

**MAGNON TRANSPORT IN NON-COLLINEAR MAGNETIC
STRUCTURES.**

BY

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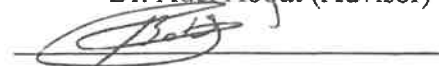


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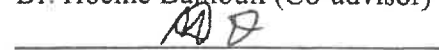
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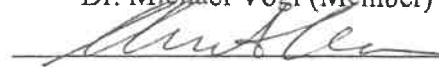
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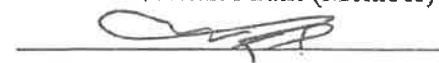
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MAGNON TRANSPORT IN NON-COLLINEAR MAGNETIC STRUCTURES.

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*To my husband Ibrahim,
without you, it wouldn't have been done.*

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List of Abbreviations

LLG	Landau–Lifshitz–Gilbert equation
FM	Ferromagnetic
AFM	Antiferromagnetic
SDW	Spin density waves
SSDW	Superposition of spin density waves
RW-AFM	Row-wise antiferromagnetic
DMI	Dzyaloshinskii–Moriya interaction

Abstract

In this research, we explore the phase space of magnetic structures and investigate the properties of the corresponding ground states. We use Holstein-Primakoff transformations to find the band structure of magnons both analytically and numerically. The study presents an analytical and numerical examination of magnons in non-collinear magnetic structures, encompassing ferromagnetic or antiferromagnetic systems in one, two, and three dimensions. Consequently, this research aspires to provide fundamental insights into the behavior of magnetic materials at both the microscopic and macroscopic levels, paving the way for innovative applications in areas such as information storage, spintronics, and quantum computing.

Keywords: Magnetic Structure, Ground States, Holstein-Primakoff Transformation, Magnons, Band Structure.

ملخص الرسالة

في هذه الدراسة، نستكشف فضاء الطور للتراكيب المغناطيسية وندرس الخصائص المرتبطة بها. نستخدم تحويلات هولشتاين-بريماكوف لتحديد بنية النطاقات الطيفية للماغنونات باستخدام طرق تحليلية وعددية. تقدم الدراسة تحليلاً وتقييماً عددياً للماغنونات ضمن التراكيب المغناطيسية غير المتوازية، وتشمل الدراسة مختلف الأنظمة الفيرومغناطيسية والأنتيفيرومغناطيسية في الأبعاد المختلفة الواحد والثنائي والثلاثي. هذا البحث يلقي الضوء على أسس سلوك المواد المغناطيسية على المستويين المجهرى والماكروسكوبى، والذي بدوره يفتح آفاقاً لتطوير تطبيقات مبتكرة في مجالات عدة مثل تخزين البيانات، التقنيات الدورانية، والحوسبة الكمومية.

الكلمات المفتاحية: البنية المغناطيسية، تحويل هولشتاين-بريماكوف، الماغنونات.

Chapter 1

Introduction

1.1 Motivation

The thesis on "Magnon Transport in Non-Collinear Magnetic Structures" aims to explore and understand the intricate behaviors of magnons—quanta of spin waves—within materials that exhibit complex magnetic textures beyond the traditional parallel alignments. This investigation is critical for advancing our knowledge in condensed matter physics, particularly in understanding how magnons behave in structures where spins are neither parallel nor antiparallel but arranged in more complex patterns.

The significance of this research lies in its potential to uncover new physical phenomena and mechanisms of magnon transport, which could lead to revolutionary applications in the realms of spintronics, quantum computing, and energy-efficient information processing. Spintronics, which leverages the spin of electrons in addition to their charge, stands to benefit immensely from insights into magnon transport, as magnons offer a promising pathway to transmit information with minimal energy loss.

The thesis is inspired by foundational studies in the field, which have explored magnonic behaviors in various settings, utilizing models such as the Landau-Lifshitz-Gilbert equation to simulate the dynamics of magnons under different physical in-

teractions and external conditions. Despite significant advancements, the dynamics of magnons in non-collinear and non-coplanar magnetic structures remain less understood, presenting an opportunity for ground breaking discoveries.

By employing both analytical and numerical methods to model and investigate these complex magnetic systems, the research seeks to bridge the gap between micro-level quantum interactions and macroscopic magnetic properties. This approach not only aims to expand our theoretical understanding of magnonic systems but also envisions the development of new technological applications that leverage the unique properties of magnons for improved performance and functionality of future electronic devices.

In summary, we endeavor to push the boundaries of current magnonic research by delving into the uncharted territories of non-collinear and non-coplanar magnetic structures. Through a combination of analytical rigor and numerical analysis, it aims to contribute valuable insights into magnon transport phenomena, opening new avenues for innovation in technology and material science.

1.2 Organisation of Thesis

The structure of this is designed to provide a comprehensive overview of the research and its context within the broader field, facilitating a clear understanding for readers. **Introduction:** This initial chapter introduces the motivations behind the study, and describes the thesis's objectives.

Advancements in Magnonic Systems: This chapter reviews crucial studies and contributions to magnonics, exploring innovative research directions in noncollinear and noncoplanar magnon systems.

Fundamentals of Magnon Dynamics in Magnetic Structures: Here, the fundamental concepts such as magnetic structures, magnetic moments, and types of magnetic materials are discussed. The chapter further delves into Bloch's theorem, magnons, the atomistic spin model, the Landau-Lifshitz-Gilbert equation, the fourier transform of Heisenberg model energy and Holstein-Primakoff transformations. It also Explores practical applications such as magnonic crystals for waveguides and logic devices, spintronics, and quantum information processing with magnons.

Advanced Analytical Approaches to Magnon Dynamics: Explores sophisticated analytical methods to understand magnon dynamics further, including non-AFM dynamics, Zeeman energy, anisotropy energy, Dzyaloshinskii-Moriya Interaction, pseudodipolar energy, and effects of an oscillating magnetic field. It includes a detailed examination of the dynamics of two spins out of phase.

Discretization of the Schrödinger Equation: Transitions to a mathematical implementation of the Hamiltonian matrix on the context of a Hermitian Hamiltonian framework for lattice systems. Presents a theoretical model for ferromagnetic spins on a honeycomb lattice.

Numerical Analysis of Magnon Dynamics: Focuses on the numerical techniques used to integrate the LLG equation and compares these methods with exact solutions. It includes discussions on the dynamics of single spins subject to a z-axis field and random spin orientations in ferromagnets.

Conclusion and Future Work: The final chapter summarizes the findings and suggests future research directions that could advance further the field of magnonics.

Chapter 2

Advancements in Magnonic Systems

Research in the field of condensed matter physics has significantly advanced our understanding of magnonic systems, particularly through the exploration of magnetic topological states. These studies have paved the way for revolutionary applications in magnonics, leveraging the exotic properties of topological insulators. The unique characteristic of these materials—unidirectional and topologically protected surface or edge states—promises robustness against perturbations, making them ideal candidates for low-energy, high-coherence information carriers in spintronics.

2.1 Key Studies and Contributions

Historical Foundations

1. **Felix Bloch (1930s)**: Introduced the concept of quantized spin waves in ferromagnetic materials, which laid the groundwork for the modern understanding of magnons [4].
2. **Theodore Holstein and Henry Primakoff (1940s)**: Developed a transformation that is foundational in magnon theory, allowed to quantitatively describe the collective excitations in a spin system [5].

3. **T. Nagamiya, K. Yosida, and R. Kubo (1950s):** Extended magnon concepts into complex spin arrangements like antiferromagnets and helimagnets, which enhanced the understanding of magnon dispersion relations and interactions [6].

Key Theoretical Advances

Technological Applications and Modern Research

1. **Magnonic Crystals (2000s-present):** Research into magnonic crystals has shown how these structures can manipulate magnon flow, leading to potential applications in wave-based computing and data storage technologies [7].
2. **Quantum Magnonics (2010s-present):** Investigates the interaction between magnons and quantum systems, such as qubits, to develop quantum information technologies [8].

Latest Innovations

Several pivotal studies have explored magnons dynamics within various systems, employing the Landau-Lifshitz-Gilbert (LLG) equation:

1. **Exploration of Ferromagnetic Spins:** In 2016, X. S. Wang, Ying Su, and X. R. Wang explored the nearest-neighbor ferromagnetic spins on a two-dimensional honeycomb lattice. They described the system by a classical Hamiltonian, which encompasses various interaction terms, including exchange interactions, anisotropy energy the pseudodipolar exchange interaction, and Zeeman energy introduced by an external magnetic field B along the z direction. The magnons dynamics were obtained by considering small deviations of the magnetic moments and applying the LLG equation [9].
2. **DMI Interaction and Spin Waves:** Building on their previous work, X. S. Wang, H. W. Zhang, and X. R. Wang in 2017 studied again the ferromagnetic spins in a (2D) honeycomb lattice using the (LLG) equation focusing

on the Dzyaloshinskii-Moriya Interaction (DMI) and pseudodipolar interaction from spin-orbit coupling. They unveiled that the bulk spin waves of this system possess nontrivial Chern numbers, which give rise to spin waves that are topologically protected, and have gapless edge states that propagate unidirectionally in a plane perpendicular to the magnetization direction [10].

3. **Topological Magnon Insulators:** Andreas Rückriegel, Arne Brataas, and Rembert A. Duine studied the topological magnon insulators and investigated their spin transport properties [11]. They calculated the electronic spin current through a normal metal in the presence and absence of random lattice defects. They also explored the effects of temperature, random lattice defects, and Gilbert damping on the spin current [11]. A topological magnon insulator described by the Hamiltonian living on a honeycomb lattice. Their Hamiltonian takes into account the nearest-neighbors exchange interaction, the next nearest-neighbors Dzyaloshinskii-Moriya interaction (DMI), and the Zeeman energy by a z-direction external magnetic field to stabilize the ferromagnetic ground state [11].
4. **Spin-Wave Propagation in Hexagonal Lattices:** The research by S. Mamica and M. Krawczyk on cylindrical cobalt inclusions arranged in a hexagonal lattice. They studied the impact of external magnetic field and squeezing on the magnons within this hexagonal lattice-based structure, to understand how these factors affect the spin-wave spectrum and magnonic band gaps. They used the LLG equation with exchange field, static external magnetic field, magnetostatic field, and a damping term described by a Gilbert damping parameter to study the dynamics of the magnons in their system [12].
5. **Classical J_1-J_2 Heisenberg Antiferromagnet:** In 2019, Tokuro Shimokawa, Tsuyoshi Okubo, and Hikaru Kawamura explored the classical J_1-J_2 honeycomb-lattice Heisenberg antiferromagnet [13]. Utilizing Monte Carlo simulations, mean-field analysis, and low-temperature expansion techniques to explore the

emergence of multiple-q states under moderate temperatures and magnetic fields. The investigation reveals a phase diagram in the temperature-magnetic field plane, showcasing various ordered states and transitions. The analysis is supported by specific heat measurements, which identify transition points corresponding to the emergence of different ordered states, such as the ring-liquid paramagnetic state and various double-q states. The findings shed light on the intricate behavior of frustrated spin systems, particularly in the context of classical Heisenberg spin systems on a honeycomb lattice [13].

6. **Multiply Periodic States and Skyrmion Crystals:** A.O. Leonov and M. Mostovoy's research into anisotropic frustrated magnets revealed distinct multiply periodic states, including skyrmion crystals. Their research identified five distinct multiply periodic states, including the skyrmion crystal, and elucidated the mechanisms behind their stabilization. The findings suggest potential observations of these states through magnetic resonance and electric polarization measurements [14]. They discussed magnetic skyrmions, emphasizing their topological significance and practical applications in skyrmionics. The study delves into the stabilization mechanisms of these states, particularly focusing on the role of magnetic anisotropy. By exploring a frustrated triangular magnet, the research uncovers eight different phases, with a significant portion occupied by the skyrmion crystal. The results indicate that frustrated magnets can host skyrmions with distinct properties, provided specific conditions are met [14]. These conditions include spiral spin ordering, symmetry axes, commensurate wave vectors, and magnetic anisotropy. The study suggests potential candidates for observing incommensurate magnetic orders and discusses the tunability of magnetocrystalline anisotropy in certain materials [14].

2.2 Innovative Directions in Noncollinear and Noncoplanar Magnonics

Despite these significant advancements, previous studies have not extensively addressed the dynamics of noncollinear and noncoplanar magnonic systems. We introduce a novel approach by employing local coordinates system that is more useful to the non collinear types of structures , which allows for an in-depth exploration of such complex magnetic structures. This innovative methodology not only enriches the theoretical framework of magnonics but also opens new pathways for the experimental realization and manipulation of magnons in noncollinear and noncoplanar configurations.

Our contribution fills a critical gap in the field by extending the study of magnonic systems to encompass noncollinear and noncoplanar states, offering new perspectives on spin dynamics and topological phenomena in condensed matter physics.

Chapter 3

Fundamentals of Magnon

Dynamics in Magnetic Structures

3.1 Magnetic Structures

Magnetic structures refer to the spatial arrangement of magnetic moments within a material, reflecting the distribution of magnetic domains and their interactions. At the atomic level, magnetic moments arise from the intrinsic spin of electrons, giving rise to a magnetic dipole. These dipoles can align parallel or antiparallel to each other, resulting in different magnetic structures. Ferromagnetism, for instance, is characterized by parallel alignment of magnetic moments, leading to strong overall magnetization [15]. Antiferromagnetic materials exhibit antiparallel alignment, causing cancellation of macroscopic magnetic moments. Ferrimagnetism, a combination of ferro- and antiferromagnetic characteristics, is found in materials with distinct magnetic sublattices. The arrangement of magnetic domains, regions with uniform magnetization, plays a crucial role in determining a material's macroscopic magnetic behavior. Understanding magnetic structures is essential for various technological applications, such as data storage, sensors, and magnetic materials design, as it allows for the manipulation and control of magnetic properties for specific functionalities. Advanced techniques, including neutron diffraction, magnetic resonance

imaging, and scanning tunneling microscopy, enable the detailed investigation of magnetic structures at the atomic and nanoscale levels [15].

3.1.1 Magnetic Moments

Magnetic moments refer to the property of a particle, that gives rise to a magnetic field. This property is associated with the intrinsic angular momentum or spin of the particle. Particles have an intrinsic angular momentum, and their spin is associated with a magnetic moment. The magnetic moment is a vector quantity. The magnetic moment is aligned with the axis of rotation or spin of the particle. The magnitude of the magnetic moment is proportional to the magnitude of the spin. The interactions between magnetic moments play a crucial role in determining the magnetic behavior of materials, leading to phenomena such as ferromagnetism, antiferromagnetism, or ferrimagnetism.

The magnetic moment is a vector quantity that represents the magnetic strength and orientation of a magnet or other object that produces a magnetic field. It is a fundamental property of particles such as electrons, atomic nuclei, and molecules, and it is also a property of larger objects like planets or pieces of magnetic materials [16].

For a particle, the magnetic moment is usually associated with its intrinsic spin and orbital angular momentum. For example, electrons have a magnetic moment both because they spin and because they orbit the nucleus in an atom. The combination of these movements generates a tiny magnetic field, which is characterized by the magnetic moment.

The magnetic moment μ is commonly given by:

$$\mu = g \frac{q}{2m} \mathbf{J} \quad (3.1.1)$$

where: $\mathbf{J}$ is the total angular momentum vector (combining both spin and orbital angular momentum), q is the charge of the particle, m is the mass of the particle, g

is the g-factor, which is a dimensionless quantity that differs between particles and accounts for differences in their magnetic properties (for an electron in an atom, this is known as the Landé g-factor) [16].

The unit of the magnetic moment in the International System of Units (SI) is the ampere-square meter ($\text{A} \cdot \text{m}^2$), but it is often also expressed in terms of the Bohr magneton (μ_B) for atomic scale magnetic moments.

We can define a quantity, called the magnetization $\mathbf{M}$, which is the magnetic moment per unit volume V of a solid, hence [17]:

$$\mathbf{m} = \int_V \mathbf{M} \, dV \quad (3.1.2)$$

3.1.2 Types of Magnetic Material

Ferromagnetic Materials

Ferromagnetic spin order refers to the alignment of magnetic moments, or spins, in a material where neighboring spins align parallel to each other as seen in figure 3.1, resulting in a net magnetization even in the absence of an external magnetic field (a spontaneous magnetic moment). In a ferromagnetic material, the individual magnetic moments interact strongly with each other, leading to a collective alignment of spins that persists over macroscopic distances.

At the microscopic level, ferromagnetic order arises primarily due to the exchange interaction between neighboring magnetic moments, which energetically favors parallel alignment of spins. This interaction is influenced by quantum mechanical principles, including those encapsulated by the Pauli exclusion principle and Coulomb interactions, which are reflected in Hund's rules within individual atoms. Hund's rules contribute to maximizing the total spin of electrons in partially filled orbitals, producing significant atomic magnetic moments. When these moments in a material interact via the exchange interaction, they tend to align parallel to each other, leading to a macroscopically ordered ferromagnetic state below the Curie temperature[18].

Ferromagnetic materials exhibit a spontaneous magnetization below the Curie temperature, above which thermal energy disrupts the ordered spin arrangement, causing the material to lose its magnetic properties. Below the Curie temperature, the ferromagnetic material forms magnetic domains, each with its own uniform spin orientation. The alignment of these domains contributes to the overall magnetization of the material [18].

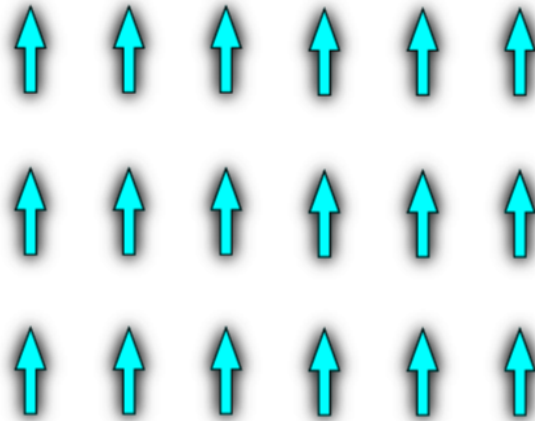


Figure 3.1: Ferromagnetic spin order.

Antiferromagnetic Materials

Antiferromagnetic spin order refers to a magnetic ordering in which neighboring magnetic moments align antiparallel to each other as seen in figure 3.2, resulting in a vanishing net magnetization. In an antiferromagnetic material, adjacent spins pair up and point in opposite directions, canceling out each other's magnetic moments. At the microscopic level, antiferromagnetic spin order arises from the exchange interaction between neighboring magnetic moments, which tends to align them antiparallel to each other. Unlike ferromagnetic materials, where neighboring spins align parallel, in antiferromagnetic materials, neighboring spins align antiparallel, leading to a cancellation of the magnetization.

Antiferromagnetic materials typically have a Néel temperature below which they

exhibit antiferromagnetic order. Below this temperature, the spins within the material form antiferromagnetic domains, where adjacent spins align antiparallel to each other within each domain. However, neighboring domains may have opposite orientations, resulting in a zero net magnetization for the entire material [19].

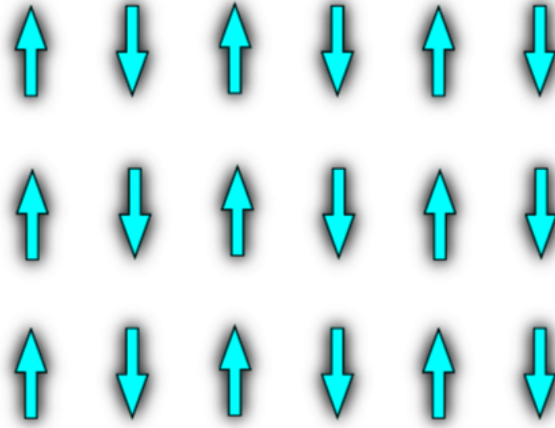


Figure 3.2: Antiferromagnetic spin order.

Ferrimagnetic Materials

Ferrimagnetic spin order is a type of magnetic ordering in which neighboring magnetic moments align antiparallel to each other, but unlike antiferromagnetic ordering, there is a net magnetization due to the unequal magnitude of the magnetic moments as seen in figure 3.3. In ferrimagnetic materials, two or more sublattices of magnetic ions or atoms are present, and these sublattices have different magnetic moments. As a result, even though the neighboring spins align antiparallel, the unequal magnitudes of the moments lead to a net magnetic moment for the material. This unequal magnitude of magnetic moments arises due to different types of ions or atoms in the sublattices, resulting in different magnetic moments for each sublattice. The antiparallel alignment of neighboring moments contributes to a cancellation effect, but because the magnitudes are different, there remains a net magnetic moment.

Ferrimagnetic materials exhibit spontaneous magnetization below a characteristic

temperature known as the Curie temperature. Above this temperature, thermal energy disrupts the ordered magnetic alignment, leading to loss of ferrimagnetic order [20].

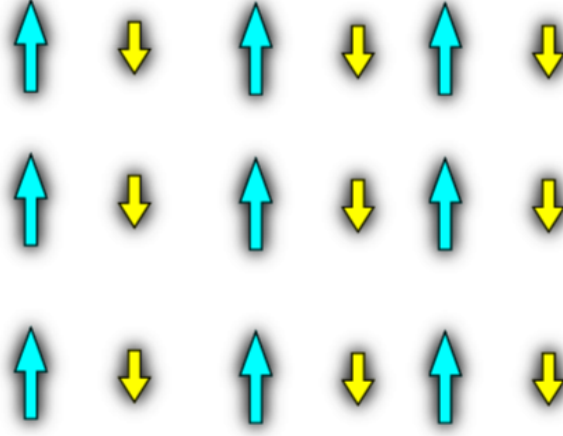


Figure 3.3: Ferrimagnetic spin order.

3.2 Bloch's Theorem

Bloch's theorem in quantum mechanics and solid-state physics describes a fundamental property of the wavefunction of the electrons moving through a regular lattice of atoms -a crystal. According to this theorem, the wave functions $\psi(r)$ of electrons in a periodic lattice can be expressed as the product of a plane wave and a function that has the same periodicity as the crystal lattice. Considering a solid with the periodic potential $V(\mathbf{r} + \mathbf{R}) = V(\mathbf{r})$. Bloch's theorem states that the wavefunctions of the one electron Hamiltonian $H = -(\hbar^2/2m) \nabla^2 + V(\mathbf{r})$ can be chosen to have the form of a plane wave times a function with the periodicity of the lattice:

$$\psi_{nk}(\mathbf{r}) = e^{i\mathbf{k} \cdot \mathbf{r}} u_{nk}(\mathbf{r}) \quad (3.2.3)$$

where

$$u_{nk}(r + R) = u_{nk}(r) \quad (3.2.4)$$

and where the subscript n refers to the n th state associated with the wavevector $\mathbf{k}$, which is the wavevector associated with the electron, $\mathbf{r}$ is the position vector, $e^{i\mathbf{k}\cdot\mathbf{r}}$ is the plane wave component, which describes the free part of the electron's motion, $u_{n\mathbf{k}}(\mathbf{r})$ is a function with the periodicity of the lattice [21].

Bloch's theorem implies that electrons in a crystal do not move entirely freely but are modulated by the periodic potential of the lattice. This modulation leads to the formation of energy bands and band gaps in solids, which are crucial for understanding the electronic properties of materials, including their conductivity, semiconducting behavior, and insulating properties.

We may also state Bloch's theorem in an alternate (but equivalent) form ¹

$$\psi_{n\mathbf{k}}(\mathbf{r} + \mathbf{R}) = e^{i\mathbf{k}\cdot\mathbf{R}}\psi_{n\mathbf{k}}(\mathbf{r}) \quad (3.2.5)$$

Two key points that emerge from Bloch's theorem are discussed below:

1. Variation in Electron Density Within a Unit Cell: In a crystal, where atoms are arranged periodically, periodically the density of electrons $|\psi_{n\mathbf{k}}(\mathbf{r})|^2$ varies from one point to another within the unit cell. This is because $u_{n\mathbf{k}}(\mathbf{r})$ is not a constant but periodic.

$$|\psi_{n\mathbf{k}}(\mathbf{r})|^2 = |e^{i\mathbf{k}\cdot\mathbf{r}}|^2 |u_{n\mathbf{k}}(\mathbf{r})|^2 = |u_{n\mathbf{k}}(\mathbf{r})|^2 \quad (3.2.6)$$

Moreover, due to the periodicity of the $u_{n\mathbf{k}}$ the electron density at a given position $\mathbf{r}$ in a unit cell is the same as at a position $\mathbf{r} + \mathbf{R}$ in different unit cell.

2. Empty Lattice Model: For empty space (i.e. zero potential), electron waves move freely. According to Bloch's theorem, the wavefunctions are plane waves $\psi_{\mathbf{k}} = e^{i\mathbf{k}\cdot\mathbf{r}}$ with energy $E = \hbar^2 k^2 / 2m$. This concept helps us understand how electrons would behave in a perfectly periodic, but empty, structure. Bloch's theorem suggests that in a crystal, electrons behave as if they are both being influenced by the crystal's periodic structure and moving freely at the same time [22].

Bloch's theorem is a versatile principle that applies to a wide range of excitations

¹The proof of Bloch's theorem can be found in several texts such as Ashcroft and Mermin.

within a crystal, including electrons, phonons (vibrations of the crystal lattice), and other forms of excitations. This means that not only the behavior of electrons moving through the periodic potential of a crystal lattice can be described by Bloch's theorem, but also the collective movements and vibrations of atoms within the lattice (phonons), as well as other quasiparticles or disturbances that propagate through the solid's periodic structure. Bloch's theorem provides a unified framework to understand how these various types of excitations exhibit wave-like properties and are modulated by the periodicity of the crystal, leading to the formation of distinctive bands of allowed and forbidden energies, which are crucial for understanding the physical properties of materials [23].

3.3 3Q State

The 3Q state is of considerable interest in condensed matter physics because it represents a compromise between different magnetic interactions and can host interesting phenomena such as chiral magnetic states and skyrmions, which are topologically stable configurations that have potential applications in the fields of magnetic memory and spintronic devices.

The 3Q state, is a noncollinear magnetic structure that can emerge in a two-dimensional triangular lattice due to competing exchange interactions among itinerant electron spins as demonstrated in figure 3.4. This kind of magnetic ordering is notable because the interactions do not favor a simple parallel or antiparallel alignment of spins as seen in ferromagnetic or antiferromagnetic orders, respectively.

Instead, the 3Q state is characterized by the superposition of three spiral spin-density waves (SSDWs), each with a distinct finite wave vector, denoted as $\mathbf{Q}^{(i)}$ for $i = 1, 2, 3$. These vectors describe the periodicity and direction of the spirals in reciprocal space. The superposition of these three SSDWs results in a complex spin texture where the spins are spatially modulated in a way that does not give rise to any net spin magnetization across the lattice [24].

The absence of net magnetization means that, while locally spins might exhibit a

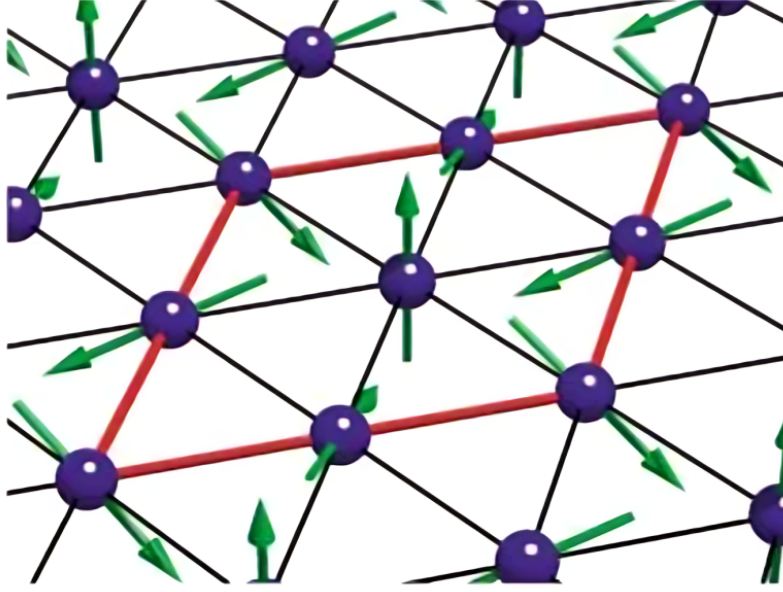


Figure 3.4: The arrangement of magnetic spins in three dimensions within a two-dimensional plane of atoms[1].

complex ordered pattern, the overall magnetic moments cancel out when averaged over the entire lattice. Such a state is energetically favorable in some systems where the competition between different magnetic interactions prevents the spins from aligning in a simple ferromagnetic or antiferromagnetic order, leading to what is known as magnetic frustration [24].

The 3Q state can also be defined as a complex, three-dimensional arrangement of spins where each of the surface's unit cells, composed of four identical atoms, displays noncollinear spin orientation. This intricate spin configuration is constructed as a linear superposition of three separate RW-AFM² structures, each corresponding to one of the three distinct $\mathbf{Q}^i$ wave vectors located at the M points of the Brillouin zone. These RW-AFM components are mutually orthogonal in the spin space, which means that they combine in such a way that their spin directions are perpendicular to one another, creating a rich tapestry of spin textures across the lattice [1].

