Quantum Theory Of Spin-wave Excitations In Ferromagnetic Layered Structures

Linjie Jiang

Follow this and additional works at: https://ir.lib.uwo.ca/digitizedtheses

Recommended Citation
https://ir.lib.uwo.ca/digitizedtheses/2614

This Dissertation is brought to you for free and open access by the Digitized Special Collections at Scholarship@Western. It has been accepted for inclusion in Digitized Theses by an authorized administrator of Scholarship@Western. For more information, please contact tadam@uwo.ca, wlswadmin@uwo.ca.
QUANTUM THEORY OF SPIN-WAVE EXCITATIONS
IN FERROMAGNETIC LAYERED STRUCTURES

by

Linjie Jiang

Department of Physics

Submitted in partial fulfilment
of the requirements for the degree of
Doctor of Philosophy

Faculty of Graduate Studies
The University of Western Ontario
London, Ontario
August 1995

© Linjie Jiang 1995
The author has granted an irrevocable non-exclusive licence allowing the National Library of Canada to reproduce, loan, distribute or sell copies of his/her thesis by any means and in any form or format, making this thesis available to interested persons.

L'auteur a accordé une licence irrévocable et non exclusive permettant à la Bibliothèque nationale du Canada de reproduire, prêter, distribuer ou vendre des copies de sa thèse de quelque manière et sous quelque forme que ce soit pour mettre des exemplaires de cette thèse à la disposition des personnes intéressées.

The author retains ownership of the copyright in his/her thesis. Neither the thesis nor substantial extracts from it may be printed or otherwise reproduced without his/her permission.

L'auteur conserve la propriété du droit d'auteur qui protège sa thèse. Ni la thèse ni des extraits substantiels de celle-ci ne doivent être imprimés ou autrement reproduits sans son autorisation.

ISBN 0-612-09866-4
ABSTRACT

The study of low-dimensional magnetic microstructures has become increasingly active and important because of the recent advances in sample growth techniques and the potential applications of these structures to technology. The theoretical study of the spin-wave excitations in these magnetic structures is important to understand many physical properties of these structures. The aim of this thesis is to study the exchange-dominated spin waves in ferromagnetic layered structures, especially those structures with one-dimensional (1D) translational symmetry.

The general method used in this thesis is a standard quantum-mechanical Green function theory formulated within a microscopic approach. However, a particular matrix diagonalization technique is developed to calculate analytically the spin-spin Green functions for the layered structures with 1D and 2D translational symmetry.

The ferromagnetic single-layered structures investigated are complete films, perpendicularly truncated films (including long rods or wires), perpendicular interfaces in "binary" films with uniform thickness, and thin films with surface steps; whereas the ferromagnetic multilayer structures investigated are conventional superlattices (with 2D translational symmetry) and perpendicularly truncated (or cleaved) superlattices. The spin-spin Green function expressions are obtained for these layered structures. The dispersion relations and spectral intensities of the bulk and surface spin-wave modes in these ferromagnetic structures are then calculated explicitly. The
finite-size effects on the spin waves are discussed by numerical examples and the asymptotic behavior of the spin waves is examined in various types of geometrical limits.

The Green function results obtained in this thesis are also useful in calculating many other experimentally observable quantities besides the spin-wave spectra and intensities; some examples would be the cross section for inelastic light scattering and the absorption strength in spin wave resonance. The possibilities of some extensions and applications of the theoretical results are briefly discussed.
ACKNOWLEDGEMENTS

I wish to thank Professor Michael G. Cottam, my academic supervisor, for his conscientious guidance, constant encouragement, and financial aid. It has been my pleasure for the last three years to work with Prof. Cottam and his assistants. My scientific custom of approaching problems and accomplishing projects, established with the help of Prof. Cottam, will continue to be beneficial to me in my future career.

I would also like to extend my gratitude to Drs. Niu-Niu Chen, Igor Rojdestvenski, and Paula Heron for their helpful comments on some topics in this thesis. Finally, the scholarships from the UWO Faculty of Graduate Studies are gratefully acknowledged.

Linjie Jiang

London, Ontario, Canada

August 1995
# Table of Contents

<table>
<thead>
<tr>
<th>Chapter</th>
<th>Title</th>
<th>Page</th>
</tr>
</thead>
<tbody>
<tr>
<td>1</td>
<td>General Introduction</td>
<td>1</td>
</tr>
<tr>
<td></td>
<td>1.1 Spin Waves</td>
<td>2</td>
</tr>
<tr>
<td></td>
<td>1.2 Low-Dimensional Structures</td>
<td>4</td>
</tr>
<tr>
<td></td>
<td>1.3 Outline of the Thesis</td>
<td>14</td>
</tr>
<tr>
<td>2</td>
<td>The Green Function Formalism for Ferromagnets</td>
<td>17</td>
</tr>
<tr>
<td></td>
<td>2.1 Introduction</td>
<td>17</td>
</tr>
<tr>
<td></td>
<td>2.2 The Heisenberg Model for Ferromagnets</td>
<td>19</td>
</tr>
<tr>
<td></td>
<td>2.3 The Green Functions for Ferromagnets</td>
<td>22</td>
</tr>
<tr>
<td></td>
<td>2.4 The Fluctuation-Dissipation Theorem</td>
<td>24</td>
</tr>
<tr>
<td></td>
<td>2.5 Example: An Infinite Ferromagnet</td>
<td>26</td>
</tr>
<tr>
<td>3</td>
<td>Perpendicularly Truncated Films</td>
<td>30</td>
</tr>
<tr>
<td></td>
<td>3.1 Films With 2D Translational Symmetry</td>
<td>31</td>
</tr>
<tr>
<td></td>
<td>3.2 Perpendicularly Truncated Films</td>
<td>42</td>
</tr>
<tr>
<td></td>
<td>3.3 Films With Two Parallel Truncations</td>
<td>54</td>
</tr>
<tr>
<td>4</td>
<td>Films With Perpendicular Interfaces and Steps</td>
<td>62</td>
</tr>
<tr>
<td></td>
<td>4.1 Two Films Coupled at Truncations</td>
<td>63</td>
</tr>
<tr>
<td></td>
<td>4.2 Perpendicular Interfaces in Films</td>
<td>69</td>
</tr>
<tr>
<td></td>
<td>4.3 Steps on the Surfaces of Thin Films</td>
<td>80</td>
</tr>
<tr>
<td>5</td>
<td>Perpendicularly Cleaved or Truncated Superlattices</td>
<td>92</td>
</tr>
<tr>
<td></td>
<td>5.1 Infinite Superlattices With 2D Translational Symmetry</td>
<td>94</td>
</tr>
<tr>
<td></td>
<td>5.2 Semi-Infinite Superlattices</td>
<td></td>
</tr>
<tr>
<td></td>
<td>With 2D Translational Symmetry</td>
<td>107</td>
</tr>
</tbody>
</table>
5.3 Perpendicularly Cleaved Infinite Superlattices .......... 117
5.4 Perpendicularly Cleaved Semi-Infinite Superlattices ...... 131

CHAPTER 6 - CONCLUSIONS ........................................ 140
   6.1 Summary of Results ...................................... 140
   6.2 Some Possible Extensions ................................. 142

APPENDIX A INVERTING SOME PARTITIONED MATRICES .......... 147
APPENDIX B DERIVATION OF THE GREEN FUNCTIONS
   FOR AN INFINITE SUPERLATTICE .............................. 150

REFERENCES ............................................................. 154

VITA ................................................................. 159
CHAPTER 1
GENERAL INTRODUCTION

The study of the collective behavior of basic excitations in magnetically ordered systems provides an effective way of thoroughly understanding many of the properties of magnetic materials. The present work is dedicated to the quantum-mechanical theory of spin-wave excitations in ferromagnets with various types of layer and multilayer geometries. Recent advances in growth techniques have made possible the fabrication of such artificial microstructures and nanostructures, and the spin waves can be studied experimentally (e.g., by light scattering and spin wave resonance).

In this introductory chapter we shall present a general review of studies of spin-wave excitations and outline the scope and arrangements of the material in the remainder of this thesis. The pioneering efforts to explain the properties of ordered magnetic materials date back to early this century when Weiss (1907) proposed the mean field theory of ferromagnetism. By introducing the concept of an effective field acting on spins to account for the correlation between spin orientations, Weiss was able to explain the temperature dependence of magnetization and the phase transition at the Curie temperature. The mean field theory was later extended to antiferromagnets by Néel (1932). Although successful in explaining the overall static properties of magnetic materials in the vicinity of critical temperatures, the mean field theory becomes less applicable at lower temperatures (e.g., in explaining the temperature dependence of the magnetization and specific
heat).

It was only after the advent of the quantum theory that the origin of the correlation between spin orientations in magnetic materials was correctly understood. As a result of the indistinguishability of identical particles, the spins align (anti)parallelly in the (anti)ferromagnetic ground state to achieve the minimum energy of the system. The dependence of energy on spin alignments is due to the so-called exchange interaction. Following the initial study of the exchange interaction by Heisenberg (1928), Bogolyubov and Tyablikov (1949) derived an exchange Hamiltonian for magnetically ordered systems. The exchange interaction is generally discussed in most standard textbooks on nonrelativistic quantum mechanics (e.g., Schiff 1955) or magnetism (e.g., Mattis 1965) and reviewed in details by Anderson (1963) and Herring (1966) for magnetic insulators and metals respectively. In addition to the exchange interaction, there are also dipole-dipole interactions between the magnetic moments of spins and anisotropy due to spin-orbit interactions or magnetoelastic effects, etc. (see Akhiezer et al 1968 for more details). In many cases these additional interactions are relativistic in origin and therefore are typically much weaker than the exchange interaction.

§ 1.1 Spin Waves

The dynamic picture of magnetically ordered systems came after the concept of spin wave introduced by Bloch (1930), who proposed that the deviations of spins from their ground-state orientations should propagate with a wavelike behavior throughout the magnetic crystal in
the presence of mainly the exchange interaction. Analogous to the ideas of lattice vibrational wave versus phonon and electromagnetic wave versus photon, the spin waves are quantized with the basic quantum being referred to as the magnon. The concepts of spin wave and magnon exhibit the dual wave-particle nature of low-lying excitations in magnetic crystals at low temperatures compared with the critical temperature. The theoretical results based on spin-wave excitations were confirmed by the measurements of thermodynamic properties due to Fallot (1936) and Weiss (1937). The first direct observations of magnons at zero and nonzero wavevectors were made by Griffith (1946) with ferromagnetic resonance and by Seavey and Tannenwald (1958) with spin wave resonance.

The nature of spin waves in a certain wavevector region is controlled by the particular type(s) of interactions that dominate in the region. In what is called the exchange region, covering the vast majority of the first Brillouin zone from about $10^8 \text{ m}^{-1}$ to the boundary (typically $10^{10} \text{ m}^{-1}$), the exchange interaction is dominant in strength. The dipole-dipole interactions become dominant over the exchange interaction in the so-called magnetostatic region where spin waves have wavevector smaller than about $10^7 \text{ m}^{-1}$ and are specifically referred to as magnetostatic waves (provided electromagnetic retardation effects can be ignored). In the intermediate wavevector region (roughly from $10^7 \text{ m}^{-1}$ to $10^8 \text{ m}^{-1}$), known as the dipole-exchange region, the dipole-dipole and exchange interactions are comparable in strength. The division of these wavevector regions is due to the fact that the exchange interaction is of short range and the dipole-dipole
interactions are of long range. Although the boundaries between these regions may be slightly different from material to material, the exchange region always occupies the majority of the entire Brillouin zone except for a small wavevector sphere, whose radius is about 1% of the dimension of the first Brillouin zone.

There have been a number of different ways of formulating spin-wave theory. For example, the semiclasical theory (Heller and Kramers 1934) and quantum theory (for a review, see Prutton 1964) interpret the spins in the magnetic crystal as precessing vectors and incommutable operators, respectively. While many other quantum mechanical formulations involve transforming spin operators into other operators such as boson creation and annihilation operators (Holstein and Primakoff 1940, Dyson 1956), the one that we have chosen to use throughout this thesis is to work directly with the spin operators. In general, the magnetic crystal should be treated as a discrete lattice. This point of view leads to the microscopic approach, with which the entire work in this thesis is carried out. However, in cases where wavelengths are much larger than the interatomic distances, the crystal can be approximated to a continuous medium and this is the basis of the macroscopic approach, which is particularly suitable for the magnetostatic and dipole-exchange regions.

§ 1.2 Low-Dimensional Structures

The behavior of spin waves is also dramatically affected by the geometries of magnetic systems. It is well understood that, in an infinite medium, all the spin-wave excitations are simply characterized
by a real wavevector and an amplitude varying in a wavelike manner in all directions. Spin waves with these propagational features are known as bulk spin waves. In materials with one or more surfaces there may also exist, in general, surface spin waves that are localized near the surfaces. In the direction normal to a surface the amplitudes of surface spin waves decrease (typically exponentially) with distance from the surface. Moreover, the bulk spin waves are modified in the presence of surfaces because the translational symmetry normal to the surfaces is violated and boundary conditions must be satisfied. The same general features hold for interfaces as for surfaces.

The theoretical studies of surface spin waves started with the semi-infinite cases, where only one surface (or interface) was considered (see Figs. 1.1(a) and 1.1(c)). Surface magnetostatic waves in thin-film and semi-infinite geometries were first predicted by Mercereau and Feynman (1956), Walker (1957) and Damon and Eshbach (1961). Subsequently, they were experimentally studied by microwave techniques (Brundle and Freedman 1968). Surface spin waves in the exchange region were first considered theoretically by Fillipov (1967), Wallis et al (1967) and DeWames and Wolfram (1969) for semi-infinite ferromagnets and by Mills and Saslow (1968) and DeWames and Wolfram (1969) for semi-infinite antiferromagnets. The first unambiguous experimental observation of the exchange-dominated surface spin waves was reported by Yu et al (1975). The effects of a surface on thermodynamic properties such as specific heat were first computed by Mills and Maradudin (1967) and Fujiwara et al (1968). The theory of interface spin waves between two different semi-infinite ferromagnets
Fig. 1.1 Schematic representation of some previously-studied low-dimensional magnetic structures: (a) surface of a semi-infinite sample, (b) thin film, (c) interface between two semi-infinite samples, and (d) right-angle wedge.
(as shown in Fig. 1.1(c)) was given by Camley and Maradudin (1982) in the magnetostatic region and by Yaniv (1983) in the exchange region. Since these early studies, a lot of methods, both theoretical and experimental, have been developed to investigate surface waves. The results obtained are enormous. There are several reviews of theoretical work (e.g., see Wolfram and DeWames 1972, Mills 1984, and Cottam and Maradudin 1984) and of experimental studies (e.g., see Sandercock 1982, Grünberg 1985, and Cottam and Lockwood 1986).

Further to the semi-infinite cases, a lot of research has been done on spin waves in magnetic thin films (see Fig. 1.1(b)) and multilayers, where two (or more) complete surfaces are involved. In the magnetostatic region, the previously-mentioned theory for the semi-infinite case was already applicable to ferromagnetic films. Its extension to antiferromagnetic films was given by Stamps and Camley (1984). The ferromagnetic double-layered structure with a nonmagnetic spacer in between was first considered by Grünberg (1980). Spin waves in magnetic films were also experimentally studied, particularly by Brillouin scattering (e.g., see Grünberg and Metawe 1977, Grünberg et al 1982 and Vernon et al 1984) and spin wave resonance (e.g., see Dutcher 1994). In the exchange region, reviews of spin waves in films include those by Puszkarski (1979) and Lévy (1981). The Green function calculations were extended from the semi-infinite case (Cottam 1976) to films by Cottam and Kontos (1980) and by Moul and Cottam (1983), in microscopic and macroscopic approaches respectively.

Since the 1980’s many efforts have been devoted to the studies of spin waves in magnetic multilayer structures in which an array of
parallel interfaces are embodied between different constituent materials. This is propelled by the recent advances in epitaxial growth techniques that made possible the artificial fabrication of high-quality multilayer structures and by the potential applications of these structures to technologies. One special type of multilayer structure is the so-called superlattice, in which an alternating arrangement of different individual slabs (or films) is repeated periodically (see Fig. 1.2). Due to this artificial periodicity, superlattices are technically easy to fabricate and theoretically relatively simple to treat, and have thus been studied intensively over the past decade. Magnetostatic waves in superlattices consisting of alternating ferromagnetic and nonmagnetic slabs were first studied theoretically by Camley et al (1983) and Grünberg and Mika (1983) and experimentally by Grimsditch et al (1983) and Kueny et al (1984). The exchange-dominated spin waves in ferromagnetic superlattices have been analyzed with several different theoretical methods (e.g., see Albuquerque et al 1986, Dobrzynski et al 1986, and Puszkarski 1988). With practical applications in mind, the theoretical studies of magnetic superlattices are not limited to infinitely extended structures. Semi-infinite superlattices with an outmost surface and finite superlattices enfolded within two parallel surfaces have also become an active subject of recent theoretical research (e.g., see Barnas 1994).

The important role that the translational symmetry of a magnetic systems plays in theoretical studies can not be overemphasized. The spin-wave excitations have wavelike propagational features in all
Fig. 1.2 Schematic representation of conventional two-component superlattices with 2D translational symmetry: (a) infinite (unlimited in both directions perpendicular to the interfaces), (b) semi-infinite (limited by vacuum or substrate on one side).
directions in which the translational symmetry of the magnetic system is preserved. This is a consequence of Bloch's theorem (see, e.g., Kittel 1986). Owing to the translational symmetry, a Fourier transformation from lattice space (or site space) to wavevector space can be made. In an infinite homogeneous magnetic medium with translational symmetry in three dimensions, spin waves are characterized by a three-dimensional (3D) real wavevector. Most magnetic systems that have been studied to date, whether they be of homogeneous substances or periodic multilayer structures, possess translational symmetry in two dimensions, resulting in a two-dimensional (2D) real wavevector for spin waves. The theoretical treatment of these systems is basically confined to dealing with finite-difference equations (within a microscopic approach) or differential equations (within a macroscopic approach) and essentially becomes a one-dimensional (1D) problem perpendicular to the surfaces (or interfaces) from a mathematical point of view. A mathematically two-dimensional problem arises in the case where translational symmetry of a system is violated in two dimensions. Because of their mathematical complexity, theories of magnetic systems in this category, other than calculations of exchange-dominated spin-wave spectra for a semi-infinite right-angle ferromagnetic wedge shown in Fig. 1.1(d) (e.g., see Sharon and Maradudin 1973 and Maradudin et al 1977), have been left largely unexplored. In this thesis we shall mainly study the exchange-dominated spin waves in a variety of ferromagnetic layered structures with only 1D translational symmetry. The geometries of these structures are schematically illustrated by the examples in Figs. 1.3
and 1.4. The experimental studies of these magnetic structures with nanometer-scale of dimensions (e.g., see Gibson et al 1991, Lederman et al 1993, Meada et al 1994) have recently become very active because of the development of new artificial fabrication techniques such as chemical vapor deposition, molecular-beam epitaxy, electron-beam lithography, and scanning tunneling microscope.

