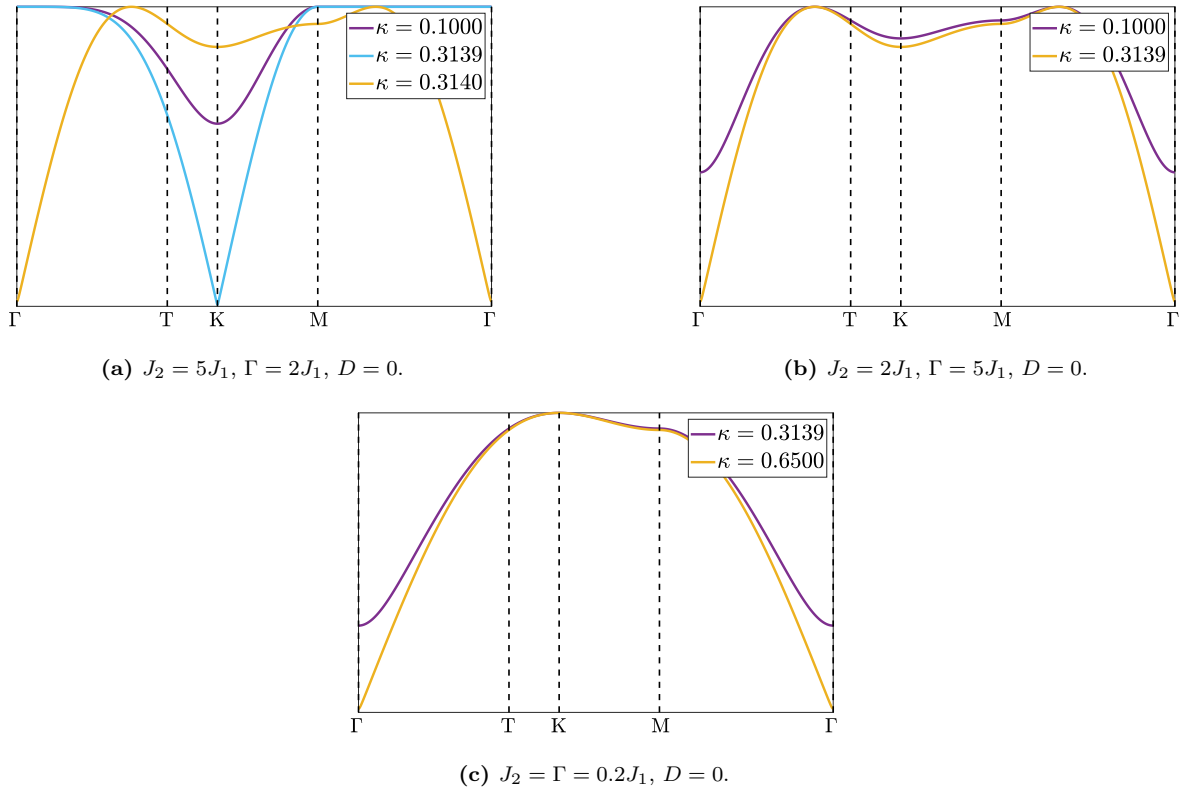
$$E_{\vec{k}}^{\pm} = \sqrt{\mu^2 \pm \sqrt{\Xi_{\vec{k}}^- - |\psi_{\vec{k}}|^2 - |\tilde{\eta}_{\vec{k}}|^2 - |\tau_{\vec{k}}|^2}} \mapsto \sqrt{\left| \mu^2 \pm \sqrt{\Xi_{\vec{k}}^- - |\psi_{\vec{k}}|^2 - |\tilde{\eta}_{\vec{k}}|^2 - |\tau_{\vec{k}}|^2} \right|}. \quad (5.4.80)$$

Based on 5.4.78, the transition parameter between gapped and gapless phases was defined as:

$$t_S := \left| \frac{\mu^2 - \sqrt{\Xi_{\vec{k}_0}^- - |\psi_{\vec{k}_0}|^2 - |\tilde{\eta}_{\vec{k}_0}|^2 - |\tau_{\vec{k}_0}|^2}}{\mu^2} \right|, \quad (5.4.81)$$