²Row-wise antiferromagnetic (RW-AFM) order is a specific type of magnetic ordering observed in certain crystalline materials. In this arrangement, the magnetic moments of the atoms are aligned antiparallel to each other within a single row, meaning that each spin points in the opposite direction to its immediate neighbors along that row. Adjacent rows maintain the same antiferromagnetic alignment, creating a regular pattern of alternating spins when viewed along the rows as shown in figure 3.5 [25].

The wave vectors associated with these SDWs typically have the same magnitude but point in different directions that are usually related by the symmetry of the underlying lattice. For example, in a hexagonal lattice, the three wave vectors could be separated by 120 degrees in the reciprocal space.

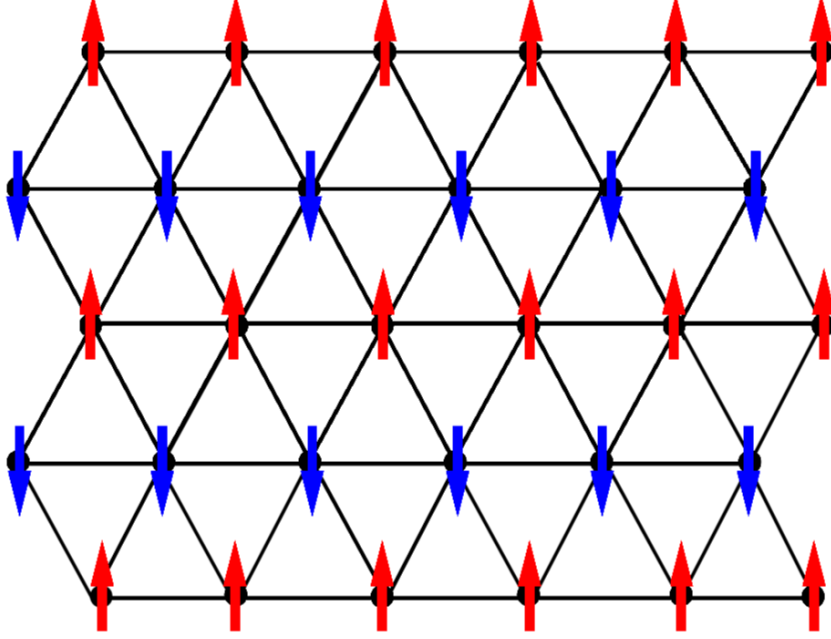


Figure 3.5: The row-wise antiferromagnetic structure shows alternating magnetic moments in opposite directions along each row of atoms. This arrangement cancels out the net magnetization, resulting in no overall magnetic moment.

Talking about 3Q state it is important to incorporate the discussion the role of four-spin interactions in the context of the Landau–Lifshitz–Gilbert (LLG) equation and their impact on complex magnetic states such as the 3Q state. One must consider the delicate interplay between various energy contributions within the system. The 3Q state is notable for its enlarged unit cell in reciprocal space, a manifestation of competing interactions and reduced symmetry within the magnetic system. The emergence of this state is a direct consequence of the intricate balance between exchange interaction, magnetic anisotropy, and, crucially, higher-order interactions like four-spin exchanges [26, 27].

In antiferromagnetic systems, these four-spin interactions can be especially significant. They often come into play in scenarios where the conventional pairwise exchange interactions fail to determine a unique ground state due to magnetic frus-

tration [28]. Here, the four-spin terms can relieve degeneracy by selecting nontrivial orders, potentially giving rise to multifaceted phenomena such as multiferroicity or spin-driven electrical polarization, which have been observed in various antiferromagnetic materials [29].

These higher-order interactions are also sensitive to the geometry of the lattice and can be influenced by the spin-orbit coupling within the material, affecting both the electronic structure and the stability of complex magnetic configurations [30]. This sensitivity underlines the necessity for a comprehensive understanding of the material's underlying physical properties when considering the effects of four-spin interactions on its magnetic states.

3.4 Landau–Lifshitz–Gilbert equation

The LLG equation is a semi-classical equation that is used to describe the dynamics of classical spins that are described by the unit vectors. The LLG equation is used to study the dynamics of magnetization for many materials and structures. Materials acquire magnetization if they are subjected to a nearby a magnetic field. The behavior of local moments is influenced by various interactions, such as spin-spin exchange, magnetocrystalline anisotropy, applied magnetic field, and other weak interactions [31].

The LLG equation was first introduced in 1935 by Landau and Lifshitz and later in 1954, Gilbert developed it further. It takes into account relativistic interactions such as spin orbit coupling effect and includes a damping term, LLG equation is given by [32]:

$$\frac{d\mathbf{m}_i}{dt} = -\gamma_o (\mathbf{H}_{\text{eff}} \times \mathbf{m}_i) + \alpha \left(\mathbf{m}_i \times \frac{d\mathbf{m}_i}{dt} \right) \quad (3.4.7)$$

where $\mathbf{m}_i = \mathbf{m}_i(\mathbf{t})$ is the atom's magnetic moment at site i within the lattice, and $\mathbf{H}_{\text{eff}}$ is the total effective field felt by the local moments due to the different fields like the anisotropy field, external field, demagnetization field, and α is a damping

parameter. The H_{eff} is given by:

$$\mathbf{H}_{\text{eff}} = -\frac{1}{\mu} \frac{\partial \mathcal{H}}{\partial \mathbf{m}} \quad (3.4.8)$$

where $\mathcal{H}$ is the Hamiltonian.

The LLG equation is a partial differential equation, and its solutions provide insights into the behavior of magnetization as it relaxed to the ground state or responds to external stimuli. The LLG equation is particularly important in the study of magnetic switching and relaxation processes, as well as in the design of magnetic devices such as magnetic memories and sensors [33].

The first term resembles the equation that describes how a free spinning object behaves in a magnetic field. The interaction between particles can be described as there is a magnetic field affecting them. This concept is quite useful and has been used a lot in the study of quantum physics in materials [34].

The second term describes how a system returns back to its stable state.

Furthermore, the equation is of special relevance because it solved some important problems in the field of magnetism. Firstly, it helped to figure out how a magnet reacts to changes in an applied magnetic field. This is a problem that is typically treated with linear response theory, and by studying it, scientists predicted a specific frequency at which magnets vibrate and how fast these vibrations fade away. These vibrations were predicted earlier by Bloch in 1930, but Landau and Lifshitz's approach made it easier to understand how things like magnetic ground state orders and the surrounding magnetic field affect these vibrations[34]. Secondly, the Landau-Lifshitz equation was applied to understand how domain walls move. A domain wall is a boundary separating different magnetic domains where the direction of magnetization changes significantly. By considering relaxation in the equation, we could figure out how these domain walls move when influenced by an outside force, and how fast they move. This equation became really important for understanding magnetic structures like solitons, which are localized waves of magnetization that

move around [34].

3.5 Fourier Transform $\mathbf{J}(\mathbf{q})$

In this section, we apply the Fourier Transform $\mathbf{J}(\mathbf{q})$ to analyze a magnetic system, which are fundamental to understanding the behavior of magnetic domains in materials science. The motivation for this study stems from the importance of getting the ground state of the system using fourier transform. The Fourier Transform, with its ability to break down these waveforms into simpler, analyzable components, provides a critical tool in our analysis.

Let us consider the system of spins on a triangular lattice with antiferromagnetic interactions, described by the following Hamiltonian, which is a purely classical spin Hamiltonian:

$$H = -J \sum_{\text{NN}} \mathbf{S}_i \cdot \mathbf{S}_j - \alpha J \sum_{\text{NNN}} \mathbf{S}_i \cdot \mathbf{S}_j \quad (3.5.9)$$

where NN denotes the sum over nearest-neighbor pairs of sites. NNN denotes the sum over next-to-nearest-neighbor pairs of sites. $\mathbf{S}_i$ are the spins at lattice sites. J is the nearest-neighbor exchange interaction. α is the ratio of next-nearest-neighbor exchange interaction to the nearest-neighbor exchange interaction $\alpha = \frac{J_2}{J_1}$. This only works classically because for spin operators such a transform breaks the spin algebra and S_k would not be a spin operator. It is convenient to use the Fourier transform of both terms:

$$\mathbf{S}_i = \frac{1}{\sqrt{N}} \sum_{\mathbf{k}} \mathbf{S}_{\mathbf{k}} e^{i\mathbf{R}_i \cdot \mathbf{k}} \quad (3.5.10)$$

The inverse Fourier transform would be:

$$\mathbf{S}_{\mathbf{k}} = \frac{1}{\sqrt{N}} \sum_{\mathbf{i}} \mathbf{S}_i e^{i\mathbf{R}_i \cdot \mathbf{k}} \quad (3.5.11)$$

where N is the total number of spins.

For the NN term:

$$\begin{aligned}
H &= \sum_{\mathbf{k}, \mathbf{k}'} \mathbf{S}_{\mathbf{k}} \cdot \mathbf{S}_{\mathbf{k}'} \sum_{i,j} J_{i,j} e^{i(\mathbf{k} \cdot \mathbf{R}_i + \mathbf{k}' \cdot \mathbf{R}_j)} \\
&= \sum_{\mathbf{k}, \mathbf{k}'} \mathbf{S}_{\mathbf{k}} \cdot \mathbf{S}_{\mathbf{k}'} \sum_{i,j} J_{i,j} e^{-i\mathbf{k}' \cdot (\mathbf{R}_i - \mathbf{R}_j)} \sum_i e^{i\mathbf{R}_i \cdot (\mathbf{k} + \mathbf{k}')} \\
&= \sum_{\mathbf{k}} J(\mathbf{k}) \mathbf{S}_{\mathbf{k}} \cdot \mathbf{S}_{-\mathbf{k}}
\end{aligned}$$

Where $J(\mathbf{k})$ is given by :

$$J(\mathbf{k}) = \sum_{i,j} J_{i,j} e^{i\mathbf{k} \cdot (\mathbf{R}_i - \mathbf{R}_j)} \quad (3.5.12)$$

$R_i - R_j = \delta_{ij}$, where $i = 1, 2, 3$

For a triangular lattice, we will have three NN vectors $\delta_1, \delta_2, \delta_3$ and six NNN vectors, which are linear combinations of the NN vectors. For simplicity, we are using only three NNN vectors, assuming the lattice has a symmetry that allows us to simplify the NNN sum. In a triangular lattice, each lattice site is surrounded by six next-nearest neighbors (NNN) which form a hexagon around it, taking the lattice constant $a = 1$.

NN Interaction

The NN vectors δ_n for the triangular lattice are:

$$\begin{aligned}
\delta_1 &= (1, 0) \\
\delta_2 &= \left(-\frac{1}{2}, \frac{\sqrt{3}}{2} \right) \\
\delta_3 &= \left(\frac{1}{2}, \frac{\sqrt{3}}{2} \right)
\end{aligned}$$

Using the Fourier transform of the exchange interaction:

$$J_{\text{NN}}(\mathbf{k}) = J \sum_{n=1}^3 e^{i\mathbf{k} \cdot \delta_n}$$

We plug in the vectors δ_n into the formula :

$$J_{\text{NN}}(\mathbf{k}) = J \left(e^{ik_x} + e^{-i\frac{k_x}{2}} e^{i\frac{\sqrt{3}k_y}{2}} + e^{i\frac{k_x}{2}} e^{i\frac{\sqrt{3}k_y}{2}} \right)$$

For each vector, we calculate the exponential term in the Fourier transform:

$$e^{i\mathbf{k} \cdot \delta_n} = \cos(\mathbf{k} \cdot \delta_n) + i \sin(\mathbf{k} \cdot \delta_n)$$

rewriting the equation and notice that the momentum sum have both positive and negative $\mathbf{k}$ and H is symmetric under $\mathbf{k}$ and $-\mathbf{k}$, hence $J(\mathbf{k})$ will contain only the cosines.

$$J_{\text{NN}}(\mathbf{k}) = J \left(\cos(k_x) + \cos\left(\frac{k_x}{2} + \frac{\sqrt{3}k_y}{2}\right) + \cos\left(\frac{k_x}{2} - \frac{\sqrt{3}k_y}{2}\right) \right)$$

NNN Interaction

For NNN, we would sum the contributions over vectors that connect a site to its next-to-nearest neighbors. These vectors are linear combinations of the δ_n vectors. For example, NNN vectors could include $\delta_1 - \delta_2$, $\delta_2 + \delta_3$, and $\delta_3 + \delta_1$. We use the combinations of NN vectors to define the NNN vectors δ_{NNN_n} :

$$\delta_{\text{NNN}_1} = \delta_2 + \delta_3 = (0, \sqrt{3})$$

$$\delta_{\text{NNN}_2} = \delta_3 + \delta_1 = \left(\frac{3}{2}, \frac{\sqrt{3}}{2}\right)$$

$$\delta_{\text{NNN}_3} = \delta_1 - \delta_2 = \left(\frac{3}{2}, \frac{-\sqrt{3}}{2}\right)$$

$$J_{\text{NNN}}(\mathbf{k}) = \alpha J \sum_{\text{NNN vectors}} e^{i\mathbf{k} \cdot \text{NNN vector}}$$

Again, we would apply Euler's formula and focus on the cosine terms after plugging in the NNN vectors.

$$J_{\text{NNN}}(\mathbf{k}) = J \left(e^{i\sqrt{3}k_y} + e^{i\frac{3k_x}{2}} e^{i\frac{\sqrt{3}k_y}{2}} + e^{i\frac{3k_x}{2}} e^{-i\frac{\sqrt{3}k_y}{2}} \right)$$

Using the NNN vectors and the same process:

$$J_{\text{NNN}}(\mathbf{k}) = \alpha J \left(\cos(\sqrt{3}k_y) + \cos\left(\frac{3}{2}k_x + \frac{\sqrt{3}k_y}{2}\right) + \cos\left(\frac{3}{2}k_x - \frac{\sqrt{3}k_y}{2}\right) \right)$$

Combine NN and NNN Contributions

We combine the two results to get the full expression for $J(\mathbf{k})$:

$$J(\mathbf{k}) = J_{\text{NN}}(\mathbf{k}) + J_{\text{NNN}}(\mathbf{k})$$

Now we simplify using trigonometric identities where needed. This involves using the angle sum and difference identities for cosine:

$$\cos(\alpha \pm \beta) = \cos(\alpha)\cos(\beta) \mp \sin(\alpha)\sin(\beta)$$

Applying these identities we get

$$\begin{aligned} J(\mathbf{k}) = & \cos(k_x) + 2 \cos\left(\frac{k_x}{2}\right) \cos\left(\frac{k_y\sqrt{3}}{2}\right) \\ & + \alpha \left[\cos(k_y\sqrt{3}) + 2 \cos\left(\frac{3k_x}{2}\right) \cos\left(\frac{k_y\sqrt{3}}{2}\right) \right], \end{aligned} \tag{3.5.13}$$

From eq. 3.5.9 we can notice that for small alpha ($\alpha < 1/8$), the energy minima are at the corners of the hexagonal Brillouin zone, such as point A in figure 3.6.

These correspond to the 120° Neel structure due to the favorable nearest-neighbor antiferromagnetic interactions, typical of the 3Q state with its triple-Q structure reflecting three magnon condensates with equal intensity.

As α increases but remains less than 1, the minima move to the centers of the faces of the Brillouin zone (like point B). Here, the corresponding wave vectors reflect a different kind of ordering, but still within the 3Q state framework, with a different orientation of the spins than the small α configuration.

When α becomes greater than 1, the minima move away from the boundary of the Brillouin zone, indicating a transition away from the 3Q state to incommensurate spirals, suggesting the ground state's sensitivity to changes in α . The wave vectors for these states are on the lines connecting the origin to the middle of the faces (like point C), which signifies a phase transition in the system as it deviates from the 3Q configuration.

The ground states as a function of α thus display a complex interplay of geometric frustration and spin interactions, where the 3Q state serves as a representative of the intricate magnetic ordering occurring in the system. The semiclassical analysis of the Hamiltonian provides insights into these ground states starting from the 3Q state and considering quantum corrections, which reflect the nontrivial aspects of spin configurations and their evolution with α .

3.6 Magnons

Magnons are quanta of elementary magnetic excitations in magnetic materials. They are collective excitations of the spin orientation of electrons in a magnetic solid, akin to how photons are quantized excitations of electromagnetic radiation. In simpler terms, magnons are like "particles" representing the collective behavior of magnetic spins [35].

When a magnetic material is subjected to an external perturbation, such as a magnetic field or a temperature change, the individual spins within the material can change orientation in certain way to create a wave. These aligned spins can then

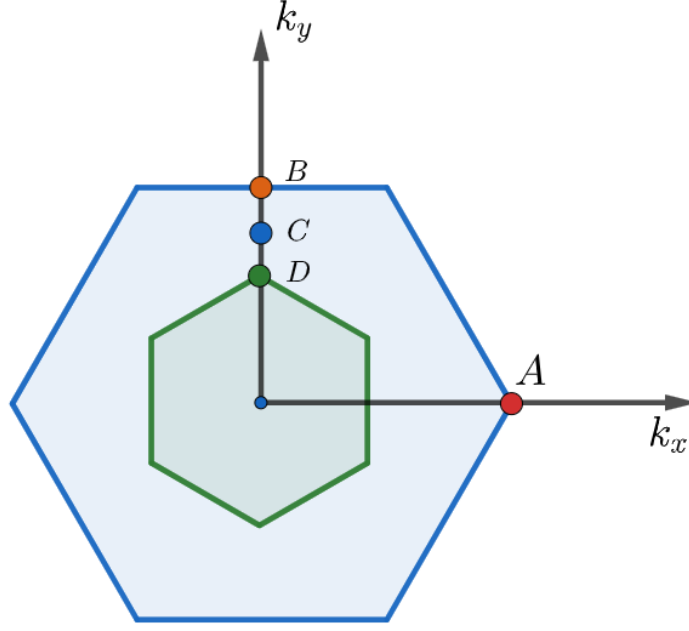


Figure 3.6: The Brillouin zone of a triangular lattice, highlighting the key wave vectors where the minima of the exchange interaction $J(\mathbf{k})$ occur as the parameter α changes. Points A, B, C, D indicate these minima.

collectively oscillate or precess, creating a wave-like disturbance known as magnons. Magnons can be described as wave packets, each carrying a certain amount of energy and momentum. Their properties, such as energy, momentum, and spin, depend on the specific characteristics of the magnetic material and its crystal structure. Magnons energy are given by $\hbar\omega_k$. From quantum mechanical principles, the magnetic moment of a system is determined by the negative gradient of its energy with respect to an applied magnetic field. Therefore, a magnon's magnetic moment is defined by the equation:

$$\mu_k = -\frac{\partial \hbar\omega_k}{\partial \mathbf{H}}, \quad (3.6.14)$$

where $\mathbf{H}$ represents the external magnetic field. This concept enables the analysis of magnetic system perturbations as the dynamics of a magnon gas, providing insightful explanations for various thermodynamic phenomena [36].

The microscopic theory implies that the exchange interaction between neighbor localized spins is dominant in determining the magnetic ground state order of crystals.

The interaction's nature, ferromagnetic or antiferromagnetic, is dictated by the sign of the exchange integral, while its magnitude influences the phase transition temperature. The vast diversity of solids displaying different types of magnetic order, such as ferromagnets and antiferromagnets, underscores the rich complexity of magnetic systems [37].

Bloch's theorem, which is applicable to electrons, phonons, and magnons, states that the wavefunction of particles in a periodic potential can be written as a product of a plane wave modulated by a function with the periodicity of the lattice as given in equation 3.2.5. This implies that for magnons, the collective excitations in a periodic solid, the probability density is expected to be periodic within the unit cell but can vary across different points within the cell. The theorem allows for understanding of the behavior of magnons in various magnetic materials, including ferromagnets, ferrimagnets, and antiferromagnets [23].

Magnons are also recognized for obeying Bose-Einstein statistics, with experiments indicating that the Stokes line in light scattering becomes more intense as the magnon energy approaches or falls below thermal energy [38]. This observation contributed to evidence supporting Bose-Einstein condensation of magnons in different magnetic materials[38].

Understanding magnons is crucial in the study of magnetic materials and their behavior, including phenomena like magnetic phase transitions, magnetic ordering, and magnetic dynamics. They play a central role in various fields such as condensed matter physics, spintronics, and magnonics, where they are exploited for applications ranging from data storage to information processing.

3.7 The Atomistic Spin Model

The foundation of the atomistic spin model lies in a discrete representation of magnetism that describes and investigates the magnetic properties of materials at the atomic level wherein each atom possesses a localized magnetic moment or spin [39]. The Heisenberg spin model is a model that describes a magnetic substance at the

atomic scale for some systems. The dynamics of a system comprising interacting atomic moments are described by a spin Hamiltonian. A standard spin Hamiltonian, denoted as $\mathcal{H}$, which encompasses Heisenberg exchange, anisotropy term, and interaction with an externally applied magnetic field, is expressed as [40]:

$$\mathcal{H} = - \sum_{i < j} J_{ij} \mathbf{m}_i \cdot \mathbf{m}_j - k \sum_i (\mathbf{m}_i \cdot \mathbf{n}_i)^2 - \sum_i \mu_i \mathbf{m}_i \cdot \mathbf{B} \quad (3.7.15)$$

The first term is the Heisenberg exchange, it accounts for the quantum mechanical exchange interaction between two neighbouring electrons with overlapping wave functions, where J_{ij} is the exchange interaction between spins, i is the local atomic site, $\mathbf{m}_i$ is the magnetic moment on atomic site i , $\mathbf{m}_j$ is on a neighboring atomic site j . k on the other hand is the uniaxial anisotropy constant on site i , $\mathbf{n}_i$ is a unit vector giving the magnetic easy axis for site i , and $\mathbf{B}$ is the external applied magnetic (Zeeman) field.

In atomistic spin models, the exchange interaction, which typically tends to be 2–4 orders of magnitude stronger than other interactions, plays a pivotal role in aligning atomic spins. In ferromagnets, characterized by positive exchange values ($J_{ij} > 0$), this strength is evident in the creation of magnetic domains, leading to well-known macroscopic magnetic properties. Conversely, in antiferromagnets with negative exchange values ($J_{ij} < 0$), atomic spins assume antiparallel order. Consequently, under the influence of weak external fields, the overall magnetization remains zero. In many cases, the most crucial aspect is the ability of a material to maintain its magnetic state without easily losing or changing it. This stability is influenced by the magnetic moments of the material to align itself along specific crystallographic directions, a characteristic often referred to as magnetocrystalline anisotropy or magnetic anisotropy energy (MAE). The most basic type of anisotropy is uniaxial, where one particular magnetic axis is favored over all others. This uniaxial anisotropy is modeled through a parameter k . [41].

3.8 Holstein-Primakoff Transformations

Holstein and Primakoff introduced a transformation that takes advantage of the highly convenient second quantization notation. This transformation is significant in interactions between magnons. The spin raising and lowering operators can be used to express the exchange term. For the j^{th} spin site,

$$\begin{aligned}\mathbf{S}_j^+ &= \mathbf{S}_j^x + i\mathbf{S}_j^y = \sqrt{2s} \left[1 - \frac{a_j^\dagger a_j}{2s} \right]^{\frac{1}{2}} a_j \\ \mathbf{S}_j^- &= \mathbf{S}_j^x - i\mathbf{S}_j^y = \sqrt{2s} a_j^\dagger \left[1 - \frac{a_j^\dagger a_j}{2s} \right]^{\frac{1}{2}} \\ \mathbf{S}_j^z &= \mathbf{S} - a_j^\dagger a_j\end{aligned}\tag{3.8.16}$$

These equations are called the Holstein-Primakoff transformation. For the case of low-temperature approximation and if the spins have classical ground state configuration, then the total number of spins that are flipped is relatively small in comparison with the total number of spins in the system, if the ground state is with all the spins along the positive, i.e. $\langle \frac{a_j^\dagger a_j}{2s} \rangle \ll 1$, then eq. 3.8.11 can be modified using binomial expansion:

$$\begin{aligned}\mathbf{S}_j^+ &= \sqrt{2s} \left(a_j - \frac{1}{4s} a_j^\dagger a_j a_j \right) \\ \mathbf{S}_j^- &= \sqrt{2s} \left(a_j^\dagger - \frac{1}{4s} a_j^\dagger a_j^\dagger a_j \right) \\ \mathbf{S}_j^z &= \mathbf{S} - a_j^\dagger a_j\end{aligned}\tag{3.8.17}$$

Keeping lowest order terms yields,

$$\begin{aligned}\mathbf{S}_j^+ &= \sqrt{2s} a_j \\ \mathbf{S}_j^- &= \sqrt{2s} a_j^\dagger\end{aligned}\tag{3.8.18}$$

$$\mathbf{S}_j^z = \mathbf{S} - a_j^\dagger a_j$$

To diagonalize the exchange Hamiltonian, Fourier transform can be used. The operators a_k^+ and a_k to create and annihilate a magnon of wavevector k , respectively [42]:

$$\begin{aligned} a_k^+ &= \frac{1}{\sqrt{N}} \sum_j e^{ik \cdot r_j} a_j^+ \\ a_k &= \frac{1}{\sqrt{N}} \sum_j e^{-ik \cdot r_j} a_j \end{aligned} \quad (3.8.19)$$

Such that:

$$[a_i, a_j^\dagger] = \delta_{ij}$$

$$[a_i, a_i] = [a_i^\dagger, a_i^\dagger] = 0$$

The Heisenberg Hamiltonian accordingly can be written as:

$$\mathcal{H} = -J \sum_{i < j} \mathbf{S}_i \cdot \mathbf{S}_j \quad (3.8.20)$$

$$= -J \sum_{i < j} \left[\mathbf{S}_i^z \mathbf{S}_j^z + \frac{1}{2} (\mathbf{S}_i^+ \mathbf{S}_j^- + \mathbf{S}_j^- \mathbf{S}_i^+) \right] \quad (3.8.21)$$

3.9 Investigation of Magnons in Magnetic Systems

In magnetic structures the collective oscillation of magnons can be used to transfer and process information, offering a novel and potentially more efficient approach compared to traditional electronic systems. These systems can significantly impact various fields such as computing, where they might allow for faster and more energy-efficient processing; data storage, enhancing capacities while reducing energy use; and healthcare, improving diagnostic imaging technologies. Each application leverages the unique properties of magnons to improve performance and efficiency

in technologies that are integral to modern life.

3.9.1 Magnonic Crystals for Waveguides and Logic Devices

Magnonic crystals are structures with a repeating pattern of magnetization. This allows them to have a similar effect on spin waves as a crystalline lattice would have for electrons. For instance, it may create band gaps that can affect the propagation of magnons. Just as photonic crystals control the flow of light with periodic variations in the refractive index, magnonic crystals use variations in magnetization to manipulate spin waves—ripples in the magnetization that can carry energy and information. These properties make magnonic crystals useful for guiding spin waves in waveguides and for processing information in logic devices, contributing to the field of spintronics where spin waves, instead of electrical current, are used for information processing tasks [43].

There’s a surge of interest in understanding how spin waves move in magnonic crystals due to their promise for tech applications like wave-based computing and communication. Interesting examples of applications can be found in microwave resonators, filters and spin wave logic devices. Magnonic crystals, which can be lines of magnetized wires or 2D patterns with magnetic properties, help manage spin waves. They can now be build with incredible precision, allowing for innovative magnetic structures and the ability to fine-tune their properties for use in tiny devices that operate at the micro or even nanoscale [44].

Magnonic crystals are gaining attraction because they might be key to innovative magnetic-based computing. Techniques like broadband ferromagnetic resonance (FMR) spectroscopy, which measures microwave absorption, are vital for studying their dynamic behavior. These methods offer in-depth insights into how magnetic structures switch and behave under different conditions. The field is moving toward using these magnetic properties for computing, where spin waves, domain walls, and nanomagnet networks can perform logic operations. With continued research, magnonic crystals could lead to advanced, on-chip magnetic devices, blending logic

functions with data storage and processing [45].

The fabrication of magnonic crystals hinges on advanced nanofabrication techniques that manipulate matter at the atomic or molecular scale. These methods include electron beam lithography, which allows for the precise patterning of nanoscale features by focusing a beam of electrons to shape or change the properties of a material. Another method is focused ion beam milling, which uses ions to precisely etch materials. Additionally, techniques like molecular beam epitaxy and chemical vapor deposition enable the controlled growth of crystal structures. The materials commonly used in these processes range from yttrium iron garnet, known for its excellent magnetic properties, to alloys like permalloy, which have desirable magnonic behaviors. The choice of material and fabrication technique directly influences the magnonic crystal's ability to manipulate spin waves for applications in waveguides and logic devices [46].

3.9.2 Spintronics and Magnon Spintronics

Spintronics, a blend of spin-based electronics, utilizes electron spin controlled by external magnetic fields to polarize electrons, thus manipulating electric current. This field aims to create semiconductors that can manage electron magnetism, enhancing future electronics with greater functionality. Originating in the late '80s with the discovery of the giant magnetoresistance effect, Spintronics could usher in devices with advanced electrical and optical characteristics, including improved memory and sensors. In traditional electronic devices, data is stored and transferred through the movement of electrons, with binary codes represented by the presence or absence of these particles. Spintronics, however, uses the electron's spin—intrinsic angular momentum of electron that points either up or down—to encode this information. Spins generally are randomly oriented, hence an external magnetic field is applied to align the spins. This method enables a novel form of data storage, where binary zeros and ones are depicted by the direction of electron spins. The concept emerged from the invention of the spin valve, a layered material structure that changes elec-

trical resistance with applied magnetic fields to control current flow [47].