Before outlining the arrangements of contents in this thesis we will describe the general scope of the thesis, in terms of the systems considered, assumptions made, and theoretical methods employed. The single layered structures (or films) considered in this thesis have only 1D translational symmetry parallel to their surfaces. The loss of translational symmetry in the other dimension parallel to their surfaces may result from either perpendicular truncations, interfaces, or surface steps (see Fig. 1.3). The multilayer structures considered in this thesis are conventional superlattices (with 2D in-plane translational symmetry) as in Fig. 1.2 and perpendicularly cleaved superlattices (with lower symmetry) as in Fig. 1.4. For convenience, all the substances in these layered structures are assumed to be ferromagnetic crystals and all the crystals are assumed to be of simple cubic lattice structure with the same lattice parameter a and surface (or interface) orientation (100). The extension to other lattice structures and surface orientations is straightforward in principle. Since the exchange interaction is of short range, we also assume that the exchange integral is significant only between the nearest neighbors and negligible otherwise. The sample temperature is assumed to be low enough (compared with the Curie temperature) that the spin wave modes
Fig. 1.3 Schematic representation of some single-layered structures with only 1D translational symmetry: (a) perpendicularly truncated film, (b) rod (or wire) with rectangular cross section, (c) two perpendicularly truncated films coupled to each other.
Fig. 1.4 Schematic representation of perpendicularly cleaved or truncated superlattices: (a) infinite, (b) semi-infinite.
or magnons under our consideration are non-interacting elementary excitations. By employing a microscopic approach we have systematically studied spin wave excitations in these layered structures in the absence of dipole-dipole interaction and anisotropy. We have concentrated on the Green functions between spin operators to calculate spectral intensities in addition to dispersion relations. These same Green function would also yield the cross section for light scattering, or the absorption strength in spin wave resonance.

§ 1.3 Outline of the Thesis

Having presented in this Chapter 1 a general review and the general scope, we now outline the arrangement of chapters in this thesis. As a general comment we may point out that Chapter 2 gives a development of the standard theoretical methods used throughout this thesis and that Chapters 3 and 4 deal with single layered structures (or films) while Chapter 5 deals with multilayer structures (superlattices). Discussion of some extensions goes in Chapter 6.

In Chapter 2 we briefly describe the Heisenberg model for ferromagnets and introduce the Heisenberg Hamiltonian. Then we present in more detail the Green function formalism for ferromagnets, including some basic definitions, equations of motion, and the random phase approximation. We also discuss correlation functions and the Fluctuation-Dissipation theorem, through which the experimentally observable quantities can be calculated from the Green functions.

In Chapter 3 we briefly reestablish some known results of spin waves in a complete film. Then we derive the spin-spin Green functions
for films with one or two perpendicular truncations (see Figs. 1.3(a) and 1.3(b)). For this, we develop an analytical procedure for diagonalizing matrices that can be partitioned into a tridiagonal form with submatrix blocks. The spin-wave spectra (dispersion relations) are deduced from the poles of the Green functions and their spectral intensities are then calculated numerically. The techniques used in this chapter also have a pedagogical value, since they are extended and used analogously in the following chapters.

In Chapter 4 we first present a general formulation for two truncated films (as considered in Chapter 3) that are exchange-coupled to each other at their truncations (see Fig. 1.3(c)). Then we elaborate upon two special cases of this complicated structure. One is where the two truncated films of different materials have the same thickness. The other is where the two films have different thickness but are made up of the same material. The latter case allows a numerical study of how spin waves are affected by a step on the surface of a film.

In Chapter 5 we first consider ferromagnetic superlattices with 2D translational symmetry parallel to the interfaces (as in Fig. 1.2). For general cases, we derive the spin-spin Green functions, from which the superlattice spin-wave spectra and their spectral intensities are calculated. Then we consider a new type of superlattices that are limited within two parallel free surfaces perpendicular to their interfaces (Fig. 1.4). The corresponding Green functions are obtained with an appropriate extension of the matrix technique developed in Chapters 3 and 4. The superlattice spin-wave spectra are hence calculated explicitly.
In Chapter 6 we summarize the theoretical results obtained for the spin-wave excitations in the ferromagnetic layered structures considered. As conclusions, we also make brief comments on some possibilities of applications and extensions of the present work.
Chapter 2

The Green Function Formalism for Ferromagnets

§ 2.1 Introduction

The Green functions, when appropriately formulated and constructed, can serve to unveil a variety of static and dynamic properties of excitations in many-body systems (e.g., spin waves in magnetic materials and phonons in crystals). The Green functions are often known as the response functions since they relate the resultant linear responses of a system to small external stimuli. It is worth noting that the response functions (or the Green functions) are characteristic of the system itself and independent, in general, of external stimuli. A wealth of information about the excitations in the system is contained in the Green functions. For example, many experimentally observable quantities, such as the light scattering cross section, can be calculated from the Green functions (via correlation functions). As a matter of fact, the Green function method has become a very comprehensive and powerful tool for theoretical study of spin waves and many other excitations. General accounts of the Green function method can be found in many textbooks on many-body theory (e.g., see Fetter and Walecka 1971 and Rickayzen 1980) and the application to surface problems has been reviewed by Cottam and Maradudin (1984).

In order to calculate the excitation spectra or dispersion relations (i.e., the excitation frequency versus wavevector relations) only, one may simply choose to start with a set of homogeneous
equations, representing the equations of motion for the excitation amplitudes derived from the Hamiltonian of the system. Substitution of the appropriate wavelike or decaying solutions (for bulk or surface modes, respectively) into these equations yields the dispersion relations and eigenfunction solutions. In the case of a superlattice, one may further construct from the equations of motion the transfer matrices relating the amplitudes from one unit cell to the next. The excitation spectra of the superlattice can then be deduced from the transfer matrices when the periodicity is taken into account.

In contrast to the above-mentioned simple dispersion relation calculations, the Green functions can provide spectral information about the excitation strengths for arbitrary values of frequency and wavevector. The intensities of excitations as well as their dispersion relations can be calculated from the Green functions for the system by a standard procedure. By using the Fluctuation-Dissipation theorem, the correlation functions can also be calculated from the Green functions. Consequently, many physical quantities (such as the specific heats and light scattering cross sections) can be deduced from the correlation functions.

In general, the Green functions can be formulated and calculated in a variety of more or less equivalent ways. Besides directly evaluating the linear response of the system to given external stimuli (see, e.g., Barker and Loudon 1972 and Cottam and Maradudin 1984 for a general discussion on linear-response theory), one can formulate quantum-mechanical commutator Green functions in a standard way (see Zubarev 1960). In magnetic systems, the Green functions can be
constructed in terms of either spin operators directly or boson operators equivalently. The latter operators might result, for example, from use of the Holstein-Primakoff transformation (Holstein and Primakoff 1940) or Dyson-Maleev transformation (Dyson 1956 and Maleev 1957). The Green function calculations can be performed with either the equation-of-motion method in the standard quantum mechanics (plus some decoupling or linearization approximation) or with the diagrammatic perturbation methods in quantum field theory.

The purpose of this chapter is to expound a Green function formalism in a particular format appropriate to the ferromagnetic systems with which we shall be concerned in this thesis. The outline of this chapter is as follows. In § 2.2 we discuss Heisenberg ferromagnetism and give the form of the total Hamiltonian. In § 2.3 we give the definition of the retarded commutator Green function and derive its equation of motion. We also introduce the Random-Phase Approximation in ferromagnetism. In § 2.4 we discuss the Fluctuation-Dissipation theorem. In § 2.5 we give a simple example, showing the application of the Green function theory to an infinite ferromagnet.

§ 2.2 The Heisenberg Model for Ferromagnets

As we mentioned in Chapter 1, the exchange interaction, which is responsible for the parallel alignment of the spins in a ferromagnet, is a direct result of the indistinguishability of identical particles. To have a simple idea of the electrostatic origin of the exchange interaction, we consider two magnetic ions (labeled by 1 and 2), each
with one electron. Since the electrons have spin \( \frac{1}{2} \) and obey the Fermi-Dirac statistics, the total wave function, which can be written as a product of an orbital part \( \Psi \) and a spin part \( \chi \), must be antisymmetric with respect to interchange of the electrons. This means that the antisymmetric spin singlet \( \chi^- (S = 0) \) and symmetric spin triplet \( \chi^+ (S = 1) \) correspond respectively to the symmetric \( (\Psi_\uparrow) \) and antisymmetric \( (\Psi_\downarrow) \) orbital wave functions. The interaction Hamiltonian \( V_{12} \) has the expectation values \( V_\pm = C \pm \frac{1}{2} J_{12} \) in the \( \Psi_\pm \) states. The quantity \( C \) is the Coulomb energy and \( J_{12} \) represents the exchange integral due to an overlap of the two individual orbitals associated with the two electrons. The fact that the operator \( -(S_1 \cdot S_2 + \frac{1}{4}) \) has eigenvalues \( \pm \frac{1}{2} \) in the \( \chi_\pm \) states (see Phillips and Rosenberg 1966) makes it possible to represent \( V_{12} \) in terms of the spin operators \( S_1 \) and \( S_2 \) of the two electrons as \( V_{12} = (C - \frac{1}{4} J_{12}) - J_{12} S_1 \cdot S_2 \). Now we see that the interaction between the two magnetic ions can be represented, up to a constant, by a Hamiltonian (Dirac 1929)

\[
H_{12} = - J_{12} S_1 \cdot S_2
\]

(2.1)

describing the exchange coupling of \( S_1 \) and \( S_2 \).

The magnitude of \( J_{12} \) typically falls off exponentially as the distance between the two ions increases. This is why the exchange interaction is of short range. In principle, \( J_{12} \) can be either positive or negative. If \( J_{12} > 0 \) (< 0), the ground state has \( S = 1 \) (= 0), corresponding to a parallel (antiparallel) alignment of the spins as in a ferromagnet (antiferromagnet). This model of ferromagnetism is due to Heisenberg (1928).
When the above argument is generalized to the whole system of spins in a ferromagnet, we obtain an exchange Hamiltonian for the ferromagnet (see, e.g., Bogolyubov and Tyablikov 1949)

\[ H_{ex} = -\frac{1}{2} \sum_{\mathbf{r}, \mathbf{r}'} J(\mathbf{r}, \mathbf{r}') \mathbf{S}_\mathbf{r} \cdot \mathbf{S}_{\mathbf{r}'} \]  

(2.2)

where the factor \( \frac{1}{2} \) is included to compensate for the double counting of each pair of spins \( \mathbf{S}_\mathbf{r} \) and \( \mathbf{S}_{\mathbf{r}'} \), at sites \( \mathbf{r} \) and \( \mathbf{r}' \) respectively, in the summation. The exchange integral \( J(\mathbf{r}, \mathbf{r}') \) is also called the exchange constant in an isotropic ferromagnet, where the dependence of \( J(\mathbf{r}, \mathbf{r}') \) on \( \mathbf{r} \) and \( \mathbf{r}' \) in the bulk is through \( |\mathbf{r} - \mathbf{r}'| \) only. Since \( J(\mathbf{r}, \mathbf{r}') \) decreases rapidly with \( |\mathbf{r} - \mathbf{r}'| \), it is often sufficient to consider the exchange coupling only between the nearest neighbors. For simplicity, \( J(\mathbf{r}, \mathbf{r}') \) is regarded in this thesis as being zero unless \( \mathbf{r} \) and \( \mathbf{r}' \) are nearest neighbor sites. This assumption includes taking \( J(\mathbf{r}, \mathbf{r}) = 0 \).

When the ferromagnet is placed in an external magnetic field \( H_0 \) (along the \( z \) direction), the Zeeman energy describing the coupling of the net magnetic moment \( \sum_\mathbf{r} g_\mu_B \mathbf{S}_\mathbf{r} \) with \( H_0 \) should be included in the total Hamiltonian for the ferromagnet

\[ H = -\frac{1}{2} \sum_{\mathbf{r}, \mathbf{r}'} J(\mathbf{r}, \mathbf{r}') \mathbf{S}_\mathbf{r} \cdot \mathbf{S}_{\mathbf{r}'} - g_\mu_B H_0 \sum_\mathbf{r} \mathbf{S}_\mathbf{r}^2 \]  

(2.3)

where \( g \) is the Landé \( g \)-factor and \( \mu_B \) is the Bohr magneton.

More generally, we should include in the total Hamiltonian additional terms describing other interactions as discussed at the beginning of Chapter 1, e.g.,

\[ H_d = -\frac{1}{2} (g_\mu_B)^2 \sum_{\mathbf{r}, \mathbf{r}'} \left[ \frac{\mathbf{S}_\mathbf{r} \cdot \mathbf{S}_{\mathbf{r}'}}{|\mathbf{R}|^3} - \frac{3(\mathbf{S}_\mathbf{r} \cdot \mathbf{R})(\mathbf{S}_{\mathbf{r}'} \cdot \mathbf{R})}{|\mathbf{R}|^5} \right] \]  

(2.4)
for the dipole-dipole interaction (where \( R = r - r' \)) and

\[
\mathcal{H}_a = -g\mu_B \sum_r H_A(r) S^z_r
\]  

(2.5)

for the Zeeman energy due to an effective uniaxial anisotropy field \( H_A(r) \) in the z direction. However, these terms are often small and negligible in comparison with the exchange interaction except in the long-wavelength limit. Therefore, the Heisenberg Hamiltonian (2.3) is basically used as the total Hamiltonian throughout this thesis, while the effects of the surface anisotropy in the form of (2.5) are included where appropriate.

§ 2.3 The Green Functions for Ferromagnets

For any two quantum-mechanical operators \( X \) and \( Y \) in the Heisenberg picture, the retarded commutator Green function (Zubarev 1960) is defined as follows

\[
\langle\langle X(t); Y(t') \rangle\rangle = -i\Theta(t-t')\langle [X(t), Y(t')] \rangle
\]  

(2.6)

where \( \Theta \) is the Heaviside step function. \( [\cdots, \cdots] \) denotes a commutator and \( \langle\cdots\rangle \) a thermal average \( \text{Tr}(\rho \cdots) \) in which \( \rho \) is the density matrix of the system.

To calculate the Green function we usually turn to its equation of motion (Zubarev 1960)

\[
\frac{d}{dt} \langle\langle X(t); Y(t') \rangle\rangle = -i\Theta(t-t')\langle [X(t), Y(t')] \rangle - i\langle\langle [X(t), \mathcal{H}; Y(t')] \rangle\rangle
\]  

(2.7)

where \( \mathcal{H} \) is the Hamiltonian of the system. Using the cyclic invariance property of trace, we can prove that \( \langle\langle X(t); Y(t') \rangle\rangle \) and \( \langle\langle [X(t), \mathcal{H}; Y(t')] \rangle\rangle \) depend on \( t \) and \( t' \) only through the difference
(t-t'). This allows a Fourier transformation

\[ \langle \langle X(t); Y(t') \rangle \rangle_E = \int_{-\infty}^{\infty} \langle \langle X; Y \rangle \rangle_E \exp[-iE(t-t')] \, dE \]  

(2.8)

to be made and (2.7) to be written in terms of the Fourier components

\[ E \langle \langle X; Y \rangle \rangle_E = \frac{1}{2\pi} \langle \langle X, Y \rangle \rangle + \langle \langle X, H; Y \rangle \rangle_E \]  

(2.9)

For a ferromagnetic system we work directly with the spins of the atoms (or molecules). The spin operators are neither bosons nor fermions, but satisfy the commutation relations

\[ [S^\alpha_r, S^\beta_{r'}] = i\epsilon_{\alpha\beta\gamma} S^\gamma_r \delta_{rr'}, \]  

(2.10)

where \( \epsilon_{\alpha\beta\gamma} \) \( (\alpha, \beta, \gamma = x, y, z) \) is the Levi-Civita tensor. Usually it is more convenient to use another set of operators \( S^\pm_r = S^x_r \pm iS^y_r \) and \( S^z_r \), which satisfy the following commutation relations derived from (2.10):

\[ [S^+_r, S^-_{r'}] = 2S^z_r \delta_{rr'}, \quad [S^z_r, S^\pm_{r'}] = \pm S^\pm_r \delta_{rr'}, \]  

(2.11)

Let \( X = S^+_r, Y = S^-_{r'}, \) and \( H \) be the Hamiltonian (2.3). Then (2.9) becomes

\[ (E - gH_0) \langle \langle S^+_r, S^-_{r'} \rangle \rangle_E = \frac{\langle \langle S^z \rangle \rangle}{\pi} \delta_{rr'} + \sum_{r',r''} J(r,r'') \langle \langle (S^+_r S^-_{r'} - S^-_{r'} S^+_r) ; S^-_{r''} \rangle \rangle_E \]  

(2.12)

The higher order Green functions on the right-hand side of (2.12) can be decoupled by means of the Random-Phase Approximation (see, e.g., Bonch-Bruevich and Tyablikov 1962) as follows:

\[ \langle \langle S^z_{r'} S^+_r ; S^-_{r''} \rangle \rangle_E = \langle \langle S^z_{r''} \rangle \rangle \langle \langle S^+_r ; S^-_{r''} \rangle \rangle_E \]  

(2.13a)

\[ \langle \langle S^z_{r'} S^-_{r''} ; S^-_{r''} \rangle \rangle_E = \langle \langle S^z_{r''} \rangle \rangle \langle \langle S^-_{r''} ; S^-_{r''} \rangle \rangle_E \]  

(2.13b)

Essentially, this involves neglecting the fluctuations in each \( S^z_r \).
operator (about $\langle S^z_\mathbf{r} \rangle$) compared with the fluctuations in the $S^z$ (or $S^-$) operator at a different site. The replacement of the $S^z$ operators by their thermal averages as in (2.13) is a reasonable approximation at low temperatures where relatively few spin waves are thermally excited. With the use of the Random-Phase Approximation, (2.12) is rearranged as

$$
\left[ -(E - g \mu_B H_0) + \sum_{\mathbf{r}, \mathbf{r}''} J(r, r'') \langle S^z_{\mathbf{r}''} \rangle \right] \langle \langle S^+_{\mathbf{r}} ; S^-_{\mathbf{r}'} \rangle \rangle_E 
- \langle S^z_{\mathbf{r}} \rangle \sum_{\mathbf{r}, \mathbf{r}''} J(r, r'') \langle \langle S^+_{\mathbf{r}''} ; S^-_{\mathbf{r}'} \rangle \rangle_E = - \frac{\langle S^z_{\mathbf{r}} \rangle}{\pi} \delta_{r r'},
$$

(2.14)

This equation is the basis for calculating Green functions for the ferromagnetic systems in the entire thesis.

