MATHEMATICAL MODELLING OF FERROMAGNETIC OVERLAYER WITH SOFTENED EXCHANGE SURFACE INTEGRAL

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To my respected supervisor;

Assoc. Prof. Dr. Shamsuddin bin Ahmad

my beloved parents;

En. Aladdin Bin Abd Rahaman and Hjh.Samsiah Bte Mohamed Noor

and my beloved wife;

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For your patience and support

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ABSTRACT

Spin waves theory is one of important concept in surface physics study. Its concept becomes a method to study the low-temperature properties of magnetic materials with ordered magnetic moments. In this study, our scope will be on the discussion of spin wave theory at ferromagnetic overlayer. Green's function is used to find a mathematical model of simple one overlayer system for ferromagnetic material. From the model, the density of states (DOS) of spin waves is studied according to their exchange interactions at the surface. The surface softened effect will be taken into consideration to see any significant impact on different ratio of surface exchange integral values.

ABSTRAK

Teori gelombang spin adalah satu konsep yang penting dalam kajian fizik permukaan. Konsep ini menjadi cara untuk mengkaji sifat bahan magnet pada suhu rendah dengan momen magnet tersusun. Dalam kajian ini, skop kita adalah perbincangan tentang teori gelombang spin pada lapisan tambahan Ferromagnet. Fungsi Green di gunakan untuk mendapatkan model matematik mudah untuk system lapisan tambahan untuk bahan ferromagnet. Dari model ini, ketumpatan keadaan gelombang spin akan di kaji berdasarkan kepada interaksi tukarganti pada permukaan. Kesan perbandingan nisbah nilai tukarganti akan di pertimbangkan untuk jika terdapat kesan pada perbezaan nisbah di nilai interaksi tukarganti.

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LIST OF SYMBOLS

a	-	lattice constant
E	-	energy
ec	-	complex energy
$f(x)$	-	arbitrary general function
G	-	Green function
H	-	Hamiltonian
i	-	imaginary unit
Im	-	imaginary part
J_{nm}	-	exchange integral
k	-	wave vector
m	-	integer
n	-	integer
N	-	integer
$N(E)$	-	density of states in terms of energy E
nc	-	number of Cunningham points
p	-	wave vector
q	-	wave vector
Q_n^+	-	spin raising operator
Q_m	-	spin lowering operator

$\boldsymbol{R}$	-	lattice vector
S_n	-	localized spin
T_C	-	Curie temperature
U	-	perturbation
V	-	perturbation
W	-	perturbation
ε	-	imaginary part in the complex energy, *ec*
δ	-	positive infinitesimal
$\hbar$	-	Planck constant
$\rho(E)$	-	density of states in terms of energy E
$\Im$	-	left hand side
$\Re$	-	right hand side
μ_β	-	Bohr magneton
ψ	-	wave function
$\| \ \rangle$	-	column matrix
$\langle \ \|$	-	row matrix
$\perp$	-	perpendicular
□ or //	-	parallel

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CHAPTER 1

RESEARCH FRAMEWORK

1.1 Introduction

In solid state physics, a crystal can be defined as a regular, ordered arrangement of atoms over a large scale. The atoms may be of a single type or the repetition of a complex arrangement of different types of atoms. The crystal can be thought of as consist of two separate parts: The lattice and the basis. The lattice is an ordered arrangement of points in space, while the basis consists of simplest arrangement of atoms which is repeated at every point in the lattice to build up the crystal structure. Many crystals have an ordered magnetic structure. This means that in the absent of an external field, the mean magnetic moment of at least one of the atoms in each unit cell of the crystal is non-zero. These magnetic moments interact to give cooperative magnetic phenomena like ferromagnetism in situations where these are a large number of atoms together in solids.

Besides, the mean magnetic moment of all Ferromagnetic material has the same orientation and polarity provided that the temperature of the ferromagnetic material does not exceed a critical value, which is called Curie temperature. The Curie temperature T_c is the temperature above which the spontaneous magnetization vanishes (Kittel.C.,1998). This implies an existence of an internal field of more accurately the atomic field. The field originates from quantum mechanical interactions between electrons. The magnetic order in ferromagnetic material is the result of correlation between the directions of the electron spins on individual atoms. This correlation is in turn due to the fact that the space symmetry of the wave function depends on the magnitude of the resultant spin of the system of electron.

Nowadays, as the technology has become the backbones of human’s life, magnetic material plays an important role in human’s life. The applications of magnetic material can be seen through the interplay of magnetism in branches of physics and technology such as in electrical appliances, industrial machineries, business, communication appliances, transportation, medical technologies and further knowledge research and development.

Magnetism is an example of how advancement in science could shape future technologies for human being. Although the phenomenon was known from ancient times and important development in its understanding came in nineteenth century, it was only with the advancement of quantum mechanics in the late 1920’s that the full understanding of the magnetic properties of solids was achieved. From that understanding it has been possible to design and use new magnetic materials which are fundamental for technology advancement.