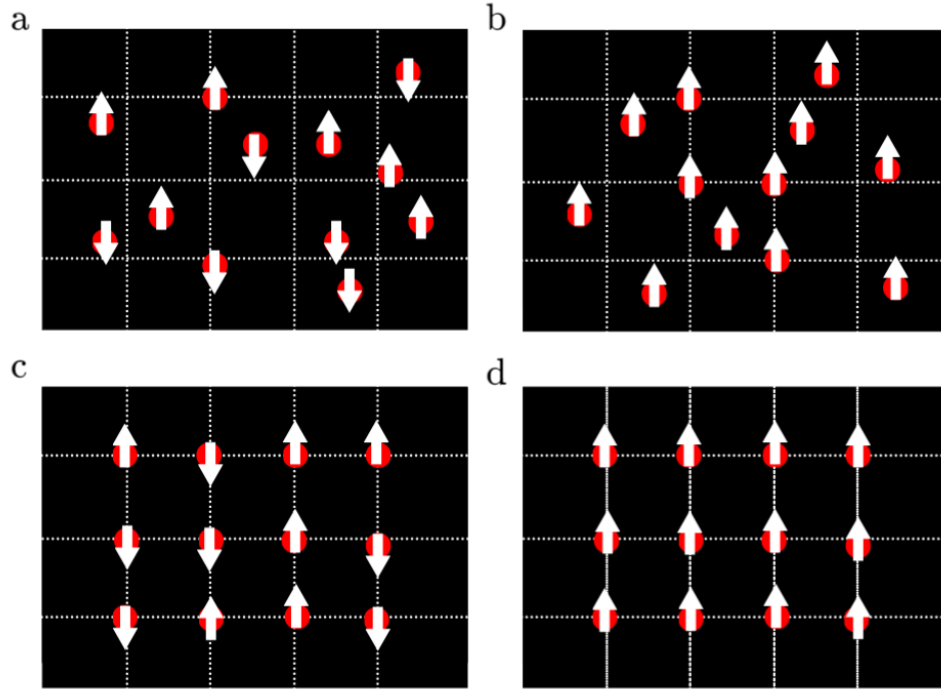


Figure 3.7: Spins possess the capability to organize into different configurations, a characteristic of significant relevance for Spintronics apparatus. a. The spins are located randomly throughout the material without a specific order. b. spins are located randomly but all in same direction (spin alignment). c. the spins are located in ordered manner on a crystal lattice forming a nonmagnetic material. d. the spins are aligned as in a magnetic material.

Since the 1970s, electronic components have become significantly smaller, advancing from the first integrated circuits to modern chips with billions of transistors. However, we're nearing a limit where shrinking these components further will be impossible due to the fundamental laws of quantum physics. Issues such as electricity leakage, increased power consumption, and heat generation become more problematic as transistors get tinier and more densely packed on chips. As electronic devices shrink, we're beginning to encounter the strange world of quantum mechanics, where electrons exhibit wave-like behavior. Spintronics, combined with nanotechnology, appears to be a promising solution to the challenges of miniaturization, exploring the realm of extremely small scales, much thinner than a strand of human hair. This approach could address issues like electric current leakage and excessive heat generation by leveraging the quantum properties of electron spin [48].

3.9.3 Quantum Information Processing with Magnons

The fields of spintronics and quantum information science are merging to create new ways of processing information using solid-state platforms. This merger allows for exploring quantum phenomena and accomplishing various quantum tasks. Traditionally, there was a divide between spintronics, which deals with classical magnetization, and quantum information science, which operates with quantum bits (qubits). Recent years have seen this gap close due to advancements in utilizing magnons for information encoding and processing, along with better understanding and creation of entangled quasi-particles, high-quality qubits, and photonic cavities. This convergence has given rise to the field of quantum magnonics. Quantum magnonics is a groundbreaking field that brings together the world of magnon spintronics with the realm of quantum information science. It's where the study of magnons meets with the advanced principles of quantum mechanics, like entanglement and superposition, used in quantum computing. This area combines traditional spintronics—which is all about manipulating the spin of electrons for electronics—with the understanding of magnons from magnonics, the control and use of light in quantum optics, and the futuristic concepts of quantum computing and information science [49]. This overview looks into the latest on magnons' quantum states and their integration with established quantum systems. Topics include the basics of magnons and entanglement, how to create and control magnonic quantum states like single-magnon and squeezed states, and quantum many-body phenomena such as Bose-Einstein condensation leading to spin superfluidity [50]. As we mentioned magnons are the fundamental excitations of the spin structure in magnetically ordered materials. They can be visualized as collective oscillations of electron spin alignments in a crystal lattice, behaving much like particles in quantum mechanics. This wave-particle duality makes them suitable for quantum applications, as they can carry spin information across a magnetic material without the movement of charge [51].

Quantum information processing aims to exploit the principles of quantum mechan-

ics, such as superposition and entanglement, to perform tasks that are impossible or highly inefficient for classical systems [52]. Magnons, with their inherent quantum nature, offer a unique pathway to manipulate quantum states of spin. By controlling magnon excitations, it's possible to encode, process, and transfer information in ways that leverage their quantum mechanical properties.

Chapter 4

Advanced Analytical Approaches to Magnon Dynamics

In the realm of condensed matter physics, the study of magnetic systems occupies a pivotal role, offering profound insights into the fundamental properties of matter. Among the myriad configurations that magnetic systems can realize, non-collinear and non-coplanar structures represent a particularly intriguing class.

The focus of this investigation is on elucidating the mathematical underpinnings and physical implications of such arrangements. A case in point is the so-called 3Q state, a specific arrangement wherein each unit cell comprises four spins, with each spin engaging with $2z = 6$ neighbors. This configuration epitomizes the antiferromagnetic principle that the vector sum of the spins within a defined neighborhood—specifically, $(z + 1)$ vectors—equates to zero. This condition is emblematic of the antiferromagnetic order, wherein opposing magnetic moments balance each other, resulting in no net magnetization at the macroscopic level.

To advance our understanding of these complex magnetic structures, we embark on a methodical analysis, beginning with foundational definitions and progressing towards the derivation of equations that accurately describe the energetics and dynamics of non-collinear, non-coplanar antiferromagnets.

In this study, we will employ two distinct methodologies to conduct our investi-

gation. The initial approach employs spherical coordinates for analysis, while the subsequent approach leverages the coordinate ξ for examination as detailed below.

4.1 Dynamical System Analysis in Spherical Coordinates

Considering a small deviation from the ground state the magnetic moment can be written as:

$$\mathbf{m}_i = \mathbf{m}_i^\circ + \delta\mathbf{m}_i$$

The LLG equation (3.4.7) becomes after taking the damping factor $\alpha = \mathbf{0}$ and $H_{\text{eff}} = \sum_{i \neq p} \mathbf{m}_i$:

$$\begin{aligned} \frac{d\delta\mathbf{m}_p}{dt} &= -\mathbf{m}_p \times \sum_{i \neq p} \mathbf{m}_i \\ &= -(\mathbf{m}_p^\circ + \delta\mathbf{m}_p) \times \left(\sum_{i \neq p} \delta\mathbf{m}_i - 2\mathbf{m}_p^\circ \right) \end{aligned} \quad (4.1.1)$$

For the case of AFM, we have $\sum_{i \neq p} \mathbf{m}_i^\circ = -2\mathbf{m}_p^\circ$, gives

$$\frac{d\delta\mathbf{m}_p}{dt} = -\mathbf{m}_p^\circ \times \sum_i \alpha_{ip} \delta\mathbf{m}_i \quad (4.1.2)$$

Where $\alpha_{ip} = 1 + \delta_{ip}$ (δ is the kronecker delta). This takes into account the fact that we have $2\mathbf{m}_p^\circ$.

Next, multiplying by $\mathbf{e}_{\theta_p}$ to get the component along $\mathbf{e}_{\theta_p}$. Note that $\mathbf{e}_{\theta_p}$ and $\mathbf{e}_{\phi_p}$ are the spherical coordinates

$$\begin{aligned} d\theta_p &= -\mathbf{e}_{\theta_p} \cdot \left(\mathbf{m}_p^\circ \times \sum_i \alpha_{ip} \delta\mathbf{m}_i \right) \\ &= -\sum_i \alpha_{ip} \delta\mathbf{m}_i \cdot (\mathbf{e}_{\theta_p} \times \mathbf{m}_p^\circ) \\ &= +\sum_i \alpha_{ip} \delta\mathbf{m}_i \cdot \mathbf{e}_{\phi_p} \end{aligned} \quad (4.1.3)$$

using $\delta \mathbf{m} = d\theta \mathbf{e}_\theta + d\phi \mathbf{e}_\phi$ we can write explicitly

$$d\theta_p = \sum_i \alpha_{ip} \left(d\theta_i (\mathbf{e}_{\theta_i} \cdot \mathbf{e}_{\phi_p}) + \mathbf{d}\tilde{\phi}_i (\mathbf{e}_{\phi_i} \cdot \mathbf{e}_{\phi_p}) \right) \quad (4.1.4)$$

Similarly multiplying 4.1.2 by $\mathbf{e}_{\phi_p}$ and defining $d\tilde{\phi} = \sin \theta d\phi$ to get $d\phi$ component

$$d\tilde{\phi} = - \sum_i \alpha_{ip} \delta \mathbf{m}_i \cdot \mathbf{e}_{\theta_p} \quad (4.1.5)$$

Which can be written explicitly as

$$d\tilde{\phi}_p = - \sum_i \alpha_{ip} \left(d\theta_i (\mathbf{e}_{\theta_i} \cdot \mathbf{e}_{\theta_p}) + \mathbf{d}\tilde{\phi}_i (\mathbf{e}_{\phi_i} \cdot \mathbf{e}_{\theta_p}) \right) \quad (4.1.6)$$

Using

$$\psi_i^\pm = \frac{d\theta_i + i d\tilde{\phi}_i}{\sqrt{2}} \quad (4.1.7)$$

$d\theta$ and $d\tilde{\phi}$ given by

$$d\theta_i = \frac{\psi_i^+ + \psi_i^-}{\sqrt{2}}, d\tilde{\phi}_i = \frac{\psi_i^+ - \psi_i^-}{i\sqrt{2}} \quad (4.1.8)$$

Hence we can write using ξ , where $\xi_p = \frac{\mathbf{e}_{\theta_p} + i\mathbf{e}_{\phi_p}}{\sqrt{2}}$

$$\begin{aligned} \delta \mathbf{m}_i &= d\theta_i \mathbf{e}_{\theta_i} + \mathbf{d}\tilde{\phi}_i \mathbf{e}_{\phi_i} \\ &= \psi_i^+ \xi_i^* + \psi_i^- \xi_i \end{aligned} \quad (4.1.9)$$

Substituting for $d\theta$ and $d\tilde{\phi}$ to get $\frac{d\psi_p^+}{dt}$

$$\begin{aligned} \frac{d}{dt} \delta \mathbf{m}_p &= \frac{d}{dt} (\psi_p^+ \xi_p^* + \psi_p^- \xi_p) \\ &= -\mathbf{m}_p \circ \sum_i \alpha_{ip} \delta \mathbf{m}_i \end{aligned} \quad (4.1.10)$$

Dot product with ξ_p from the right

$$\begin{aligned}
\frac{d\psi_p^+}{dt} &= \frac{1}{\sqrt{2}} \sum_i \alpha_{ip} \left(d\theta_i \mathbf{e}_{\theta_i} + \mathbf{d}\tilde{\phi}_i \mathbf{e}_{\phi_i} \right) (\mathbf{e}_{\phi_p} - i\mathbf{e}_{\theta_p}) \\
&= \frac{1}{2} \sum_i \alpha_{ip} \left((\psi_i^+ + \psi_i^-) \mathbf{e}_{\theta_i} - i(\psi_i^+ - \psi_i^-) \mathbf{e}_{\phi_i} \right) (\mathbf{e}_{\phi_p} - i\mathbf{e}_{\theta_p}) \\
&= -\frac{i}{2} \sum_i \alpha_{ip} \left\{ \psi_i^+ (\mathbf{e}_{\theta_i} - i\mathbf{e}_{\phi_i}) + \psi_i^- (\mathbf{e}_{\theta_i} + i\mathbf{e}_{\phi_i}) \right\} (\mathbf{e}_{\theta_p} + i\mathbf{e}_{\phi_p})
\end{aligned} \tag{4.1.11}$$

$$\Rightarrow i \frac{d\psi_p^+}{dt} = \sum_i \alpha_{ip} \left\{ \psi_i^+ \boldsymbol{\xi}_i^* \boldsymbol{\xi}_p + \psi_i^- \boldsymbol{\xi}_i \boldsymbol{\xi}_p \right\} \tag{4.1.12}$$

Similarly for $\frac{d\psi_p^-}{dt}$

$$\Rightarrow i \frac{d\psi_p^-}{dt} = - \sum_i \alpha_{ip} \left\{ \psi_i^+ \boldsymbol{\xi}_i^* \boldsymbol{\xi}_p^* + \psi_i^- \boldsymbol{\xi}_i \boldsymbol{\xi}_p^* \right\} \tag{4.1.13}$$

using $\psi_i^+ = \psi_i^+ e^{i(kR_i - \omega t)}$, $\psi_i^- = \psi_i^- e^{i(kR_i - \omega t)}$, we get

$$\begin{aligned}
\omega \psi_p^+ &= \sum_i \alpha_{ip} \left\{ \psi_i^+ \boldsymbol{\xi}_i^* \boldsymbol{\xi}_p + \psi_i^- \boldsymbol{\xi}_i \boldsymbol{\xi}_p \right\} e^{i\mathbf{k}\mathbf{R}_{pi}} \\
\omega \psi_p^- &= - \sum_i \alpha_{ip} \left\{ \psi_i^+ \boldsymbol{\xi}_i^* \boldsymbol{\xi}_p^* + \psi_i^- \boldsymbol{\xi}_i \boldsymbol{\xi}_p^* \right\} e^{i\mathbf{k}\mathbf{R}_{pi}}
\end{aligned} \tag{4.1.14}$$

where we defined $\mathbf{R}_{pi} = \mathbf{R}_i - \mathbf{R}_p$, which are used to define the vectors connecting neighbors.

4.1.1 Non AFM

In the case of the presence of a non-zero net magnetization vector, denoted as $(\sum \mathbf{m}_i = \mathbf{M})$, this introduces an additional term in our mathematical formulation. Then the exchange term in the LLG equation will be written as:

$$- (\mathbf{m}_p^\circ + \delta \mathbf{m}_p) \times 2\mathbf{M} \tag{4.1.15}$$

In the equilibrium state, the net torque exerted on each spin must be nullified, indicating that the cross product of the equilibrium magnetization vector, $\mathbf{m}_p^\circ$, with the

total magnetization vector, $\mathbf{M}$, equals zero: $\mathbf{m}_p^\circ \times \mathbf{M} = \mathbf{0}$. This condition underscores the fundamental principle of torque equilibrium in magnetic systems. We can get θ and ϕ components by:

$$\begin{aligned}
-(\mathbf{m}_p^\circ + \delta\mathbf{m}_p) \times 2\mathbf{M} \cdot \mathbf{e}_{\theta_p} &= -\mathbf{e}_{\theta_p} \cdot ((\mathbf{m}_p^\circ + \delta\mathbf{m}_p) \times 2\mathbf{M}) \\
&= -2\mathbf{M} \cdot (\mathbf{e}_{\theta_p} \times (\mathbf{m}_p^\circ + \delta\mathbf{m}_p)) \\
&= +2\mathbf{M} \cdot \mathbf{e}_{\phi_p} - 2\delta\mathbf{m}_p \cdot (\mathbf{M} \times \mathbf{e}_{\theta_p}) \\
-(\mathbf{m}_p^\circ + \delta\mathbf{m}_p) \times 2\mathbf{M} \cdot \mathbf{e}_{\phi_p} &= -2\mathbf{M} \cdot \mathbf{e}_{\theta_p} - 2\delta\mathbf{m}_p \cdot (\mathbf{M} \times \mathbf{e}_{\phi_p})
\end{aligned} \tag{4.1.16}$$

Hence we can write ψ^+ as:

$$i \frac{d\psi_p^+}{dt} = 2\mathbf{M} \cdot \boldsymbol{\xi}_p - 2i\delta\mathbf{m}_p \cdot (\mathbf{M} \times \boldsymbol{\xi}_p) \tag{4.1.17}$$

using $\delta\mathbf{m}_p = \psi_p^+ \boldsymbol{\xi}_p^* + \psi_p^- \boldsymbol{\xi}_p$

$$i \frac{d\psi_p^+}{dt} = 2\mathbf{M} \cdot \boldsymbol{\xi}_p - 2i\psi_p^+ \mathbf{M} \cdot (\boldsymbol{\xi}_p^* \times \boldsymbol{\xi}_p) - 2i\psi_p^- \mathbf{M} \cdot (\boldsymbol{\xi}_p \times \boldsymbol{\xi}_p^*) \tag{4.1.18}$$

using $(\boldsymbol{\xi}_p \times \boldsymbol{\xi}_p) = \mathbf{0}$ and $(\mathbf{m}_p^\circ \times \mathbf{M} = 0 \Rightarrow \mathbf{M} \cdot \boldsymbol{\xi}_p = 0)$ yields an additional term to the previous result:

$$\begin{aligned}
i \frac{d\psi_p^+}{dt} &= \dots - 2\psi_p^+ (\mathbf{M} \cdot \mathbf{e}_{r_p}) \\
i \frac{d\psi_p^-}{dt} &= \dots + 2\psi_p^- (\mathbf{M} \cdot \mathbf{e}_{r_p})
\end{aligned} \tag{4.1.19}$$

4.2 Analysis in the Local ξ Coordinate System

Taking a general Hamiltonian H , the LLG equations gives:

$$\begin{aligned}
\frac{d\delta\mathbf{m}}{dt} &= -(\mathbf{m}^\circ + \delta\mathbf{m}) \times (\mathbf{H}^\circ + \delta\mathbf{H}) \\
&= -\mathbf{m}^\circ \times \mathbf{H}^\circ - \mathbf{m}^\circ \times \delta\mathbf{H} - \delta\mathbf{m} \times \mathbf{H}^\circ - \delta\mathbf{m} \times \delta\mathbf{H} \\
&\approx -\mathbf{m}^\circ \times \delta\mathbf{H} - \delta\mathbf{m} \times \mathbf{H}^\circ
\end{aligned} \tag{4.2.20}$$

In the approximation step, the cross-product term $\delta\mathbf{m} \times \delta\mathbf{H}$ is dropped, assuming it is of second order and thus negligible for small perturbations. This simplification assumes linear response theory, where only first-order terms are considered. Moreover, we used the fact that the torque at equilibrium vanishes. ($\mathbf{m}_p^\circ \times \mathbf{H}^\circ = \mathbf{0}$)

Given $\delta\mathbf{m}_p = \psi^+ \boldsymbol{\xi}^* + \psi^- \boldsymbol{\xi}$, we derive:

$$\frac{d}{dt}(\psi^+ \boldsymbol{\xi}^* + \psi^- \boldsymbol{\xi}) = -\mathbf{m}_p^\circ \times \delta\mathbf{H} - (\psi^+ \boldsymbol{\xi}^* + \psi^- \boldsymbol{\xi}) \times \mathbf{H}^\circ \quad (4.2.21)$$

Dot product of (eq. 4.2.21) with $\boldsymbol{\xi}$ from right gives:

$$\frac{d}{dt}(\psi^+ \boldsymbol{\xi}^* + \psi^- \boldsymbol{\xi}) \cdot \boldsymbol{\xi} = -\mathbf{m}_p^\circ \times \delta\mathbf{H} \cdot \boldsymbol{\xi} - (\psi^+ \boldsymbol{\xi}^* + \psi^- \boldsymbol{\xi}) \times \mathbf{H}^\circ \cdot \boldsymbol{\xi} \quad (4.2.22)$$

Using $\boldsymbol{\xi} \cdot \boldsymbol{\xi} = 0$, $\boldsymbol{\xi} \cdot \boldsymbol{\xi}^* = 1$, we simplify:

$$\Rightarrow \frac{d\psi_p^+}{dt} = -\mathbf{m}_p^\circ \times \delta\mathbf{H}_p \cdot \boldsymbol{\xi}_p - \psi_p^+ \boldsymbol{\xi}_p^* \times \mathbf{H}_p^\circ \cdot \boldsymbol{\xi}_p - \psi_p^- \boldsymbol{\xi}_p \times \mathbf{H}_p^\circ \cdot \boldsymbol{\xi}_p \quad (4.2.23)$$

Now using $\boldsymbol{\xi} \times \mathbf{m}_p^\circ = i\boldsymbol{\xi}$ and $\boldsymbol{\xi}^* \times \mathbf{H}^\circ \cdot \boldsymbol{\xi} = \mathbf{H}^\circ \cdot (-i\mathbf{e}_r)$

$$\Rightarrow i \frac{d\psi_p^+}{dt} = \delta\mathbf{H}_p \cdot \boldsymbol{\xi}_p - \psi_p^+ \mathbf{H}_p^\circ \cdot \mathbf{e}_{r_p} \quad (4.2.24)$$

Similarly, to get the equation for ψ_p^- , we multiply (eq. 4.2.21) by $\boldsymbol{\xi}^*$ from right, after some calculations we get:

$$\Rightarrow i \frac{d\psi_p^-}{dt} = \delta\mathbf{H} \cdot \boldsymbol{\xi}^* - \psi^- \mathbf{H}^\circ \cdot \mathbf{e}_r \quad (4.2.25)$$

Now considering the Hamiltonian as representative of the exchange energy, the underlying dynamics of the system:

Example 4.1 : For the case of exchange interaction,

we have $\delta H_p^{\text{ex}} = J \sum_q \delta m_q = J \sum_q \psi_q^+ \boldsymbol{\xi}_q^* + \psi_q^- \boldsymbol{\xi}_q$.

Substituting into 4.24 yields:

$$\begin{aligned} \Rightarrow i \frac{d\psi^+}{dt} &= J \left(\sum_q \psi_q^+ \boldsymbol{\xi}_q^* + \psi_q^- \boldsymbol{\xi}_q \right) \cdot \boldsymbol{\xi}_p - \psi^+ \mathbf{H}_p^\circ \cdot \mathbf{e}_{r_p} \\ i \frac{d\psi^+}{dt} &= J \left(\sum_{q \neq p} \psi_q^+ \boldsymbol{\xi}_q^* \boldsymbol{\xi}_p + \psi_q^- \boldsymbol{\xi}_q \boldsymbol{\xi}_p \right) - \psi^+ \mathbf{H}_p^\circ \cdot \mathbf{e}_{r_p} \end{aligned}$$

Similarly substituting into 4.25 to get the equation of ψ^- gives:

$$i \frac{d\psi_p^-}{dt} = -J \left(\sum_{q \neq p} \psi_q^+ \boldsymbol{\xi}_q^* \boldsymbol{\xi}_p^* + \psi_q^- \boldsymbol{\xi}_q \boldsymbol{\xi}_p^* \right) + \psi_p^- \mathbf{H}_p^\circ \cdot \mathbf{e}_{r_p}$$

4.3 Additional Terms

This section introduces and discusses several key energy contributions that play pivotal roles in the dynamics and stability of magnetic systems. Each of these energy terms contributes uniquely to the overall behavior of magnetic materials, influencing their properties under various special conditions. First we will consider each term separately to derive the corresponding LLG equation. Then we will combine different terms to study some systems.

4.3.1 Zeeman Energy

The Zeeman energy, which results from the interaction between a magnetic moment and an external magnetic field is given by the formula:

$$\mathcal{H}_{\text{Zeeman}} = -\mathbf{m} \cdot \mathbf{B} \quad (4.3.26)$$

where $\mathbf{m}$ is the magnetic moment of the atom and $\mathbf{B}$ is the external magnetic field.

The negative sign indicates that the energy is minimized when the magnetic moment aligns with the magnetic field.

The LLG equation of the zeeman inte are expressed as:

$$\begin{aligned}
\mathbf{m}_i \times \mathbf{B} &= (\mathbf{m}_i^\circ + \delta\mathbf{m}_i) \times \mathbf{B} \\
&= \mathbf{m}_i^\circ \times \mathbf{B} + \delta\mathbf{m}_i \times \mathbf{B} \quad \text{where,} \quad \delta\mathbf{m}_i = \psi^+ \boldsymbol{\xi}^* + \psi^- \boldsymbol{\xi} \quad (4.3.27) \\
\text{hence, } \mathbf{H}^\circ &= \frac{\mathbf{B}}{\mu}, \quad \delta\mathbf{H} = \mathbf{0}
\end{aligned}$$

This yields,

$$\begin{aligned}
i \frac{d\psi_p^+}{dt} &= \delta\mathbf{H}_p \cdot \boldsymbol{\xi}_p - \psi_p^+ \mathbf{H}_p^\circ \cdot \mathbf{e}_{r_p} \\
&= -\psi_p^+ \mathbf{B} \cdot \mathbf{e}_{r_p}. \quad (4.3.28)
\end{aligned}$$

$$\begin{aligned}
\Rightarrow i \frac{d\psi_p^+}{dt} &= \dots - \frac{1}{\mu} \psi_p^+ \mathbf{B} \cdot \mathbf{e}_{r_p} \\
i \frac{d\psi_p^-}{dt} &= \dots + \frac{1}{\mu} \psi_p^- \mathbf{B} \cdot \mathbf{e}_{r_p} \quad (4.3.29)
\end{aligned}$$

Which can be written in a matrix form as:

$$i \frac{d}{dt} \begin{bmatrix} \psi_p^+ \\ \psi_p^- \end{bmatrix} = \frac{1}{\mu} \begin{bmatrix} -\mathbf{B} \cdot \mathbf{e}_{r_p} & 0 \\ 0 & \mathbf{B} \cdot \mathbf{e}_{r_p} \end{bmatrix} \begin{bmatrix} \psi_p^+ \\ \psi_p^- \end{bmatrix}$$

These equations describe the wavefunctions resulting from considering the Zeeman interaction in the LLG equation. As we can see we have only the onsite potential.

4.3.2 Anisotropy Energy

In our exploration of the anisotropy energy within a general framework, we express the anisotropy term as follows:

$$\mathcal{H} = -k \sum_i (\mathbf{n}_i \cdot \mathbf{m}_i)^2, \quad \mathbf{n}_i = n_r \mathbf{e}_r + \frac{n_\perp}{\sqrt{2}} (\mathbf{e}^{i\phi_n} \boldsymbol{\xi}_i^* + \mathbf{e}^{-i\phi_n} \boldsymbol{\xi}_i), \quad (4.3.30)$$

where k represents the anisotropy constant, $\mathbf{n}_i$ is a unitary vector that denotes the anisotropy direction, and $\mathbf{m}_i$ stands for the magnetization vector at site i . The

anisotropy direction is further decomposed into radial and perpendicular components relative to a chosen reference frame. Upon calculating the gradient of the Hamiltonian with respect to the magnetization, we obtain the effective field resulting from anisotropy contributions:

$$\frac{1}{\mu} \frac{\partial \mathcal{H}}{\partial \mathbf{m}_i} = -\frac{2k}{\mu} \sum_i (\mathbf{n}_i \cdot \mathbf{m}_i) \mathbf{n}_i. \quad (4.3.31)$$

Substituting these expressions into equations 4.2.24 and 4.2.25, where

$$\mathbf{H}_p^\circ = \frac{2k}{\mu} (\mathbf{n}_p \cdot \mathbf{m}_p) \mathbf{n}_p, \quad \delta \mathbf{H}_p = \frac{2k}{\mu} (\mathbf{n}_p \cdot \delta \mathbf{m}_p) \mathbf{n}_p, \quad \delta \mathbf{m}_p = \psi_p^+ \boldsymbol{\xi}_p^* + \psi_p^- \boldsymbol{\xi}_p, \quad (4.3.32)$$

we obtain the following equation:

$$\begin{aligned} i \frac{d\psi^+}{dt} &= \frac{2k}{\mu} \left[\psi_p^+ (\boldsymbol{\xi}_p^* n_p) (\boldsymbol{\xi}_p n_p) + \psi_p^- (\boldsymbol{\xi}_p n_p) \right] - \frac{2k}{\mu} \psi_p^+ (n_p \cdot \mathbf{e}_{r_p})^2 \\ &= \dots + \frac{k}{\mu} n_\perp^2 [\psi_p^+ + \psi_p^- e^{2i\phi_n}] - \frac{2k}{\mu} \psi_p^+ n_{r_p}^2 \end{aligned} \quad (4.3.33)$$

and similarly,

$$i \frac{d\psi^-}{dt} = \dots - k n_\perp^2 [\psi_p^- + \psi_p^+ e^{-2i\phi_n}] + 2k \psi_p^- n_{r_p}^2 \quad (4.3.34)$$

the equation can be cast into a form as bellow

$$i \frac{d}{dt} \begin{bmatrix} \psi_p^+ \\ \psi_p^- \end{bmatrix} = \begin{bmatrix} k n_\perp^2 - 2k n_{r_p}^2 & k n_\perp^2 e^{2i\phi_n} \\ -k n_\perp^2 e^{-2i\phi_n} & - (k n_\perp^2 - 2k n_{r_p}^2) \end{bmatrix} \begin{bmatrix} \psi_p^+ \\ \psi_p^- \end{bmatrix},$$

with the relations:

$$n_\perp^2 = 1 - n_r^2, \quad n_\perp^2 = n_\theta^2 + n_\varphi^2, \quad \varphi_n = \tan^{-1} \left(\frac{n_\varphi}{n_\theta} \right).$$

or for numerical purposes, it can be useful to rewrite the equation in the following form:

$$i \frac{d}{dt} \begin{bmatrix} \psi_p^+ \\ \psi_p^- \end{bmatrix} = \frac{2k}{\mu} \begin{bmatrix} (\boldsymbol{\xi}_p^* \cdot \mathbf{n}_p) (\boldsymbol{\xi}_p \cdot \mathbf{n}_p) & (\boldsymbol{\xi}_p \cdot \mathbf{n}_p) (\boldsymbol{\xi}_p \cdot \mathbf{n}_p) \\ -(\boldsymbol{\xi}_p^* \cdot \mathbf{n}_p) (\boldsymbol{\xi}_p^* \cdot \mathbf{n}_p) & -(\boldsymbol{\xi}_p \cdot \mathbf{n}_p) (\boldsymbol{\xi}_p^* \cdot \mathbf{n}_p) \end{bmatrix} \begin{bmatrix} \psi_p^+ \\ \psi_p^- \end{bmatrix} - \frac{2k}{\mu} \begin{bmatrix} (\mathbf{n}_p \cdot \mathbf{e}_{r_p})^2 & 0 \\ 0 & -(\mathbf{n}_p \cdot \mathbf{e}_{r_p})^2 \end{bmatrix} \begin{bmatrix} \psi_p^+ \\ \psi_p^- \end{bmatrix}$$

using this equation we can get the effective magnetic field that is resulted from anisotropy interaction in any direction.