§ 2.4 The Fluctuation-Dissipation Theorem

As we mentioned before, the correlation functions are directly used in studying many properties of a magnetic system, for example, thermodynamic properties such as the temperature dependence of magnetization (see, e.g., Akhiezer 1968) and the cross sections for the inelastic scattering of light or neutrons from magnons (see, e.g., Cottam and Lockwood 1986 for more details). The connection between Green functions and correlation functions is established by the Fluctuation-Dissipation theorem.

The right-hand side of (2.6) involves the correlation functions $\langle X(t)Y(t') \rangle$ and $\langle Y(t')X(t) \rangle$, which are related by (Zubarev 1960)

$$
\langle X(t)Y(t') \rangle = \langle Y(t')X(t + \beta) \rangle
$$

(2.15)

with $\beta = \frac{1}{k_B T}$. Similar to (2.8), a Fourier transformation
\[ \langle X(t)Y(t') \rangle = \int_{-\infty}^{\infty} \langle XY \rangle_E \exp[-iE(t-t')] \, dE \quad (2.16) \]

can be made and (2.15) implies
\[ \langle XY \rangle_E = \langle YX \rangle_E \exp(\beta E) \quad (2.17) \]

Hence, we can express (2.6) in terms of the Fourier components as
\[ \langle \langle X; Y \rangle \rangle_E = \frac{1}{2\pi} \int_{-\infty}^{\infty} \frac{\langle XY \rangle_{E'} \exp(\beta E') - 1}{E - E' + i\nu} \, dE' \quad (2.18) \]

where \( \nu \) is a positive real infinitesimal (\( \nu \to 0 \)). This can be regarded as a limit of the analytically continued Green function
\[ \langle \langle X; Y \rangle \rangle_E = \frac{1}{2\pi} \int_{-\infty}^{\infty} \frac{\langle XY \rangle_{E'} \exp(\beta E') - 1}{E - E'} \, dE' \quad (2.19) \]

as \( E \) approaches the real axis from the upper half of the complex plane. The right-hand side of (2.19) can be separated into its real and imaginary parts by using the following identity (see, e.g., Parry 1973)
\[ \frac{1}{E - E'} = \frac{1}{E - E' + i\nu} = \mathcal{P}\left( \frac{1}{E - E'} \right) - i\Re(E - E') \quad (2.20) \]

where \( \mathcal{P} \) means that the principal value is taken in any integration over \( E' \). By taking the imaginary part of each side of (2.19), we get the Fluctuation-Dissipation theorem, i.e.,
\[ \langle XY \rangle_E = -2n(E) \, \Im(\langle \langle X; Y \rangle \rangle_E) \quad (2.21) \]

where \( n(E) = [\exp(\beta E) - 1]^{-1} \) is the Bose-Einstein factor.

In terms of the spin operators, (2.21) becomes, for example,
\[ \langle S^+_{\tau}, S^+_{\tau'} \rangle_E = -2n(E) \, \Im(\langle \langle S^+_{\tau}; S^+_{\tau'} \rangle \rangle_E) \quad (2.22) \]

Form (2.17) we can also get
\[ \langle S^+_r S^-_r \rangle_E = -2[n(E)+1] \text{ Im} \langle \langle S^+_r ; S^-_r \rangle \rangle_E \] (2.23)

These forms of correlation functions are particularly useful in calculating from the Green function results many of the measurable quantities such as the temperature dependence of magnetization.

§ 2.5 Example: An Infinite Ferromagnet

As an elementary example of the application of the Green function theory to ferromagnetic systems, we may consider an infinite ferromagnet with the simple cubic lattice structure. Because of the translational symmetry in three dimensions, \( \langle S^z_r \rangle \) is independent of site \( r \) (as such it is denoted simply as \( \langle S^z \rangle \)) and we can make a three-dimensional (3D) Fourier transformation to a wavevector representation

\[ \langle \langle S^+_r ; S^-_r \rangle \rangle_E = \frac{1}{N_3} \sum \limits_{\mathbf{q}} G(E, q) \exp[i \mathbf{q} \cdot (r-r')] \] (2.24)

\[ \langle S^z_r, S^z_r \rangle_E = \frac{1}{N_3} \sum \limits_{\mathbf{q}} F(E, q) \exp[i \mathbf{q} \cdot (r-r')] \] (2.25)

where \( N_3 \) is the total number (macroscopically large) of spins in the ferromagnet.

We can rewrite (2.14) in the 3D wavevector space as follows:

\[ [-\langle E - \mu H_0 \rangle + 6J \langle S^z \rangle] G(E, q) = 2J \langle S^z \rangle [\cos(q_x a) + \cos(q_y a) + \cos(q_z a)] G(E, q) \]

\[ = - \frac{\langle S^z \rangle}{n} \] (2.26)

and solve for the analytically continued Green function \( G(E, q) \), obtaining

\[ G(E, q) = \frac{\langle S^z \rangle}{\pi |E - E(q)|} \] (2.27)
where
\[ E(q) = g\mu_B H_0 + 2J\langle S_z \rangle \Lambda_3(q) \quad (2.28) \]

with
\[ \Lambda_3(q) = 3 - [\cos(q_x a) + \cos(q_y a) + \cos(q_z a)] . \quad (2.29) \]

This Green function has one pole at \( E = E(q) \), which gives the dispersion relation of spin waves in the ferromagnet. At low temperatures \( T < T_C \) where \( \langle S^z \rangle \to S \), (2.28) reproduces the standard expression (e.g., see Kittel 1986) for the linear (i.e., non-interacting) spin-wave modes in a simple cubic ferromagnet. For later comparison, we express this standard result (i.e., (2.28) with \( \langle S^z \rangle \to S \)) graphically in Fig. 2.1 (in three equivalent ways). The dispersion relation is simply a straight line (see Fig. 2.1(a)) when the spin-wave frequency is plotted against \( \Lambda_3(q) \), i.e., in terms of the 3D wavevector \( q \). However, when the frequency is plotted versus just one or two components of the wavevector, the bulk spin-wave frequency spectrum becomes a continuum band (see Figs. 2.1(b) and 2.1(c)), since the remaining components of \( q \) can range from 0 to \( \frac{\pi}{a} \).

From (2.22), (2.24), (2.25), and (2.27) we obtain the spectral intensity
\[ F(E, q) = -2n(E) \text{Im} \left( \frac{\langle S^z \rangle}{\pi i [E - E(q)]} \right) = \frac{2\langle S^z \rangle}{\exp(\beta E) - 1} \delta[E - E(q)] \quad (2.30) \]

and the correlation function
\[ \langle S^z_{r'}(t')S^z_r(t) \rangle = \int_{-\infty}^{\infty} \frac{1}{N^3} \sum_{q} F(E, q) \exp[iq \cdot (r - r')] \exp[-iE(t-t')] \, dE \quad (2.31) \]

At \( r = r' \) and \( t = t' \) the above equation becomes
Fig. 2.1 The dispersion relations for spin waves in an infinite simple-cubic ferromagnet represented in three ways. The dimensionless frequencies are plotted against: (a) $\Lambda_3(q)$ defined in (2.29), (b) $\Lambda_2(q_x, q_y) = 2 - [\cos(q_x a) + \cos(q_y a)]$, and (c) $\Lambda_1(q_z) = 1 - \cos(q_z a)$. In the latter two cases the spin-wave modes form continua (shown by the shaded areas).
\[ \langle S_r S_r^* \rangle = \frac{2\langle S^z \rangle}{N^2} \sum_q \frac{1}{\exp[\beta E(q)] - 1} \]  

(2.32)

For the special case of \( S = \frac{1}{2} \), we have the identity

\[ S_r^z S_r^{z*} = \frac{1}{2} - S_r^z \]  

(2.33)

From (2.32), together with (2.28) and (2.33), we can calculate the temperature dependence of \( \langle S^z \rangle \) (and hence of the magnetization and spectrum (2.28)). Also the Curie temperature \( T_c \) is readily obtained by seeking the asymptotic value of \( T \) at which \( \langle S^z \rangle \rightarrow 0 \) when \( H_0 = 0 \).

An infinite ferromagnet is probably the simplest example. The general methods developed in this chapter are specifically applied to various ferromagnetic structures with limited geometries in the chapters that follow. The main difference in these latter applications is that there is no longer translational symmetry in all three spatial dimensions. This greatly complicates the method of solution of the Green function equations and makes the spin-wave spectra much more complex and interesting.
Chapter 3
Perpendicularly Truncated Films

The behavior of spin-wave excitations in Heisenberg ferromagnetic films with two-dimensional (2D) translational symmetry (see Fig. 1.1(b)) has been investigated by means of the Green function formalism (e.g., see Cottam and Kontos 1980 and Moul and Cottam 1983). Due to the finite thickness, the bulk spin waves are quantized with the wavevector components perpendicular to the surfaces taking discrete values. Also localized surface spin waves may occur if the exchange constants on the surfaces are sufficiently different from those in the bulk.

In this chapter we study the spin waves in a ferromagnetic film terminated by one or more truncations perpendicular to the two film surfaces (see Figs. 1.3(a) and (b)). The presence of an extra truncated surface may give rise to surface spin wave modes that decay with distances from the truncation. In order to thoroughly investigate the effects of the truncated surfaces, we choose to neglect the variation of the exchange constants on the two original surfaces from those in the bulk. This free surface simplification also allows the exact analytic solutions of surface spin waves due to the truncations to be obtained.

The outline of this chapter is as follows. In § 3.1 we briefly re-derive, for completeness and later comparison, the known results of spin waves in a complete film with either unperturbed or perturbed surface parameters. This formalism is generalized in § 3.2 where we investigate the bulk and surface spin-wave modes in a film with a pair
of parallel free surfaces and one perpendicularly truncated surface. In § 3.3 we continue our investigation by considering the application to a film with two perpendicularly truncated surfaces, parallel to each other. The analytic theory in each case is illustrated by numerical examples.

§ 3.1 Films With 2D Translational Symmetry

We consider an $N$-layer ferromagnetic film of the simple cubic lattice structure with a pair of (001) surfaces and another $N-2$ interior atomic layers (see Fig. 3.1). The spin at any atomic site has the position vector

$$ r = (r_{\parallel}, (n-1)a) \quad (1 \leq n \leq N) \quad (3.1) $$

where $r_{\parallel}$ is the in-plane component (parallel to the xy plane) of the position vector and $a$ is the lattice parameter.

The Hamiltonian of the system in an external magnetic field $H_0$ (along the $z$ direction) is given by (2.3) with the exchange constant $J(r,r')$ between the nearest neighbors being $J_s$ if $r$ and $r'$ are both in either of the two (001) surfaces and $J$ otherwise. If $J_s$ is different from $J$, this allows for a simple perturbation of the surfaces in a symmetric film. The equation of motion for the spin-spin Green function is given by (2.14). At low temperatures the thermal average $\langle S_p^z \rangle$ is approximately equal to the spin quantum number $S$ and is therefore site independent.

Since the film has translational symmetry in the xy plane, we can make the 2D Fourier transformations

$$ \langle \langle S_p^+ : S_{p'}^- \rangle \rangle_E = \frac{1}{D^2} \sum q_{\parallel} G(n,n' | E, q_{\parallel}) \exp[i q_{\parallel} \cdot (r_1 - r_2)] \quad (3.2) $$
Fig. 3.1 Schematic diagram of a ferromagnetic film with 2D translational symmetry (in the x and y directions) and finite thickness (N atomic layers) in the z direction.
\[ \langle S_{F}^{z}, S_{F}^{z} \rangle_{E} = \frac{1}{N_{E}} \sum_{q_{\parallel}} F(n; n' \mid E, q_{\parallel}) \exp[iq_{\parallel} \cdot (r_{n} - r_{n'})] \] (3.3)

where \( q_{\parallel} = (q_{x}, q_{y}) \) is a 2D wavevector and \( N_{E} \) is the number (macroscopically large) of spins in any atomic layer parallel to the \( xy \) plane. We next rewrite (2.14) in the film geometry as a set of finite-difference equations that depend on the layer indices:

\[
\begin{align*}
(d - c) \ G(1; n') - G(2; n') &= - \frac{1}{\pi J} \delta_{1n'} \quad (3.4a) \\
(\ d \ G(n; n') - G(n-1; n') - G(n+1; n') &= - \frac{1}{\pi J} \delta_{nn'} \quad (1 < n < N) \quad (3.4b) \\
(d - c) \ G(N; n') - G(N-1; n') &= - \frac{1}{\pi J} \delta_{Nn'} \quad (3.4c)
\end{align*}
\]

where \( G(n; n') \) is the Fourier component as in (3.2) but, for convenience, its dependence on \( E \) and \( q_{\parallel} \) has not been explicitly written down. The coefficients \( d \) and \( c \) are

\[
\begin{align*}
d &= \omega_{0} - \omega + 2[1 + \Lambda_{2}(q_{\parallel})] \quad (3.5) \\
c &= 1 - \omega_{AS} + 2(1 - \epsilon)\Lambda_{2}(q_{\parallel}) \quad (3.6)
\end{align*}
\]

where

\[
\begin{align*}
\omega &= \frac{E}{JS} \quad (3.7) \\
\omega_{0} &= \frac{g_{\mu_{B}} H_{0}}{JS} \quad (3.8) \\
\omega_{AS} &= \frac{g_{\mu_{B}} H_{AS}}{JS} \quad (3.9) \\
\Lambda_{2}(q_{\parallel}) &= 2[\cos(q_{x}a) + \cos(q_{y}a)] \quad (3.10) \\
\epsilon &= \frac{J_{s}}{J} \quad (3.11)
\end{align*}
\]

We have considered the effects of uniaxial surface anisotropy by
including (2.6) into the total Hamiltonian with an effective anisotropy field in layers 1 and $N$ only:

$$H_A(r) = H_A(n) = H_{as}(\delta_{n1} + \delta_{nn'})$$  \hspace{1cm} (3.12)

When we regard $G(n;n')$ as the element $(G)_{nn'}$ of an $N \times N$ matrix $G$ in the $n$th row and $n'$th column, (3.4) is equivalently expressed in the matrix form

$$(A - C) G = -\frac{1}{\mu J}$$  \hspace{1cm} (3.13)

where $A$, $C$, and $I$ are $N \times N$ matrices with elements being

$$A(n;n') = (A)_{nn'} = d \delta_{nn'} - \delta_{n-1,n'} - \delta_{n+1,n'}$$  \hspace{1cm} (3.14)

$$C(n;n') = (C)_{nn'} = c(\delta_{n1} \delta_{n'1} + \delta_{nn} \delta_{n'n})$$  \hspace{1cm} (3.15)

and $(I)_{nn'} = \delta_{nn'}$. It is known that the inverse of the finite tridiagonal matrix $A$ (denoted by $A^{-1} = B$) is given by (see, e.g., Cottam and Kontos 1980)

$$B(n;n') = (B)_{nn'} = \frac{x^{n+n'} - x^{|n-n'|} + x^{2(N+1)-(n+n')} - x^{2(N+1)-|n-n'|}}{(1-x^{2(N+1)})(x-x^{-1})}$$  \hspace{1cm} (3.16)

where $x$ is a complex parameter defined by

$$x + x^{-1} = d \hspace{1cm} (0 < |x| \leq 1)$$  \hspace{1cm} (3.17)

if $|d| \neq 2$ and

$$B(n;n') = (B)_{nn'} = \left(\frac{d}{|d|}\right)^{n-n'-1}\left(\frac{n + n' - |n-n'|}{2} - \frac{nn'}{N+1}\right)$$

if $|d| = 2$. In the limit of $N \rightarrow \infty$ the factors involving $x^{2(N+1)}$ in (3.16) will vanish for values of $x$ within the unit circle on the complex plane, and we recover the expression (see, e.g., Cottam 1976)
for the semi-infinite ferromagnet, i.e.,

\[ B(n; n') = \frac{x^{n+n'} - x^{n-n'}}{x - x^{-1}} \quad (N \to \infty) \]  

(3.18)

We note that the matrix \( B \) in (3.16) satisfies the symmetry properties

\[ B(n; n') = B(n'; n) = B(N-n+1; N-n'+1) \]  

(3.19)

The required Green functions \( G(n; n') \) are then obtained by noting that

\[ G = -\frac{1}{\pi J} (A - C)^{-1} = -\frac{1}{\pi J} (I - BC)^{-1} B \]  

(3.20)

The matrix \((I-BC)^{-1} B\) can be calculated straightforwardly using (3.15) and (3.16) (see Cottam and Kontos 1980). Alternatively, we can write down the formal solution of (3.13) with the help of the Dyson equation

\[ G = -\frac{B}{\pi J} + BCG \]  

(3.21)

or (in terms of the elements)

\[ G(n; n') = -\frac{B(n; n')}{\pi J} + c[B(n; 1)G(1; n') + B(n; N)G(N; n')] \]  

(3.22)

To express \( G(n; n') \) in terms of \( B(n; n') \), we need to solve for \( G(1; n') \) and \( G(N; n') \) on the right-hand side of (3.22). This can be done from

\[
\begin{pmatrix}
1-cB(1; 1) & -cB(1; N) \\
-cB(N; 1) & 1-cB(N; N)
\end{pmatrix}
\begin{pmatrix}
G(1; n') \\
G(N; n')
\end{pmatrix} = -\frac{1}{\pi J}
\begin{pmatrix}
B(1; n') \\
B(N; n')
\end{pmatrix}
\]  

(3.23)

which is obtained by setting \( n = 1 \) and \( n = N \) in (3.22). By substituting the solution of (3.23) into (3.22), we obtain the Green functions \( G(n; n') \) in terms of \( B(n; n') \) as

\[ G(n; n') = -\frac{B(n; n')}{\pi J}\]

\[-\frac{c}{\pi J} \{ [1-cB(N; N)]B(n; 1)B(1; n') + cB(1; N)B(n; 1)B(N; n') \}

\[ + cB(N; 1)B(n; N)B(1; n') + [1-cB(1; 1)]B(n; N)B(N; n') \}\]  

(3.24)
where

\[ W_0 = [1 - cB(1; 1)][1 - cB(N; N)] - c^2B(1; N)B(N; 1) \]  \hspace{1cm} (3.25)

We also note that the matrix \( G \) satisfies the same symmetry properties as those for \( B \), i.e.,

\[ G(n; n') = G(n'; n) = G(N-n+1; N-n'+1) \]  \hspace{1cm} (3.26)

After substituting (3.16) into (3.24) and (3.25), we eventually obtain

\[ G(n; n') = -\frac{\{\sin((N-n+1)ka) - \sin((N-n)ka)\}\{\sin(n'ka) - \sin((n'-1)ka)\}}{W\sin(ka)} \]  \hspace{1cm} (n \neq n')

(3.27)

where

\[ W = \sin((N+1)ka) - 2\sin(Nka) + c^2\sin((N-1)ka) \]  \hspace{1cm} (3.28)

Here we have, for convenience, introduced another complex parameter \( k \) defined in terms of \( x \) by

\[ x = \exp(ika) \hspace{1cm} (\text{Im}(k) \neq 0) \]  \hspace{1cm} (3.29)

By analogy to (2.27) in the case of an infinite ferromagnet, the dispersion relations for the spin-wave modes in the film are determined by the poles of the Green function matrix \( G \), i.e., the solutions of \( W = 0 \). But by contrast to (2.27), the number of the physical spin-wave poles of \( G \) (for a fixed in-plane wavevector \( q_\parallel \)) will be equal to the number of atomic layers \( N \) across the thickness. These \( N \) discrete spin waves may represent either bulk or surface modes.