Started from the ancient world until recent technological development, magnetism has been a mysterious, almost magical phenomenon. The miners who obtained the ore to underpin the iron age were familiar with the extraordinary properties of one component of their product. This substance which we call magnetite, derived from its ancient Greek name, it is known to be a special oxide of iron. The piece of this material would attract or repel each other depending on the way in which they were oriented, and if suspended freely appeared to align relative to the north/south axis of the earth. The fact that this direction coincide with the polester suggested that heavenly forces were at play and let to it being characterized as a lodestone. Moreover, it was found that these properties could be transmitted to metallic iron either by rubbing it with lodestone or working it in a special way but these properties were unique to these materials and were not found in other rocks or in metals such as silver and gold. (Dan Wei,2008)

Magnetic phenomenon had been detected and researched since the early time of human civilization. This field is the second oldest research field in the world (Howson, 1994). The first magnetic effect was found with the discovery of a mineral magnetite material. This material was named lodestone. The material has been utilized for basic components in compass which function as reference for North-South direction. Since then, the research in magnetism never stops to decipher more properties and behavior of this mysterious material. The first scientific research on magnetism was done by an English scientist, William Gilbert (1540-1603) who published a book named *De Magnete*. He had carried out various type of experiment to study the properties of magnetic materials and finally he made a conclusion that the earth itself is a giant magnet which has north and south pole (Jorgensen, 1996). In 19 century, the scientists have found the relation of magnet and electricity. Since this great discovery, the research of electromagnetism has become very popular topic and expanded vastly until it gives impact on industrial evolution in Europe. The creation of electric generator and electric motor has become a cornerstone of industrial advancement.

Research and development activity in magnetism never stop. In 20th century, scientists discovered the electrons and atoms in the magnet from the view of quantum mechanics. The magnetic properties of the atom and molecules had been an interest to the researches. This modern quantum physics explained that the two major effects which contribute to the magnetism of an atom are the electron spin and the movement of electron in the orbital. From this understanding, new field of research created. It is called surface magnetism. This field focuses on the thermodynamics properties variance at the surface of the material.

By comparison, the research in surface magnetism is still new. In brief, magnetic surface waves are excitation of the transverse component of the magnetization, whose amplitude is localized near the surface of a magnetically ordered system. These waves are characterized by wave vector $\mathbf{k}_{||}$ parallel to the surface, and one or more (sometimes complex) attenuation constants, which describe the excitation amplitude as a function of distance into the crystal normal to the surface.

Magnetic surface waves are predicted by both microscopic and macroscopic theories. In the microscopic Heisenberg theory, surface spin waves occur because of abrupt changes in the exchange interactions at and near the surface. In macroscopic magnetostatic theory, they are associated with shape dependent demagnetization fields. In general, dipolar, exchange, crystal orientation, applied magnetic field orientation, size and shape effects influence the magnetic surface wave dispersion (Shamsuddin Ahmad,1990)

The name surface magnon or surface spin wave is used for surface waves for which the exchange interaction is the dominant energy at low temperature, T=0. Surface spin waves of ferromagnets have been the subject of extensive study.

1.2 Research Background

Recently, the study of ferromagnetic surface and interface has become the field of interest to many physicists, mathematicians and industrialist. The application of magnetism has become the cornerstone of new technology discovery. Generally, there are three types of magnetic materials which are ferromagnet, antiferromagnet, paramagnet and diamagnet. Most of surface magnetism researches are interested in ferromagnets because of its vast application in technology.

Ferromagnetism is the basic mechanism by which certain materials form permanent magnets and exhibit strong interactions with magnets; it is responsible for most phenomena of magnetism encountered in everyday life for example, electric motor operation.

The attraction between a magnet and ferromagnetic material is the quality of magnetism first apparent to the ancient world, and to us today. Ferromagnetism leads the study of spin waves. In terms of the history of solid state physics, the concept of spin waves has been established a long time ago, starting from 1930 by Bloch’s work but in the past the ideas have generally proved to be of theoretical rather than of experimental interest. However, recently results of experimental work demonstrate that spin waves really do exist in magnetic materials and that they are more than merely a mathematical entity. The spin wave theory is a method for investigating low temperature properties of magnetic materials with ordered magnetic moments. The method consists essentially in the description of low-lying energy levels of a system of an enormous number of strongly interacting spin moments in terms of spin waves or magnons.

The spin of an electron, combined with its orbital angular momentum, results in a magnetic dipole moment and creates a magnetic field. The classical analogue of quantum-mechanical spin is a spinning ball of charge but quantum has distinct differences, such as the fact that it has discrete up and down states that are not described by a vector; similarly for orbital motion, whose classical analogue is a current loop. In many materials specifically, those with a filled electron shell, however, the total dipole moment of all the electrons is zero that is the spins are in up or down pairs. Only atoms with partially filled shells (i.e., unpaired spin) can experience a net magnetic moment in the absence of an external field. Ferromagnetic materials contain many atoms with unpaired spins. When these tiny magnetic dipoles are aligned in the same direction, they create a measurable macroscopic field.