4.3.3 Dzyaloshinskii-Moriya Interaction

The Dzyaloshinskii-Moriya Interaction (DMI) represents a pivotal extension to the Heisenberg model, introducing an asymmetry in the exchange interaction that stems from spin-orbit coupling. This interaction is crucial for understanding complex non-collinear spin textures such as chiral magnetic skyrmions. The impact of DMI on magnon dynamics—quasiparticle excitations in magnets—is profound, leading to nonreciprocal magnon dispersion relations and the stabilization of topological magnonic phases [53].

The DMI energy, represented by $\mathcal{H} = -\sum \mathbf{D}_{ij} \cdot (\mathbf{m}_i \times \mathbf{m}_j)$, accounts for noncollinear spin arrangements. This is due to the nature of the interaction, which depends on the cross product of neighboring magnetic moments $\mathbf{m}_i$ and $\mathbf{m}_j$, modulated by the DMI vector $\mathbf{D}_{ij}$. The effective field generated by this interaction, $\mathbf{H} = \frac{1}{\mu} \sum_j (\mathbf{m}_j \times \mathbf{D}_{ij})$, and its variation, $\delta \mathbf{H} = \frac{1}{\mu} \sum_j (\delta \mathbf{m}_j \times \mathbf{D}_{ij})$, depend on the cross products involving the DMI vectors and magnetic moment changes.

Decomposing the DMI vector $\mathbf{D}_{pq}$ into parallel ($\parallel$) and perpendicular ($\perp$) components relative to a reference frame allows us to express it as a combination of alignment along the radial direction ($\mathbf{e}_{r_p}$) and a component that involves the spin orientation variables $\boldsymbol{\xi}_p$ and $\boldsymbol{\xi}_p^*$, modulated by the angle ϕ_{pq} ,

$$\mathbf{D}_{\text{pq}} = \mathbf{D}_{\text{pq}}^{\parallel} \cdot \mathbf{e}_{\text{rp}} + \frac{\mathbf{D}_{\text{pq}}^{\perp}}{\sqrt{2}} \left((\mathbf{e}^{+i\phi_{\text{pq}}} \boldsymbol{\xi}_{\text{p}}^* + \mathbf{e}^{-i\phi_{\text{pq}}} \boldsymbol{\xi}_{\text{p}}) \right).$$

$$\begin{aligned} H_p^{\circ} \cdot \mathbf{e}_{\text{rp}} &= \frac{\lambda}{\mu} \sum_q (\mathbf{e}_{\text{rq}} \times \mathbf{D}_{\text{pq}}) \cdot \mathbf{e}_{\text{rp}} \\ &= \frac{\lambda}{\mu} \sum_q \mathbf{e}_{\text{rq}} \cdot (\mathbf{D}_{\text{pq}} \times \mathbf{e}_{\text{rp}}) \end{aligned} \quad (4.3.35)$$

$$\begin{aligned} \delta H_p &= \frac{\lambda}{\mu} \sum_q (\delta m_q \times \mathbf{D}_{\text{pq}}) \\ &= \frac{\lambda}{\mu} \sum_q (\psi_q^+ \boldsymbol{\xi}_q^* \times \mathbf{D}_{\text{pq}} + \psi_q^- \boldsymbol{\xi}_q \times \mathbf{D}_{\text{pq}}) \end{aligned} \quad (4.3.36)$$

Now using 4.2.24 and 4.2.25 yields,

$$\begin{aligned} i \frac{d\psi_p^+}{dt} &= \dots + \frac{\lambda}{\mu} \sum_q (\psi_q^+ \boldsymbol{\xi}_q^* \times \mathbf{D}_{\text{pq}} + \psi_q^- \boldsymbol{\xi}_q \times \mathbf{D}_{\text{pq}}) \cdot \boldsymbol{\xi}_p \\ &\quad - \frac{\lambda}{\mu} \psi_p^+ \mathbf{e}_{\text{rq}} \cdot (\mathbf{D}_{\text{pq}} \times \mathbf{e}_{\text{rp}}) \end{aligned} \quad (4.3.37)$$

$$\begin{aligned} i \frac{d\psi_p^-}{dt} &= \dots - \frac{\lambda}{\mu} \sum_q \left(\psi_q^- \boldsymbol{\xi}_q \times \mathbf{D}_{\text{pq}} + \frac{1}{\mu} \psi_q^+ \boldsymbol{\xi}_q^* \times \mathbf{D}_{\text{pq}} \right) \cdot \boldsymbol{\xi}_p^* \\ &\quad + \frac{\lambda}{\mu} \psi_p^- \mathbf{e}_{\text{rq}} \cdot (\mathbf{D}_{\text{pq}} \times \mathbf{e}_{\text{rp}}) \end{aligned} \quad (4.3.38)$$

In matrix form we find:

$$\begin{aligned} i \frac{d}{dt} \begin{bmatrix} \psi_p^+ \\ \psi_p^- \end{bmatrix} &= \frac{\lambda}{\mu} \begin{bmatrix} \boldsymbol{\xi}_q^* \times \mathbf{D}_{\text{pq}} \cdot \boldsymbol{\xi}_p & \boldsymbol{\xi}_q \times \mathbf{D}_{\text{pq}} \cdot \boldsymbol{\xi}_p \\ -\boldsymbol{\xi}_q^* \times \mathbf{D}_{\text{pq}} \cdot \boldsymbol{\xi}_p^* & -\boldsymbol{\xi}_q \times \mathbf{D}_{\text{pq}} \cdot \boldsymbol{\xi}_p^* \end{bmatrix} \begin{bmatrix} \psi_q^+ \\ \psi_q^- \end{bmatrix} \\ &\quad - \frac{\lambda}{\mu} \begin{bmatrix} \sum_q \mathbf{e}_{\text{rq}} \cdot (\mathbf{D}_{\text{pq}} \times \mathbf{e}_{\text{rp}}) & 0 \\ 0 & -\sum_q \mathbf{e}_{\text{rq}} \cdot (\mathbf{D}_{\text{pq}} \times \mathbf{e}_{\text{rp}}) \end{bmatrix} \begin{bmatrix} \psi_p^+ \\ \psi_p^- \end{bmatrix} \end{aligned}$$

The above equations provide insight into how the wave functions of the system evolve over time when the system is affected by the DMI.

4.3.4 Pseudodipolar Energy

Pseudodipolar energy refers to an energy term that arises in certain magnetic systems, particularly those with complex, non-collinear magnetic structures. Unlike the

classical dipolar energy, which originates from the magnetic dipole-dipole interactions and depends on the inverse cube of the distance between magnetic moments, pseudodipolar energy often emerges from often quantum mechanical, interactions within the system [54].

Pseudodipolar often emerging from superexchange and atomistic spin-orbit interactions. This form of energy is pivotal in understanding materials where the orientation and interaction of atomic spins play a crucial role. Superexchange is a mechanism where magnetic interactions occur indirectly through an intermediary, non-magnetic atom, leading to either ferromagnetic or antiferromagnetic ordering. Atomistic spin-orbit interaction, on the other hand, involves the coupling between an electron's spin and its orbital motion around the nucleus, influencing magnetic anisotropy and the overall magnetic properties of the material [55].

The pseudodipolar energy is: $\mathcal{H}_{pseudo} = F (\mathbf{m}_i \cdot \mathbf{e}_{ij}) (\mathbf{m}_j \cdot \mathbf{e}_{ij})$, where F is the interaction strength.

Below we find expression for H_p° and δH_p for this type of Hamiltonian. These results are subsequently used in Eq. (4.2.24) and (4.2.25),

$$\mathbf{H}_p^\circ = \mathbf{e}_{pq} (\mathbf{m}_q^\circ \cdot \mathbf{e}_{pq}), \quad \delta \mathbf{H}_p = \mathbf{e}_{pq} (\delta \mathbf{m}_q \cdot \mathbf{e}_{pq}), \quad \mathbf{e}_{pq} = \left(a, \frac{b}{\sqrt{2}} e^{i\phi} \boldsymbol{\xi}_q^*, \frac{b}{\sqrt{2}} e^{-i\phi} \boldsymbol{\xi}_q \right).$$

Where $\mathbf{e}_{pq}$ is the direction between spins p and q .

For different projections of the total effective field $\mathbf{H}$ and its variation $\delta \mathbf{H}$ we find

$$\mathbf{H}_p \cdot \mathbf{e}_{rp} = \frac{F}{\mu} \sum_q (\mathbf{e}_{rp} \cdot \mathbf{e}_{pq}) (\mathbf{e}_{rq} \cdot \mathbf{e}_{pq}), \quad \delta \mathbf{H}_p \cdot \boldsymbol{\xi}_p = \frac{F}{\mu} \sum_q ((\psi_q^+ \boldsymbol{\xi}_q^* + \psi_q^- \boldsymbol{\xi}_q) \cdot \mathbf{e}_{pq}) (\boldsymbol{\xi}_p \cdot \mathbf{e}_{pq}).$$

Hence ψ_p^+ and ψ_p^- are determined by the following dynamic equations:

$$\begin{aligned} i \frac{d\psi_p^+}{dt} = & \dots \frac{F}{\mu} \sum_q \left(\frac{b}{\sqrt{2}} e^{-i\varphi} \psi_q^+ + \frac{b}{\sqrt{2}} e^{i\varphi} \psi_q^- \right) \left(a \boldsymbol{\xi}_p \cdot \mathbf{e}_q + \frac{b}{\sqrt{2}} e^{i\varphi} \boldsymbol{\xi}_p \cdot \boldsymbol{\xi}_q^* + \frac{b}{\sqrt{2}} e^{-i\varphi} \boldsymbol{\xi}_p \cdot \boldsymbol{\xi}_q \right) \\ & - \frac{F}{\mu} \sum_q \psi_p^+ (\mathbf{e}_{pq} \cdot \mathbf{e}_{rp}) (\mathbf{e}_{pq} \cdot \mathbf{e}_{rp}), \end{aligned} \tag{4.3.39}$$

$$\begin{aligned}
i\frac{d\psi_p^-}{dt} = \dots - \frac{F}{\mu} \sum_q \left(\frac{b}{\sqrt{2}} e^{-i\varphi} \psi_q^+ + \frac{b}{\sqrt{2}} e^{i\varphi} \psi_q^- \right) \left(a \boldsymbol{\xi}_p^* \cdot \mathbf{e}_{\mathbf{r}_q} + \frac{b}{\sqrt{2}} e^{-i\varphi} \boldsymbol{\xi}_p^* \boldsymbol{\xi}_q + \frac{b}{\sqrt{2}} e^{i\varphi} \boldsymbol{\xi}_p^* \cdot \boldsymbol{\xi}_q^* \right) \\
+ \frac{F}{\mu} \sum_q \psi_p^- (\mathbf{e}_{\mathbf{p}q} \cdot \mathbf{e}_{\mathbf{r}_p}) (\mathbf{e}_{\mathbf{p}q} \cdot \mathbf{e}_{\mathbf{r}_p}).
\end{aligned} \tag{4.3.40}$$

or for numerical purposes the equations could be rewritten as:

$$i\frac{d\psi^+}{dt} = \dots - \frac{F}{\mu} \sum_q (\mathbf{e}_{\mathbf{r}_p} \cdot \mathbf{e}_{\mathbf{p}q}) (\mathbf{e}_{\mathbf{r}_q} \cdot \mathbf{e}_{\mathbf{p}q}) + \frac{F}{\mu} \sum_q ((\psi_q^+ \boldsymbol{\xi}_q^* + \psi_q^- \boldsymbol{\xi}_q) \cdot \mathbf{e}_{\mathbf{p}q}) (\boldsymbol{\xi}_p \cdot \mathbf{e}_{\mathbf{p}q}). \tag{4.3.41}$$

$$i\frac{d\psi^-}{dt} = \dots + \frac{F}{\mu} \sum_q (\mathbf{e}_{\mathbf{r}_p} \cdot \mathbf{e}_{\mathbf{p}q}) (\mathbf{e}_{\mathbf{r}_q} \cdot \mathbf{e}_{\mathbf{p}q}) - \frac{F}{\mu} \sum_q ((\psi_q^- \boldsymbol{\xi}_q + \psi_q^+ \boldsymbol{\xi}_q^*) \cdot \mathbf{e}_{\mathbf{p}q}) (\boldsymbol{\xi}_p^* \cdot \mathbf{e}_{\mathbf{p}q}). \tag{4.3.42}$$

For the pseudodipolar interaction the equation can be cast into the following matrix form:

$$\begin{aligned}
i\frac{d}{dt} \begin{bmatrix} \psi_p^+ \\ \psi_p^- \end{bmatrix} = \frac{F}{\mu} \sum_q \begin{bmatrix} (\boldsymbol{\xi}_q^* \cdot \mathbf{e}_{\mathbf{p}q}) (\boldsymbol{\xi}_p \cdot \mathbf{e}_{\mathbf{p}q}) & (\boldsymbol{\xi}_q \cdot \mathbf{e}_{\mathbf{p}q}) (\boldsymbol{\xi}_p \cdot \mathbf{e}_{\mathbf{p}q}) \\ -(\boldsymbol{\xi}_q^* \cdot \mathbf{e}_{\mathbf{p}q}) (\boldsymbol{\xi}_p^* \cdot \mathbf{e}_{\mathbf{p}q}) & -(\boldsymbol{\xi}_q \cdot \mathbf{e}_{\mathbf{p}q}) (\boldsymbol{\xi}_p^* \cdot \mathbf{e}_{\mathbf{p}q}) \end{bmatrix} \begin{bmatrix} \psi_q^+ \\ \psi_q^- \end{bmatrix} \\
+ \frac{F}{\mu} \sum_q \begin{bmatrix} -(\mathbf{e}_q \cdot \mathbf{e}_{\mathbf{p}q}) (\mathbf{e}_p \cdot \mathbf{e}_{\mathbf{p}q}) & 0 \\ 0 & (\mathbf{e}_q \cdot \mathbf{e}_{\mathbf{p}q}) (\mathbf{e}_p \cdot \mathbf{e}_{\mathbf{p}q}) \end{bmatrix} \begin{bmatrix} \psi_p^+ \\ \psi_p^- \end{bmatrix}
\end{aligned}$$

These equations give the dynamic equations of a system under the influence of pseudodipolar interaction.

4.3.5 Four-Spin Interaction

The four-spin interaction can be analyzed through its contribution to the perturbation in the Hamiltonian, δH_p° , which is demonstrated for a plaquette p and spins located at vertices q , k , and l forming the plaquette. The interaction is modulated by a coupling constant K over the magnetic moment μ , reflecting the interplay between multiple spin sites within the system.

The four spin system is demonstrated in figure 4.1 below:

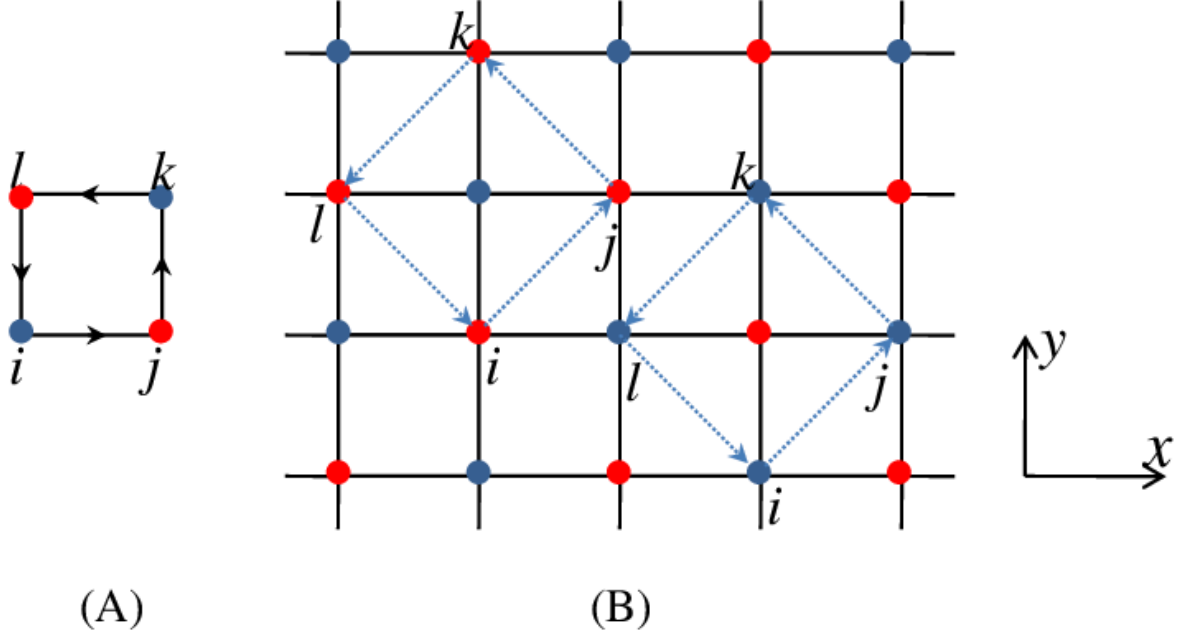


Figure 4.1: Schematic illustration of four spin interactions, each spin is interacted only once: (A) only nearest neighbor hopping shows interactions between adjacent spins, highlighting immediate spin coupling; (B) only next nearest neighbor hopping depicts interactions between spins separated by one site, emphasizing longer-range spin coupling effects [2].

$$\mathcal{H}_{4spin} = -K \sum_{pqkl} (\mathbf{m}_p \cdot \mathbf{m}_q) (\mathbf{m}_k \cdot \mathbf{m}_l) \quad \Rightarrow \quad \frac{-1}{\mu} \frac{\partial \mathcal{H}_{4spin}}{\partial \mathbf{m}_p} = \frac{K}{\mu} \sum_{qkl} \mathbf{m}_q (\mathbf{m}_k \cdot \mathbf{m}_l),$$

$$\mathbf{H}_p^\circ + \delta \mathbf{H}_p = \frac{K}{\mu} \sum_{qkl} (\mathbf{m}_q^\circ + \delta \mathbf{m}_q) ((\mathbf{m}_k^\circ + \delta \mathbf{m}_k) \cdot (\mathbf{m}_l^\circ + \delta \mathbf{m}_l)),$$

where $\mathbf{H}_p^\circ = \frac{K}{\mu} \sum_{qkl} \mathbf{m}_q^\circ (\mathbf{m}_k^\circ \cdot \mathbf{m}_l^\circ)$ represents the unperturbed Hamiltonian due to four-spin interaction, and $\delta \mathbf{H}_p$ encapsulates the perturbation resulting from fluctuations in spin orientations:

$$\delta \mathbf{H}_p = \frac{K}{\mu} \sum_{qkl} (\delta \mathbf{m}_q (\mathbf{m}_k^\circ \cdot \mathbf{m}_l^\circ) + \mathbf{m}_q^\circ (\mathbf{m}_k^\circ \cdot \delta \mathbf{m}_l) + \mathbf{m}_q^\circ (\delta \mathbf{m}_k \cdot \mathbf{m}_l^\circ)).$$

For all the neighbors we have:

$$\begin{aligned}
\delta \mathbf{H}_p^\circ \cdot \boldsymbol{\xi}_p &= \frac{K}{\mu} \sum_{qkl} \left[\psi_q^+(\boldsymbol{\xi}_q^* \cdot \boldsymbol{\xi}_p)(e_{\mathbf{r}_k} \cdot e_{\mathbf{r}_l}) + \psi_q^-(\boldsymbol{\xi}_q \cdot \boldsymbol{\xi}_p)(e_{\mathbf{r}_k} \cdot e_{\mathbf{r}_l}) \right. \\
&\quad + \psi_k^+(e_{\mathbf{r}_q} \cdot \boldsymbol{\xi}_p)(\boldsymbol{\xi}_k^* \cdot e_{\mathbf{r}_l}) + \psi_k^-(e_{\mathbf{r}_q} \cdot \boldsymbol{\xi}_p)(\boldsymbol{\xi}_k \cdot e_{\mathbf{r}_l}) \\
&\quad \left. + \psi_l^+(e_{\mathbf{r}_q} \cdot \boldsymbol{\xi}_p)(e_{\mathbf{r}_k} \cdot \boldsymbol{\xi}_l^*) + \psi_l^-(e_{\mathbf{r}_q} \cdot \boldsymbol{\xi}_p)(e_{\mathbf{r}_k} \cdot \boldsymbol{\xi}_l) \right],
\end{aligned} \tag{4.3.43}$$

where $\delta \mathbf{m}_q$, $\mathbf{m}_k^\circ$, and $\mathbf{m}_l^\circ$ are the fluctuations and equilibrium magnetizations at sites q , k , and l , respectively. $\boldsymbol{\xi}_p$, $\boldsymbol{\xi}_q^*$, and $\boldsymbol{\xi}_l$ are the corresponding coordinates. This four-spin interaction influences the time evolution of the magnon modes, which can be described through the following matrix equation:

$$\begin{aligned}
i \frac{d}{dt} \begin{bmatrix} \psi_p^+ \\ \psi_p^- \end{bmatrix} &= \frac{K}{\mu} \sum_{\substack{qkl \\ \in p}} \begin{bmatrix} (\boldsymbol{\xi}_q^* \cdot \boldsymbol{\xi}_p)(\mathbf{e}_{\mathbf{r}_l} \cdot \mathbf{e}_{\mathbf{r}_l}) & (\boldsymbol{\xi}_q \cdot \boldsymbol{\xi}_p)(\mathbf{e}_{\mathbf{r}_l} \cdot \mathbf{e}_{\mathbf{r}_l}) \\ -(\boldsymbol{\xi}_q^* \cdot \boldsymbol{\xi}_p^*)(\mathbf{e}_{\mathbf{r}_l} \cdot \mathbf{e}_{\mathbf{r}_l}) & -(\boldsymbol{\xi}_q \cdot \boldsymbol{\xi}_p^*)(\mathbf{e}_{\mathbf{r}_l} \cdot \mathbf{e}_{\mathbf{r}_l}) \end{bmatrix} \begin{bmatrix} \psi_q^+ \\ \psi_q^- \end{bmatrix} \\
&\quad + \begin{bmatrix} (\mathbf{e}_{\mathbf{r}_q} \cdot \boldsymbol{\xi}_p)(\boldsymbol{\xi}_k^* \cdot \mathbf{e}_{\mathbf{r}_l}) & (\mathbf{e}_{\mathbf{r}_q} \cdot \boldsymbol{\xi}_p)(\boldsymbol{\xi}_k \cdot \mathbf{e}_{\mathbf{r}_l}) \\ -(\mathbf{e}_{\mathbf{r}_q} \cdot \boldsymbol{\xi}_p^*)(\boldsymbol{\xi}_k^* \cdot \mathbf{e}_{\mathbf{r}_l}) & -(\mathbf{e}_{\mathbf{r}_q} \cdot \boldsymbol{\xi}_p^*)(\boldsymbol{\xi}_k \cdot \mathbf{e}_{\mathbf{r}_l}) \end{bmatrix} \begin{bmatrix} \psi_k^+ \\ \psi_k^- \end{bmatrix} \\
&\quad + \begin{bmatrix} (\mathbf{e}_{\mathbf{r}_q} \cdot \boldsymbol{\xi}_p)(\mathbf{e}_{\mathbf{r}_l} \cdot \boldsymbol{\xi}_l^*) & (\mathbf{e}_{\mathbf{r}_q} \cdot \boldsymbol{\xi}_p)(\mathbf{e}_{\mathbf{r}_l} \cdot \boldsymbol{\xi}_l) \\ -(\mathbf{e}_{\mathbf{r}_q} \cdot \boldsymbol{\xi}_p^*)(\mathbf{e}_{\mathbf{r}_l} \cdot \boldsymbol{\xi}_l^*) & -(\mathbf{e}_{\mathbf{r}_q} \cdot \boldsymbol{\xi}_p^*)(\mathbf{e}_{\mathbf{r}_l} \cdot \boldsymbol{\xi}_l) \end{bmatrix} \begin{bmatrix} \psi_l^+ \\ \psi_l^- \end{bmatrix}.
\end{aligned} \tag{4.3.44}$$

The equations describe how the components ψ_p^+ and ψ_p^- evolve over time through interactions with neighboring states indexed by q , k , and l . It is capturing the influence of neighboring states on the current state. The diagonal elements describe direct effects on the same component, while off-diagonal elements represent cross-coupling between the two components. The summation over indices indicates that the time evolution of a state is affected by interactions with neighboring states.

4.3.6 Oscillating Magnetic Field

An oscillating magnetic field is a magnetic field that varies in time. It's commonly used in various scientific and industrial applications, including magnetic resonance imaging (MRI) in medicine, where it helps in generating detailed images of organs

and tissues in the body. In the context of magnetic systems and spin dynamics, an oscillating magnetic field can influence the behavior of magnetic moments or spins, leading to phenomena like resonance or changes in the state of the system. This dynamic interplay between the oscillating field and magnetic moments is fundamental to understanding and manipulating the properties of magnetic materials for technological applications.

To understand the influence of oscillating magnetic field on the dynamics of the system, we begin with the Hamiltonian:

$$\begin{aligned}\mathcal{H} &= (\mathbf{m}_p^\circ + \delta\mathbf{m}_p) \times (\mathbf{h}(\mathbf{t})) \\ &= \mathbf{m}_p^\circ \times \mathbf{h}(\mathbf{t}) + \delta\mathbf{m}_p \times \mathbf{h}(\mathbf{t})\end{aligned}\tag{4.3.45}$$

$$H_p^\circ = -\frac{1}{\mu}\mathbf{h}(\mathbf{t}), \quad \delta H_p = \mathbf{0}\tag{4.3.46}$$

$$\delta H_p \cdot \boldsymbol{\xi}_p = \mathbf{0}\tag{4.3.47}$$

$$H_p^\circ \cdot \mathbf{e}_{\mathbf{r}_p} = -\frac{1}{\mu}\mathbf{h}(\mathbf{t}) \cdot \mathbf{e}_{\mathbf{r}_p}\tag{4.3.48}$$

Note that we Take the parallel part of the oscillating magnetic field. Subsequently, we derive the dynamical equations for ψ_p^+ and ψ_p^- , reflecting the influence of the oscillating field on the magnetic system's state, as illustrated below:

$$i\frac{d\psi_p^+}{dt} = \dots - \psi_p^+ \mathbf{h}(\mathbf{t}) \cdot \mathbf{e}_{\mathbf{r}_p}\tag{4.3.49}$$

$$i\frac{d\psi_p^-}{dt} = \dots + \psi_p^- \mathbf{h}^\circ(\mathbf{t}) \cdot \mathbf{e}_{\mathbf{r}_p}.\tag{4.3.50}$$

These equations give the Schrödinger equation equation in which the Hamiltonian includes the oscillating magnetic field, as we can see we have only the onsite potential and there is no hopping term.

4.4 Holstein-Primakoff Method for a Triangular Lattice

To properly describe the system using the Holstein-Primakoff transformation in a triangular lattice with four sites per unit cell as given in figure 4.2, it is essential to specify that the system is in the 3Q state. This state configuration plays a critical role in the spatial arrangement and interactions within the unit cell.