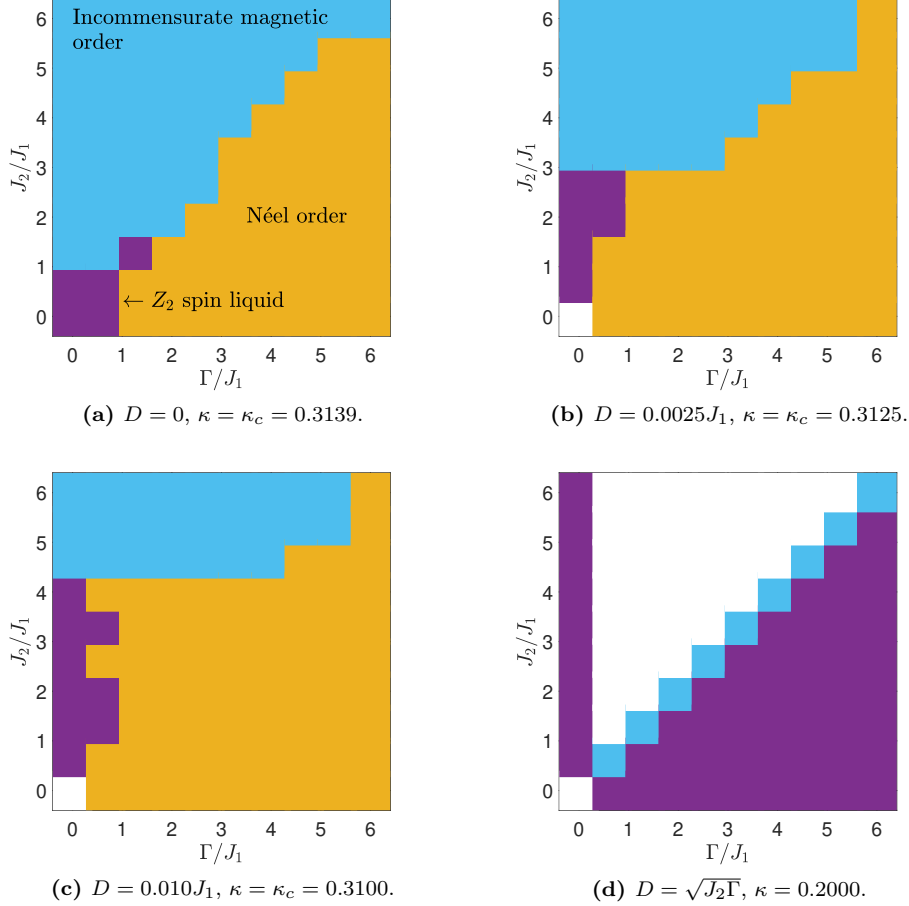
where we numerically defined a phase as gapless if  $t_S < 0.0005$ . In addition, we had to determine a suitable value for boson density,  $\kappa$ . As expected from the quantum nature of spin liquids, a low  $\kappa$ -value (quantum limit) tended to give pure  $Z_2$  phase diagrams. On the other hand, a higher  $\kappa$ -value (closer to classical limit) tended to turn IMO into NO by a first-order phase transition (as expected from reference[28]), and  $Z_2$  into NO by a second-order phase transition. The transitions for  $D = 0$  are illustrated in figure 9.

<sup>25</sup>After some numerical experiments, we found that no alternative solutions were introduced with this transformation. However, the probability of finding a physical solution increased.



**Figure 9:** Normalized plots of the dispersion  $E_k^-$  in 5.4.78 for different boson densities  $\kappa$  when no Dzyaloshinskii-Moriya interactions are present. The critical value  $\kappa_c \sim 0.3139$  seems to reproduce results from reference [2] in the best way. Purple color represents zero-flux  $Z_2$  spin liquid (gapped), yellow color represents Néel order (gapless at  $\Gamma$ -point) and cyan color represents incommensurate magnetic order (gapless between T- and K-point). When approaching extreme quantum limit  $\kappa \ll \kappa_c$ , the entire phase diagram tends to take a continuous second-order transition into spin liquid, as seen from figures 9a, 9b, 9c. Above critical value, as seen in figure 9a, the incommensurate order phase tends to take a discontinuous first-order transition into Néel order phase (mathematically, this is because the dispersion enters imaginary plane at condensation point, and all such solutions suddenly become unphysical). Closer to the classical limit ( $\kappa \gg \kappa_c$ ), the liquid phase continuously turns into Néel order phase, which for  $D = 0$  happens at approximately  $\kappa \sim 0.65$ , as seen in figure 9c. For  $\kappa = \kappa_c$ , we achieve a phase diagram with all three phases, as will be seen in figure 10a. The mean-field parameters were found by solving self-consistency equations and picking a solution with lowest total energy.

The critical boson density  $\kappa_c$ , as defined in figure 9, changed as function of  $D$  - with higher  $D$  giving lower  $\kappa_c$ . In other words, higher DMI introduced more order to the system. Because of that, no such quantity could be defined for the case, where  $D$  is given by 5.2.10. The phase diagrams for different  $D$  and  $\kappa$  can be seen in figure 10.