**Numerical results and discussion**

It has been proven (see, e.g., Puszkarski 1979 and Cottam and Kontos 1980) that there may be, at most, one or two surface spin-wave modes in the film, depending on the surface parameter \( c \). However, if \( |c| \leq 1 \) (e.g., if \( 1 \leq c \leq \frac{5}{4} \) and \( H_{as} = 0 \) at any value of \( q_\parallel \)), there
are no surface modes. The bulk modes, known as standing spin waves in a film, are associated with the solutions of $\hat{W} = 0$ for $x$ on the upper half of unit circle $|x| = 1$ and the surface modes are associated with the solutions for $x$ on the real axis $|x| < 1$. Equivalently from (3.29), the bulk modes have discrete real values for $k$, acting as the $z$ component of wavevector, within the interval $[0, \frac{n}{a}]$ and the acoustic (or optical) surface modes have complex $k$ in the form of $k = i\xi$ (or $\frac{n}{a} + i\xi$) with $\xi > 0$. The parameter $\xi$ is called the reciprocal attenuation length of the surface spin waves and is determined by $\exp(-\xi a) = |x| < 1$.

As numerical examples, we now give in Figs. 3.2(a) and (b) the dispersion relation curves for spin waves in a 5-layer film with $J_z = 0.5J$ and $J_z = 1.5J$, respectively. We see that acoustic (optical) surface modes lie below (above) the region for the bulk modes, whose lower and upper edges (the dotted lines) correspond to $k = 0$ and $k = \frac{n}{a}$ respectively. In the special case of free surfaces ($J_z = J$, i.e., $\epsilon = 1$), there are five bulk modes (the lowest one coincides with the lower edge of the bulk mode region) and no surface modes (see Fig. 3.3(a)). In this film with finite thickness ($N = 5$), the bulk spin-wave modes are "quantized", with the $z$ component of wavevector $k$ taking discrete real values. As one could expect, the bulk modes would fill up the bulk mode region (which is identical to that in Fig. 2.1(b)) and form a bulk-mode continuum in the limit when $N \rightarrow \infty$. Particularly, the bulk modes correspond to $q_z = \frac{(n-1)\pi}{Na}$ (with $n = 1, 2, \cdots, N$) in the case of $J_z = J$.

An alternative way of displaying the dispersion relations is now
Fig. 3.2 The dispersion relation curves (the solid lines) for spin waves in a ferromagnetic film with $N = 5$: (a) $J_s = 0.5J$ showing two acoustic surface branches below the bulk mode region, (b) $J_s = 1.5J$ showing two optical surface branches above the bulk mode region. The edges of the bulk mode region are shown by the dotted lines.
Fig. 3.3 The dispersion relations for spin waves in a 5-layer ferromagnetic film with free surfaces ($J_z = J$). The edges of the bulk mode region are shown by the dotted lines. The dimensionless frequencies are plotted against: (a) $\Lambda_2(q_{||})$ for the five bulk modes (the lowest coincides with the lower edge of the bulk mode region), and (b) $\Lambda_1(q_x)$ for the bulk mode $B_5$. In the latter case the bulk mode $B_5$ forms a continuum (shown by the shaded area).
discussed for later comparison. If we choose to plot the frequency of
each bulk mode found in Fig. 3.3(a) against $\Lambda_1(q_x) = 1 - \cos(q_x a)$, then
the bulk modes broaden into bands or continua (which may partly
overlap), since $q_y$ can take continuous values from 0 to $\frac{\pi}{a}$. For
example, we illustrate in Fig. 3.3(b) the broadened bulk-mode continuum
corresponding to the bulk mode marked by $B_5$ in Fig. 3.3(a). The edges
of the total bulk mode region (dotted lines) in this representation are
shown for comparison.

From the Fluctuation-Dissipation theorem (2.18), together with
(3.2) and (3.3), we immediately get the connection between the Fourier
components of the correlation function and the analytically continued
Green function (with $E = E + i \nu$)

$$ F(n; n' \mid E, q_y) = -2n(E) \lim_{\nu \to 0} \text{Im}[G(n; n' \mid E + i \nu, q_y)] $$

(3.30)

We note that the dependence of $F(n; n' \mid E, q_y)$ on $E$ has two factors: the
Bose-Einstein factor and the imaginary part of the Green function
component. The latter factor contains important information about the
intensities of the spin-wave modes while $n(E)$ is just a thermal
population factor, and so we shall concentrate on $\text{Im}[G(n; n' \mid E + i \nu, q_y)]$. Since
the correlation functions of spin operators at the equal time and
equal site (i.e., $t = t'$ and $r = r'$) are of particular importance in
many applications such as (2.32), we shall concentrate on this case.

For brevity and consistency, we introduce the following notation

$$ Y(n; \omega - \omega_0, \Lambda_2) = -\lim_{\nu \to 0} \text{Im}[G(n; n \mid E + i \nu, q_y)] $$

(3.31)

Similar to (2.30), $F(n; n \mid E, q_y)$ is expected to have peaks at those
values of $\omega - \omega_0$ and $\Lambda_2(q_y)$ that satisfy the dispersion relations.
Fig. 3.4  The spin wave intensities (calculated from the imaginary part of the Green function component in 2D wavevector space) in a ferromagnetic film with 2D translational symmetry. The assumed parameters are \( N = 5, n = 2 \) (the equal site), \( J_s = J \), and \( A_2(q_4) = 1.5 \).
For example, we plot $\gamma(2; \omega - \omega_0, 1.5)$ against $\omega - \omega_0$ for $N = 5$ and $\epsilon = 1$ in Fig. 3.4. We see that five peaks occur at precisely the five values of $\omega - \omega_0$ on the dispersion relation curves (Fig. 3.3(a)) at $A_2(q_x) = 1.5$. In principle, the theoretical peaks are $\delta$-function contributions, but for the purpose of numerical calculation we have included a small intrinsic width (damping). The integrated areas under the peaks, together with the Bose-Einstein factor $n(E)$, determine the spectral intensities of the spin-wave modes.

§ 3.2 Perpendicularly Truncated Films

Now we consider an $N$-layer ferromagnetic film with an additional truncated (010) surface at $y = 0$ (see Fig. 3.5). In this perpendicularly truncated film, the spin of any atom has the position vector

$$r = (x, (m-1)a, (n-1)a) \quad (1 \leq m < \infty, 1 \leq n \leq N) \quad (3.32)$$

The system extends to $\pm\infty$ in the $x$ direction. The exchange constants are taken to be $J_z$ if the nearest neighbors are both in the truncated surface and $J$ otherwise. This simplification implies that the two (001) surfaces are taken here to be free surfaces.

The Hamiltonian of this truncated film is again given by (2.3) and the equation of motion for the spin-spin Green function is given by (2.14). Unlike the complete film, however, there is only one-dimensional (1D) translational symmetry, which is in the $x$ direction. So we can only make the 1D Fourier transformations

$$\langle \langle S^+_r; S^-_{r'} \rangle \rangle_E = \frac{1}{Q^1} \sum_{Q_x} G(m, n; m', n' | E, q_x) \exp[iq_x(x-x')] \quad (3.33)$$
Fig. 3.5  Schematic diagram of a perpendicularly truncated $N$-layer ferromagnetic film, showing the assumed exchange interactions.
\[ \langle S^{-}_{m}, S^{+}_{m'} \rangle_E = \frac{1}{Q_1} \sum_{q_x} F(m, n; m', n' \mid E, q_x) \exp[iq_x(x-x')] \]  

(3.34)

where \( Q_1 \) is the number (macroscopically large) of spins in any crystalline axis in the \( x \) direction. After substituting (3.33) into (2.14), we can rewrite the equations of motion for the Green function components \( G(m, n; m', n' \mid E, q_x) \) as an infinite set of finite difference equations that depend on the layer indices \( m \) and \( n \). If we regard the Green function components as the elements of such a partitioned matrix \( G \) that \( G(m, n; m', n' \mid E, q_x) \) enters in the \( mn \)th row and \( n'n' \)th column of the submatrix in the \( mn \)th row and \( mm' \)th column, we can express the equations of motion compactly in the matrix form

\[ (A - R) G = -\frac{i}{\hbar} \]  

(3.35)

This has the same form as (3.13) except that \( A \) and \( R \) are partitioned matrices with elements defined by

\[ A(m, n; m', n') = (D)_{mn'} \delta_{m=m'} - \delta_{nn'} (\delta_{m-1, m'} + \delta_{m+1, m'}) \]  

(3.36)

\[ R(m, n; m', n') = (C)_{nn'} \delta_{m=1} \delta_{m'=1} \]  

(3.37)

where

\[ (D)_{mn'} = (d - \delta_{n1} - \delta_{nN}) \delta_{nn'} - \delta_{n-1, n'} - \delta_{n+1, n'} \]  

(3.38)

\[ (C)_{nn'} = c \delta_{nn'} - (1-\epsilon)[(\delta_{n1} + \delta_{nN}) \delta_{nn'} + \delta_{n-1, n'} + \delta_{n+1, n'}] \]  

(3.39)

are the elements of the \( N \times N \) matrices \( D \) and \( C \). Here the coefficients \( d \) and \( c \) are given by

\[ d = \omega - \omega_0 + 2[2+\Lambda_1(q_x)] \]  

(3.40)

\[ c = 1 + 2(1-\epsilon)[1+\Lambda_1(q_x)] \]  

(3.41)

where \( \omega, \omega_0 \), and \( \epsilon \) are defined by (3.7), (3.8), and (3.11),
respectively, and \( \Lambda_1(q_x) \) is

\[
\Lambda_1(q_x) = 1 - \cos(q_x a)
\]

(3.42)

The submatrices \( D \) and \( C \) can be simultaneously diagonalized by similarity transformations (involving the same orthogonal matrix), so that

\[
V^{-1} D V = D'
\]

(3.43)

\[
V^{-1} C V = C'
\]

(3.44)

where the diagonal matrices \( D' \) and \( C' \) have the elements

\[
(D')_{nn'} = d_n \delta_{nn'} = \left( d - 2 \cos \left( \frac{(n-1)\pi}{N} \right) \right) \delta_{nn'}
\]

(3.45)

\[
(C')_{nn'} = c_n \delta_{nn'} = \left( c - 2(1-c) \cos \left( \frac{(n-1)\pi}{N} \right) \right) \delta_{nn'}
\]

(3.46)

and the orthogonal matrix \( V \) has the elements

\[
(V)_{nn'} = \left( \frac{2-\delta_{n'1}}{N} \right)^{1/2} \cos \left( \frac{(2n-1)(n'-1)\pi}{2N} \right)
\]

(3.47)

Now we can construct a partitioned matrix \( U \) with elements

\[
U(m,n;m',n') = (V)_{nn'} \delta_{mm'}
\]

(3.48)

and transform \( A, R, \) and \( G \) into a representation in which all the submatrices are diagonal. In this new representation (which we shall henceforth refer to as the subdiagonal representation), (3.35) remains formally the same, \( i.e., \)

\[
(A' - R') G' = -\frac{1}{kJ}
\]

(3.49)

where

\[
A' = U^{-1} A U
\]

(3.50)

\[
R' = U^{-1} R U
\]

(3.51)

\[
G' = U^{-1} G U
\]

(3.52)

The introduction of the above "subdiagonal" representation makes
it possible to extend the standard technique of inverting the ordinary tridiagonal matrices (see, e.g., Wax 1954 and Cottam 1976) to partitioned matrices. Since diagonal matrices can be operated on algebraically in the same way as ordinary c-numbers, we can simply replace the ordinary elements in the standard results by the corresponding diagonal submatrices of partitioned matrices involved and then deal with the internal structure of the submatrices separately. This basic idea is mathematically analogous to a procedure followed by Wolfram and DeWames (1969) in their analysis of a semi-infinite two-sublattice antiferromagnet.

In the "subdiagonal" representation produced by \(U\), the inverse of \(A'\) (denoted by \(B' = A'^{-1}\)) has the elements

\[
B'(m, n; m', n') = \frac{x_n^{m+m'} - x_n^{m-m'}}{x_n^{m} - x_n^{-m}} \delta_{nn'}
\]

(3.53)

This is obviously an extension of (3.18) to the partitioned matrix \(B'\).

In particular, putting \(m' = 1\), we have

\[
B'(m, n; 1, n') = B'(1, n; m, n') = x_n^m \delta_{nn'}
\]

(3.54)

Here the complex parameters \(x_n\) (\(0 < |x_n| \leq 1\)) are the elements of the diagonal matrix \(X'\) defined by an extended form of (3.17), i.e.,

\[
X' + X'^{-1} = 0'
\]

(3.55)

or, specifically,

\[
x_n + x_n^{-1} = d_n = \omega - \omega + 2\left[2 - \cos \frac{(n-1)\pi}{N} + \chi(q_x)\right]
\]

(0 < |x_n| \leq 1)

(3.56)

Similar to (3.21), we can write the formal solution of (3.49) as

\[
G' = -\frac{B'}{\pi J} + B' \quad R' \quad G'
\]

(3.57)

or (in terms of the elements)
\[ G'(m, n; m', n') = -\frac{B'(m, n; m', n')}{\pi J} \cdot c_n B'(m, n; 1, n') G'(1, n; m', n') \]  \hspace{1cm} (3.58)

By taking \( m = 1 \) in (3.57), we get

\[ G'(1, n; m', n') = -\frac{B'(1, n; m', n')}{\pi J \left[ 1 - c_n B'(1, n; 1, n') \right]} \]  \hspace{1cm} (3.59)

and eventually

\[ G'(m, n; m', n') = -\frac{1}{\pi J} \left[ B'(m, n; m', n') + \frac{c_n x_n^{m+m'}}{1 - c_n x_n} \right] \delta_{nn'} \]  \hspace{1cm} (3.60)

By transforming \( G'(m, n; m', n') \) back to the original representation, we get the required Green function components in the form

\[ G(m, n; m', n' \mid E, q_x) = \sum_{n'} \langle \Psi \rangle_{nn'} \langle \Psi \rangle_{n'n''} G'(m, n''; m', n'') \]  \hspace{1cm} (3.61)

The dispersion relations of the spin-wave modes in this truncated film are determined by the poles of \( G(m, n; m', n' \mid E, q_x) \). Particularly, the surface spin-wave modes are given (see (3.60) and (3.61)) by

\[ x_{n''} = c_n^{-1} \quad (n'' = 1, \ldots, N) \]  \hspace{1cm} (3.62)

The explicit results for the dispersion relations of the surface spin waves are therefore

\[ \omega = \omega_0 + 2 \left[ 2 - \cos \left( \frac{(n''-1)\pi}{N} \right) + \Lambda(q_x) \right] - (c_{n''} + c_n^{-1}) \]  \hspace{1cm} (3.63)

where

\[ c_{n''} = 1 + 2(1-c) \left[ 1 - \cos \left( \frac{(n''-1)\pi}{N} \right) + \Lambda(q_x) \right] \]  \hspace{1cm} (3.64)

**Numerical results and discussion**

Due to the restriction \(|x_{n''}| \leq 1\) (which is a condition for localization near the truncation), these surface spin-wave modes exist only for such values of \( c \) and \( \Lambda(q_x) \) that \(|c_{n''}| \approx 1\). More specifically,
it follows that there exist \( N \) acoustic surface spin-wave modes across the entire Brillouin zone if \( c < 1 \). However, in the case of \( c \gg 1 \), the \( n^{\text{th}} \) optical surface spin-wave mode exists (for large enough \( q_z \)) only if \( c > 1 + \left( 3 - \cos \left( \frac{(n-1)\pi}{N} \right) \right)^{-1} \). For example, we give in Fig. 3.6 the dispersion relations of the 5 optical surface spin-wave modes (marked by \( O_1 \) to \( O_5 \)) in a truncated 5-layer film with \( J_z = 1.5J \). Due to the localization condition, all the optical surface spin-wave modes in this case terminate at a characteristic frequency \( \omega_c \) given by

\[
\omega_c = \omega_0 + 4 - \frac{2}{1 - c} \quad (3.65)
\]

For comparison, we show by the dotted lines the edges of the bulk mode region for the corresponding film without truncation.