The Hamiltonian for spin exchange interactions on a triangular lattice is given by:

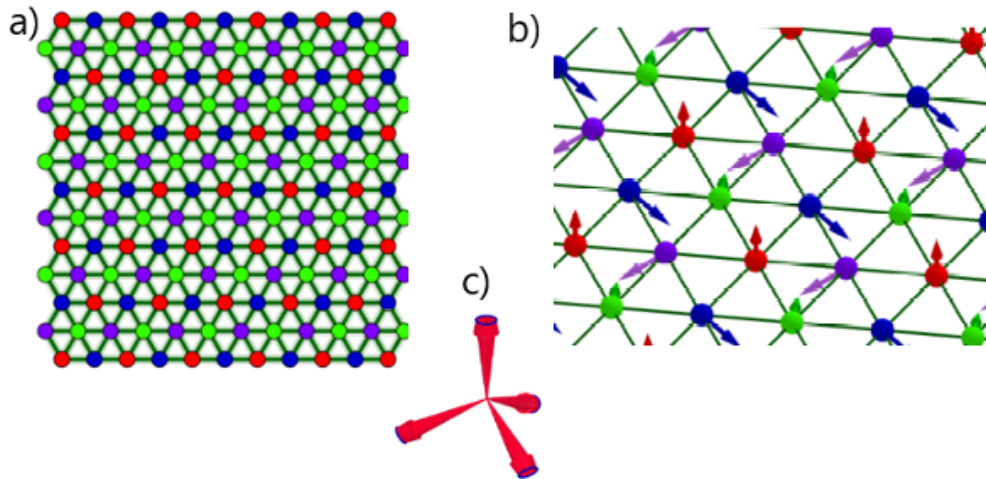


Figure 4.2: Lattice model for the 3Q state. a) The triangular lattice with 4 sites unit cell. b) The local spins configuration. All the spins are non-collinear and noncoplaner. c) The four different local spins of a unit cell plotted from the same origin. The angles between each two local spins are the same [3].

$$\mathcal{H} = -J \sum_{\mathbf{p} \in \{a,b,c,d\}} \mathbf{S}_{\mathbf{p}} \cdot \sum_{\mathbf{q} \in \mathbf{p} + \delta} \mathbf{S}_{\mathbf{q}}, \quad (4.4.51)$$

where J represents the exchange interaction strength, (a, b, c, d) are the spins' sites of the unit cell, delta represents the distance to the nearest neighbor, $\mathbf{S}_{\mathbf{p}}$ and $\mathbf{S}_{\mathbf{q}}$ are the spin vectors at sites $\mathbf{p}$ and $\mathbf{q}$, respectively, and δ denotes the nearest neighbor vectors.

Considering the Holstein-Primakoff transformation to delve into the intricacies of

magnon interactions within a magnetically ordered system, let's define interaction term $\mathbf{S}_p \cdot \mathbf{S}_q$ the interaction I ,
Note that $\mathbf{S}_p$ is given by:

$$\mathbf{S}_p = \begin{bmatrix} \mathbf{S}_x \\ \mathbf{S}_y \\ \mathbf{S}_z \end{bmatrix}$$

where

$$\begin{aligned} \mathbf{S}_+ &= \mathbf{S}_x + i\mathbf{S}_y, \\ \mathbf{S}_- &= \mathbf{S}_x - i\mathbf{S}_y \end{aligned} \tag{4.4.52}$$

This gives, $\mathbf{S}_x = \frac{\mathbf{S}_+ + \mathbf{S}_-}{2}$ and $\mathbf{S}_y = \frac{\mathbf{S}_+ - \mathbf{S}_-}{2i}$

using lowest order approximation discussed in section 3.8, hence I can be represented as:

$$I = \begin{bmatrix} \sqrt{2s} \frac{a+a^\dagger}{2} \\ \sqrt{2s} \frac{a-a^\dagger}{2i} \\ s - a^\dagger a \end{bmatrix} \cdot \begin{bmatrix} \sqrt{2s} \frac{b+b^\dagger}{2} \\ \sqrt{2s} \frac{b-b^\dagger}{2i} \\ s - b^\dagger b \end{bmatrix} \tag{4.4.53}$$

This gives (Note that here we have non vanishing value of the dot product between different unit vectors because each corresponds to different site):

$$\begin{aligned} I &= \frac{s}{2} ((a + a^\dagger)(b + b^\dagger) (\mathbf{e}_{\theta_a} \cdot \mathbf{e}_{\theta_b}) - (a - a^\dagger)(b - b^\dagger) (\mathbf{e}_{\phi_a} \cdot \mathbf{e}_{\phi_b})) \\ &\quad + (s^2 - s(a^\dagger a + b^\dagger b))(\mathbf{e}_{r_a} \cdot \mathbf{e}_{r_b}) \\ &\quad + \frac{s}{2i} ((a + a^\dagger)(b - b^\dagger)(\mathbf{e}_{\theta_a} \cdot \mathbf{e}_{\phi_b}) + (a - a^\dagger)(b + b^\dagger)(\mathbf{e}_{\phi_a} \cdot \mathbf{e}_{\theta_b})) \\ &\quad + \frac{s\sqrt{2s}}{2} ((a + a^\dagger)(\mathbf{e}_{\theta_a} \cdot \mathbf{e}_{r_b}) - i(a - a^\dagger)(\mathbf{e}_{\phi_a} \cdot \mathbf{e}_{r_b}) \\ &\quad \quad + (b + b^\dagger)(\mathbf{e}_{r_a} \cdot \mathbf{e}_{\theta_b}) - i(b - b^\dagger)(\mathbf{e}_{r_a} \cdot \mathbf{e}_{\phi_b})) \end{aligned} \tag{4.4.54}$$

for the term of the order $s\sqrt{2s}$, we will need to do the calculations for all the pairs that consider the nearest neighbor vectors i.e. for (a, b) , (a, c) , (a, d) and all the other rotations for different atoms b,c,d. This will lead to terms like $(a + a^\dagger) (\mathbf{e}_{\theta_a} \cdot (\mathbf{e}_{r_b} + \mathbf{e}_{r_c} + \mathbf{e}_{r_d})) = (a + a^\dagger) (\mathbf{e}_{\theta_a} \cdot (-\mathbf{e}_{r_a})) = \mathbf{0}$, this is because we have AFM, hence cancelling terms of

the order $s\sqrt{s}$ yields:

Hence:

$$\begin{aligned}
(I) = & + \frac{s}{2} (ab + a^\dagger b^\dagger + ab^\dagger + a^\dagger b) (\mathbf{e}_{\theta_a} \cdot \mathbf{e}_{\theta_b}) \\
& - \frac{s}{2} (ab + a^\dagger b^\dagger - ab^\dagger - a^\dagger b) (\mathbf{e}_{\phi_a} \cdot \mathbf{e}_{\phi_b}) \\
& + (s^2 - sa^\dagger a - sb^\dagger b) (\mathbf{e}_{r_a} \cdot \mathbf{e}_{r_b}) \\
& + \frac{s}{2i} (ab - a^\dagger b^\dagger - ab^\dagger + a^\dagger b) (\mathbf{e}_{\theta_a} \cdot \mathbf{e}_{\phi_b}) \\
& + \frac{s}{2i} (ab - a^\dagger b^\dagger + ab^\dagger - a^\dagger b) (\mathbf{e}_{\phi_a} \cdot \mathbf{e}_{\theta_b}).
\end{aligned} \tag{4.4.55}$$

we find:

$$\begin{aligned}
I = & + \frac{s}{2} (ab + a^\dagger b^\dagger) (\mathbf{e}_{\theta_a} \cdot \mathbf{e}_{\theta_b} - \mathbf{e}_{\phi_a} \cdot \mathbf{e}_{\phi_b}) \\
& + \frac{s}{2} (ab^\dagger + a^\dagger b) (\mathbf{e}_{\theta_a} \cdot \mathbf{e}_{\theta_b} + \mathbf{e}_{\phi_a} \cdot \mathbf{e}_{\phi_b}) \\
& + (s^2 - sa^\dagger a - sb^\dagger b) (\mathbf{e}_{r_a} \cdot \mathbf{e}_{r_b}) \\
& + \frac{s}{2i} (ab - a^\dagger b^\dagger) (\mathbf{e}_{\theta_a} \cdot \mathbf{e}_{\phi_b} + \mathbf{e}_{\phi_a} \cdot \mathbf{e}_{\theta_b}) \\
& - \frac{s}{2i} (ab^\dagger - a^\dagger b) (\mathbf{e}_{\theta_a} \cdot \mathbf{e}_{\phi_b} - \mathbf{e}_{\phi_a} \cdot \mathbf{e}_{\theta_b})
\end{aligned} \tag{4.4.56}$$

collecting the similar terms

$$\begin{aligned}
I = & + \frac{s}{2} (ab) (\mathbf{e}_{\theta_a} \cdot \mathbf{e}_{\theta_b} - \mathbf{e}_{\phi_a} \cdot \mathbf{e}_{\phi_b} - \mathbf{i} (\mathbf{e}_{\theta_a} \cdot \mathbf{e}_{\phi_b} + \mathbf{e}_{\phi_a} \cdot \mathbf{e}_{\theta_b})) \\
& + \frac{s}{2} (a^\dagger b^\dagger) (\mathbf{e}_{\theta_a} \cdot \mathbf{e}_{\theta_b} - \mathbf{e}_{\phi_a} \cdot \mathbf{e}_{\phi_b} + \mathbf{i} (\mathbf{e}_{\theta_a} \cdot \mathbf{e}_{\phi_b} + \mathbf{e}_{\phi_a} \cdot \mathbf{e}_{\theta_b})) \\
& + \frac{s}{2} (ab^\dagger) (\mathbf{e}_{\theta_a} \cdot \mathbf{e}_{\theta_b} + \mathbf{e}_{\phi_a} \cdot \mathbf{e}_{\phi_b} + \mathbf{i} (\mathbf{e}_{\theta_a} \cdot \mathbf{e}_{\phi_b} - \mathbf{e}_{\phi_a} \cdot \mathbf{e}_{\theta_b})) \\
& + \frac{s}{2} (a^\dagger b) (\mathbf{e}_{\theta_a} \cdot \mathbf{e}_{\theta_b} + \mathbf{e}_{\phi_a} \cdot \mathbf{e}_{\phi_b} - \mathbf{i} (\mathbf{e}_{\theta_a} \cdot \mathbf{e}_{\phi_b} - \mathbf{e}_{\phi_a} \cdot \mathbf{e}_{\theta_b})) \\
& + (s^2 - s(a^\dagger a + b^\dagger b)) (\mathbf{e}_{r_a} \cdot \mathbf{e}_{r_b})
\end{aligned} \tag{4.4.57}$$

writing the vectors in terms of different $\xi's$

$$\begin{aligned}
I = & + s(ab) (\boldsymbol{\xi}_a^* \cdot \boldsymbol{\xi}_b^*) + s(a^\dagger b^\dagger) (\boldsymbol{\xi}_a \cdot \boldsymbol{\xi}_b) \\
& + s(ab^\dagger) (\boldsymbol{\xi}_a^* \cdot \boldsymbol{\xi}_b) + s(a^\dagger b) (\boldsymbol{\xi}_a \cdot \boldsymbol{\xi}_b^*) \\
& + (s^2 - s(a^\dagger a + b^\dagger b)) (\mathbf{e}_{r_a} \cdot \mathbf{e}_{r_b}).
\end{aligned} \tag{4.4.58}$$

We need to do the same calculation for the couples (a, b),(a, c),(a, d),(b, a),(b,

c),(b, d),(c, a),(c, b),(c, d),(d, a), (d, b), (d, c). The last term in equation 4.4.60 for the NN of atom a lead:

$$\begin{aligned} & \left(s^2 - s(a^\dagger a) \right) \left(\mathbf{e}_{\mathbf{r}_a} \cdot \left(\mathbf{e}_{\mathbf{r}_b} + \mathbf{e}_{\mathbf{r}_c} + \mathbf{e}_{\mathbf{r}_d} \right) \right) - s \left(\mathbf{b}^\dagger \mathbf{b} (\mathbf{e}_{\mathbf{r}_a} \cdot \mathbf{e}_{\mathbf{r}_b}) + \mathbf{c}^\dagger \mathbf{c} (\mathbf{e}_{\mathbf{r}_a} \cdot \mathbf{e}_{\mathbf{r}_c}) + \mathbf{d}^\dagger \mathbf{d} (\mathbf{e}_{\mathbf{r}_a} \cdot \mathbf{e}_{\mathbf{r}_d}) \right) \\ & = - \left(s^2 - s(a^\dagger a) \right) - s \left(b^\dagger b (\mathbf{e}_{\mathbf{r}_a} \cdot \mathbf{e}_{\mathbf{r}_b}) + \mathbf{c}^\dagger \mathbf{c} (\mathbf{e}_{\mathbf{r}_a} \cdot \mathbf{e}_{\mathbf{r}_c}) + \mathbf{d}^\dagger \mathbf{d} (\mathbf{e}_{\mathbf{r}_a} \cdot \mathbf{e}_{\mathbf{r}_d}) \right) \end{aligned} \quad (4.4.59)$$

where we used the following relation to simplify equations:

$$(\mathbf{e}_{\mathbf{r}_a} \cdot \mathbf{e}_{\mathbf{r}_b} + \mathbf{e}_{\mathbf{r}_a} \cdot \mathbf{e}_{\mathbf{r}_c} + \mathbf{e}_{\mathbf{r}_a} \cdot \mathbf{e}_{\mathbf{r}_d}) = (\mathbf{e}_{\mathbf{r}_a} \cdot (\mathbf{e}_{\mathbf{r}_b} + \mathbf{e}_{\mathbf{r}_c} + \mathbf{e}_{\mathbf{r}_d})) = \mathbf{e}_{\mathbf{r}_a} \cdot (-\mathbf{e}_{\mathbf{r}_a}) = -1$$

here we expand the last term in equation 4.4.60 for the atoms b, c, and d we get :

$$-4s^2 + 2s(a^\dagger a + b^\dagger b + c^\dagger c + d^\dagger d) \quad (4.4.60)$$

after these calculations the interaction I can be written as:

$$\begin{aligned} I &= -4s^2 + 2s(a^\dagger a + b^\dagger b + c^\dagger c + d^\dagger d) \\ &+ s \sum_{p \in (a,b,c,d)} \sum_{q \in (a,b,c,d), q \neq p} \left((pq) (\boldsymbol{\xi}_p^* \cdot \boldsymbol{\xi}_q^*) + (p^\dagger q^\dagger) (\boldsymbol{\xi}_p \cdot \boldsymbol{\xi}_q) + (pq^\dagger) (\boldsymbol{\xi}_p^* \cdot \boldsymbol{\xi}_q) + (p^\dagger q) (\boldsymbol{\xi}_p \cdot \boldsymbol{\xi}_q^*) \right) \\ &= -4s^2 + 2s(a^\dagger a + b^\dagger b + c^\dagger c + d^\dagger d) \\ &+ s \sum_{p \in \zeta} \sum_{q \in \zeta} + \{ (pq) (\boldsymbol{\xi}_p^* \cdot \boldsymbol{\xi}_q^*) + (\mathbf{p}^\dagger \mathbf{q}^\dagger) (\boldsymbol{\xi}_p \cdot \boldsymbol{\xi}_q) + (\mathbf{p} \mathbf{q}^\dagger) (\boldsymbol{\xi}_p^* \cdot \boldsymbol{\xi}_q) + (\mathbf{p}^\dagger \mathbf{q}) (\boldsymbol{\xi}_p \cdot \boldsymbol{\xi}_q^*) \} \delta_{\mathbf{p}\mathbf{q}} \end{aligned} \quad (4.4.61)$$

with $\zeta = \{a, b, c, d\}$ Since the operators are Bosons, we have $[a, a^\dagger] = 1$ and therefore $2aa^\dagger = aa^\dagger + a^\dagger a + 1$. We therefore put $2aa^\dagger$ inside the sum ($\boldsymbol{\xi}_p \boldsymbol{\xi}_p = \boldsymbol{\xi}_p^\dagger \boldsymbol{\xi}_p^\dagger = 0$ and $\boldsymbol{\xi}_p \boldsymbol{\xi}_p^\dagger = 1$) and get:

$$I = -4s^2 + 4s + s \sum_{p \in \zeta} \sum_{q \in \zeta} \{ (\mathbf{p}\mathbf{q}) (\boldsymbol{\xi}_p^* \cdot \boldsymbol{\xi}_q^*) + (\mathbf{p}^\dagger \mathbf{q}^\dagger) (\boldsymbol{\xi}_p \cdot \boldsymbol{\xi}_q) + (\mathbf{p}\mathbf{q}^\dagger) (\boldsymbol{\xi}_p^* \cdot \boldsymbol{\xi}_q) + (\mathbf{p}^\dagger \mathbf{q}) (\boldsymbol{\xi}_p \cdot \boldsymbol{\xi}_q^*) \}$$

where δ_{pq} is taken out since $p = q$ is allowed in the sum let us define a vector operator: $\tilde{\mathbf{p}} = \mathbf{p}\boldsymbol{\xi}_p^*$ the interaction I becomes:

$$I = -4s^2 + 4s + s \sum_{p \in \zeta} \sum_{q \in \zeta} \{ (\tilde{\mathbf{p}}\tilde{\mathbf{q}}) + (\tilde{\mathbf{p}}^\dagger \tilde{\mathbf{q}}^\dagger) + (\tilde{\mathbf{p}}\tilde{\mathbf{q}}^\dagger) + (\tilde{\mathbf{p}}^\dagger \tilde{\mathbf{q}}) \} \quad (4.4.62)$$

The above equation means that now, we can reduce the unit cell and that the result is universal and depends only on the lattice.

4.5 Tilted Ferromagnet

Exploring the dynamics of 1D magnons we will investigate the case involving two tilted spins per unit, each oriented at angles of θ and $-\theta$ respectively, shown in figure 4.3 below:

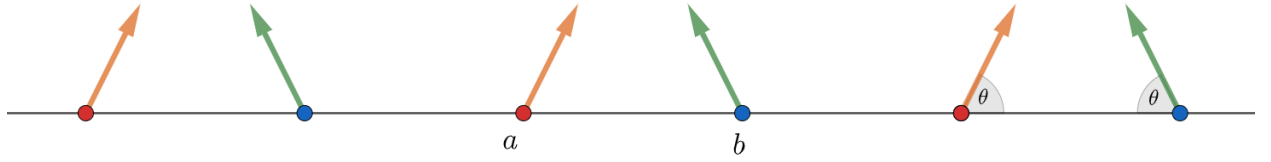


Figure 4.3: The case study of 2 spins in one dimension titled at angles of θ and $-\theta$ degrees shows two spins oriented at opposite diagonal angles in a one-dimensional lattice. This configuration illustrates the interaction dynamics and angular dependence of spin coupling in simplified systems.

The spin Hamiltonian is given by, note that this Hamiltonian leads to the above order

$$\mathcal{H} = -J \sum_{ij} \mathbf{m}_i \cdot \mathbf{m}_j - k \sum_i (\mathbf{m}_i \cdot \mathbf{e}_z)^2 - \sum_i \mathbf{B}_i \cdot \mathbf{m}_i, \quad (4.5.63)$$

where J denotes the exchange interaction strength, k is a constant describing the strength of an anisotropic spin spin interaction, and $\mathbf{B}_i$ is the external magnetic field.

The effective field, $\mathbf{H}_{\text{eff}}$, derived from $\mathcal{H}$ and taking $\mu = 1$ is, by using equation 3.4.8

$$H_{\text{eff}} = J \sum_{ij} \mathbf{m}_j + 2k \mathbf{e}_z (\mathbf{m}_i \cdot \mathbf{e}_z) + B \quad (4.5.64)$$

$$\text{with } \mathbf{H}_a \cdot \mathbf{e}_{r_a} = 2J \cos 2\theta + 2k \cos^2 \theta + B \cos \theta = A. \quad (4.5.65)$$

For magnon dynamics, we find

$$i \frac{d\psi_a^+}{dt} = \sum_b (\psi_b^+ \xi_a^* \xi_b + \psi_b^- \xi_a \xi_b^*) + A\psi_a^+, \quad (4.5.66)$$

$$i \frac{d\psi_a^-}{dt} = - \sum_b (\psi_b^- \xi_a^* \xi_b + \psi_b^+ \xi_a \xi_b^*) - A\psi_a^- \quad (4.5.67)$$

Note that this is the LLG equation with the damping constant is zero.

Introducing magnon wavefunctions as

$$\psi^+ = \psi_a^+ e^{i(k \cdot r_a - \omega t)}, \quad \psi^- = \psi_a^- e^{-i(k \cdot r_a - \omega t)}, \quad (4.5.68)$$

We can see that equations have the form of a Schrodinger equation for a spinor $\psi = (\psi^+, \psi^-)$. Although it has the form of a Schrodinger equation this is a classical dynamic equation.

The dispersion relation of these magnons, given by the frequency ω , is determined through their coupling in the lattice, characterized by the displacement vectors δ , the dispersion relation at site a is given by:

$$\begin{aligned} \omega \psi_a^+ &= \sum_{\delta} e^{ik \cdot \delta} (\psi_b^+ \xi_b \xi_a^* + \psi_b^- \xi_a \xi_b^*) + A\psi_a^+, \\ \omega \psi_a^- &= - \sum_{\delta} e^{-ik \cdot \delta} (\psi_b^- \xi_a \xi_b^* + \psi_b^+ \xi_b^* \xi_a^*) - A\psi_a^-. \end{aligned} \quad (4.5.69)$$

For the magnons at site b , the frequency is also ω , with dispersion relations:

$$\begin{aligned} \omega \psi_b^+ &= \sum_{\delta} e^{-ik \cdot \delta} (\psi_a^+ \xi_a \xi_b^* + \psi_a^- \xi_b \xi_a^*) + A\psi_b^+, \\ \omega \psi_b^- &= - \sum_{\delta} e^{ik \cdot \delta} (\psi_a^- \xi_b \xi_a^* + \psi_a^+ \xi_b^* \xi_a^*) - A\psi_b^- \end{aligned} \quad (4.5.70)$$

Note that $\sum_{\delta} e^{-ik \cdot \delta} = \sum_{\delta} e^{ik \cdot \delta} = 2 \cos ka$, because $\delta = +a, -a$

we can represent them in a matrix form as:

$$\omega \begin{pmatrix} \psi_a^+ \\ \psi_b^+ \\ \psi_a^- \\ \psi_b^- \end{pmatrix} = 2 \cos ka \begin{bmatrix} A & \xi_b \xi_a^* & 0 & \xi_a \xi_b \\ \xi_a \xi_b^* & A & \xi_b \xi_a & 0 \\ 0 & -\xi_b^* \xi_a^* & -A & -\xi_a \xi_b^* \\ -\xi_b^* \xi_a^* & 0 & -\xi_b \xi_a^* & -A \end{bmatrix} \begin{pmatrix} \psi_a^+ \\ \psi_b^+ \\ \psi_a^- \\ \psi_b^- \end{pmatrix}$$

The graph in figure 4.4 illustrates the dispersion relation of magnons in a two-spin system on a honeycomb lattice. The plot displays a variety of bands, each represented by a different color, indicating the existence of multiple magnon energy bands in the system.

A key feature observable in the graph is the existence of a band gap, an energy interval where magnon states are absent. The depicted graph illustrates a set of bands that exhibit symmetrical behavior about the energy axis. One curve ascends from negative to positive energy values with increasing wave vector k , while its counterpart descends symmetrically. This symmetry suggests a correspondence between a magnon and its antimagnon within the system—akin to the relationship between an electron and a hole in electronic systems.

The curve representing the magnon (ascending curve) shows how the energy of these quasiparticles increases with their momentum. Conversely, the symmetrically descending curve, representing the antimagnon, indicates an energy decrease as the momentum increases. This band reflects the energy state of the system when a magnon is annihilated or reabsorbed, leading to the recovery of the ordered spin state.

Note that if we compare the magnon energies in this case with the ones that appear as excitations in the Holstein primakoff Hamiltonian, we can see that the energies here can be negative. However, in the Holstein Primakoff case negative energy excitations would be a problem. This is because magnons are bosons and negative energy excitations in bosonic systems like magnons would imply that the ground state of the system is not stable because adding more bosons to these states would

indefinitely lower the energy of the system. According to Bose-Einstein statistics:

$$\text{If } \epsilon < 0, \text{ then } E = \sum_i n_i \epsilon \rightarrow -\infty \text{ as } n_i \rightarrow \infty$$

where ϵ is the excitation energy and n_i is the number of bosons in state i .

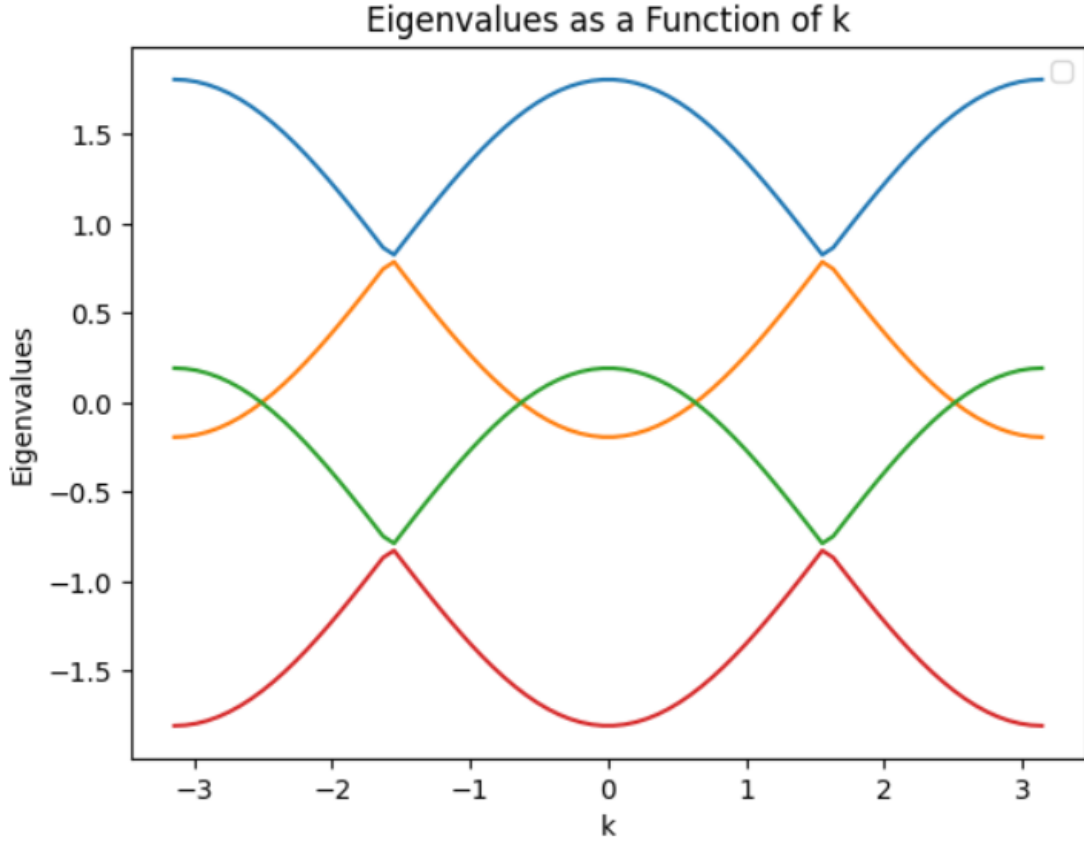


Figure 4.4: The band gap energy of a system of 2 spins titled at angles of 45 and -45 degrees.

Chapter 5

Discretization of the Schrödinger Equation

The Schrödinger equation is a fundamental equation in quantum mechanics that provides a way to predict the behavior and characteristics of particles at the quantum level. It describes the wave function of the system and how it evolves over time, essentially offering a mathematical model for the texture of quantum states within a quantum system governed by a specific Hamiltonian. This equation comes in two forms: time-dependent, which describes how the quantum state changes over time, and time-independent, which focuses on the stationary states and their energy levels of the system. Through the Schrödinger equation, one can determine the probabilities of finding particles in various states or locations [56]. In this section we aim to map the Schrödinger equation onto an effective tight binding model.

Considering the time-independent Schrödinger equation in one dimension:

$$i\hbar \frac{\partial \Psi(x, t)}{\partial t} = -\frac{\hbar^2}{2\mu} \frac{\partial^2 \Psi(x, t)}{\partial x^2} + V(x)\Psi(x, t), \quad (5.0.1)$$

where μ is the effective mass, $V(x)$ is the potential energy, i is the imaginary number, $\hbar$ is the Planck constant and $\psi(x, t)$ is the wave function.

To discretize this equation, we introduce a spatial grid with points $x_j = j\Delta x$, where Δx is the grid spacing and j is an integer. The first derivative of the wavefunction

ψ with respect to x can be approximated as follows:

$$\begin{aligned}\frac{\partial\psi}{\partial x} &\approx \frac{\psi(x + \Delta x) - \psi(x)}{\Delta x} \\ &= \frac{\psi(x_{j+1}) - \psi(x_j)}{\Delta x},\end{aligned}\tag{5.0.2}$$

The second derivative can be approximated as:

$$\begin{aligned}\frac{\partial^2\psi}{\partial x^2} &\approx \frac{\frac{\psi(x+\Delta x)-\psi(x)}{\Delta x} - \frac{\psi(x)-\psi(x-\Delta x)}{\Delta x}}{\Delta x} \\ &= \frac{\psi(x_{j+1}) - 2\psi(x_j) + \psi(x_{j-1}))}{(\Delta x)^2}.\end{aligned}\tag{5.0.3}$$

Substituting these approximations into the Schrödinger equation yields:

$$i\hbar \frac{d\Psi_j(t)}{dt} = -\frac{\hbar^2}{2\mu a^2} (\Psi_{j+1}(t) - 2\Psi_j(t) + \Psi_{j-1}(t)) + V_j \Psi_j(t)\tag{5.0.4}$$

where for a step a , $\psi_j(t) = \psi(ja, t)$ [57].