**Figure 10:** Phase diagrams for the extended Kane-Mele-Hubbard model, obtained with Schwinger boson zero-flux mean-field theory for different Dzyaloshinskii-Moriya interactions  $D$  and boson densities  $\kappa$ . Purple color corresponds to zero-flux  $Z_2$  spin liquid phase, yellow color corresponds to Néel order, cyan color corresponds to incommensurate magnetic order, and white color corresponds to no found solution. For all cases, we used  $\mathcal{N} = 20$ , which gives 800 lattice sites in total. The resolution is only  $10 \times 10$  due to long computation time.

Figure 10a agrees quite well with the results from reference [2], except for that the  $Z_2$ -area is somewhat closer to the origin in our case (the difference might be due to different numerical approaches). From the figures 10a, 10b, 10c, we see that as  $D$  increases, the IMO phase becomes less achievable for weak isotropic NNN interactions,  $J_2$ . At the same time, the  $Z_2$ -area becomes longer, and a spin liquid can be achieved for higher  $J_2$ , when anisotropic interaction  $\Gamma$  is small. However, the  $\kappa$ -value for our phase diagrams is decreasing with increasing  $D$ , meaning that for a constant  $\kappa$ , the order in the system is generally increasing when DMI is introduced.

Constructing a phase diagram with  $D$  as function of  $J_2$  and  $\Gamma$  for a  $\kappa$  close to the ones used in other cases was challenging numerically, as the probability of finding a solution decreased. Therefore, based on the results from figures 9 and 10a, we propose that a such phase diagram would reassemble figure 10a close to the axes, and having NO phase otherwise. After some numerical experiments, we did however discover an interesting result with  $D = 2\sqrt{J_2\Gamma}$  and  $\kappa \sim 0.2$ , as seen in figure 10d. For this particular low value of  $\kappa$ , IMO phase condensed when  $J_2 = \Gamma$ .

## 5.5 Discussion

In this section, we want to briefly discuss the results obtained with Abrikosov fermion mean-field theory and Schwinger boson mean-field zero-flux theory. As discussed in reference [2], the gapless and topologically gapped spin liquids might be suppressed by gauge fluctuations and instanton effects. However, the chiral gapped phase is stable due to nontrivial topology. Thus, although further investigations about the former two spin liquids are needed, the gap opening in Abrikosov fermion mean-field approach might suggest lattice ordering when DMI is introduced. At the same time, for intermediate DMI (when 5.2.10 is not valid), the chiral gapped phase becomes available in some  $\Gamma > J_2$ -areas.

The argument about lattice ordering is further suggested by the Schwinger boson mean-field approach. However, we should still remember that mean-field theories at best are qualitative, and that rigorous conclusions cannot be made.

## 6 Conclusion and outlook

In this thesis, we have considered derivation of a spin-Hamiltonian, the general idea behind bosonization and fermionization, and symmetry in quantum mechanics. We then applied Abrikosov fermion and Schwinger boson mean-field theories to an extended Kane-Mele-Hubbard model, where Dzyaloshinskii-Moriya interactions were included. Based on these theories, we constructed phase diagrams that possibly suggest increased ordering.

Our next goal is to analyze the extended model with other approaches. In particular, we would like to construct a phase diagram by using a classical approach, such as Luttinger-Tisza method[29][30][31][32][33][34] or classical Monte-Carlo simulations[35]. In addition, we would like to extend our Kane-Mele-Hubbard model even further, by introducing a scalar spin chirality interaction term, defined by[36][37]:

$$\hat{\vec{S}}_i \cdot (\hat{\vec{S}}_j \times \hat{\vec{S}}_k), \tag{6.0.1}$$

and repeat the approach in this thesis. In addition, we would like to discuss thermal Hall effect, and how our results can be connected with experiments[38][39].

## A Some important mathematical theorems

**Theorem A.1** (Baker-Hausdorff theorem). Given two operators  $\hat{A}$  and  $\hat{B}$  in the same space, following relation holds:

$$e^{-\hat{B}}\hat{A}e^{\hat{B}} = \sum_{n=0}^{\infty} \frac{1}{n!} [\hat{A}, \hat{B}]_n, \quad (\text{A.0.1})$$

where

$$[\hat{A}, \hat{B}]_0 = \hat{A}; \quad [\hat{A}, \hat{B}]_n = [[\hat{A}, \hat{B}]_{n-1}, \hat{B}]. \quad (\text{A.0.2})$$

**Theorem A.2** (Completeness relation for Pauli matrices). Following identity is true for Pauli matrices:

$$\vec{\sigma}_{\alpha\beta} \cdot \vec{\sigma}_{\gamma\delta} := \sum_{i=1}^3 \sigma_{\alpha\beta}^{(i)} \sigma_{\gamma\delta}^{(i)} = 2\delta_{\alpha\delta}\delta_{\beta\gamma} - \delta_{\alpha\beta}\delta_{\gamma\delta} \quad (\text{A.0.3})$$

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