These permanent dipoles often called simply “spins” even though they also generally include orbital angular momentum tend to align in parallel to an external magnetic field, an effect called paramagnetism. A related but much weaker effect is diamagnetism, due to the orbital motion induced by an external field, resulting in a dipole moment opposite to the applied field. Ferromagnetism involves an additional phenomenon, however the dipoles tend to align spontaneously, without any applied field. This is a purely quantum-mechanical effect.

According to classical electromagnetism, two nearby magnetic dipoles will tend to align in opposite directions (which would create an antiferromagnetic material). In a ferromagnet, however, they tend to align in the same direction because of the Pauli Principle tow electrons with the same spin cannot also have the same position, which effectively reduces the energy of their electrostatic interaction compared to electrons with opposite spin. Mathematically, this is expressed more precisely in term of the spinstatistics theorem because electrons are fermions with half-integer spin, their wave functions are antisymmetric under interchange of particle positions. This difference in energy is called the exchange energy. (Jiles D.,1998).To study surface ferromagnetism, we have to use Green function. Green function will give a better calculation in ferromagnetic surface and overlayer since it is more understandable.

1.3 Problem statement

This research will study the density of state at one overlayer semi infinite ferromagnet substrate by considering only nearest neighbor atom. The research also will focus on the soften effect of exchange integral of $\frac{J_{\perp}}{J}$.

1.4 Research Objectives

This study embarks on the following objectives:

1.4.1 To derive a mathematical model for one overlayer ferromagnet

1.4.2 To find the density of state (DOS) of spin waves at semi-infinite surface of ferromagnet and investigate the softened effect

1.5 Scope of research

This study uses the Heisenberg Model. An assumption has been made that is the electrons of the atom in ferromagnetic materials are moving within their atoms. This study only considers the nearest atoms will affect the density of states (DOS) of spin waves.

In this study, Green function is applied to explore the properties of density of states (DOS) of spin waves. We consider the spin waves where their excitations only exist at low temperature. If the total number of spin waves present in a system is relatively small, and this so at low temperature, interactions between spin waves are insignificant and thus low-lying energy eigenvalues of the system are additively obtained from the energy of the spin waves. If the energies of free spin waves and their mutual interactions are known, it is possible to calculate with accuracy the thermodynamic properties of the system at low temperature such as the spontaneous magnetization. At low temperature, only long-wavelength spin waves will excite thermally.

Generally, spin waves theory can be discussed based on two mutually exclusive model: the localized moment model (Heisenberg Hamiltonian model) and the band or itinerant model (Hubbard Hamiltonian model). In the Heisenberg model, ferromagnetism properties are assumed to be affected by localized electrons at each atom in the crystal where the electrons move locally at one significant ion. On the other hand, in Hubbard model, the electron are said to move freely from one ion to another in the narrow energy band. It is found experimentally that the d-electron I transition metals have properties of both itinerant model and localized model. However, for long-wavelength spin waves we can map the spin wave problem for a metallic ferromagnet described by the itinerant model onto an equivalent problem described by Heisenberg model of a ferromagnetic insulator (Mathon, et.al. 1994). Since we are only interested in long-wavelenght spin waves, we shall assume throughout this thesis that the Heisenberg model is applicable.

1.6 Significant of Research

The purpose of this study is to find the density of states of spin waves at ferromagnet surface and which contribute to the determination of temperature dependence of magnetization according to exchange interactions. The result obtained from this study will enrich the technical reports, references and reading material in the field of surface physics. The better understanding in surface magnetization will help the industry to enhance the quality of magnetic products. Experts believe that one day tiny magnets could be implanted on a computer central processing unit (CPU) chip because system data could be recorded in magnets. Consequently, computer would never need to boot up. Therefore this research is very important in order to explore the better properties of ferromagnetic surface.

1.7 Thesis Layout

In chapter one, research framework will be discussed. The brief introduction of this research contains the important explanation of ferromagnetic surface and overlayer. This chapter also includes the objectives, scope, significance and thesis layout.

In chapter two, the in concept of magnetism and physics of solid state material will be studied in detail. Furthermore, the Heisenberg model of ferromagnetism will be explored in this chapter since this topic is very useful for the next chapter. This chapter also covers other important topics that will be used in the next chapter to give the first view of what this research is all about.

Chapter three will start with the brief description of ferromagnetism. Then it is followed by explanation of spin waves theory. Furthermore, this chapter will also cover the topic of Green function that will be applied in the discussion of spin waves theory in infinite and semi-infinite ferromagnet Heisenberg crystal.

Chapter four will explain Green function derivation of the ferromagnetic system in one layer. The calculation also will lead to density of state (DOS) equations for semi infinite and the softening effect will be taken into consideration to see how difference in exchange integral ration could affect the density of state of a system.

Chapter five will discuss the result and conclusion of the research findings.

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