To derive the parameter t from the discretized Schrödinger Hamiltonian, we need to focus on the kinetic part of the Hamiltonian. The parameter t' represents the hopping parameter in the tight-binding model, which is a measure of the quantum mechanical tunneling probability between adjacent lattice sites.

In the discretization process, the continuous Hamiltonian's kinetic energy term, which involves second-order partial derivatives, is approximated by finite differences on a lattice. The hopping parameter t is related to the kinetic energy operator in the continuous case of one dimensional Schrödinger equation $-\frac{\hbar^2}{2\mu}\Delta^2 = -\frac{\hbar^2}{2\mu} \frac{\psi(x_{j-1}) - 2\psi(x_j) + \psi(x_{j+1}))}{(a)^2}$, this gives the hopping parameter t' ,

$$t' = \frac{\hbar^2}{2\mu a^2}\tag{5.0.5}$$

This expression shows that t' scales with the inverse of the mass and the square of the lattice spacing, meaning that heavier particles or larger lattice spacing will result in a smaller hopping parameter, and thus a lower probability for tunneling between lattice sites.

5.1 The Hamiltonian Matrix

In this section we want to obtain the Hamiltonian matrix for different systems, and then identify a general form of these matrices.

Hamiltonian Matrix for Hopping and On-Site Potentials Between Cells and Strips

We start with the Hamiltonian matrix for hopping and on site potential between cells as well as between a strip and another strip as demonstrated in figure 5.1.

The Hamiltonian below is demonstrating the magnons hopping on the lattice, which is given by:

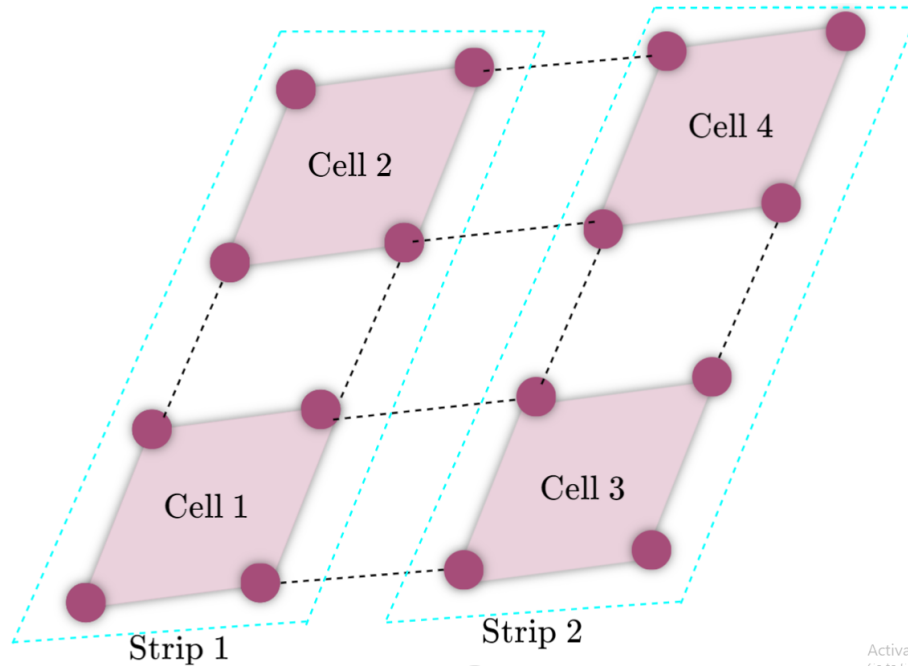


Figure 5.1: Configuration of two strips, each containing two cells, showing a lattice structure with cells labeled 1 through 4. Strip 1 includes Cell 1 and Cell 2, while Strip 2 comprises Cell 3 and Cell 4, highlighting the spatial arrangement and connectivity within the system.

$$\omega \begin{pmatrix} \psi_1 \\ \psi_2 \\ \psi_3 \\ \psi_4 \\ \psi_5 \\ \psi_6 \\ \psi_7 \\ \psi_8 \\ \psi_9 \\ \psi_{10} \\ \psi_{11} \\ \psi_{12} \\ \psi_{13} \\ \psi_{14} \\ \psi_{15} \\ \psi_{16} \end{pmatrix} = \begin{bmatrix} \epsilon & -t & 0 & -t & 0 & \dots & 0 & \dots & 0 & 0 & \dots & 0 & 0 & \dots & 0 & 0 \\ -t & \epsilon & -t & 0 & 0 & 0 & \dots & 0 & -t & 0 & \dots & 0 & \dots & 0 & 0 & 0 \\ 0 & -t & \epsilon & -t & 0 & -t & 0 & \dots & 0 & \dots & 0 & -t & \dots & 0 & 0 & 0 \\ \vdots & \vdots & \vdots & \ddots & \vdots & \vdots & \dots & \vdots & \vdots & \dots & \vdots & \vdots & \dots & \vdots & \vdots & \vdots \\ -t & 0 & 0 & \dots & \epsilon & -t & \dots & 0 & 0 & \dots & 0 & 0 & \dots & 0 & 0 & -t \\ 0 & 0 & 0 & -t & \epsilon & -t & 0 & -t & 0 & \dots & 0 & 0 & \dots & 0 & 0 & 0 \\ \vdots & \vdots & \vdots & \dots & \vdots & \vdots & \ddots & \vdots & \vdots & \dots & \vdots & \vdots & \dots & \vdots & \vdots & \vdots \\ 0 & 0 & 0 & \dots & 0 & -t & 0 & -t & \epsilon & 0 & \dots & 0 & \dots & 0 & 0 & 0 \\ 0 & -t & 0 & 0 & 0 & \dots & 0 & 0 & \epsilon & -t & 0 & -t & 0 & \dots & 0 & 0 \\ \vdots & \vdots & \vdots & \dots & \vdots & \vdots & \dots & \vdots & \vdots & \ddots & \vdots & \vdots & \dots & \vdots & \vdots & \vdots \\ 0 & 0 & 0 & \dots & 0 & 0 & \dots & 0 & 0 & -t & \epsilon & -t & 0 & -t & 0 & 0 \\ 0 & 0 & -t & 0 & \dots & 0 & \dots & 0 & -t & 0 & -t & \epsilon & -t & 0 & 0 & 0 \\ \vdots & \vdots & \vdots & \dots & \vdots & \vdots & \dots & \vdots & \vdots & \dots & \vdots & \vdots & \ddots & \vdots & \vdots & \vdots \\ 0 & 0 & 0 & \dots & 0 & 0 & \dots & 0 & \dots & 0 & -t & 0 & -t & \epsilon & -t & 0 \\ 0 & 0 & 0 & \dots & 0 & 0 & \dots & 0 & 0 & \dots & 0 & 0 & \dots & -t & \epsilon & -t \\ 0 & 0 & 0 & \dots & 0 & 0 & -t & 0 & \dots & 0 & \dots & 0 & -t & 0 & -t & \epsilon \end{bmatrix} \begin{pmatrix} \psi_1 \\ \psi_2 \\ \psi_3 \\ \psi_4 \\ \psi_5 \\ \psi_6 \\ \psi_7 \\ \psi_8 \\ \psi_9 \\ \psi_{10} \\ \psi_{11} \\ \psi_{12} \\ \psi_{13} \\ \psi_{14} \\ \psi_{15} \\ \psi_{16} \end{pmatrix}$$

The diagonal terms ϵ represent the on-site energy, while the off-diagonal terms $-t$ correspond to the hopping energy, indicating the likelihood of a particle moving between neighboring sites.

Governing Equations for Hopping Terms Between Atoms in a Unit Cell

Now consider a unit cell of four atoms given by figure 5.2, the governing equations for

the hopping terms between atoms a and b are given by:

$$i \frac{d\psi_a^+}{dt} = \sum \psi_b^+ \xi_a \xi_b^* + \sum \psi_b^- \xi_a \xi_b \quad (5.1.6)$$

$$\text{Let } \psi_a^+ = \psi_a^+ e^{i(kr_a - \omega t)}, \psi_a^- = \psi_a^- e^{i(kr_a - \omega t)}$$

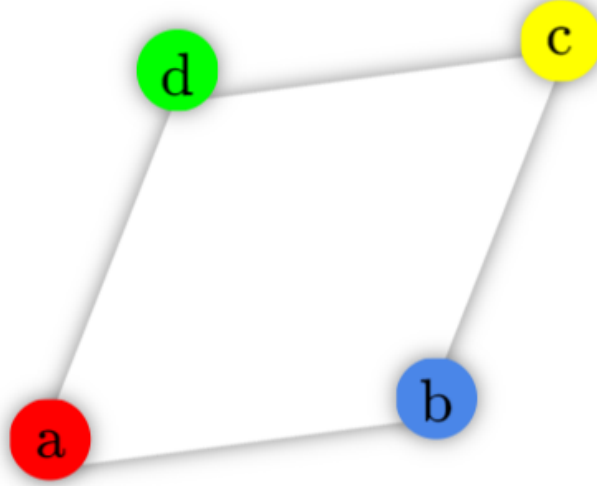


Figure 5.2: Unit cell with four atoms, labeled as a (red), b (blue), c (yellow), and d (green), showing the basic repeating structure in a lattice.

$$\psi_b^+ = \psi_b^+ e^{i(kr_b - \omega t)}, \psi_b^- = \psi_b^- e^{i(kr_b - \omega t)}$$

hence, the equations for wave functions a and b are given by:

$$\begin{aligned} \omega \psi_a^- &= -J \sum_{\delta} e^{ik \cdot \delta} \psi_b^* \xi_{ab}^* - J \sum_{\delta} e^{ik \cdot \delta} \psi_b \xi_a \xi_b^*, \\ \omega \psi_a^+ &= J \sum_{\delta} e^{ik \cdot \delta} \psi_b^+ \xi_a \xi_b^* + J \sum_{\delta} e^{ik \cdot \delta} \psi_b^- \xi_a \xi_b, \\ \omega \psi_b^+ &= J \sum_{\delta} e^{-ik \cdot \delta} \psi_a^+ \xi_b \xi_a^* + J \sum_{\delta} e^{-ik \cdot \delta} \psi_a^- \xi_b \xi_a, \\ \omega \psi_b^- &= -J \sum_{\delta} e^{-ik \cdot \delta} \psi_a^- \xi_b^* \xi_a^* - J \sum_{\delta} e^{-ik \cdot \delta} \psi_a^+ \xi_b^* \xi_a^*. \end{aligned} \tag{5.1.7}$$

where J is the exchange interaction constant, $\delta = r_b - r_a$

Similarly, we can find the equations of atoms c and d. Accordingly all these equations can be summarized in the following matrix:

$$\begin{bmatrix} A & J \sum e^{ik \cdot \delta} \xi_b^* \xi_a & 0 & J \sum e^{ik \cdot \delta} \xi_d^* \xi_a & 0 & J \sum e^{ik \cdot \delta} \xi_a \xi_b & 0 & J \sum e^{ik \cdot \delta} \xi_a \xi_d \\ J \sum e^{-ik \cdot \delta} \xi_b \xi_a^* & A & J \sum e^{-ik \cdot \delta} \xi_b \xi_c^* & 0 & J \sum e^{-ik \cdot \delta} \xi_a \xi_b & 0 & J \sum e^{-ik \cdot \delta} \xi_c \xi_b & 0 \\ 0 & J \sum e^{ik \cdot \delta} \xi_b^* \xi_c & A & J \sum e^{ik \cdot \delta} \xi_d^* \xi_c & 0 & J \sum e^{-ik \cdot \delta} \xi_a \xi_c & 0 & J \sum e^{ik \cdot \delta} \xi_d \xi_c \\ J \sum e^{-ik \cdot \delta} \xi_d \xi_a^* & 0 & J \sum e^{-ik \cdot \delta} \xi_d \xi_c^* & A & J \sum e^{ik \cdot \delta} \xi_a \xi_d & 0 & J \sum e^{-ik \cdot \delta} \xi_c \xi_d & 0 \\ 0 & -J \sum e^{ik \cdot \delta} \xi_b^* \xi_a & 0 & -J \sum e^{ik \cdot \delta} \xi_d^* \xi_a^* & A & -J \sum e^{ik \cdot \delta} \xi_a \xi_b^* & 0 & -J \sum e^{ik \cdot \delta} \xi_a \xi_d^* \\ -J \sum e^{-ik \cdot \delta} \xi_b \xi_a^* & 0 & -J \sum e^{ik \cdot \delta} \xi_b^* \xi_c^* & 0 & -J \sum e^{ik \cdot \delta} \xi_a^* \xi_b & A & -J \sum e^{ik \cdot \delta} \xi_c^* \xi_b & 0 \\ 0 & -J \sum e^{ik \cdot \delta} \xi_b^* \xi_c & 0 & -J \sum e^{ik \cdot \delta} \xi_d^* \xi_c^* & 0 & -J \sum e^{ik \cdot \delta} \xi_b^* \xi_c & A & J \sum e^{ik \cdot \delta} \xi_d^* \xi_c \\ -J \sum e^{ik \cdot \delta} \xi_d \xi_a^* & 0 & -J \sum e^{ik \cdot \delta} \xi_d^* \xi_c^* & 0 & -J \sum e^{ik \cdot \delta} \xi_a^* \xi_d & 0 & -J \sum e^{ik \cdot \delta} \xi_c^* \xi_d & 0 \end{bmatrix} \tag{5.1.8}$$

where A is a constant representing the onsite potential.

From the above matrices, we can see that generally the Hamiltonian matrix has the following form:

$$\begin{bmatrix} f_{aa} & f_{ba} & f_{ca} & f_{da} & \cdot & g_{aa} & g_{ba} & g_{ca} & g_{da} \\ f_{ab} & f_{bb} & f_{cb} & f_{db} & \cdot & g_{ab} & g_{bb} & g_{cb} & g_{db} \\ f_{ac} & f_{bc} & f_{cc} & f_{dc} & \cdot & g_{ac} & g_{bc} & g_{cc} & g_{dc} \\ f_{ad} & f_{bd} & f_{cd} & f_{dd} & \cdot & g_{ad} & g_{bd} & g_{cd} & g_{dd} \\ \cdot & \cdot & \cdot & \cdot & \cdot & \cdot & \cdot & \cdot & \cdot \\ -g_{aa}^* & -g_{ba}^* & -g_{ca}^* & -g_{da}^* & \cdot & -f_{aa}^* & -f_{ba}^* & -f_{ca}^* & -f_{da}^* \\ -g_{ab}^* & -g_{bb}^* & -g_{cb}^* & -g_{db}^* & \cdot & -f_{ab}^* & -f_{bb}^* & -f_{cb}^* & -f_{db}^* \\ -g_{ac}^* & -g_{bc}^* & -g_{cc}^* & -g_{dc}^* & \cdot & -f_{ac}^* & -f_{bc}^* & -f_{cc}^* & -f_{dc}^* \\ -g_{ad}^* & -g_{bd}^* & -g_{cd}^* & -g_{dd}^* & \cdot & -f_{ad}^* & -f_{bd}^* & -f_{cd}^* & -f_{dd}^* \end{bmatrix}$$

Here f and g are functions that gives the hopping and onsite potential between different atoms. It is clear that $f_{qp} = f^*(qp)$ and $g_{qp} = g_{pq}$. This shows that the total matrix can be written as:

$$\begin{bmatrix} H & \gamma \\ -\gamma^\dagger & -H^T \end{bmatrix}$$

where T is the transpose of the matrix, H is the onsite potential matrix and γ is the hoping potential matrix.

The matrix that describe the onsite potential for atom a alone is given by:

$$\omega \begin{pmatrix} \psi_a^+ \\ \psi_a^- \end{pmatrix} = \begin{pmatrix} A & 0 \\ 0 & A \end{pmatrix} \begin{pmatrix} \psi_a^+ \\ \psi_a^- \end{pmatrix}$$

Hopping matrix from atom a to atom b ($a \rightarrow b$)

$$\omega \begin{pmatrix} \psi_a^+ \\ \psi_a^- \end{pmatrix} = \begin{pmatrix} J\xi_a\xi_b^* & J\xi_a\xi_b \\ -J\xi_a^*\xi_b^* & J\xi_a^*\xi_b \end{pmatrix} \begin{pmatrix} \psi_b^+ \\ \psi_b^- \end{pmatrix}$$

Hopping matrix from atom b to atom a ($b \rightarrow a$)

$$\omega \begin{pmatrix} \psi_b^+ \\ \psi_b^- \end{pmatrix} = \begin{pmatrix} J\xi_b\xi_a^* & J\xi_a\xi_b \\ -J\xi_a^*\xi_b^* & -J\xi_b^*\xi_a^* \end{pmatrix} \begin{pmatrix} \psi_a^+ \\ \psi_a^- \end{pmatrix}$$

5.2 Hermitian Hamiltonian Framework for a Lattice System

In exploring the dynamics of lattice systems, the Hamiltonian framework plays a pivotal role, encompassing on-site energy interactions and directional hopping phenomena. We introduce a Hamiltonian, denoted by H , to capture on-site interactions within a lattice system. Additionally, we define τ and τ' as the hopping parameters between nearest neighbor cells in distinct directions. The overall energy expression is given by:

$$E = H + \tau e^{ik\delta} + \tau' e^{-ik\delta}. \quad (5.2.9)$$

The matrix of on site and hopping matrices:

$$\omega \begin{pmatrix} \vdots \\ \psi_{n-1} \\ \psi_n \\ \psi_{n+1} \\ \vdots \end{pmatrix} \begin{pmatrix} v_a & \tau_{ab} & \tau_{ac} & 0 & \cdots & 0 \\ \tau_{ba} & v_b & \cdots & \cdots & \cdots & 0 \\ \tau_{ca} & \cdots & v_c & \cdots & \cdots & 0 \\ \vdots & \vdots & \vdots & \ddots & \cdots & 0 \\ \cdots & \cdots & \cdots & \cdots & \cdots & v_n \end{pmatrix} = E \begin{pmatrix} \vdots \\ \psi_{n-1} \\ \psi_n \\ \psi_{n+1} \\ \vdots \end{pmatrix}$$

Specifically, if the onsite potential of all the strips is the same i.e. ($v_a = v_b = \cdots = H$) and the hoping between any 2 strips is τ or τ' (it is τ if it is from a to b and τ' from b to a and so on), we can express the energy of a system involving hopping

from site n to its nearest neighbors as:

$$i \begin{pmatrix} \vdots \\ \psi_{n-1} \\ \psi_n \\ \psi_{n+1} \\ \vdots \end{pmatrix} \begin{pmatrix} H & \tau & 0 & 0 & \cdots & 0 \\ \tau' & H & \tau & 0 & \cdots & 0 \\ 0 & \tau' & H & \tau & 0 & \cdots \\ \vdots & \vdots & \vdots & \ddots & \tau & 0 \\ 0 & \cdots & \cdots & 0 & \tau' & H \end{pmatrix} = E \begin{pmatrix} \vdots \\ \psi_{n-1} \\ \psi_n \\ \psi_{n+1} \\ \vdots \end{pmatrix}$$

If we take a component of the matrix it gives,

$$\tau' \psi_{n-1} + H \psi_n + \tau \psi_{n+1} = E \psi_n \quad (5.2.10)$$

where τ and τ' represent the hopping parameters, H denotes the onsite Hamiltonian, and ψ_n is the wave function at site n .

Upon introducing the wave vector k and angular frequency ω , we represent the wave functions as phase-shifted across different sites:

$$\psi_n = \psi e^{i(nk - \omega t)},$$

leading to a refined expression for the energy:

$$E = H + \tau e^{ik} + \tau' e^{-ik} \quad (5.2.11)$$

where E here represents the eigenvalues of the right handed part of equation 5.2.11. However, this formulation challenges the Hermitian property of the Hamiltonian. Since we use Kwant (which is dealing only with Hermitian matrices), we want to make this matrix Hermitian. This will be done by employing an extended Pauli matrix $\tilde{\sigma}_z$, ensuring a Hermitian construct:

$$\tilde{\sigma}_z = \begin{bmatrix} \sigma_z & 0 & \cdots & 0 \\ 0 & \sigma_z & \cdots & 0 \\ \vdots & \vdots & \ddots & \vdots \\ 0 & 0 & \cdots & \sigma_z \end{bmatrix}, \quad (5.2.12)$$

with $\sigma_z = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}$ denoting the z-component of Pauli spin matrices. This formulation introduces $\tilde{\sigma}_z E'$ [58], where E' is manifestly Hermitian, reconciling the non-Hermitian discrepancy. Note that this procedure is valid only when τ and τ' are related like in the case:

$$\tilde{\sigma}_z E' = \tilde{\sigma}_z \left[\tilde{H}_H + \tilde{\tau} e^{ik\delta} + \tilde{\tau}^\dagger e^{-ik\delta} \right], \quad (5.2.13)$$

where $\tau = \sigma_z \tilde{\tau}$

$$\left[\tilde{H}_H + \tilde{\tau} e^{ik} + \tilde{\tau}^\dagger e^{-i\mu} \right]^\dagger = \tilde{H}_H + \tilde{\tau}^\dagger e^{-ik} + \tau e^{ik}, \quad \text{i.e is Hermitian.}$$

Incorporating the Hermitian Hamiltonian matrix within the framework of Kwant, a computational software designed for quantum transport simulations. Kwant's architecture is particularly tuned to handle Hermitian matrices.

By leveraging the Hermitian Hamiltonian matrix constructed through the $\tilde{\sigma}_z$ extension, we can utilize Kwant to accurately simulate the quantum dynamics of various lattice configurations. Diagonalization of the Hamiltonian matrix within Kwant facilitates the precise determination of energy eigenvalues across the Brillouin zone, revealing the band gap of the system. One of the primary objectives of such simulations is to find the band structure of the material, a critical factor in understanding its electronic properties and potential applications in semiconductor physics, topological insulators, and beyond [59]. Now we want to implement this theoretical framework for Ferromagnetic Spins on a Honeycomb Lattice.

5.3 Example of Ferromagnetic Spins on a Honeycomb Lattice

The honeycomb lattice, a two-dimensional lattice structure realized in graphene, exhibits fascinating electronic properties due to its unique topology and symmetry. When considering ferromagnetic ordering within such a lattice, spins align uniformly across the lattice sites, which can lead to interesting magnetic properties and electronic band structures. In this section, we explore the configuration of ferromagnetic spins on a honeycomb lattice, and the resulting band gap energies.

5.3.1 Theoretical Model

Our theoretical framework begins with the construction of a tight-binding Hamiltonian that accounts for the exchange interactions between adjacent spins, the Zeeman energy, the pseudodipolar energy, and the anisotropy. The lattice is modeled using the kwant toolkit, which allows for the explicit definition of lattice vectors and sublattice positions, enabling a precise representation of the honeycomb structure as shown in figure 5.3.

Hamiltonian Formulation

The spin Hamiltonian for the system is given by

$$\begin{aligned}\mathcal{H} = & -\frac{J}{2} \sum_{\langle i,j \rangle} \mathbf{m}_i \cdot \mathbf{m}_j - \frac{1}{2} \sum_{\langle i,j \rangle} \mathcal{F}(\mathbf{m}_i, \mathbf{m}_j, \mathbf{e}_{ij}) \\ & - \sum_i \frac{K}{2} m_z^2 - \mu B \sum_i \mathbf{m}_z\end{aligned}\tag{5.3.14}$$

where J is the exchange coupling constant, $\mathcal{F}(\mathbf{m}_i, \mathbf{m}_j, \mathbf{e}_{ij}) = F(\mathbf{m}_i \cdot \mathbf{e}_{ij})(\mathbf{m}_j \cdot \mathbf{e}_{ij})$ where F is the interaction strength, K is the anisotropy constant, B is the external magnetic field, and $\mathbf{m}_i$ represents the spin on site i . This Hamiltonian captures the essential physics of ferromagnetic ordering in the system, where the first term de-

scribes the nearest-neighbor ferromagnetic interaction, the second term represents the pseudodipolar energy, the third term is the anisotropy energy, and the last term corresponds to the Zeeman energy in an external magnetic field.

The LLG equation

This is the LLG equation corresponding to the Hamiltonian above equation (5.3.14)

$$\begin{aligned} \frac{\partial \mathbf{m}_i}{\partial t} = -\mathbf{m}_i \times & \left[J \sum_j \mathbf{m}_j + F \sum_j (\mathbf{m}_j \cdot \mathbf{e}_{ij}) \mathbf{e}_{ij} \right. \\ & \left. + K m_{iz} \mathbf{e}_z + B \mathbf{e}_z \right], \end{aligned} \quad (5.3.15)$$

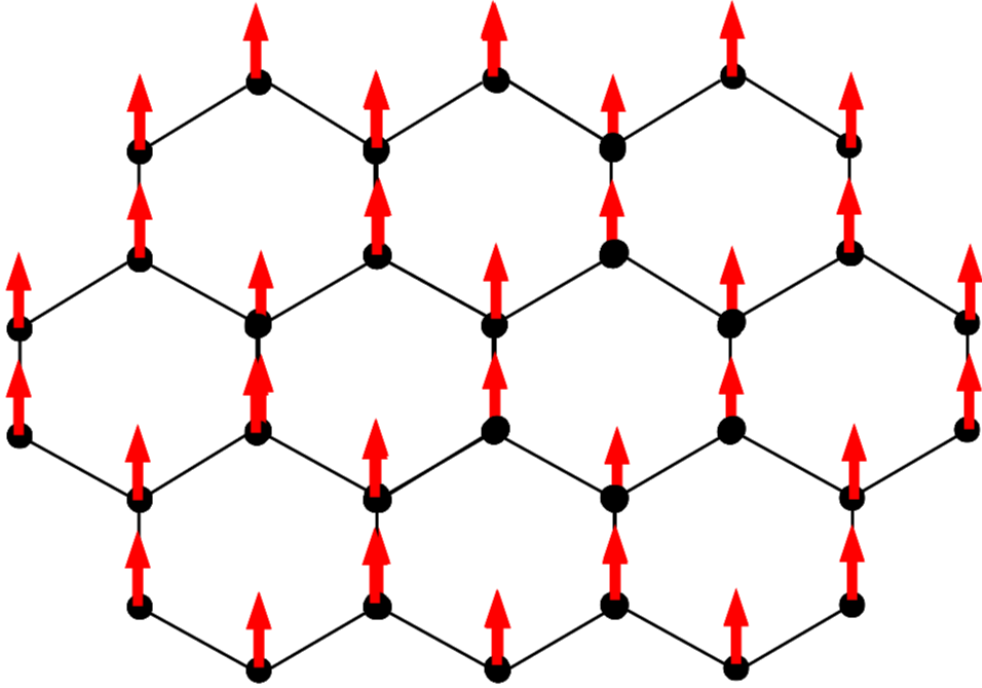


Figure 5.3: Schematic diagram of ferromagnetic spins on a honeycomb lattice, illustrating the arrangement of spins in a two-dimensional hexagonal structure where each spin is aligned in the same direction, demonstrating ferromagnetic order.

This system is a long graphene strip. We analyzed the system's Hamiltonian and identified the associated Landau-Lifshitz-Gilbert (LLG) equation. To simulate it, we used KWANT. We applied our derived equations for exchange, anisotropy, pseudodipolar, and Zeeman interactions. Since these equations are not Hermitian, we

used the method outlined in Section 5.1 to ensure the matrices are Hermitian. KWANT helped us set up the system, identify its nearest neighbors, and determine the band gap.

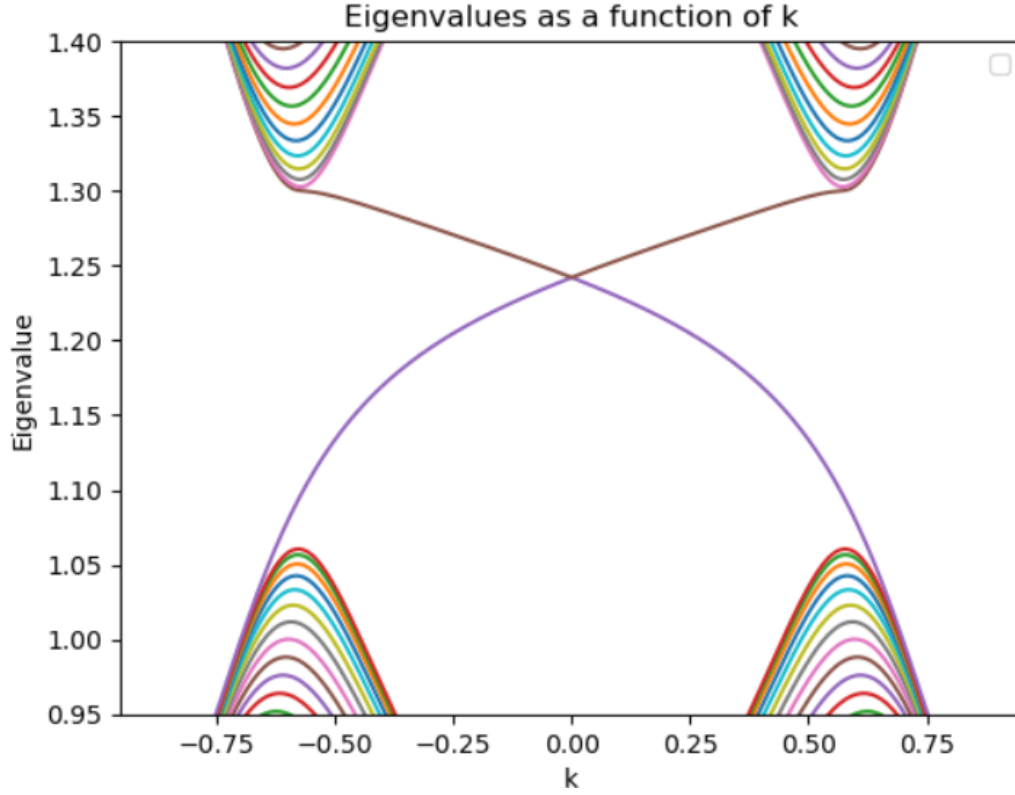


Figure 5.4: The band gap energy of a system of ferromagnetic spins on a honeycomb lattice.