As one could expect, the surface modes would increase in number to form a continuum band in the limit of \( N \rightarrow \infty \). This can be verified by replacing \( \frac{(n-1)\pi}{N} \) on the right-hand sides of (6.63) and (6.64) by \( q_z a \) ranging from 0 to \( \pi \). Physically, when the film thickness becomes effectively infinite, the truncated film recovers 2D translational symmetry parallel to the truncated surface. Consequently, a 2D Fourier transformation can be made from the 2D lattice space (parallel to the truncated surface) to the 2D wavevector space. In this 2D wavevector representation, the dispersion relations of the surface modes become expressed more simply as:

\[
\omega = \omega_0 + 2[1 + \Lambda_2(q_z, q_x)] - (c + c^{-1}) \quad (3.66)
\]

where

\[
c = 1 + 2(1-c)\Lambda_2(q_z, q_x) \quad (3.67)
\]

and \( \Lambda_2(q_z, q_x) = 2 - [\cos(q_z a) + \cos(q_x a)] \). This is just the standard result for the surface spin waves in a semi-infinite ferromagnet (see,
Fig. 3.6 The dispersion relation curves for surface spin waves in a perpendicularly truncated ferromagnetic film. For $N = 5$ and $J_s = 1.5J$ the optical surface spin-wave modes (marked by $O_1$ to $O_5$) are cut off in dimensionless frequency at $\omega - \omega_0 = 8$ (see text). For comparison, the edges of the bulk mode region for the corresponding film without truncation are shown by the dotted lines.
Fig. 3.7 The dispersion relation curve for surface spin waves in a semi-infinite ferromagnet. The dimensionless frequencies are plotted against $A_2(q_x, q_y)$. For $J_s = 1.5J$ the optical surface spin-wave mode is cut off in dimensionless frequency at $\omega - \omega_0 = 8$. The edges of the bulk mode region are shown by the dotted lines.
e.g., Wolfram and Dewames 1972). For comparison with Fig. 3.6, we plot in Fig. 3.7 the dispersion relation curve for the optical surface mode (3.66), again taking \( c = 1.5 \).

Similar to (3.30), the Fourier components of the correlation functions in a truncated film are related to \( \text{Im}[G(m,n; m', n'| E + i\nu, q_x)] \) by

\[
F(m,n; m', n'| E, q_x) = -2n(E) \text{Im}[G(m,n; m', n'| E + i\nu, q_x)] \bigg|_{\nu \to 0} \quad (3.68)
\]

As in § 3.1, we investigate only the equal-site components and use a notation similar to (3.31):

\[
Y(m,n; \omega - \omega_0, \Lambda_1) = -\text{Im}[G(m,n; m, n'; E + i\nu, q_x)] \bigg|_{\nu \to 0} \quad (3.69)
\]

As examples we plot \( Y(m,2; \omega - \omega_0, 1.5) \) against \( \omega - \omega_0 \) for the same physical parameters as in Fig. 3.6 and for three different values of the layer index \( m \) (see Figs. 3.8 and 3.9). First, we notice from Fig. 3.8 for \( m = 1 \) that three peaks occur precisely at the three values of \( \omega - \omega_0 \) on the dispersion relation curves (Fig. 3.6) at \( \Lambda_1(q_x) = 1.5 \). These three peaks are expected to shrink in intensity and eventually vanish as \( m \) increases (because the surface spin waves are localized near the truncated surface), leaving contributions to the intensity coming only from the standing bulk spin waves of the film. This is confirmed by our corresponding numerical calculations for \( m = 3 \) and \( m = 50 \) (Figs. 3.9(a) and (b)).

When \( m \gg N \) (as in Fig. 3.9(b)), \( Y(m,n; \omega - \omega_0, \Lambda_1) \) becomes essentially independent of \( \varepsilon \) and \( m \), as expected. In Fig. 3.9(b) we see that the spin wave intensities distribute in the frequency region which precisely covers the physical bulk-mode continua for a complete film.
Fig. 3.8  The spin wave intensities (calculated from the imaginary part of the Green functions) in a perpendicularly truncated ferromagnetic film. The assumed parameters are $m = 1$ (the site is in the truncated surface), $n = 2$, $\Lambda_1(q_x) = 1.5$, and the same as in Fig. 3.6 otherwise.
Fig. 3.9  As in Fig. 3.8 but with the site chosen to be: (a) in the third atomic layer from the truncation ($m = 3$), (b) far away from the truncation ($m = 50$).
(see Fig. 3.3) at $\Lambda_1(q_x) = 1.5$. As a further check on the large-$m$
limit, we can compare with results in § 3.1 for the complete film. If
the Fourier component of the Green function (3.27) is transformed from
the wavevector $q_y$ space back to the real $y$ space, we could take the
imaginary part of the new Fourier component $G(y, n; y', n'; E + iv, q_x)$
to calculate the spectral intensities of the spin-wave modes. Note that
$G(y, n; y', n'; E + iv, q_x)$ depends on $y$ and $y'$ only through the difference
$y - y'$ because of the translational symmetry. In Figs. 3.10(a) and (b) we
present two examples of $\gamma(y, 2; \omega - \omega_0, \Lambda_1) = -\text{Im}[G(y, 2; y, 2; E + iv, q_x)] |_{v \to 0}$
(which is independent of $y$) plotted against $\omega - \omega_0$ for the spin waves in
a complete 5-layer film with free surfaces. We note in Fig. 3.10 that
the spin wave intensities distribute in the frequency regions
corresponding to the physical bulk-mode continua for a complete film
(e.g., see Fig. 3.3). It can now be seen explicitly that the
intensities shown in Fig. 3.9(b) for $m > N$ tend to resume the intensity
distributions for the spin waves in the corresponding complete 5-layer
film with free surfaces (see Fig. 3.10(a)). Therefore, we can conclude
that, at large enough distances away from the truncated surface, the
spin waves behave as if the film were not truncated, i.e., they do not
"feel" the existence of the truncated surface if it is far enough away.

§ 3.3 Films With Two Parallel Truncations

In this section we generalize the results of § 3.2 to an $N$-layer
ferromagnetic film with two parallel truncations, perpendicular to the
original pair of free surfaces (see Fig. 3.11). The two truncated (010)
surfaces are located at $y = 0$ and $y = (N-1)a$, respectively. The spin of
Fig. 3.10  The spin wave intensities (calculated from the imaginary part of the Green function component in 1D wavevector space) in a complete ferromagnetic film with 2D translational symmetry. The assumed parameters are $N = 5$, $n = 2$, $J_s = J$, and (a) $\Lambda_1(q_x) = 1.5$, (b) $\Lambda_1(q_x) = 1$. 
Fig. 3.11 Schematic diagram of an $N$-layer ferromagnetic film with two perpendicular truncations, parallel to each other, showing the assumed exchange interactions.
any atom in this film has the position vector

\[ r = (x, (m-1)a, (n-1)a) \quad (1 \leq m \leq N, \ 1 \leq n \leq N) \]  

(3.70)

The exchange constants are assumed to be \( J_s \) if the nearest neighbors are both in either of the two truncated surfaces and \( J \) otherwise. Equivalently, this structure may be viewed as a long ferromagnetic rod or wire, with rectangular cross section of \( M \) atoms by \( N \) atoms.

The Hamiltonian and the equation of motion for the spin-spin Green function are given respectively by (2.3) and (2.14) as before. Also, as in § 3.2, we can only make the 1D Fourier transformations (3.33) and (3.34). Consequently, we can express the equations of motion for the Green function components \( G(m,n;m',n';E,q_x) \) in the same matrix form as (3.35) and make the same type of similarity transformations to "subdiagonalize" the partitioned matrices. Actually, the expressions (3.36), (3.38) - (3.52), and (3.55) - (3.57) apply in this section provided \( m \) and \( m' \) are restricted to the range from 1 to \( M \). For the film with two truncations, the expressions for the partitioned matrices \( R \) and \( B'(m; A^{-1}) \) are modified as follows:

\[ R(m,n;m',n') = (C)_{nm'}(\delta_{m1} \delta_{m'1} + \delta_{mM} \delta_{m'M}) \]  

(3.71)

\[ B'(m,n;m',n') = \frac{x^{m+m'} - x^{|m-m'|} + x^{2(N+1)-(m+m')} - x^{2(N+1)-|m-m'|}}{(1 - x^{2(N+1)})(x_n - x_n^{-1})} \delta_{nm'} \]  

(3.72)

(3.72) is obviously analogous to (3.16) and is a generalization of (3.53) to the finite-dimensional partitioned matrix \( B' \) in this case. When written in terms of the matrix elements, (3.57) becomes
\[ G'(m, n; m', n') = - \frac{B'(m, n; m', n')}{\omega J} \]

\[ + c_n [B'(m, n; 1, n') \ G'(1, n; m', n') + B'(m, n; M, n') \ G'(M, n; m', n')] \] (3.73)

By taking \( m = 1 \) and \( m = M \) in (3.73), we get

\[ \begin{pmatrix}
1-c_n B'(1, n; 1, n') & -c_n B'(1, n; M, n') \\
-c_n B'(M, n; 1, n') & 1-c_n B'(M, n; M, n')
\end{pmatrix}
\begin{pmatrix}
G'(1, n; m', n') \\
G'(1, n; M, n')
\end{pmatrix} = - \frac{1}{\omega J}
\begin{pmatrix}
B'(1, n; m', n') \\
B'(1, n; M, n')
\end{pmatrix} \] (3.74)

Next, by substituting the solution of (3.74) back into (3.73), we obtain

\[ G'(m, n; m', n') = - \frac{B'(m, n; m', n')}{\omega J} \]

\[ - \frac{c_n \delta_{nn'}}{\omega J} \left\{ [1-c_n B'(M, n; M, n')]B'(m, n; 1, n')B'(1, n; m', n') \right. \]

\[ + c_n B'(1, n; M, n')B'(m, n; 1, n')B'(M, n; m', n') \]

\[ + c_n B'(M, n; 1, n')B'(m, n; M, n')B'(1, n; m', n') \]

\[ + [1-c_n B'(1, n; 1, n')]B'(m, n; M, n')B'(M, n; m', n') \} \] (3.75)

where

\[ w_n^{(0)} = [1-c_n B'(1, n; 1, n')][1-c_n B'(M, n; M, n')]-c_n^2 B'(1, n; M, n')B'(M, n; 1, n') \] (3.76)

After substituting (3.72) into (3.75) and (3.76), we eventually obtain the required Green function results as:

\[ G'(m, n; m', n') \]

\[ = \frac{\{\sin[(M-m+1)k_a]-c_n \sin[(M-m)k_a]\}\{\sin(m k_a)-c_n \sin((m'-1)k_a)\}}{\omega J w_n \sin(k_a) \sin(k_{n'})} \delta_{nn'} \]

\( (m \geq m') \) (3.77)
where
\[ w_n = \sin[(M+1)k_n a] - 2c_n \sin(Mk_n a) + c_n^2 \sin[(M+1)k_n a] \]  \hspace{1cm} (3.78)

Here we have introduced \( N \) parameters \( k_n \) defined by
\[ x_n = \exp(ik_n a) \hspace{1cm} \text{[\( \text{Im}(k_n) > 0 \)]} \hspace{1cm} (3.79) \]
in a similar manner to (3.29). The Green function components \( G(m, n; m', n' | E, q) \) are readily obtained by transforming \( G'(m, n; m', n') \) back to the original representation as in (3.61). Since (3.53) is a limiting case of (3.72) for \( M \to \infty \), we can verify algebraically that the above Green function expressions would recover the corresponding results of § 3.2 as \( M \to \infty \).

**Numerical results and discussion**

The dispersion relations in this case are determined by the poles of \( G(m, n; m', n' | E, q) \), i.e., the solutions of \( w_n = 0 \) for \( n' = 1, 2, \ldots, N \). As a numerical example, we plot, for \( J_s = 0.5J \), the dispersion relation curves for spin waves in a film with two truncations (see Fig. 3.12). This example corresponds to \( M = 4 \) and \( N = 5 \), i.e., there are 20 branches to the spectrum as expected. In general, the number of the branches (i.e., the number of the Green function poles) should be \( MN \). By analogy with the argument that leads to (3.66) from (3.63) in § 3.2, we can verify that, as \( M \to \infty \) (while \( M \) is kept fixed), the \( MN \) spin-wave modes group up and condense into \( M \) continuum bands, all of which would become the bulk-mode continua for a complete film in the case of \( J_s = J \).

Again, we point out that the spectral intensities of the spin waves in this ferromagnetic structure can be obtained by calculating the imaginary part of the Green function components in the forms of
Fig. 3.12 The dispersion relation curves for spin waves in a ferromagnetic film with two parallel truncations perpendicular to the free surfaces. The assumed parameters are $M = 4$, $N = 5$, and $J_5 = 0.5J$. 
(3.61) and (3.77). Following the same procedure as in § 3.2, we could calculate the intensities of the spin-wave modes shown in Fig. 3.12. The numerical calculations involved are straightforward in principle but tedious because of the large number of branches. We shall omit such computations and continue to use the procedures developed in this chapter (and in Chapter 2) to study the spin wave behavior in geometrically more complicated ferromagnetic structures.
CHAPTER 4

FILMS WITH PERPENDICULAR INTERFACES AND STEPS

As we have seen in the last chapter, the dispersion relations and intensities of spin wave modes in homogeneous films with perpendicular truncation(s) can be calculated with a matrix procedure which we refered to as "subdiagonalization". The same type of procedure may also be applied to a more complicated case (see Fig. 1.3(c)) where two truncated films are ferromagnetically coupled at their truncated surfaces to form an interface. The dispersion relations and intensities of spin wave modes in this complicated system can, in principle, be calculated. Since many parameters are involved in this more complex geometry, we shall first give a formulating scheme for the calculations in general. More attention is then paid to two special cases of particular interest, i.e., where the two truncated films are either equally thick or made up of the same material. Results are worked out explicitly in these two special cases.

In the first case, when the two films are equally thick but are made up of different materials, we are in effect considering a film with a perpendicular interface. This can also be viewed as a perpendicularly cleaved structure formed from two coupled semi-infinite ferromagnets. The spin waves at an interface between two semi-infinite ferromagnets in the absence of perpendicular cleavage was first studied theoretically by Yaniv (1983).

On the other hand, in the case when the two films are made up of the same material but have different thickness, we are essentially dealing with a homogeneous film with a steplike discontinuity on its
surface. This model is important because surfaces can never be perfectly flat in reality and the existence of atomic steps on surfaces is known to occur in practice (see, e.g., Magnan et al 1991 and Evans 1991). Recently, Stamps et al (1992 and 1993) considered the spin wave transmission and reflection in a ultrathin film with a surface step. However, theoretical research in this direction is still at a very early stage.

The outline of this chapter is as follows. In § 4.1 we use the "subdiagonalization" procedure in a matrix formalism to establish a scheme for calculating the dispersion relations and intensities of spin waves in two truncated films coupled ferromagnetically at the truncations. In § 4.2 we carry out the detailed calculations in the special case where the two films of different materials are equally thick. Next, § 4.3 is dedicated to the other special case where the two materials are identical but the mismatch of the thickness results in a step of arbitrary height on one of the surfaces.

§ 4.1 Two Films Coupled at Truncations

As a general model, we consider two truncated ferromagnetic films coupled ferromagnetically at their truncations (see Fig. 4.1). The two different materials labelled by the index \( \kappa \) (= 1, 2) are assumed, for simplicity, to have the simple cubic lattice structure with the same lattice parameter \( a \). The spins at adjacent sites across the interface between the two truncated surfaces are separated by the same distance \( a \) and coupled through an exchange constant denoted by \( J_{12} \). In the film 1 (with \( N_1 \) atomic layers) the spin of any atom has the position vector

\[
r = (x, -ma, (n-1)a) \quad (1 \leq m < \infty, 1 \leq n \leq N_1)
\]  (4.1)
Fig. 4.1  Schematic diagram of two truncated ferromagnetic films coupled ferromagnetically to each other through exchange constant $J_{12}$. 
and the spin quantum number is $S_z$. The exchange constants are taken to be $J_{S_1}$ if the nearest neighbors are both on the truncated surface and $J_1$ otherwise. In the film 2 (with $N_2$ atomic layers) the spin of any atom has the position vector

$$\mathbf{r} = (x, (m-1)a, (n-1)a) \quad (1 \leq m < \omega, 1 \leq n \leq N_2)$$  \hspace{1cm} (4.2)

and the spin quantum number is $S_z$. Without loss of generality, we assume that the film labelled by the index 2 is thicker, i.e., $N_1 \leq N_2$. For the nearest-neighbor spins on the truncated surface ($m = 1$) of the film 2, there are three possibilities in general for the exchange constants (see Fig. 4.1): the exchange constants are denoted by $J_{S_2}$ if neither of the nearest neighbors exceeds $z = (N_1-1)a$, by $J_C$ if both of the nearest neighbors are in the "corner" corresponding to $z = (N_2-1)a$, and by $J_S$ otherwise. Likewise, the exchange constants are $J_2$ if the nearest neighbors are not both on the truncated surface.