Figure 5.4 displays the eigenvalue spectrum as a function of the wave vector k . The plot showcases a series of colorful bands representing the eigenvalues across different values of k , which spans symmetrically from negative to positive values. The presence of multiple bands suggests a system with multiple energy levels. We used the following values for the constants $J=0.1$, $k=0.4$, $F=0.5$, the magnetic field and the anisotropy are both along the z -axis.

Crucially, the plot reveals a band gap: a region where no eigenvalues exist, indicating an energy range where no electronic states can be occupied. This band gap is most noticeable around $k = 0$, where the upper and lower bands diverge, leaving a clear band separation between them. The existence of a band gap is a defining characteristic of semiconductors and insulators and determines the electronic and

optical properties of the material.

The lower bands, which are tightly packed and approach each other near the edges of the plot, might correspond to the valence band of the material, indicating the range of energy levels that are filled with electrons. Above the band gap, the sparsely separated lines represent the conduction band, which dictates the energy levels that electrons can occupy when the material is doped or when energy is applied.

Chapter 6

Numerical Analysis of Magnon Dynamics

6.1 Time Integration of the LLG equation

Time integration of the LLG equation is a critical procedure in computational micromagnetics, allowing for the simulation of magnetic dynamics over time. This process typically involves discretizing the LLG equation temporally and solving it iteratively, with the aim of understanding how magnetic moments in materials evolve under various conditions, including the presence of magnetic fields, thermal fluctuations, and material anisotropies. Common numerical methods for this purpose include the Euler method, Runge-Kutta methods, and more sophisticated schemes designed to conserve the magnitude of the magnetic moment vector and adhere to the constraints of the LLG equation.

6.1.1 Stochastic Landau-Lifshitz-Gilbert Equation

An interesting model to consider for magnetic systems is the so-called Brown-Kubo-Hashitsume model. In the Brown-Kubo-Hashitsume model, we begin with a formula that describes how a magnetic moment $\mathbf{m}$, moves in a random manner [60]. This formula is known as the stochastic Gilbert equation. it is adjusted to fit the clas-

the Landau-Lifshitz framework, creating what is known as the stochastic Landau-Lifshitz-Gilbert equation, we are using this method to simulate the LLG equation [60]. The stochastic LLG equation is given by:

$$\frac{\partial \mathbf{S}_i}{\partial t} = -\frac{\gamma}{(1 + \lambda^2)} [\mathbf{S}_i \times \mathbf{H}_{\text{eff}}^i + \lambda \mathbf{S}_i \times (\mathbf{S}_i \times \mathbf{H}_{\text{eff}}^i)] \quad (6.1.1)$$

where $\mathbf{S}_i$ symbolizes the direction of a magnetic spin at site i , γ represents the gyromagnetic ratio, and $\mathbf{H}_{\text{eff}}^i$ denotes the effective magnetic field acting on each spin, it is derived from the negative gradient of the spin Hamiltonian with respect to the spin $\mathbf{S}_i$, highlighting the role of the local spin moment in shaping this field.

$$\mathbf{H}_{\text{eff}}^i = -\frac{1}{\mu_S} \frac{\partial \mathcal{H}}{\partial \mathbf{S}_i} + \mathbf{H}_{\text{th}}^i \quad (6.1.2)$$

When considering thermal effects, it is essential to adopt Langevin Dynamics, especially for modeling temperature-induced fluctuations. This method introduces a thermal field represented by a Gaussian white noise term, which grows with temperature, affecting the magnetic behavior of the system.

$$\mathbf{H}_{\text{th}}^i = \Gamma(t) \sqrt{\frac{2\lambda k_B T}{\gamma \mu_s \Delta t}} \quad (6.1.3)$$

The Langevin Dynamics approach integrates a thermal field into the LLG equation to mimic the influence of temperature on spin dynamics. The technique assumes that at each timestep, every spin experiences an instantaneous thermal field based on a Gaussian distribution. This incorporation of thermal effects allows for a more comprehensive simulation of spin dynamics across various temperature conditions [61].

These equations are necessary to study the time evolution of a system of spins numerically. Different integration schemes can be used provided that during the simulations the moment vector $\mathbf{m}_i$ has to be normalized after each new integration step to assure the conservation of the magnetic moment [62]. The Heun method,

known for enabling larger time step usage due to its predictor-corrector algorithm, will be employed here.

6.1.2 Heun's Method

To simulate the LLG equation we use Heun's method, which is a numerical technique used to solve ordinary differential equations (ODEs). It is a type of predictor-corrector method that improves upon the basic Euler method by making a preliminary step (the predictor) and then using this to make a more informed final step (the corrector). The Heun method begins by predicting a new direction for each spin, $\mathbf{S}'_i$, using the initial spin $\mathbf{S}_i$ and the effective magnetic field $\mathbf{H}_{\text{eff}}^i$ through an initial Euler step:

$$\mathbf{S}'_i = \mathbf{S}_i + \Delta\mathbf{S}\Delta t, \quad (6.1.4)$$

we are solving an LLG equation with a step, this step $\Delta\mathbf{S}$, is defined as:

$$\Delta\mathbf{S} = -\frac{\gamma}{1 + \lambda^2} \left[\mathbf{S}_i \times \mathbf{H}_{\text{eff}}^i + \lambda \mathbf{S}_i \times (\mathbf{S}_i \times \mathbf{H}_{\text{eff}}^i) \right]. \quad (6.1.5)$$

This process doesn't maintain the magnitude of the spin, necessitating normalization after both the initial prediction and the final correction to ensure the spin remains a unit vector. Following the prediction, the effective field is recalculated due to the altered spin positions, though the random thermal field remains constant. The next position of the spin, $\mathbf{S}_i^{t+\Delta t}$, is determined with a correction step that averages the initial and updated changes in spin:

$$\mathbf{S}_i^{t+\Delta t} = \mathbf{S}_i + \frac{1}{2} [\Delta\mathbf{S} + \Delta\mathbf{S}'] \Delta t, \quad (6.1.6)$$

where $\Delta\mathbf{S}'$ is calculated similarly to $\Delta\mathbf{S}$ but using the predicted spin $\mathbf{S}'_i$ and the updated effective field $\mathbf{H}_{\text{eff}}^{i'}$:

$$\Delta\mathbf{S}' = -\frac{\gamma}{1 + \lambda^2} \left[\mathbf{S}'_i \times \mathbf{H}_{\text{eff}}^{i'} + \lambda \mathbf{S}'_i \times (\mathbf{S}'_i \times \mathbf{H}_{\text{eff}}^{i'}) \right]. \quad (6.1.7)$$

This process is applied sequentially to each spin before updating the entire system. The Heun method, while designed for equations with stochastic noise, simplifies to a conventional second-order Runge-Kutta method in noise-free scenarios.

In certain scenarios, employing spherical coordinates simplifies the computation. For these instances, it is advantageous to represent the change in spin, $\Delta \mathbf{S}$, using spherical coordinates for ease of analysis and calculation.

Starting from 6.1.5, absorbing the factor $\frac{\gamma}{(1+\lambda^2)}$ in the time variable. Then, we write:

$$\frac{\partial \mathbf{S}_i}{\partial t} = \frac{d\theta}{dt} \mathbf{e}_\theta + \sin \theta \frac{d\phi}{dt} \mathbf{e}_\phi \quad (6.1.8)$$

By multiplying the whole equation with $\mathbf{e}_\theta$, we get:

$$\begin{aligned} \frac{d\theta}{dt} &= -\mathbf{e}_\theta \cdot [\mathbf{S}_i \times \mathbf{H}_{\text{eff}}^i] - \mathbf{e}_\theta \cdot [\lambda \mathbf{S}_i \times (\mathbf{S}_i \times \mathbf{H}_{\text{eff}}^i)] \\ &= -\mathbf{H}_{\text{eff}}^i \cdot [\mathbf{e}_\theta \times \mathbf{S}_i] - (\mathbf{S}_i \times \mathbf{H}_{\text{eff}}^i) \cdot [\mathbf{e}_\theta \times \lambda \mathbf{S}_i] \\ &= \mathbf{H}_{\text{eff}}^i \cdot \mathbf{e}_\phi + \lambda \mathbf{e}_\phi \cdot (\mathbf{S}_i \times \mathbf{H}_{\text{eff}}^i) \\ &= \mathbf{H}_{\text{eff}}^i \cdot \mathbf{e}_\phi + \lambda \mathbf{H}_{\text{eff}}^i \cdot (\mathbf{e}_\phi \times \mathbf{S}_i) \\ &= \mathbf{H}_{\text{eff}}^i \cdot \mathbf{e}_\phi + \lambda \mathbf{H}_{\text{eff}}^i \cdot \mathbf{e}_\theta \end{aligned} \quad (6.1.9)$$

By multiplying the same equation with $\mathbf{e}_\phi$, we get:

$$\begin{aligned} \frac{d\tilde{\phi}}{dt} &= -\mathbf{e}_\phi \cdot [\mathbf{S}_i \times \mathbf{H}_{\text{eff}}^i] - \mathbf{e}_\phi \cdot [\lambda \mathbf{S}_i \times (\mathbf{S}_i \times \mathbf{H}_{\text{eff}}^i)] \\ &= -\mathbf{H}_{\text{eff}}^i \cdot [\mathbf{e}_\phi \times \mathbf{S}_i] - (\mathbf{S}_i \times \mathbf{H}_{\text{eff}}^i) \cdot [\mathbf{e}_\phi \times \lambda \mathbf{S}_i] \\ &= -\mathbf{H}_{\text{eff}}^i \cdot \mathbf{e}_\theta - \lambda \mathbf{e}_\theta \cdot (\mathbf{S}_i \times \mathbf{H}_{\text{eff}}^i) \\ &= -\mathbf{H}_{\text{eff}}^i \cdot \mathbf{e}_\theta - \lambda \mathbf{H}_{\text{eff}}^i \cdot (\mathbf{e}_\theta \times \mathbf{S}_i) \\ &= -\mathbf{H}_{\text{eff}}^i \cdot \mathbf{e}_\theta + \lambda \mathbf{H}_{\text{eff}}^i \cdot \mathbf{e}_\phi \end{aligned} \quad (6.1.10)$$

If we use our usual variables ψ and ξ , we find:

$$\frac{d\psi}{dt} = (\lambda - i) \mathbf{H}_{\text{eff}}^i \cdot \xi_i \quad (6.1.11)$$

6.2 Comparison of the Stochastic Numerical Methods with Exact Solutions

6.2.1 Dynamics of a Single Spin Subject to a field along the z-axis

This section explores the dynamics of a single spin initially aligned along the x-axis within a ferromagnetic system, subject to an external magnetic field directed along the z-axis as given in figure 6.1[63]. Here again we are using Kwant library to construct the lattice for mathematical operations. The Hamiltonian of this system can be written as

$$\mathcal{H} = -J \sum \mathbf{S}_i \cdot \mathbf{S}_j - \sum \mathbf{B} \cdot \mathbf{S}_i \quad (6.2.12)$$

where J is the exchange interaction and $\mathbf{B}$ is the external magnetic field. We are simulating the time evolution of the spins through the application of the Landau-Lifshitz-Gilbert (LLG) equation, considering both exchange interactions and the influence of an external magnetic field.

For the specific case where a single spin is initially aligned with the x-axis and subject to a field along the z-axis, the predicted time evolution can be described as follows [63]:

$$\begin{aligned} S_x(t) &= \text{sech} \left(\frac{\lambda \gamma H}{1 + \lambda^2} t \right) \cos \left(\frac{\gamma H}{1 + \lambda^2} t \right) \\ S_y(t) &= \text{sech} \left(\frac{\lambda \gamma H}{1 + \lambda^2} t \right) \sin \left(\frac{\gamma H}{1 + \lambda^2} t \right) \\ S_z(t) &= \tanh \left(\frac{\lambda \gamma H}{1 + \lambda^2} t \right) \end{aligned} \quad (6.2.13)$$

The mathematical framework provided predicts the behavior of the spin components over time, capturing the essence of their dynamical evolution due to the applied field. Specifically, the equations outline how the x and y components of the spin undergo a damping and precessional motion, while the z component exhibits a change in magnitude, illustrating the spin's alignment or misalignment with the field over time.

In our simulation, we initialize the magnetic moments to align along the x-axis. The effective field acting on each spin is computed by summing contributions from neighboring spins and the external magnetic field. The LLG equation's integration over time is achieved through a predictor-corrector method, ensuring the conservation of the magnitude of each magnetic moment while accurately capturing the dynamics of the system.

Figures included visually complement the theoretical predictions by showcasing the initial setup of the magnetization vector relative to the applied field, and graphically representing the temporal evolution of the spin's x-component. This simulation results not only validates the stochastic numerical methods employed but also offers an intuitive understanding of the spin dynamics under the influence of an external magnetic field. Through this comparison, we aim to underscore the reliability and accuracy of the Heun's method approach in replicating complex quantum mechanical behaviors.

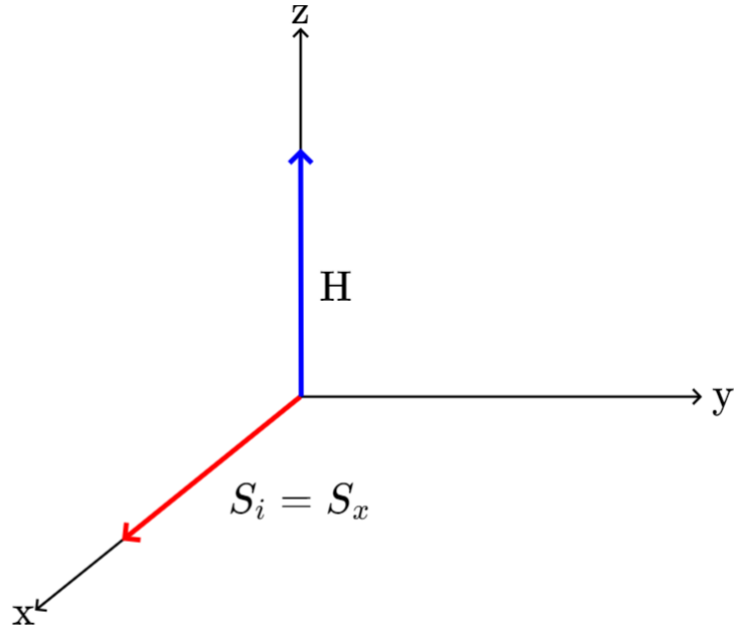


Figure 6.1: Initial orientation of the magnetization vector and the applied field for the simulation, depicting the starting alignment of magnetic moments and the direction of the external magnetic field used to study the system's response.

Figure 6.2 illustrates a remarkable congruence between the simulation results and the analytical solution, demonstrating an exact match in their trajectories.

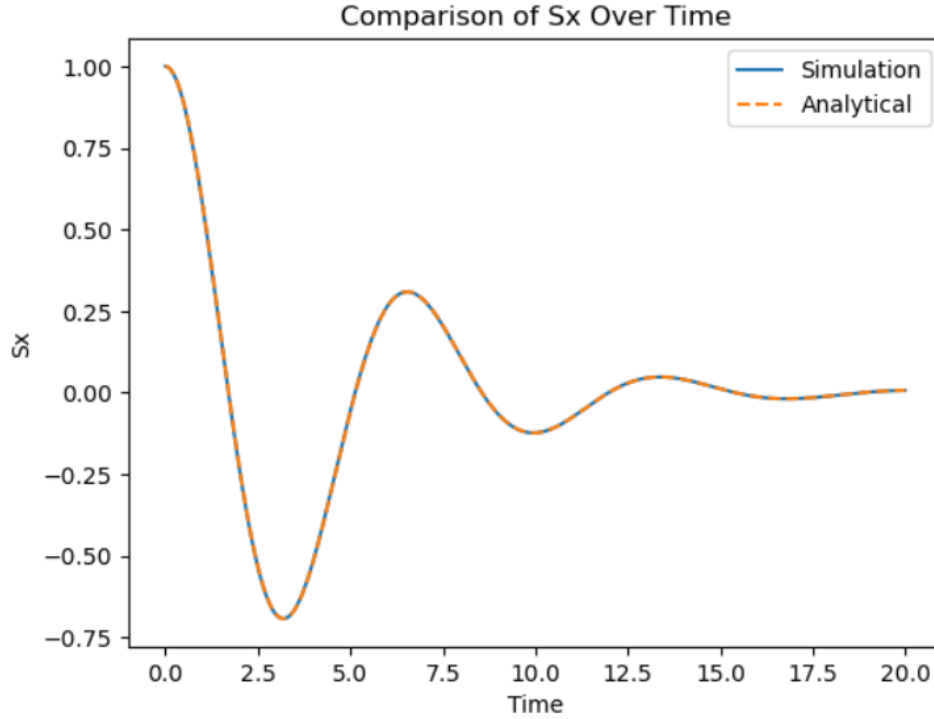


Figure 6.2: Time evolution of a single spin in an applied field, showing the magnetization vector precessing around the x-axis component, illustrating the dynamic behavior of the spin under the influence of the external field.

In simulations, we used lattice of spins because this allows us to model more accurately the real conditions in a magnetic material where no spin exists in isolation. Each spin on the lattice influences and is influenced by its neighbors, leading to a more realistic representation of magnetic behaviors. Each spin in a lattice is influenced by an effective field resulting from the sum of external magnetic fields and the fields due to neighboring spins. This makes the behavior of any single spin dependent on the state and alignment of other spins in the lattice, effectively linking each spin's dynamics to the lattice as a whole. In simulations, especially those aiming to understand magnetic properties and reactions to external fields or stochastic elements, treating a spin in isolation would yield inaccurate results. Thus, when we speak about the time evolution of a single spin as part of a lattice, we are essentially zooming in on one part of a much larger, interconnected system where the collective behavior and interactions dominate the dynamics observed.

We can see that the equations and the solution are only valid for a single spin with-

out any interactions. On the other hand, if we consider a lattice with neighbor interactions, and an initial value where all the spins are parallel to each other, we will get the same result because $\mathbf{s}_i$ will be constantly the same as $\mathbf{s}_j$ and therefore $\mathbf{S}_i \times \mathbf{S}_j = \mathbf{0}$.

6.2.2 Random Spin Orientation in Ferromagnets

This subsection explores the dynamic behavior of spins within a ferromagnetic system characterized by random initial orientations. Utilizing the Kwant library, we construct a lattice-based simulation to analyze how individual spins evolve over time under the influence of various interactions such as exchange, anisotropic, and external magnetic fields. The core of our approach is to numerically solve the stochastic Landau-Lifshitz-Gilbert (LLG) equation, which governs the precessional motion and damping of magnetic moments.

Our simulation begins with the initialization of magnetic moments in random directions to mimic the disordered state of spins. We apply a uniform external magnetic field along the z-axis, alongside considering the effects of anisotropy and exchange interactions among neighboring spins. Through iterative application of the LLG equation, we track the evolution of these spins, focusing on the x-component as a measure of the magnetization's dynamic response as shown in figure 6.3.

The process involves a predictor-corrector method to ensure the accurate integration of spins' trajectories over time while maintaining their magnitudes constant. This method allows us to observe the transition from random orientations towards a more ordered state, underpinning the complex interplay between thermal fluctuations and magnetic interactions within ferromagnetic materials.

The precessional behavior of spin observed in the graph is indicative of the rotational motion of the spin vector under the influence of an effective magnetic field. This behavior is characterized by the periodic oscillations in the S_x component of the spin, which result from the spin's motion around the axis of the magnetic field. The

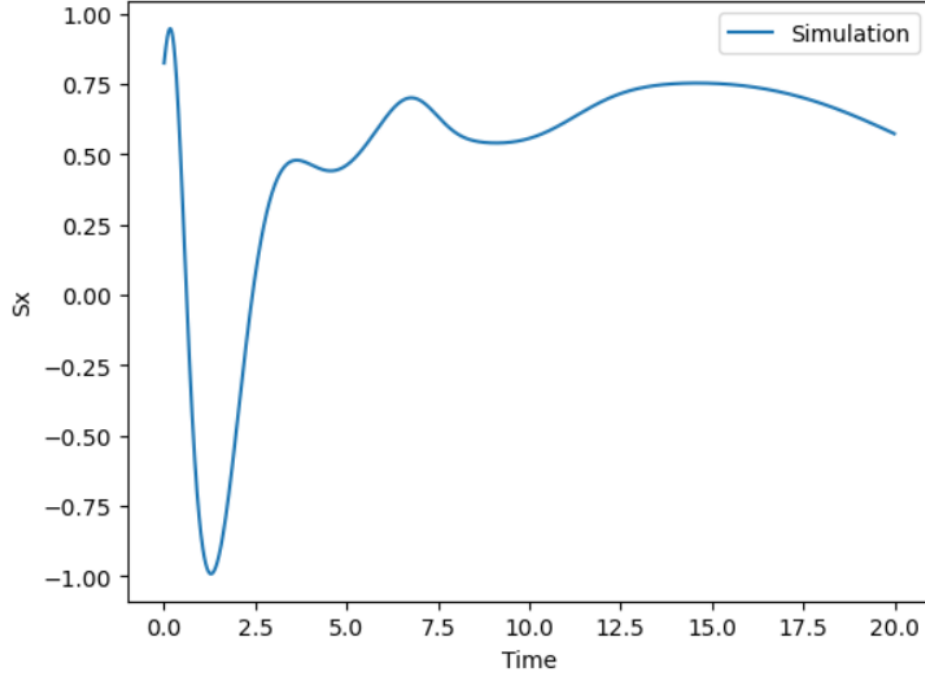


Figure 6.3: Time evolution of spin orientations in a ferromagnetic system subject to an external magnetic field, highlighting the precessional movement and eventual alignment of spins along the x-component.

amplitude and frequency of these oscillations provide insights into the strength of the magnetic interactions and the damping effects within the system, characterized by the parameter λ in the LLG equation.

The total effective magnetic field that each spin experiences is the sum of the exchange field, the external field, and the anisotropy field. The effective field determines the torque that acts on each spin, causing the spins to precess. This precession is evident from the oscillations in S_x over time, reflecting the periodic change in the projection of the spin vector onto the x-axis as it rotates around the effective field direction.

Chapter 7

Conclusion and Future Work

7.1 Conclusion

In this thesis, we have delved into the intricate world of magnonic systems and dynamics, exploring key studies, fundamental principles, advanced analytical approaches, and numerical analysis techniques. Our journey has led us to unravel the complexities of magnon dynamics in magnetic structures, from Bloch's theorem to the Holstein-Primakoff transformations. We have also discussed the application of magnonic systems in various domains such as waveguides, spintronics, and quantum information processing.

Through our exploration of advanced analytical approaches, including discretization of the Schrödinger equation and numerical integration methods, we have gained deeper insights into the behavior of magnons in different configurations and under varying physical conditions. By comparing stochastic numerical methods with exact solutions, we have enhanced our understanding of the dynamics of magnetic systems, both at the level of single spins and within ferromagnetic materials.

7.2 Future Work

While our study has shed light on many aspects of magnonic systems, there remain several avenues for future exploration and research. One promising direction is the development of more efficient numerical techniques for simulating magnon dynamics, especially in complex systems, is essential for advancing our understanding and to enable practical utilization of magnonic devices. Integrating of theoretical models with experimental validations will also be crucial for bridging the gap between theoretical predictions and real-world applications. For example, simulating LLG equation in spherical coordinates with reduced memory usage is one of the promising avenues for future research. It involves the development of efficient numerical methods for simulating the Landau-Lifshitz-Gilbert (LLG) equation in spherical coordinates. By employing only two variables, azimuthal and polar angles, instead of the traditional Cartesian coordinates, memory usage can be significantly reduced while maintaining accuracy. This approach could enable simulations of larger systems and longer time scales, facilitating the exploration of complex magnonic phenomena. Moreover, another important aspect of future work is the inclusion of four-spin interactions in simulation codes. While current models often consider pairwise interactions, incorporating higher-order interactions, such as the four-spin interaction, can lead to a more comprehensive understanding of magnonic systems. By capturing the collective behavior of multiple spins, these interactions may reveal emergent phenomena and exotic phases that are inaccessible in pairwise interaction models. Despite significant progress, several deep questions remain unanswered in the field of magnonics. One such question pertains to the precise mechanisms governing magnon transport and relaxation in complex magnetic structures. Understanding how magnons interact with defects, interfaces, and nonuniform magnetic fields is essential for optimizing the performance of magnonic devices. Additionally, the quest for efficient methods of magnon manipulation and control poses a significant challenge. While magnonic devices hold promise for various ap-

plications, such as information processing fast and efficient computing, realizing their full potential requires the development of reliable techniques for manipulating magnon currents, switching magnetization states, and modulating magnon properties with high precision and energy efficiency.

Furthermore, the exploration of exotic magnonic states, such as topological magnon insulators and skyrmion-mediated magnon transport, presents exciting opportunities for both fundamental research and technological innovation. Unraveling the underlying physics of these states and harnessing their unique properties could lead to transformative advancements in magnonics and spin-based technologies.

In summary, future research in magnonics should focus on developing efficient simulation techniques, incorporating higher-order interactions, and addressing deep unresolved questions in the field. By tackling these challenges, we can advance our understanding of magnonic phenomena and pave the way for groundbreaking discoveries and technological breakthroughs.

Appendix A

A.1 Useful Relations

The variable ξ is employed as a local coordinate to characterize each spin configuration. Furthermore, ξ is subject to the following relationships:

$$\xi_{\mathbf{k}} \cdot \xi_{\mathbf{k}} = 0$$

$$\xi_{\mathbf{k}} \times \xi_{\mathbf{k}} = 0$$

$$\xi_{\mathbf{k}} \cdot \xi_{\mathbf{k}}^* = 1$$

$$\mathbf{e}_{\mathbf{r}_{\mathbf{k}}} \cdot \xi_{\mathbf{k}} = \mathbf{e}_{\mathbf{r}_{\mathbf{k}}} \cdot \xi_{\mathbf{k}}^* = 0$$

$$\xi_{\mathbf{k}} \times \xi_{\mathbf{k}}^* = -i (\mathbf{e}_{\theta_{\mathbf{k}}} \times \mathbf{e}_{\phi_{\mathbf{k}}}) = -i \mathbf{e}_{\mathbf{r}_{\mathbf{k}}}$$

$$\xi_{\mathbf{k}} = i \mathbf{e}_{\mathbf{r}_{\mathbf{k}}} \times \xi_{\mathbf{k}}$$

$$\xi_{\mathbf{k}} \cdot \xi_{\mathbf{k}'}^* = i \mathbf{e}_{\mathbf{r}_{\mathbf{k}}} \cdot (\xi_{\mathbf{k}} \times \xi_{\mathbf{k}'}^*)$$

$$\xi_{\mathbf{k}}^* \cdot \xi_{\mathbf{k}'} = i \mathbf{e}_{\mathbf{r}_{\mathbf{k}}} \cdot (\xi_{\mathbf{k}'} \times \xi_{\mathbf{k}}^*)$$

$$\xi_{\mathbf{k}} \cdot \xi_{\mathbf{k}'} = i \mathbf{e}_{\mathbf{r}_{\mathbf{k}}} \cdot (\xi_{\mathbf{k}} \times \xi_{\mathbf{k}'})$$

Consider the differential equation describing the dynamics of the system, given by:

A.2 Some Detailed Calculations

The following is the detailed calculations of equation 4.1.11 :

$$\begin{aligned}
\frac{d}{dt}\psi_p^+ &= -\mathbf{m}_p^\circ \times \sum_i \alpha_{ip} \delta \mathbf{m}_i \cdot \xi_p \\
&= -\sum_i \alpha_{ip} \delta \mathbf{m}_i \cdot (\xi_p \times \mathbf{m}_p^\circ) \\
&= -i \sum_i \alpha_{ip} \delta \mathbf{m}_i \cdot \xi_p \quad (\text{using } \xi_p \times \mathbf{m}_p^\circ = i\xi_p) \\
&= -i \sum_i \alpha_{ip} (d\theta_i \mathbf{e}_{\theta_i} + d\tilde{\phi}_i \mathbf{e}_{\phi_i}) \left(\frac{1}{\sqrt{2}} \right) (\mathbf{e}_{\theta_p} + i\mathbf{e}_{\phi_p}) \quad (\text{substituting } \xi_p) \\
&= \frac{1}{\sqrt{2}} \sum_i \alpha_{ip} \left(d\theta_i \mathbf{e}_{\theta_i} + d\tilde{\phi}_i \mathbf{e}_{\phi_i} \right) (\mathbf{e}_{\phi_p} - i\mathbf{e}_{\theta_p}) \\
&= \frac{1}{2} \sum_i \alpha_{ip} \left\{ (\psi_i^+ + \psi_i^-) \mathbf{e}_{\theta_i} + \frac{(\psi_i^+ - \psi_i^-)}{i} \mathbf{e}_{\phi_i} \right\} (\mathbf{e}_{\phi_p} - i\mathbf{e}_{\theta_p}) \quad (\text{substituting } d\theta_i \text{ and } d\tilde{\phi}_i) \\
&= \frac{1}{2} \sum_i \alpha_{ip} \left\{ \psi_i^+ (\mathbf{e}_{\theta_i} - i\mathbf{e}_{\phi_i}) + \psi_i^- (\mathbf{e}_{\theta_i} + i\mathbf{e}_{\phi_i}) \right\} (\mathbf{e}_{\phi_p} - i\mathbf{e}_{\theta_p}) \quad (\text{rearranging terms}) \\
&= -i \sum_i \alpha_{ip} (\psi_i^+ \xi_i^* + \psi_i^- \xi_i) \xi_p^* \quad (\text{substituting } \xi \text{ and } \xi^*)
\end{aligned} \tag{A.2.1}$$

Here, $\xi_p = \frac{1}{\sqrt{2}}(\mathbf{e}_{\theta_p} + i\mathbf{e}_{\phi_p})$ represents the complex spin vector, and ξ^* denotes its complex conjugate.