As in Chapter 3, the equations of motion for the spin-spin Green function are obtained using (2.14). Due to the 1D translational symmetry of this system in the $x$ direction, we can make the following 1D Fourier transformations by analogy with (3.33) and (3.34):

$$\langle \langle S_r^z S_{r'}^z \rangle \rangle_E = \frac{1}{D_1} \sum q_x G(k, m, n; \kappa', m', n' \parallel E, q_x) \exp [iq(x-x')] \hspace{1cm} (4.3)$$

$$\langle S_r^z S_{r'}^z \rangle_E = \frac{1}{D_1} \sum q_x F(k, m, n; \kappa', m', n' \parallel E, q_x) \exp [iq(x-x')] \hspace{1cm} (4.4)$$

where $r$ (or $r'$) is a site in the film of material $\kappa$ (or $\kappa'$) and $D_1$ is the number (macroscopically large) of spins in any crystalline axis in the $x$ direction. In the same way as in § 3.2, the equations of motion for the Fourier components of the Green function $G(k, m, n; \kappa', m', n' \parallel E, q_x)$ can be written compactly in a partitioned matrix form, i.e.,
\[(A - R)G = - \frac{1}{K}\]  

(4.5)

where

\[A = \begin{pmatrix} J_1 A_1 & 0 \\ 0 & J_2 A_2 \end{pmatrix}\]  

(4.6)

\[R = \begin{pmatrix} J_1 R_1 & J_{12} K \\ J_{12} K^T & J_2 (R_2 + P_2) \end{pmatrix}\]  

(4.7)

Here the matrices \(A_\kappa\) and \(R_\kappa\) (\(\kappa = 1, 2\)) have the same forms as the matrices \(A\) and \(R\) on the left-hand side of (3.35). The expressions for the elements of \(A_\kappa\) and \(R_\kappa\) are the same as (3.36)–(3.39) if the material subscript \(\kappa\) is added where appropriate. Also the parameters \(d_\kappa\) and \(c_\kappa\) are given here by

\[d_\kappa = \omega_{0\kappa} - \omega_\kappa + 2[2 + \Lambda_1(q_\kappa)]\]  

(4.8)

\[c_1 = 1 + 2(1 - \varepsilon_1)[1 + \Lambda_1(q_\kappa)] - \frac{J_{12} S_2}{J_1 S_1}\]  

(4.9a)

\[c_2 = 1 + 2(1 - \varepsilon_2)[1 + \Lambda_1(q_\kappa)] - \frac{J_{12} S_1}{J_2 S_2}\]  

(4.9b)

Note that the additional terms in (4.9), compared to \(c\) in (3.41), are due to the exchange coupling between the truncated surfaces. Similarly, \(\omega_\kappa, \omega_{0\kappa},\) and \(\varepsilon_\kappa\) are defined by

\[\omega_\kappa = \frac{E}{J_\kappa S_\kappa}\]  

(4.10)

\[\omega_{0\kappa} = \frac{g H B H_0}{J_\kappa S_\kappa}\]  

(4.11)

\[\varepsilon_\kappa = \frac{J S_\kappa}{J_\kappa}\]  

(4.12)
and \( \Lambda_1(q_x) \) is given by (3.42). The matrix \( K^T \) in (4.7) means the transposition of \( K \), and \( 0 \) is a null matrix. The only submatrix (denoted by \( L \)) of \( K \) in (4.7) that is not null corresponds to \( m = m' = 1 \), i.e.,

\[
K(m, n; \tilde{m}, \tilde{n}) = (L)_{mn} \delta_{m1} \delta_{m'1} = \delta_{mn} \delta_{m1} \delta_{m'1}
\]

\[
(1 \leq n \leq N_1, \ 1 \leq n' \leq N_2)
\]  

(4.13)

The only submatrix (denoted by \( P \)) of \( F \) in (4.7) that is not null also corresponds to \( m = m' = 1 \), i.e.,

\[
P_2(m, n; \tilde{m}, \tilde{n}) = (P)_{mn} \delta_{m1} \delta_{m'1}
\]

\[
(1 \leq n \leq N_2, \ 1 \leq n' \leq N_2)
\]  

(4.14)

and its non-zero elements are listed as follows:

\[
P(N_1; N_1) = (P)_{N_1 N_1} = \varepsilon_2 - \varepsilon
\]  

(4.15a)

\[
P(n; n) = (P)_{nn} = 2(\varepsilon_2 - \varepsilon)[1 + \Lambda_1(q_x)] + \frac{J_{1z} S_1}{J_{2z} S_2} \quad (N_1 < n < N_2)
\]  

(4.15b)

\[
P(N_2; N_2) = (P)_{N_2 N_2} = \varepsilon_2 - \varepsilon + 2(\varepsilon_2 - \varepsilon) \Lambda_1(q_x) + \frac{J_{1z} S_1}{J_{2z} S_2}
\]  

(4.15c)

\[
P(n-1; n) = (P)_{n-1, n} = -(\varepsilon_2 - \varepsilon) \quad (N_1 \leq n \leq N_2)
\]  

(4.15d)

\[
P(n; n-1) = (P)_{n, n-1} = -(\varepsilon_2 - \varepsilon) \quad (N_1 \leq n \leq N_2)
\]  

(4.15e)

where we denote

\[
\varepsilon = \frac{J_{5z}}{J_{2z}}
\]  

(4.16)

\[
\varepsilon_c = \frac{J_{cz}}{J_{2z}}
\]  

(4.17)

Finally, like the the partitioned matrices \( A \) and \( R \), the partitioned matrix \( G \) is also divided into 2x2 blocks by the material indices \( \kappa \) and
\( \kappa' \). For example, \( G(1, m, n; 2, m', n' \mid E, q) \) is in the top-right block, representing a Green function component between one spin in the atomic layer labelled by \( m \) and \( n \) in film 1 and the other in the atomic layer labelled by \( m' \) and \( n' \) in film 2.

The inverse of \( A' \kappa \), denoted by \( B' \kappa \), can now be calculated in the same way as in § 3.2. The elements of \( B' \kappa = A^{-1} \kappa \)

\[
B' \kappa(m, n; m', n') = \sum_{n''} (V' \kappa)_{nn''} (V' \kappa)_{n'n''} B' \kappa(m, n''; m', n'')
\]

(4.18)

where \( V' \kappa \) is an orthogonal matrix with elements given by

\[
(V' \kappa)_{nn'} = \left( \frac{2 - \delta_{n'n''}}{N' \kappa} \right)^{1/2} \cos \frac{(2n-1)(n'-1)\pi}{2N' \kappa}
\]

(4.19)

and

\[
B' \kappa(m, n; m', n') = \frac{x_{\kappa n}^{m+m'} - x_{\kappa n}^{m-m'}}{x_{\kappa n}^{m} - x_{\kappa n}^{-m'}} \delta_{nn'}
\]

(4.20)

Here the complex parameters \( x_{\kappa n} \) (0 \( x_{\kappa n} \) \( \leq 1 \)) are the elements of the diagonal matrix \( X' \kappa \) defined by

\[
X' \kappa + X'^{-1} \kappa = D' \kappa
\]

(4.21a)

or, specifically

\[
x_{\kappa n} + x_{\kappa n}^{-1} = d_{\kappa n} = \omega_{\kappa} - \omega_{\kappa} + 2 \left[ 2 - \cos \frac{(n-1)\pi}{N' \kappa} + \Lambda_{1}(q_{\kappa}) \right]
\]

(0 \( x_{\kappa n} \) \( \leq 1 \))

(4.21b)

Obviously, \( D' \kappa \) is also a diagonal matrix with the elements given by

\[
D' \kappa(n; n') = (D' \kappa)_{nn'} = d_{\kappa n} \delta_{nn'}
\]

(4.22)

In particular, the submatrices in the first row or column of the partitioned matrix \( B' \kappa \) are simply powers in \( X' \kappa \), i.e.,

\[
B' \kappa(m, n; 1, n') = B' \kappa(1, n; m, n') = (X' \kappa)_{nn'} = [(X' \kappa)_{nn'}]^{m} = x_{\kappa n}^{m} \delta_{nn'}
\]

(4.23)
From (4.6) we see that the inverse of $A$ is simply
\[
B = (A)^{-1} = \begin{pmatrix}
\frac{B_1}{J_1} & 0 \\
0 & \frac{B_2}{J_2}
\end{pmatrix}
\] (4.24)

On recalling (3.20), we can rewrite (4.5) as
\[
G = -\frac{1}{K} (I - B R)^{-1} B
\] (4.25)

where
\[
I - B R = \begin{pmatrix}
I - B_1 R_1 & -\frac{J_2}{J_1} B_1 K \\
-\frac{J_2}{J_1} B_2 K^T & I - B_2 (R_2 + P_2)
\end{pmatrix}
\] (4.26)

As we have pointed out before, the spin wave spectra (dispersion relations) and spectral intensities can be calculated from the poles and imaginary parts of the Green function components (i.e., the appropriate matrix elements of $G$). In particular, the dispersion relations of the spin waves localized near the two truncated surfaces are determined by the singularities of $(I - B R)^{-1}$, i.e., the solutions of
\[
\text{det}(I - B R) = 0
\] (4.27)

In the most general case of the system that we have described in this section, it is extremely complicated to solve (4.27) explicitly and to calculate the inverse of $I - B R$. Therefore, it is worthwhile to simplify this general system to some special cases with more physical significance and to examine these special cases in more detail.

§ 4.2 Perpendicular Interfaces in Films

Here we consider the special case where the two truncated films
introduced in § 4.1 have the same thickness. In this special case, we shall be able to study analytically the spin wave modes localized near the perpendicular interface in a film composed of two different materials (see Fig. 4.2).

We note that this simplification (i.e., \( N_1 = N_2 = N \)) makes the matrices \( P \) and \( P_2 \) null and the matrix \( L \) becomes an \( N \times N \) identity matrix. Specifically, we need to invert the partitioned matrix \( I - \mathbf{B} \mathbf{R} \), which takes the following form in this special case:

\[
I - \mathbf{B} \mathbf{R} = \begin{pmatrix}
I - \mathbf{B} \mathbf{R}_1 & -\frac{J_{12}}{J_1} \mathbf{B} \mathbf{K} \\
\frac{J_{12}}{J_2} \mathbf{B} \mathbf{K}^T & I - \mathbf{B} \mathbf{R}_2
\end{pmatrix}
\] (4.28)

This can be easily done in the "subdiagonal" representation introduced in § 3.2. The partitioned matrices \( \mathbf{B} \), \( \mathbf{R} \), and \( \mathbf{G} \) can be simultaneously "subdiagonalized" by the following similarity transformations

\[
\mathbf{B}' = \mathbf{U}^{-1} \mathbf{B} \mathbf{U}
\] (4.29)
\[
\mathbf{R}' = \mathbf{U}^{-1} \mathbf{R} \mathbf{U}
\] (4.30)
\[
\mathbf{G}' = \mathbf{U}^{-1} \mathbf{G} \mathbf{U}
\] (4.31)

where

\[
\mathbf{U} = \begin{pmatrix}
\mathbf{U}_1 & 0 \\
0 & \mathbf{U}_2
\end{pmatrix}
\] (4.32)

As in (3.48), the partitioned matrix \( \mathbf{U}_k \) has the elements

\[
\mathbf{U}_k(m, n; m', n') = (\mathbf{V})_{mn} \delta_{mm'}
\] (4.33)

where \((\mathbf{V})_{mn}\) is given by (3.47).

In this representation, (4.25) remains formally the same, i.e.,

\[
\mathbf{G}' = -\frac{1}{N} (I - \mathbf{B}' \mathbf{R}')^{-1} \mathbf{B}'
\] (4.34)

and all the submatrices can be treated in the same way as ordinary
Fig. 4.2  Schematic diagram of a perpendicular interface between two different exchange-coupled ferromagnetic materials in a film ("binary" film).
c-numbers because they are all diagonal. Consequently, we may obtain
\((I - B'R')^{-1}\) and \(G'\) by formally replacing the ordinary c-number elements
in the known results for an interface between two semi-infinite ferromagnets (see Yaniv 1983 and Chen et al 1995), i.e., the \(N \to \infty\)
limit of our present geometry, by the corresponding diagonal \(N \times N\)
submatrices of partitioned matrices involved. The submatrices of \(B'_k\) can
be expressed in terms of \(X'_k\) defined by (4.21). The only submatrix
(denoted by \(C'_k\)) of \(R'_k\) that is not null corresponds to \(m = m' = 1\), i.e.,
\[
R'_k(m, n; m', n') = (C'_k)_{nn'} \delta_{mm'}
\]  
and its elements are
\[
(C'_k)_{nn'} = c_{kn} \delta_{nn'} \quad (1 \leq n, n' \leq N)
\]
where
\[
c_{kn} = c_k - 2(1 - c_k) \cos \frac{(n-1)\pi}{N}
\]
In inverting \(I - B'R'\) in the "subdiagonal" representation, we find out
that the following matrix must be inverted first (see the pertinent
discussion in Appendix A):
\[
W' = (I - X'_1 C'_1)(I - X'_2 C'_2) - \rho X'_1 X'_2
\]
where
\[
\rho = \frac{J^2_{12}}{J^1_{12}}
\]
Since \(W'\) is diagonal with its elements given by
\[
(W'_n)_{nn'} = w_n \delta_{nn'}
\]
where
\[
w_n = (1 - c_{1n} x_{1n})(1 - c_{2n} x_{2n}) - \rho x_{1n} x_{2n}
\]
it follows that \(W'^{-1}\) is also diagonal with its \(n\)th diagonal element
given by \(w'^{-1}_n\). It then is straightforward but tedious to invert \(I - B'R'\)
following the procedure mentioned in Appendix A and to calculate \( G' \) in (4.34) with the results for \((1-B'R')^{-1}\). Without presenting the lengthy algebraic calculations, we give only the final expressions for \( G'(\kappa, m, n; \kappa', m', n') \) here:

\[
G'(1, m, n; 1, m', n') = -\frac{1}{\pi J_1} \left[ B'_1(m, n; m', n') + \frac{c_{1n} - (c_{1n} c_{2n} - \rho) x_{2n} x_{1n}}{\nu_n} x_{m+m'} \right] \delta_{nn'} \\
(4.42a)
\]

\[
G'(2, m, n; 2, m', n') = -\frac{1}{\pi J_2} \left[ B'_2(m, n; m', n') + \frac{c_{2n} - (c_{2n} c_{1n} - \rho) x_{1n}}{\nu_n} x_{m+m'} \right] \delta_{nn'} \\
(4.42b)
\]

\[
G'(\kappa, m, n; \kappa', m', n') = -\frac{J_{12}}{\pi J_1 J_2} \frac{x_{\kappa n} x_{\kappa' n}}{\nu_n} \delta_{nn'} \quad (\kappa \neq \kappa') \\
(4.42c)
\]

By transforming \( G'(\kappa, m, n; \kappa', m', n') \) back to the original representation, we get the required Green function components in the form

\[
G(\kappa, m, n; \kappa', m', n' | E, q_x) = \sum_{n''} (V)_{nn''} (V)_{n'n''} G'(\kappa, m, n''; \kappa', m', n'') \\
(4.43)
\]

From (4.41) and (4.42), it can be easily shown that our previous results in § 3.2 are recovered when the interface coupling \( J_{12} \) is set equal to 0, as expected.

The dispersion relations of the spin waves localized near the interface are determined by the poles of \( G(\kappa, m, n; \kappa', m', n' | E, q_x) \), i.e., the solutions of

\[
\nu_{n''} = (1 - c_{1n''} x_{1n''})(1 - c_{2n''} x_{2n''}) - \rho x_{1n''} x_{2n''} = 0 \\
(n'' = 1, \ldots, N) \\
(4.44)
\]

where \( x_{\kappa n''} \) is defined by (4.21b) with \( N_\kappa = N \).
Numerical results and discussion

As a numerical example, we plot the dispersion relation curves for $N = 5$ and for a set of representative values of spin quantum numbers and exchange constants (see Fig. 4.3). The interface spin-wave modes are indicated by full lines, while we also show the boundaries of the bulk mode regions for the corresponding complete films (without truncation or interface) of material 1 (the dashed lines) and of material 2 (the dotted lines). We notice that there are two distinct groups of interface spin-wave modes in Fig. 4.3. Both are acoustic interface modes with respect to film 1 (in the sense that the $x_{1n''}$ are real with $0 < x_{1n''} \leq 1$) and optical interface modes with respect to film 2 (in the sense that the $x_{2n''}$ are real with $-1 \leq x_{2n''} < 0$). Each group has a characteristic frequency $\omega_{1C}^{(K)}$ at which the interface spin wave modes are cut off (by analogy to Fig. 3.6). The occurrence of $\omega_{1C}^{(K)}$ is due to the restriction $|x_{Kn''}| \leq 1$ (which is a condition for the spin waves to be localized near the interface). Compared with (3.65), the characteristic frequencies $\omega_{1C}^{(K)} (K = 1, 2)$ in this case also depend only on the spin quantum numbers and exchange constants, but are much more complicated algebraically than (3.65). However, it is easy to calculate $\omega_{1C}^{(K)}$ just numerically. For those values of the spin quantum numbers and exchange constants used in Fig. 4.3, we get $\omega_{1C}^{(1)} - \omega_{01} = 2.92$ for the upper group and $\omega_{1C}^{(2)} - \omega_{01} = 1.47$ for the lower group.

By analogy with the argument that leads to (3.66) from (3.63) in § 3.2, we can verify that the two groups of interface spin-wave modes in Fig. 4.3 would form two continua as $N \rightarrow \infty$. These two continua would become represented as two interface branches if the frequency were
Fig. 4.3 The dispersion relation curves (the solid lines) for interface spin waves localized near a perpendicular interface in a "binary" film composed of two ferromagnetic materials 1 and 2. The dashed and dotted lines represent the edges of bulk mode region for complete films of materials 1 and 2, respectively. The assumed parameters are $N = 5$, $S_2/S_1 = J_2/J_1 = 0.5$, $J_{31}/J_1 = 0.8$, $J_{32}/J_1 = 0.6$, $J_{12}/J_1 = 0.7$. The interface modes cut off at two characteristic frequencies (see text).
plotted against $\Lambda_2(q_z, q_x)$ instead of $\Lambda_1(q_x)$. This is the way in which our new results in this section recover the known results for an interface between two semi-infinite ferromagnets (see Yaniv 1983 and Chen et al 1995) in the limit of $N \rightarrow \infty$ (where the translational symmetry in the $z$ direction would be regained in our interface structures).

As before we examine the imaginary part of the Green function to obtain important information about the spectral intensities of the spin waves. For convenience, we introduce a notation similar to (3.67) referring to a site in material $\kappa$:

$$Y(\kappa, m, n; \omega_1 - \omega_{0_{\Sigma}}, \Lambda_1) = -\text{Im}[G(\kappa, m, n; \kappa, m, n; \mathbf{E} + i\nu, q_x)] \bigg|_{\nu \rightarrow 0} \quad (4.45)$$

As numerical examples, we plot $Y(\kappa, m, 2; \omega_1 - \omega_{0_{\Sigma}}, 1)$ against $\omega_1 - \omega_{0_{\Sigma}}$ for the same parameters as in Fig. 4.3, examining both values for $\kappa$ and three different values for $m$ (see Figs. 4.4 - 4.6). We see from Fig. 4.4 for $m = 1$, in particular, that eight peaks (corresponding to the eight interface spin-wave modes) occur precisely at the eight values of $\omega_1 - \omega_{0_{\Sigma}}$ on the dispersion relation curves (see the solid lines in Fig. 4.3) at $\Lambda_1(q_z) = 1$. As in § 3.2, these eight peaks are expected to shrink in intensity and eventually vanish as $m$ increases, leaving contributions to the spectral intensity coming only from the standing bulk spin waves in film $\kappa$. This is confirmed by our numerical calculations for $m = 2$ (see Fig. 4.5) and $m = 50$ (see Fig. 4.6). By comparing the relative change of the interface mode intensities from Fig. 4.4(a) for $\kappa = 1$ to Fig. 4.4(b) for $\kappa = 2$ (and also from Fig. 4.5(a) to 4.5(b), etc.), we find that the interface spin-wave modes within the upper and lower groups have their intensities mainly
Fig. 4.4 The intensities of spin waves modes (calculated from the imaginary part of the Green functions) in a "binary" ferromagnetic film (with the same parameters as in Fig. 4.3) at $\Lambda_1(q_x) = 1$. The site is chosen to be at the interface ($m = 1$) in: (a) material 1 (i.e., $\kappa = 1$), (b) material 2 (i.e., $\kappa = 2$).
Fig. 4.5 As in Fig. 4.4 but with $n = 2$ and: (a) $\kappa = 1$, (b) $\kappa = 2$. 
Fig. 4.6  As in Fig. 4.4 but with $m = 50$ and: (a) $\kappa = 1$, (b) $\kappa = 2$. 
associated with films 1 and 2, respectively.