Incorporate substitutions for $\psi_i^+ = \psi_i^+ e^{i(k \cdot R_i - \omega t)}$ and $\psi_i^- = \psi_i^- e^{i(k \cdot R_i - \omega t)}$, and derive the corresponding time evolution equation. Consider:

$$\begin{aligned}
\Rightarrow \quad \omega \psi_p^+ e^{i(k \cdot R_p - \omega t)} &= \sum_i \alpha_{ip} \left\{ \psi_i^+ \xi_i^* \xi_p^* + \psi_i^- \xi_i \xi_p \right\} e^{i(k \cdot R_i - \omega t)}, \\
\omega \psi_p^+ &= \sum_i \alpha_{ip} \left\{ \psi_i^+ \xi_i^* \xi_p + \psi_i^- \xi_i \xi_p \right\} e^{ik \cdot (R_i - R_p)}, \quad \text{where } R_{ip} = R_i - R_p
\end{aligned} \tag{A.2.2}$$

Defining the expressions for ψ_i^+ and ψ_i^- :

$$\begin{aligned}\psi_i^+ &= \frac{d\theta_i + id\tilde{\varphi}_i}{\sqrt{2}}, \\ \psi_i^- &= \frac{d\theta_i - id\tilde{\varphi}_i}{\sqrt{2}}, \\ d\theta_i &= \frac{\psi_i^+ + \psi_i^-}{\sqrt{2}}, \\ d\tilde{\varphi}_i &= \frac{\psi_i^+ - \psi_i^-}{i\sqrt{2}}.\end{aligned}$$

Utilizing these expressions, the differential change in ψ_p^+ over time can be derived as follows:

$$\begin{aligned}\frac{d\psi_p^+}{dt} &= \frac{1}{\sqrt{2}} \frac{d}{dt} (d\theta_p + id\tilde{\varphi}_p), \\ &= \frac{1}{\sqrt{2}} \left(\sum_i \alpha_{ip} (d\theta_i (e_{\theta_i} \cdot e_{\phi_p}) + d\tilde{\varphi}_i (e_{\phi_i} \cdot e_{\phi_p})) \right) \\ &\quad - i \left(\sum_i \alpha_{ip} (d\theta_i (e_{\theta_i} \cdot e_{\phi_p}) + d\tilde{\varphi}_i (e_{\phi_i} \cdot e_{\theta_p})) \right), \tag{A.2.3} \\ &= \frac{1}{\sqrt{2}} \frac{d}{dt} \left(\sum_i \alpha_{ip} ((\psi_i^+ + \psi_i^-) e_{\theta_i} - i(\psi_i^+ - \psi_i^-) e_{\varphi_i}) (e_{\varphi_p} - i e_{\theta_p}) \right), \\ &= -\frac{i}{2} \frac{d}{dt} \sum_i \alpha_{ip} (\psi_i^+ (e_{\theta_i} - i e_{\varphi_i}) + \psi_i^- (e_{\theta_i} + i e_{\varphi_i})) (e_{\theta_p} + i e_{\varphi_p}).\end{aligned}$$

This set of equations collectively encapsulates the time-dependent dynamics of the system, articulated through complex vector components and their interactions.

$$i \frac{d\psi_p^+}{dt} = \frac{d}{dt} \sum_i \alpha_{ip} (\psi_i^+ \xi_i^* \xi_p + \psi_i^- \xi_i \xi_i) \tag{A.2.4}$$

$$i \frac{d\psi_p^-}{dt} = -\frac{d}{dt} \sum_i \alpha_{ip} \{ \psi_i^+ \xi_i^* \xi_p^* + \psi_i^- \xi_i \xi_p^* \} \tag{A.2.5}$$

Anisotropy Energy

The dynamics of anisotropy energy are governed by the following set of equations, which delineate the interactions and effects within the system:

$$\begin{aligned}
i \frac{d\psi_p^+}{dt} &= 2k \left(n_{r_p} e_{r_p} + \frac{n_\perp}{\sqrt{2}} (e^{i\varphi_n} \xi_p^* + e^{-i\varphi_n} \xi_p) \right) \cdot (\psi_p^+ \xi_p^* + \psi_p^- \xi_p) \cdot \left(n_{r_p} e_{r_p} + \frac{n_\perp}{\sqrt{2}} (e^{i\varphi_n} \xi_p^* + e^{-i\varphi_n} \xi_p) \right) \cdot \xi_p \\
&\quad - 2k \psi_p^+ \left(\left(n_{r_p} e_{r_p} + \frac{n_\perp}{\sqrt{2}} (e^{i\varphi_n} \xi_p^* + e^{-i\varphi_n} \xi_p) \right) \cdot e_{r_p} \right)^2, \\
&= 2k \left(\frac{n_\perp}{\sqrt{2}} e^{i\varphi_n} \psi_p^- + \frac{n_\perp}{\sqrt{2}} e^{-i\varphi_n} \psi_p^+ \right) \left(\frac{n_\perp}{\sqrt{2}} e^{i\varphi_n} \right) - 2k \psi_p^+ n_{r_p} (n_{r_p}) \\
&= 2k \left(\frac{n_\perp^2}{2} e^{2i\varphi_n} \psi_p^- + \frac{n_\perp^2}{2} \psi_p^+ \right) - 2k \psi_p^+ n_{r_p}^2 \\
&= kn_\perp^2 (\psi_p^+ + e^{2i\varphi_n} \psi_p^-) - 2kn_{r_p}^2 \psi_p^+,
\end{aligned}$$

which gives:

$$i \frac{d\psi_p^+}{dt} = kn_\perp^2 (\psi_p^+ + e^{2i\varphi_n} \psi_p^-) - 2kn_{r_p}^2 \psi_p^+, \quad (\text{A.2.6})$$

$$i \frac{d\psi_p^-}{dt} = -kn_\perp^2 (\psi_p^- + e^{-2i\varphi_n} \psi_p^+) + 2kn_{r_p}^2 \psi_p^-. \quad (\text{A.2.7})$$

The terms n_{r_p} and $n_\perp$ represent the radial and perpendicular components of the anisotropy vector, respectively. The complex exponentials $e^{i\varphi_n}$ and $e^{-i\varphi_n}$ reflect phase shifts due to the anisotropy in different spatial dimensions. The equation clearly shows the coupling between the anisotropy's directional components and the spinor fields, influencing the time evolution of ψ_p^+ and ψ_p^- .

Appendix B

Source Codes

B.1 Band Gap of 2 Spins Out of Phase

```
import numpy as np
from scipy.linalg import eigvals
import matplotlib.pyplot as plt
import math

# Define functions to convert spherical to Cartesian coordinates
# ↪ to find the dot product of xi
def spherical_to_cartesian(theta_a, phi_a):
    tx_a = math.cos(theta_a) * math.cos(phi_a)
    ty_a = math.cos(theta_a) * math.sin(phi_a)
    tz_a = - math.sin(theta_a)
    return tx_a, ty_a, tz_a

def spherical_to_cartesian_c(theta_b, phi_b):
    px_b = - math.sin(phi_b)
    py_b = math.cos(phi_b)
```

```

        return px_b, py_b

# values for vectors ta, tb, pa, and pb:
theta_a = np.pi/4
phi_a = 3*(np.pi)/2
theta_b = -np.pi/4
phi_b = (np.pi)/2
tx_a, ty_a, tz_a = spherical_to_cartesian(theta_a, phi_a)
tx_b, ty_b, tz_b = spherical_to_cartesian(theta_b, phi_b)
px_a, py_a = spherical_to_cartesian_c(theta_a, phi_a)
px_b, py_b = spherical_to_cartesian_c(theta_b, phi_b)

# Define 3D vectors with zero z-component
vector_ta = np.array([tx_a, ty_a, tz_a])
vector_tb = np.array([tx_b, ty_b, tz_b])
vector_pa = np.array([px_a, py_a, 0])
vector_pb = np.array([px_b, py_b, 0])

# Define xi as a complex number
xi_a = (vector_ta + 1j * vector_pa) / np.sqrt(2)
xi_b = (vector_tb + 1j * vector_pb) / np.sqrt(2)

# Calculate the dot product
dot_product1 = np.dot(np.conjugate(xi_a), xi_b)
dot_product2 = np.dot((xi_a), xi_b)
dot_product3= np.dot(xi_a, np.conjugate(xi_b))
dot_product4 = np.dot(np.conjugate(xi_a), np.conjugate(xi_b))

# Define the number of values and the range for k

```

```

num_values = 80
k_values = np.linspace(-np.pi, np.pi, num_values)

# Initialize an empty array to store eigenvalues
eigenvalues_list = []

# Define the matrix M as a function of k
def matrix_M(k):
    ka = 0.1
    theta = np.pi/4 # Define theta
    A = 2*np.cos(2*theta) + 2*ka*np.cos(theta)**2 + np.cos(theta
    ↪ )
    M = np.array([
        [A, dot_product1* np.cos(k), 0, dot_product2 * np.cos(k)
        ↪ ],
        [dot_product3 * np.cos(k), A, dot_product2 * np.cos(k),
        ↪ 0],
        [0, -dot_product4 * np.cos(k), -A, -dot_product3 * np.
        ↪ cos(k)],
        [-dot_product4 * np.cos(k), 0, -dot_product1 * np.cos(k)
        ↪ , -A]
    ])
    return M

# Loop through each value of k
for k in k_values:
    # Get the matrix M for the current k
    M = matrix_M(k)

    # Calculate the eigenvalues of the matrix
    eigenvalues = eigvals(M)

```

```

    # Append the eigenvalues to the list
    eigenvalues_list.append(eigenvalues)

    eigenvalues_array = np.array(eigenvalues_list)

# Plot the eigenvalues as a function of k
for i in range(eigenvalues_array.shape[1]):
    plt.plot(k_values, eigenvalues_array[:, i])

# Add labels and legend
plt.xlabel("k")
plt.ylabel("Eigenvalues")
plt.legend()
plt.title("Eigenvalues as a Function of k")

# Show the plot
plt.show()

#plt.plot(k_values, eigenvalues_array)

```

B.2 Band Gap of a Honeycomb

```

import numpy as np
import kwant
from numpy import sqrt
from matplotlib import pyplot as plt
def magnitude(x, y, z):
    return np.sqrt(x**2 + y**2 + z**2)
def to_spherical(x, y, z):
    radius = magnitude(x, y, z)

```

```

    theta = np.arctan2(y, x)
    phi = np.arccos(z / radius)
    return radius, theta, phi
def to_cartesian_r(theta, phi):
    x = np.sin(theta) * np.cos(phi)
    y = np.sin(theta) * np.sin(phi)
    z = np.cos(theta)
    return x, y, z

def to_cartesian(radius, theta, phi):
    x = radius * np.cos(theta) * np.cos(phi)
    y = radius * np.cos(theta) * np.sin(phi)
    z = -radius * np.sin(theta)
    return x, y, z

def to_cartesian_c(theta, phi):
    x = -np.sin(phi)
    y = np.cos(phi)
    return x, y

def get_vector_t(theta, phi):
    x, y, z = to_cartesian(1, theta, phi)
    return np.array([x, y, z])

def get_vector_p(theta, phi):
    x, y = to_cartesian_c(theta, phi)
    return np.array([x, y, 0])

def get_xi(theta, phi):
    vector_t = get_vector_t(theta, phi)
    vector_p = get_vector_p(theta, phi)
    xi = (vector_t + 1j * vector_p) / np.sqrt(2)
    return xi

theta = np.arccos(-1/3.)

```

```

phi = np.pi / 4.
m1 = np.array([1/2. * np.sin(theta), -sqrt(3)/2. * np.sin(theta)
    ↪ , np.cos(theta)])
m2 = np.array([1/2. * np.sin(theta), sqrt(3)/2. * np.sin(theta),
    ↪ np.cos(theta)])
m3 = np.array([0, 0, 1])
m4 = np.array([-np.sin(theta), 0, np.cos(theta)])

def get_xi_from_M(m):
    (radius, theta, phi) = to_spherical(*m)
    xi = get_xi(theta, phi)
    return xi
def get_e_r_from_M(m):
    (radius, theta, phi) = to_spherical(*m)
    e_r = to_cartesian_r(theta, phi)
    return e_r

M = [m1, m2, m3, m4]
lat=kwant.lattice.honeycomb()
sublattices = lat.sublattices
a, b = sublattices
M=[m3,m3]
XI = [get_xi_from_M(m) for m in M]
n = [0,0,1]
def get_m(sublattice, M):
    return M[sublattices.index(sublattice)]

system=kwant.Builder()
# we need to create first the whole system in order to be able
    ↪ to call the neighbors

```

```

# we can not find the correct neighbors while creating the sites
    ↪ one by one
size=35
for i in range(-size,size):
    for j in range(-size,size):
        for sub in sublattices:
            system[sub(i, j)] = np.eye(2)

def get_Epq(site1,site2):
    e_pq = np.array(site2.pos) - np.array(site1.pos)
    norm=np.linalg.norm(e_pq)    # we want to make it a unit
    ↪ vector

    return np.array([e_pq[0],e_pq[1],0])/norm

def onsite(site,J,k,B_field,s,n, F):
    family = site.family
    i = sublattices.index(family)
    xi = XI[i]
    e_r = M[i] #get_e_r_from_M(M[i])
    A = np.dot(np.conjugate(xi),n)*np.dot(xi,n)
    B = np.dot(xi,n)*np.dot(xi,n)
    C = (np.dot(n,e_r))*2

    anisotropy = np.array([[A - C,B],
                            [np.conjugate(B), np.conjugate(A) - C]])

    Field=np.array([[np.dot(s,e_r),0 ],
                    [0,np.dot(s,e_r)]])

    Neighbors=system.neighbors(site)

```

```

field=np.array([0,0,0]) #from neighbors
value = 0
for site2 in Neighbors:
    family = site2.family
    j = sublattices.index(family)
    m2 = M[j]
    value += np.dot(m2,M[i])

#from pseudodipole:
A=0
for site2 in Neighbors:
    e_pq=get_Epq(site,site2)
    family = site2.family
    j = sublattices.index(family)
    m2 = M[j]
    A+=np.dot(m2,e_pq)*np.dot(e_r,e_pq)

def get_exchange_hop(xi1, xi2):
    A=np.dot(xi1.conj(),xi2)
    B=np.dot(xi2,xi1)
    return np.array([[A,B],[B.conj(),A.conj()]])

def get_pseudo_hop(xi1, xi2, epq):
    A=np.dot(xi1.conj(),epq)*np.dot(xi2,epq)
    B=np.dot(xi1,epq)*np.dot(xi2,epq)
    return np.array([[A,B],[B.conj(),A.conj()]])

def Hop1(site1, site2, J,k,B_field,s,n, F):

```

```

    family1 = site1.family
    family2 = site2.family
    i1 = sublattices.index(family1)
    xi1 = XI[i1]
    i2 = sublattices.index(family2)
    xi2 = XI[i2]

    #from pseudo
    epq = get_Epq(site1,site2)

    return J * get_exchange_hop(xi1, xi2) + F * get_pseudo_hop(
        ↪ xi1,xi2,epq)

for i in range(-size,size):
    for j in range(-size,size):
        for sub in sublattices:
            system[sub(i, j)] = onsite
system[lat.neighbors(1)] = Hop1
#system[lat.neighbors(2)] = Hop2
sys=system.finalized()

sites=system.finalized().sites

sites1=[sys.id_by_site[site] for site in sites if site.tag[0]==0
    ↪ and (abs(site.tag[1])<(size-2)) ]
sites2=[sys.id_by_site[site] for site in sites if site.tag[0]==1
    ↪ and (abs(site.tag[1])<(size-2)) ]
kwant.plot(system)

```

```

params=dict(J=.1,k=0.4,B_field=0.2,s=np.array([0,0,1]),n=np.
    ↪ array([0,0,1]), F=0.5)
ham=sys.hamiltonian_submatrix(from_sites=sites1, to_sites=sites1
    ↪ ,params=params) #to get the Hamiltonian of a cell
tau=sys.hamiltonian_submatrix(from_sites=sites1, to_sites=sites2
    ↪ ,params=params) #to get the hopping between cells
n,_=ham.shape
S = np.kron(np.eye(n//2), np.array([[1, 0], [0, -1]]))

def Hk(k):
    # Construct the full Hamiltonian matrix
    mat = ham + tau * np.exp(1j * k) + tau.T.conj() * np.exp(-1j
        ↪ * k)
    # Use eigvals for general matrices
    eigenvalues = np.linalg.eigvals(np.dot(S, mat))
    # Return the sorted eigenvalues
    return np.sort(eigenvalues.real)
momenta = np.linspace(-np.pi, np.pi,300)

eigenvalues_list = []
for k in momenta:
    # Calculate the eigenvalues of the matrix
    eigenvalues = Hk(k)
    # Append the eigenvalues to the list
    eigenvalues_list.append(eigenvalues)
    eigenvalues_array = np.array(eigenvalues_list)
# Plot the eigenvalues as a function of k
for i in range(eigenvalues_array.shape[1]):
    plt.plot(sqrt(3)*momenta/(2*np.pi), eigenvalues_array[:, i])
    plt.ylim([0.95,1.4])
plt.xlabel('k')

```

```

plt.ylabel('Eigenvalue')
plt.title('Eigenvalues as a function of k')
plt.legend()
plt.show()

```

B.3 Dynamics of a Single Spin Subject to a z-Axis Field

```

import kwant
import numpy as np
from numpy import sqrt
import matplotlib.pyplot as plt

# Define lattice parameters and sublattices
lat = kwant.lattice.general([(2, 0), (2*0.5, 2*sqrt(3)/2)],
                           [(0, 0), (1/2, sqrt(3)/2), (1, 0), (3/2, sqrt(3)/2)])
sublattices = lat.sublattices
a, b, c, d = sublattices
gamma = 1
dt = 0.01
lamda = 0.3
num_steps = 2000

def SHAPE(pos):
    x, y = pos
    return abs(x) < 5 and abs(y) < 5

sys = kwant.Builder()
sys[lat.shape(SHAPE, (0, 0))] = 0
#sys[lat.neighbors()] = 1

```

```

N = len(sites)

# Initialize magnetic moments (one spin along the x-axis)
M = np.zeros((N + 1, 3))
M[:] = np.array([1, 0, 0]) # Spin initially along x-axis
M[-1] = np.array([0, 0, 0]) # Fictitious sites with zero M.


Neighbors=[list(sys.neighbors(site)) for site in sites ]
#overwriting the Neighbours to write them in terms of their id
Neighbors=[[sysf.id_by_site[site] for site in liste] for liste
    ↪ in Neighbors]

#This is to always have neighbors of 6 (square matrix)
Neighbors=[item+(6-len(item))*[N] for item in Neighbors]
# the rank of the fictitious site is N
#This is to define the neighbors of the fictitious site.
Neighbors=Neighbors+[6*[N]]


sysf=sys.finalized()
sites=list(sysf.sites)

def normalize(vector):
    norm = np.linalg.norm(vector)
    if norm == 0:
        return vector
    else: return vector / norm

```

```

def normalize_matrix(matrix):
    norms = np.linalg.norm(matrix, axis=1)
    norms[norms == 0] = 1 # Avoid division by zero
    return matrix / norms[:, np.newaxis]

H = np.array((N + 1) * [[0, 0, 1]]) # External magnetic field
    ↪ along z-axis
H[-1] = np.array([0, 0, 0]) # External magnetic field along z-
    ↪ axis

def effective_field(M, Neighbors):
    # Effective field due to exchange interaction and external
    ↪ magnetic field along z-axis
    return np.sum(M[Neighbors], axis=1) + H

# Lists to store Sx and time values for plotting
Sx_values = []
time_values = []

# Perform the simulation steps
for step in range(num_steps):
    # Calculate effective field
    Heff = effective_field(M, Neighbors)

    # Predictor step for S
    D = np.cross(M, Heff)
    S_predictor = M + dt * (-gamma / (1 + lamda**2)) * (D +
    ↪ lamda * np.cross(M, D))

```

```

# Normalize the predictor
S_predictor = normalize_matrix(S_predictor)

# Calculate the effective field at the predicted spin
Heff = effective_field(S_predictor, Neighbors)

# Perform the corrector step
R = np.cross(S_predictor, Heff)
S_corrector = 0.5 * M + 0.5 * S_predictor + 0.5 * dt * (-
    ↪ gamma / (1 + lamda**2)) * (R + lamda * np.cross(
    ↪ S_predictor, R))

# Normalize the spin unit vectors
S_corrector_normalized = normalize_matrix(S_corrector)

# Update the magnetic moments with the corrected values
M = S_corrector_normalized

# Store Sx and time values for plotting
Sx_values.append(M[0, 0]) # Append the x-component of the
    ↪ spin
time_values.append(step * dt)

# Analytical solution for Sx
t_analytical = np.linspace(0, num_steps * dt, num_steps)
H_magnitude = 1 # Assuming H = [0, 0, 1] has magnitude 1
Sx_analytical = (1 / np.cosh(lamda * gamma * H_magnitude *
    ↪ t_analytical / (1 + lamda**2))) * \
    np.cos(gamma * H_magnitude * t_analytical / (1 +
    ↪ lamda**2))

```

```

# Plot simulation Sx as a function of time
plt.plot(time_values, Sx_values, label='Simulation')

# Plot analytical Sx as a function of time
plt.plot(t_analytical, Sx_analytical, label='Analytical',
         ↪ linestyle='--')

plt.xlabel('Time')
plt.ylabel('Sx')
plt.title('Comparison of Sx Over Time')
plt.legend()
plt.show()

```

B.4 Dynamics of Ferromagnetic Subject to a z-Axis magnetic Field

```

import kwant
import numpy as np
from numpy import sqrt
import matplotlib.pyplot as plt

# Define lattice parameters and sublattices
lat = kwant.lattice.general([(2, 0), (2*0.5, 2*sqrt(3)/2)],
                           [(0, 0), (1/2, sqrt(3)/2), (1, 0),
                           ↪ (3/2, sqrt(3)/2)])

sublattices = lat.sublattices
a, b, c, d = sublattices
gamma = 1

```

```

dt = 0.01
lamda = 0.3
num_steps = 2000

def SHAPE(pos):
    x, y = pos
    return abs(x) < 5 and abs(y) < 5

sys = kwant.Builder()
sys[lat.shape(SHAPE, (0, 0))] = 0
sys[lat.neighbors()] = 1

N = len(sites)

# Initialize magnetic moments with random directions
M = np.random.rand(N + 1, 3) # Generate random vectors
M = normalize_matrix(M) # Normalize each vector to have unit
    ↪ length
M[-1] = np.array([0, 0, 0]) # Keep the fictitious site with
    ↪ zero magnetization

Neighbors=[list(sys.neighbors(site)) for site in sites ]
Neighbors=[[sysf.id_by_site[site] for site in liste] for liste
    ↪ in Neighbors] #overwriting the Neighbours to write them in
    ↪ terms of their number(id)

#This is to always have neighbors of 6 because we have to have a
    ↪ square matrix

```

```

Neighbors=[item+(6-len(item))*[N] for item in Neighbors]# the
    ↪ rank of the fictitious site is N
#This is to define the neighbors of the fictitious site (The
    ↪ neighbors of the fictitious site is the fictitious site
    ↪ itself)
Neighbors=Neighbors+[6*[N]]

sysf=sys.finalized()
sites=list(sysf.sites)

def normalize(vector):
    norm = np.linalg.norm(vector)
    if norm == 0:
        return vector
    else: return vector / norm

def normalize_matrix(matrix):
    norms = np.linalg.norm(matrix, axis=1)
    norms[norms == 0] = 1 # Avoid division by zero
    return matrix / norms[:, np.newaxis]

# External magnetic field along z-axis
H_ext = np.array((N + 1) * [[0, 0, 1]]) # Assume a uniform
    ↪ external field for simplicity
H_ext[-1] = np.array([0, 0, 0]) # No external field on the
    ↪ fictitious site
H_anisotropy = np.zeros(N)

def effective_field(M, Neighbors, K_anisotropy=0.1, J = 1.0):

```

```

# Anisotropy field (assuming uniaxial anisotropy along z-
    ↪ axis)

#[:, np.newaxis] turns M[:, 2] into a column vector,
    ↪ resulting in each element of M[:, 2]
#being multiplied by the anisotropy field vector [0, 0, 1],
    ↪ aligning with the z-axis.

H_anisotropy = (2 * K_anisotropy)* M[:, 2][:, np.newaxis] *
    ↪ np.array([0, 0, 1])

# Total effective field including exchange, external, and
    ↪ anisotropy contributions

Heff = - J * np.sum(M[Neighbors], axis=1) + H_ext +
    ↪ H_anisotropy

return Heff

# Lists to store Sx and time values for plotting
Sx_values = []
time_values = []

# Perform the simulation steps
for step in range(num_steps):
    # Calculate effective field
    Heff = effective_field(M, Neighbors)

    # Predictor step for S
    D = np.cross(M, Heff)
    S_predictor = M + dt * (-gamma / (1 + lamda**2)) * (D +
        ↪ lamda * np.cross(M, D))

    # Normalize the predictor
    S_predictor = normalize_matrix(S_predictor)

```

```

# Calculate the effective field at the predicted spin
Heff = effective_field(S_predictor, Neighbors)

# Perform the corrector step
R = np.cross(S_predictor, Heff)
S_corrector = 0.5 * M + 0.5 * S_predictor + 0.5 * dt * (-
    ↪ gamma / (1 + lamda**2)) * (R + lamda * np.cross(
    ↪ S_predictor, R))

# Normalize the spin unit vectors
S_corrector_normalized = normalize_matrix(S_corrector)

# Update the magnetic moments with the corrected values
M = S_corrector_normalized

# Store Sx and time values for plotting
Sx_values.append(M[0, 0]) # Append the x-component of the
    ↪ spin
time_values.append(step * dt)

# Plot simulation Sx as a function of time
plt.plot(time_values, Sx_values, label='Simulation')

plt.xlabel('Time')
plt.ylabel('Sx')
plt.legend()
plt.show()

```

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August 2022 – May 2024

- Orchestrated laboratory sessions that bolstered students' comprehension and application of physics concepts.
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Teaching Assistant at Birzeit University

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- Facilitated hands-on laboratory courses, integrating practical experiments with core theoretical knowledge.

Member of the Physics Club at Birzeit University

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- Spearheaded initiatives to support peers academically, significantly enhancing resource availability through the creation of an electronic library.
- Organized multiple high-profile public lectures and educational events, fostering a community of learning and enthusiasm for physics.

Member of the Astronomy Club at Birzeit University

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- Led a series of successful public stargazing events and educational programs, highlighting celestial phenomena to a broad audience, with some events drawing more than 2000 participants.
- Utilized advanced astronomical equipment for the empirical study of celestial bodies, contributing to the club's educational outreach through detailed analytical reports published in the club's monthly digest.

Awards and Scholarships

- Received full funding for MSc programs at both KFUPM and Birzeit University.
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Academic Activities

Conference: Understanding Tropical Cyclones

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- The application of rare event sampling techniques to model severe weather events.

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- Hands-on exercises in computational physics, enhancing their understanding of molecular dynamics.

Research and Professional Experience

Quantum Teleportation

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- Investigated the practical implications and applications of quantum teleportation for energy transfer, employing advanced quantum computing techniques.

Analysis of Annealed Tungsten Oxide Thin Films

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- Conducted comprehensive studies on the physical and chemical properties of annealed WO_3 thin films to optimize their use in optical and electronic devices.

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- Performed detailed elemental analysis of various metals using LIBS, enhancing understanding of material properties for industrial applications.

Investigation of the Layer Hall Effect in Antiferromagnets

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- Explored the Layer Hall effect in two-dimensional antiferromagnetic materials, paving the way for new insights into magnetoelectric coupling and quantum materials.

The Ground State Deformation and Nuclear Magic Numbers

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- Utilized proxy-SU(3) symmetry to analyze ground state deformations and magic numbers in nuclei, contributing to advanced understanding of nuclear structure and stability.

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- Fluent in both English and Arabic.
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