When \( m \gg N \) (as in Fig. 4.6), \( Y(\kappa, m, n; \omega - \omega_{01}, \Lambda) \) becomes essentially independent of \( m \) and the physical parameters for the interface. We see in Fig. 4.6(a) that the spin wave intensities distribute in the frequency region which precisely covers the physical bulk-mode continua at \( \Lambda(q_x) = 1 \) for a complete 5-layer film with free surfaces (see Fig. 3.3). Moreover, the graph of \( Y(1, 50, 2; \omega - \omega_{01}, 1) \) tends to resume the intensity distributions for the standing bulk spin-wave modes in the corresponding complete film (for comparison, see Fig. 3.10(b)). The same features are also observed in Fig. 4.6(b) for the intensities of the spin-wave modes at large distances in film 2 from the interface (note that the dimensionless frequencies are always defined in terms of \( J_1 S_1 \) for consistancy in cases where two different materials are involved). These features strongly confirm that, at large enough distances in film \( \kappa \) away from the interface, the spin waves behave the same way as in a complete film made up of material \( \kappa \), as expected.

§ 4.3 Steps on the Surfaces of Thin Films

Finally in this section, we consider another very important special case where the two truncated films introduced in § 4.1 are made up of the same ferromagnetic material while \( N_1 \neq N_2 \), so that the system becomes equivalent to a single film with a step change in thickness at \( y = 0 \). In this special case, we shall be able to study the spin wave modes localized near the atomic step on the free surface of a film (see Fig. 4.7).

We note that this simplification (corresponding to \( J_1 = J_{s1} = J_{s2} \)
Fig. 4.7 Schematic diagram of an atomic step on a surface of a ferromagnetic film. The step is at $y = 0$ and in general its height may be any integer number of atomic layers.
\( J_{s_2} = J_2 = J \) and \( S_1 = S_2 = S \) makes the matrices \( R_\kappa \) \((\kappa = 1, 2)\) in (4.7) become null. The non-zero elements of \( P \) then become

\[
P(n_1; n_1) = (P)_{n_1, n_1} = 1 - \varepsilon \quad (4.46a)
\]

\[
P(n; n) = (P)_{n, n} = 1 + 2(1 - \varepsilon)[1 + \Lambda_1(q_x)] \quad (N_1 < n < N_2) \quad (4.46b)
\]

\[
P(n_2; n_2) = (P)_{n_2, n_2} = 2 - \varepsilon + 2(1 - \varepsilon)\Lambda_1(q_x) \quad (4.46c)
\]

\[
P(n-1; n) = (P)_{n-1, n} = -(1 - \varepsilon) \quad (N_1 \leq n \leq N_2) \quad (4.46d)
\]

\[
P(n; n-1) = (P)_{n, n-1} = -(1 - \varepsilon) \quad (N_1 \leq n \leq N_2) \quad (4.46e)
\]

where we define

\[
\varepsilon = \frac{J_s}{J} \quad (4.47)
\]

\[
\varepsilon_c = \frac{J_c}{J} \quad (4.48)
\]

For convenience, we divide (4.5) by \( J \) and rewrite it as follows

\[
(A - R)G = -\frac{1}{\pi J} \quad (4.49)
\]

so that

\[
A = \begin{pmatrix} A_1 & 0 \\ 0 & A_2 \end{pmatrix} \quad (4.50)
\]

\[
R = \begin{pmatrix} 0 & K \\ K^T & R_2 \end{pmatrix} \quad (4.51)
\]

Here the matrices \( A_\kappa \) \((\kappa = 1, 2)\), which are defined as in § 3.2 and differ only in their dimension, have the same diagonal elements

\[
d = \omega_0 - \omega + 2[2 + \Lambda_1(q_x)] \quad (4.52)
\]
where
\[ \omega = \frac{E}{JS} \quad (4.53) \]
\[ \omega_0 = \frac{g \mu \mu_0 H}{JS} \quad (4.54) \]

From (4.49), we have
\[ G = -\frac{1}{\mu J} (I - B R)^{-1} B \quad (4.55) \]
where
\[ B = (A)^{-1} = \begin{pmatrix} B_1 & 0 \\ 0 & B_2 \end{pmatrix} \quad (4.56) \]

The inverse of \( I - B R \) in (4.55) can be expressed as follows (for details, see (A.5) in Appendix A):
\[ (I - B R)^{-1} = \begin{pmatrix} 1 & -B_1 \kappa \\ -B_2 K^T & 1 - B_2 P_2 \end{pmatrix}^{-1} = \begin{pmatrix} I + B_1 K W^{-1} B_2 K^T & B_2 K W^{-1} \\ W_2^{-1} B_2 K^T & W_2^{-1} \end{pmatrix} \quad (4.57) \]
where
\[ W_2 = I - B_2 P_2 - B_2 K B_1 \quad (4.58) \]

To invert \( W_2 \), we must first invert the following \( N_2 \times N_2 \) matrix (see (A.10) in Appendix A):
\[ W = I - X_2 P - X_2 L^T X_1 L \quad (4.59) \]
where
\[ X_\kappa = V_\kappa X'_\kappa V^{-1} \quad (4.60) \]
is the submatrix corresponding to \( m = m' = 1 \) of the partitioned matrix \( B_\kappa \). Here \( V_\kappa \) and \( X'_\kappa \) are defined respectively by (4.19) and (4.21) with \( \omega_\kappa \) and \( \omega_{0\kappa} \) being replaced by \( \omega \) and \( \omega_0 \). Once the result for \( W^{-1} \) is obtained (in terms of \( W^{-1} \)), we can invert \( I - B R \) according to (4.57) and calculate \( G \) from (4.55). The results for the required Green
function components are given as follows:

\[ G(1, m, n; 1, m', n' \mid E, q_x) \]

\[ = -\frac{1}{\pi J} \left[ B_1(m, n; m', n') + B_1(m, n; 1, n_1') \tilde{W}(n_1; n_2) B_2(1, n_2; 1, n_1') B_1(1, n_1'; m', n') \right] \]  

(4.61a)

\[ G(2, m, n; 2, m', n' \mid E, q_x) \]

\[ = -\frac{1}{\pi J} \left[ B_2(m, n; m', n') + B_2(m, n; 1, n_2') P(n_2; n_2') \tilde{W}(n_2'; n_2') B_2(1, n_2'; m', n') \right] \]

\[ + B_2(m, n; 1, n_1') B_1(1, n_1', 1, n_1') \tilde{W}(n_1'; n_2) B_2(1, n_2; m', n') \]  

(4.61b)

\[ G(1, m, n; 2, m', n' \mid E, q_x) = -\frac{1}{\pi J} B_1(m, n; 1, n_1') \tilde{W}(n_1; n_2) B_2(1, n_2; m', n') \]  

(4.61c)

\[ G(2, m, n; 1, m', n' \mid E, q_x) = G(1, m', n' \mid 2, m, n \mid E, q_x) \]  

(4.61d)

where \( \tilde{W}(n_2; n_2') \) represent the matrix elements of \( \tilde{W} = W^{-1} \). In (4.61) we implicitly assume that any repeated \( n \)-indices should be summed over.

The appropriate ranges of integer values are 1 to \( N_1 \) for the index \( n_1 \) or \( n_1' \), and 1 to \( N_2 \) for \( n_2 \), \( n_2' \), or \( n_2'' \). The dispersion relations of the spin waves localized near the step on the surface of the film are determined by the poles of \( G(\kappa, m, n \mid \kappa', m', n' \mid E, q_x) \), i.e., the solutions of

\[ \det \tilde{W} = \det(1 - X_2 \overline{P} - X_2 L^T X_1 L) = 0 \]  

(4.62)

This equation can only be solved numerically. The degree of complexity in the numerical calculations here increases rapidly as \( N_2 \) increases. The most probable case of surface steps under natural circumstances is 1-atomic layer step (i.e., \( N_2 = N_1 = 1 \)), which often results if the surface formed in orientations slightly deviated from the high-symmetry crystalline planes (e.g., see Falicov et al 1990). If the thickness of
a film is large compared with the step height, a macroscopic approach becomes appropriate and the step plays a much less important role. Therefore, having employed the microscopic approach here, we shall concentrate on thin films where the thickness may be comparable with the step height (often of one or two atomic spacings).

Numerical results and discussion

By solving (4.62) numerically, we obtain the dispersion relations of the localized spin wave modes for various values of the film thickness and step parameters (see solid lines in Figs. 4.8 - 4.10). For comparison in each case, we plot with the dashed lines the edges of the bulk mode regions that would correspond to complete films in the absence of surface steps. Also, the dotted lines indicate the boundaries beyond which the localized spin waves may exist. The upper localization boundary typically lies close in frequency to the top of the bulk mode region for a complete film while the lower boundary is coincident with the lower edge of this bulk mode region. From these figures (and also from a wide range of other numerical examples too numerous to present here), we infer that at most \( N_2 - N_1 \) acoustic spin wave modes may occur when the exchange constants at the step (\( J_s \) and \( J_c \)) are smaller than the bulk value \( J \). When the exchange constants at the step (\( J_s \) and \( J_c \)) are sufficiently larger than \( J \), there may exist at most \( N_2 - N_1 + 1 \) optical spin wave modes but only \( N_2 - N_1 \) of them may be appreciably split off in frequency above the localization boundary.

As in the standard procedure used before, the spectral intensities of spin waves in a film with a step can also be calculated from the imaginary part of the Green function components in (4.61). The
Fig. 4.8 The dispersion relation curves for spin waves localized near an atomic step of a ferromagnetic film with the thickness mismatch from 2 to 3 atomic layers. The spin-wave mode localization boundaries and the edges of the bulk mode region (for films without a step) are shown respectively by the dotted and dashed lines (see text). The exchange constants are assumed to be $J_0/J = 0.85$ and $J_e/J = 0.8$ for the acoustic spin-wave mode $A$, $J_0/J = 4.5$ and $J_e/J = 5$ for the two optical spin-wave modes $O_1$ and $O_2$. 
Fig. 4.9 The dispersion relation curves for spin waves localized near an atomic step of a ferromagnetic film with the thickness mismatch from 3 to 4 atomic layers. The spin-wave mode localization boundaries and the edges of the bulk mode region (for films without a step) are shown respectively by the dotted and dashed lines (see text). The exchange constants are assumed to be $J_g/J = 0.7$ and $J_c/J = 0.5$ for the acoustic spin-wave mode $A$, $J_g/J = 2$ and $J_c/J = 3$ for the two optical spin-wave modes $O_1$ and $O_2$. 
Fig. 4.10 The dispersion relation curves for spin waves localized near an atomic step of a ferromagnetic film with the thickness mismatch from 2 to 4 atomic layers. The spin-wave mode localization boundaries and the edges of the bulk mode region (for films without a step) are shown respectively by the dotted and dashed lines (see text). The exchange constants are assumed to be $J_s/J = 0.5$ and $J_c/J = 0.4$ for the two acoustic spin-wave modes $A_1$ and $A_2$, $J_s/J = 2.5$ and $J_c/J = 3$ for the three optical spin-wave modes $O_1$, $O_2$, and $O_3$. 

\[
\Lambda_1(q_x)
\]
difficulty involved is to invert the matrix \( W \) in (4.59). Here we calculate, as a numerical example, the imaginary part of 
\[ G(2,m,n;2,m,n;E+i\nu,q_{x}) \]
for \( n = 3 \) and \( m = 1, 2, 30 \) (i.e., three different distances from the step). As a result, \( Y(2,m,3;\omega-\omega_{0},\Lambda_{1}) \)
(which is defined in the same form as (4.45)) is plotted against \( \omega-\omega_{0} \)
at \( \Lambda_{1}(q_{x}) = 1.6 \) in what is probably the simplest non-trivial case
(i.e., \( N_{1} = 2 \) and \( N_{2} = 3 \)) for \( \epsilon = 4.5 \) and \( \epsilon_{c} = 5 \). From the numerical results given in Figs. 4.11, 4.12(a) and (b) we see that the spin wave
modes localized near the step (corresponding those marked by \( O_{1} \) and \( O_{2} \)
in Fig. 4.8) decay rapidly with the distance from the step, as expected. The strong resemblance of Fig. 4.12(b) to Fig. 3.10 indicates
that, when the step is spatially far enough away (\( m \gg N_{2} \)), the behavior
of spin-wave modes here eventually becomes the same as that in a complete film without any surface step.
Fig. 4.11 The intensities of spin-wave modes (calculated from the imaginary part of the Green functions) in a ferromagnetic film with an atomic step on its surface. The thickness mismatch is from 2 to 3 atomic layers. The site is chosen to be at the "corner" of the step: (κ = 2, m = 1, n = 3). The assumed parameters are $J_z/J = 4.5$, $J_c/J = 5$, and $\Lambda (q_s) = 1.6$. 
Fig. 4.12    As in Fig. 4.11 but for: (a) $m = 2$, (b) $m = 30$. 
CHAPTER 5

PERPENDICULARLY CLEAVED OR TRUNCATED SUPERLATTICES

In the last two chapters we have examined the behavior of spin waves in single layered structures (i.e., in complete and truncated films, in "binary" films, and in stepped films). In this chapter we continue to employ the same type of Green function formalism described in Chapter 2 to study the exchange-dominated spin waves in multilayer structures. In particular, we shall re-examine the spin wave behavior in ferromagnetic superlattices with 2D translational symmetry (thereby extending previous work) and also we make the first (to our knowledge) analysis of the exchange-dominated spin waves in ferromagnetic superlattices that possess translational symmetry in only 1D.

As we mentioned in § 1.2 (see also Fig. 1.2), a typical superlattice is composed alternately of different films (or slabs). These constituent films can be regarded as grouped into unit cells and, as we move along the direction perpendicular to the interfaces, the elementary unit repeats periodically in an extended (effectively infinite) structure. As a result of this new periodicity, many of the physical properties are modified in the superlattice. A direct consequence is that a reduced Brillouin zone, associated with the new spatial period (namely the size of an elementary unit cell), is formed. Another important feature of a magnetic superlattice is that the dispersion relation curves of the spin waves (plotted against the wavevector component perpendicular to the interfaces) are "folded" back, as explained later. At the reduced Brillouin-zone boundaries,
these folded curves usually exhibit frequency gaps that are known as stop bands.

The spin waves in ferromagnetic superlattices whose constituent films are considered to be complete layers, i.e., effectively infinite in the directions parallel to the interfaces (see Fig. 1.2), have been extensively studied theoretically by the transfer matrix method (e.g., see Albuquerque et al 1986, Raj and Tilley 1987, and Barnas 1992) and to a certain extent by means of microscopic spin-spin Green functions (e.g., see Mthon 1989, Dobrzynski et al 1986, and Dobrzynski 1987). As we mentioned in § 2.1, only spin wave dispersion relations can be calculated with the standard transfer matrix method, while the Green function method can provide the spin wave spectral intensities in addition to the dispersion relations. For completeness (and later comparison with cleaved or truncated structures), we shall generalize the known results of spin waves in this conventional type of superlattices first.

We shall then consider perpendicularly cleaved (or truncated) superlattices as depicted in Fig. 1.4. The loss of translational symmetry (in the y direction) in this new type of superlattices results from a pair of cleaved surfaces perpendicular to the interfaces. The bulk spin wave modes will be "quantized" due to the finite thickness of the sample in the y direction. In general, the presence of the cleaved surfaces may give rise to surface spin waves. Since the finite-size effects on the spin wave behavior typical in conventional superlattices are our major concern, we assume here that the cleaved surfaces are free surfaces. Hence, these perpendicularly cleaved superlattices can
be regarded as being built up alternately of two different types of truncated film (which have been considered in § 3.3) along the z direction. As a result, the matrix "subdiagonalization" method developed in Chapters 3 and 4 can be extended and applied to this new type of superlattices as well.

In the direction perpendicular to the interfaces, both conventional and cleaved superlattices may or may not be terminated by an outmost surface, corresponding to semi-infinite and infinite superlattices. The content of this chapter is correspondingly arranged as follows. First, § 5.1 and § 5.2 deal with spin waves in infinite and semi-infinite superlattices with two-dimensional (2D) translational symmetry, respectively. Then § 5.3 and § 5.4 deal with spin waves in the perpendicularly cleaved infinite and semi-infinite superlattices, respectively, enabling finite-size effects to be discussed.

§ 5.1 Infinite Superlattices With 2D Translational Symmetry

In this section we shall consider an infinite ferromagnetic superlattice built up alternately from two different types of complete films (which have been studied in § 3.1) placed in an external magnetic field $H_0$ (along the z direction) perpendicular to the interfaces (see Fig. 5.1). We assume, for simplicity, that the two types of films have a simple cubic structure with the same lattice parameter $a$. It is convenient, as in § 4.1, to introduce a material index $\kappa$ (= 1, 2) to label the two types of films. Film $\kappa$ is assumed to have $N_\kappa$ (001) atomic layers across its thickness so that the spatial period of the superlattice is given by
Fig. 5.1 Schematic diagram of an infinite two-component superlattice with 2D translational symmetry (in the x and y directions), showing the exchange interactions.
\[ D = (N_1 + N_2)a \] (5.1)

The exchange constants within film \( \kappa \) are taken to be \( J_{\kappa} \) if the nearest neighbors are both in either of the film "surfaces" (i.e., the outmost atomic layers of film \( \kappa \)) and \( J_\kappa \) otherwise. The spins at adjacent sites across the interface between the neighboring "surfaces" of films 1 and 2 are assumed to be separated by the same distance \( a \) and coupled through an exchange constant denoted by \( J_{12} \). The spin quantum number of the spins in film \( \kappa \) is denoted by \( S_\kappa \). Note that, if we simplify the interfaces by taking \( J_{\kappa} = J_\kappa \) and \( S_1 = S_2 = S \), this type of superlattice reduces to that studied by Albuquerque et al (1986) and Dobrzynski et al (1986). Without loss of generality, film 2 is chosen to be on the right of film 1 within each elementary unit cell (see Fig. 5.1) so that the spin of any atom in film \( \kappa \) in the \( N \)th elementary unit cell has the position vector

\[ r = \left( r_1, (N - 1)D + (N_1 \delta_{\kappa} + n - 1)a \right) \]

\[ (-\infty < N < \infty, 1 \leq n \leq N_\kappa) \] (5.2)

The Hamiltonian of this superlattice and the equation of motion for the spin-spin Green function are still given formally by (2.3) and (2.14), respectively. Since the superlattice has 2D translational symmetry in the \( xy \) plane, we can make the 2D Fourier transformations

\[ \langle \langle S_{r+q}^+ \cdot S_{r+q}^- \rangle \rangle_E = \frac{1}{\Omega_2} \sum_{\mathbf{q}_||} G(N, \kappa, n; N', \kappa', n'; E, \mathbf{q}_||) \exp[i \mathbf{q}_|| \cdot (r_1 - r_1')] \] (5.3)

\[ \langle S_{r}^-, S_{r}^+ \rangle_E = \frac{1}{\Omega_2} \sum_{\mathbf{q}_||} F(N, \kappa, n; N', \kappa', n'; E, \mathbf{q}_||) \exp[i \mathbf{q}_|| \cdot (r_1 - r_1')] \] (5.4)

where \( \mathbf{q}_|| = (q_x, q_y) \) is a 2D wavevector and \( \Omega_2 \) is the number
(macroscopically large) of spins in any atomic layer parallel to the xy plane. For brevity, the dependence of the Fourier components of the Green functions and correlation functions on $E$ and $q_\parallel$ will not be written down explicitly where it is obvious. In the same manner as in § 3.1 and § 4.1, we can rewrite the equations of motion for the Green function components $G(N, k, n; N', k', n')$ in terms of infinite-dimensional partitioned matrices, i.e.,

$$ (A_0 - C)G = -\frac{i}{\hbar} $$

(5.5)

The matrix elements of $A_0$ are given by

$$ A_0(N, k, n; N', k', n') = J_{k, k'} n n' \delta_{k, k'} \delta_{N N'} $$

(5.6)

where the matrix $A_k$ has a similar form as the matrix $(A-C)$ on the left-hand side of (3.13) for a single film, i.e.,

$$ (A_k)_{n n'} = [d_k - c_k \left( \delta_{n1} + \delta_{n N_k} \right)] \delta_{n n'} - \delta_{n-1, n'} - \delta_{n+1, n'} $$

(5.7)

The matrix elements of $A_k$ are given here by

$$ d_k = \omega_{0k} - \omega_k + 2[1 + \Lambda_2(q_\parallel)] $$

(5.8)

$$ c_1 = 1 + 2(1 - \varepsilon_1) \Lambda_2(q_\parallel) - \frac{J_{12} S_2}{J_{11} S_1} $$

(5.9a)

$$ c_2 = 1 + 2(1 - \varepsilon_2) \Lambda_2(q_\parallel) - \frac{J_{12} S_1}{J_{22} S_2} $$

(5.9b)

Note that the additional terms in (5.9), compared to (3.6), are due to the exchange coupling between films 1 and 2. The parameters $\omega_k$, $\omega_{0k}$, and $c_k$ are defined respectively by (4.10) - (4.12) and $\Lambda_2(q_\parallel)$ by (3.10). The matrix elements of $C$ in (5.5) describe the exchange coupling across the interfaces between the two materials and are given by
\[ C(N, \kappa; n; N', \kappa', n') = J_{12} \left[ \delta_{nn_1} \delta_{n'1} \delta_{\kappa_1 \kappa'_2} + \delta_{nn_1} \delta_{n'1} \delta_{\kappa_1 \kappa_2} \delta_{NN'} + \delta_{nn_2} \delta_{n'2} \delta_{\kappa_1 \kappa'_2} \delta_{N-1, N'} + \delta_{nn_2} \delta_{n'2} \delta_{\kappa_1 \kappa'_2} \delta_{N+1, N'} \right] \] (5.10)

Finally, the partitioned matrix \( G \) has \( G(N, \kappa; n; N', \kappa', n') \) as its matrix elements, representing the Green function components between one spin in the \( n \)th atomic layer of film \( \kappa \) in the \( N \)th cell and the other in the \( n' \)th atomic layer of film \( \kappa' \) in the \( N' \)th cell of the superlattice.

From (3.26) and (3.27) we get the expression for the matrix elements of \( B_\kappa = A^{-1}_\kappa \) as follows:

\[
B_\kappa(n; n') = (B_\kappa)_{nn'} = \begin{cases} P_\kappa(n, n') & (n \geq n') \\ P_\kappa(n', n) & (n' > n) \end{cases} \] (5.11)

Here the function \( P_\kappa(n, n') \) is given by

\[
P_\kappa(n, n') = \frac{\{(\sin((N - n + 1)k_\kappa) - c_\kappa \sin((N - n)k_\kappa))\}(\sin(n'k_\kappa) - c_\kappa \sin((n' - 1)k_\kappa))}{W_\kappa \sin(k_\kappa)}
\] (5.12)

where

\[
W_\kappa = \sin((N + 1)k_\kappa) - 2c_\kappa \sin(N k_\kappa) + c_\kappa^2 \sin((N - 1)k_\kappa)
\] (5.13)

The parameter \( k_\kappa \) is defined in terms of \( x_\kappa \) by

\[
x_\kappa = \exp(ik_\kappa a) \quad [\text{Im}(k_\kappa) > 0]
\] (5.14)

and the complex parameter \( x_\kappa \) is defined by

\[
x_\kappa + x_\kappa^{-1} = \omega_\kappa - \omega_\kappa + 2[1 + \Lambda_2(q_\|)] \quad (||x_\kappa|| \leq 1)
\] (5.15)

Note that the matrix \( B_\kappa \) satisfies the same symmetry properties indicated in (3.26), i.e.,
\[ B_{\kappa}(n;n') = B_{\kappa}(n';n) = B_{\kappa}(N_{\kappa}-n+1;N_{\kappa}-n'+1) \] (5.16)

while the function \( P_{\kappa}(n,n') \) does not. By noting the block-diagonal structure of \( A \) in (5.6), we immediately obtain the matrix elements of \( B_0 = A_0^{-1} \) as follows:

\[ B_0(N,\kappa,n;N',\kappa',n') = \frac{B_{\kappa}(n;n')}{\delta_{\kappa\kappa'}\delta_{NN'}} \] (5.17)

Now the formal solution of (5.5) can be written with the help of the Dyson equation as

\[ G = -\frac{B_0}{\Pi} + B_0 C G \] (5.18)

Using the above results for \( B_0 \) and \( C \), it is straightforward to deduce the matrix elements of \( G \) (see Appendix B for the algebraic details). This involves solving finite-difference equations, such as (B.7) and (B.10), whose integer variables are the superlattice unit cell indices instead of the atomic layer indices in films. The solution of this new type of finite-difference equations results in a new complex parameter \( x \) defined by

\[ x + x^{-1} = d \quad (|x| \leq 1) \] (5.19)

where

\[ d = \frac{\rho^{-1}W_{12} - 2U_{11}W_{21}(N_1) + \rho \sin((N_1 - 1)k_a)\sin((N_1 - 1)k_a)}{\sin(k_1)\sin(k_2)} \] (5.20)

Here the function \( U_{\kappa}(n) \) is defined by

\[ U_{\kappa}(n) = \sin(nk_a) - \cos(nk_a) \] (5.21)

and \( \rho \) is given in (4.39).

After some lengthy algebra, the final results for
\[ G(N, \kappa, n; N', \kappa', n') \text{ are} \]
\[ G(N, \kappa, n; N', \kappa, n') = -\frac{B_k(n;n')}{\pi^J_k} \delta_{NN'} + \frac{P_{0k}(n,n')}{\pi^J_k} \frac{x}{x-x^{-1}} |N-N'| \]
\[ + \frac{P_k(n,n')}{\pi^J_k} \frac{x}{x-x^{-1}} |N-N'-1| + \frac{P_k(n',n)}{\pi^J_k} \frac{x}{x-x^{-1}} |N-N'+1| \]
(5.22a)

\[ G(N, 1; N', 2, n') \]
\[ = \frac{P_{12}(n,n')}{\pi^J_{12}} \frac{x}{x-x^{-1}} |N-N'| + \frac{P_{12}(N_1-n+1, N_2-n'+1)}{\pi^J_{12}} \frac{x}{x-x^{-1}} |N-N'-1| \]
(5.22b)

\[ G(N, 2, n; N', 1, n') = G(N', 1, n'; N, 2, n) \]
(5.22c)

where

\[ P_{01}(n, n') \]
\[ = \frac{1}{\sin(k_a)\sin(k_a)U_1} \left\{ U_1(N_1-n+1)U_1(N_1-n'+1) + U_1(n)U_1(n')U_2(N_2) \right\} \]
\[- \rho(U_1(N_1-n+1)\sin((N_1-n')k_a) + U_1(n)\sin((n'-1)k_1)\sin((N_2-1)k_2)) \sin((N_2-1)k_2) \]
(5.23)

and \( P_{02}(n, n') \) can be obtained from \( P_{01}(n, n') \) by interchanging the subscripts 1 and 2. Also we have

\[ P_{12}(n, n') = \frac{U_1(n)U_2(N_2-n'+1) - \rho\sin((n-1)k_1)\sin((N_2-n')k_1)\sin((N_2-1)k_2) }{\sin(k_1)\sin(k_2)\sin(k_2) } \]
(5.24)

From these expressions for the Green function components, we notice that only the new complex parameter \( x \) defined by (5.19) carries the dependence of \( G(N, \kappa, n; N', \kappa', n') \) on the elementary unit cell indices \( N \) and \( N' \) of the infinite superlattice. This is strikingly analogous to the way in which the Green functions for a film (see (3.27)) depend on
the atomic layer indices through the parameter $x$ defined by (3.17), except that the film is finite in the $z$ direction. In an infinite ferromagnet, the bulk spin-wave modes (which are given by (2.28)) can be obtained equivalently from (3.17) by equating $x$ to $\exp(iq_z a)$, as a consequence of the translational symmetry of the lattice. In the same manner, we obtain the bulk spin-wave modes in this infinite superlattice from (5.19) by relating $x$ to a wavevector component $Q$ (in the $z$ direction) with the following equation involving the superlattice period $D$:

$$x = \exp(i Q D)$$  \hspace{1cm} (5.25)

The dispersion relations for the superlattice bulk spin waves (i.e., the spin wave frequencies expressed as a function of $q_z$ and $Q$) are then determined by

$$d = 2 \cos(QD)$$  \hspace{1cm} (5.26)

Although there may exist interface spin waves (which would correspond to real $x$ between $-1$ and $1$) decaying with increasing multiples of the lattice parameter $a$ across the thickness of film $\kappa$, no surface spin waves that decay with increasing multiples of $D$ may occur in the infinite superlattice. This is because there are no poles of the Green functions (see (5.22) and (5.24)) that correspond to real values of $x$ between $-1$ and $1$. The bulk mode continua (also known as bulk bands or pass bands) of the spin waves in the superlattice correspond to $0 \leq Q \leq \frac{\pi}{D}$ (i.e., $Q$ lies within the reduced Brillouin zone).

**Numerical results and discussion**

To illustrate the dispersion relations for the superlattice bulk spin waves, we plot $\omega - \omega_{01}$ against $QD$ in Fig. 5.2 for $N_1 = 3$, $N_2 = 2$,
Fig. 5.2 The dispersion relation curves for bulk spin-wave modes in: (a) bulk sample of the constituent materials 1 and 2, (b) an infinite superlattice with 2D translational symmetry. The dimensionless frequency $\omega_1 - \omega_{01}$ is plotted against: (a) $q_x a$, (b) $QD$. The assumed parameters are $S_z/S_1 = 2, J_z/J_1 = 0.25, \Lambda_2(q_y) = 0.25$ (for both (a) and (b)); and $N_1 = 3, N_2 = 2, J_{s1}/J_1 = 0.9, J_{s2}/J_1 = 0.3, J_{12}/J_1 = 0.6$ (additionally for (b)).
and \( \Lambda_2(q_\parallel) = 0.25 \) and for a set of representative values of spin quantum numbers and exchange constants. For comparison, we first show in Fig 5.2(a) the frequencies of the bulk spin-wave modes (see (2.28)) in homogeneous materials \( \kappa = 1, 2 \) (with exchange constant \( J_\kappa \) and spin quantum number \( S_\kappa \)) plotted against \( q_\parallel a \) for \( \Lambda_2(q_\parallel) = 0.25 \) as well. We then see in Fig. 5.2(b) that the spin wave dispersion relation curves for the superlattice are "folded" back at the reduced Brillouin-zone boundary. Also there is a perturbation of the frequencies in the superlattice, leading to the occurrence of the stop bands (or "forbidden" bands). In the intermediate frequency range \( 0.5 \leq \omega_{11} - \omega_{12} \leq 2.25 \) (where the bulk mode regions of the spin waves in homogeneous materials 1 and 2 overlap), the dispersion relations for the superlattice exhibit broad pass bands and narrow stop bands. Beyond this frequency range, the pass bands become narrow and the stop bands broad. As illustrated by this numerical example, our results for the dispersion relations obtained by means of the Green function method generalize and would reproduce (should appropriate limits be taken) those reached by Albuquerque et al (1986) with the transfer matrix method.

Further to this numerical example, the dispersion relations for the superlattice bulk spin waves are illustrated in a conventional way (i.e., by plotting frequency versus \( q_\parallel \)) for the same parameters as in Fig. 5.2(b). For this example (where \( N_1 + N_2 = 5 \)) of an infinite superlattice, there are five bulk bands (whose edges are shown by the solid lines in Fig. 5.3), as expected. The bulk bands have real \( Q \) within the interval \( [0, \frac{\pi}{D}] \), whereas the stop bands would correspond to
Fig. 5.3 The edges of bulk bands $B_1$ to $B_5$ for an infinite superlattice with 2D translational symmetry. The dimensionless frequency $\omega - \omega_{01}$ is plotted against $\Lambda_2(q_{||})$. The dotted lines represent the bulk spin-wave modes corresponding to $QD = \pi/2$. The complex forms of $QD$ in the stop bands are also presented (with $\xi = D\xi > 0$). The assumed parameters are $N_1 = 3$, $N_2 = 2$, $S_2/S_1 = 2$, $J_2/J_1 = 0.25$, $J_{s1}/J_1 = 0.9$, $J_{s2}/J_1 = 0.3$, and $J_{12}/J_1 = 0.6$. 
complex $Q$ in the forms of $Q = i\xi$ and $Q = \frac{\pi}{D} + i\xi$ (with $\xi > 0$) in alternating fashion. The dotted lines corresponding to $Q = \frac{\pi}{2D}$ are plotted, for clarity, within the bulk bands. Consistent with Fig. 5.2(b), the bulk bands at small values of $q_\parallel$ are broad inside the intermediate frequency range and narrow outside. The broadness of the bulk bands decreases typically with $q_\parallel$.

The Green function results in (5.22) enable us to calculate the spin wave spectral intensities in addition to the dispersion relations. To do so, we need to calculate the imaginary part of the analytically continued Green function $G(N, \kappa, n; N', \kappa', n'; E+i\nu, q_\parallel)$. We shall consider only the equal-site components as usual and introduce the following notation for convenience:

$$Y(\kappa, n; \omega_1 - \omega_0, \Lambda_2) = -\text{Im}[G(N, \kappa, n; N, \kappa, n'; E+i\nu, q_\parallel)]_{\nu \to 0} \quad (5.27)$$

The unit cell index $N$ is omitted from the left-hand side in this notation because $G(N, \kappa, n; N, \kappa, n)$ does not depend on $N$ in an infinite superlattice. This independence and the symmetric "surfaces" of the constituent films ensure the symmetry property: $Y(\kappa, N_k - n+1; \omega_1 - \omega_0, \Lambda_2) = Y(\kappa, n; \omega_1 - \omega_0, \Lambda_2)$. As examples, in Fig. 5.4 we plot $Y(1,1; \omega_1 - \omega_0, \Lambda_2)$ and $Y(2,2; \omega_1 - \omega_0, \Lambda_2)$ against $\omega_1 - \omega_0$ for the same parameters as in Fig. 5.3 and for $\Lambda_2(q_\parallel) = 2$. By noting the changes in the relative intensity of the bulk spin waves between Fig. 5.4(a) and Fig. 5.4(b), we deduce that the bulk spin wave modes in the higher (lower) bulk bands for this example have their spectral intensities associated more strongly with film 1 (film 2). Our calculations of the spin wave spectral intensities (as well as the generalization of the superlattice structure)
Fig. 5.4  The intensities of bulk spin-waves modes (calculated from the imaginary part of the Green functions) in an infinite superlattice with 2D translational symmetry. The site is chosen to be: (a) in the "surface" \((n = 1)\) of constituent film \(1\) \((\kappa = 1)\), (b) in the "surface" \((n = 2)\) of constituent film \(2\) \((\kappa = 2)\). We take \(\Lambda_2(q_1) = 2\) and other parameters are assumed to be the same as in Fig. 5.3.
complement the previous study of ferromagnetic superlattices by Dobrzynski et al (1986) with the Green function method.

§ 5.2 Semi-Infinite Superlattices With 2D Translational Symmetry

Based on our knowledge of spin waves in infinite superlattices, we now turn to consider a semi-infinite superlattice composed of the same two types of ferromagnetic films \( \kappa (\kappa = 1, 2) \) as a generalization of § 5.1. For simplicity, we let the outmost film be the same as the constituent films of the same type in the interior region except that one of its surfaces exposed to the vacuum becomes the external surface of this semi-infinite superlattice. Without loss of generality, the outmost film is chosen to be film 1 in the first unit cell (see the right side of Fig. 5.5). The exchange constants between the nearest neighbors within this superlattice surface are allowed to be different, in general, from those within the corresponding "surfaces" in the interior region and denoted by \( J_{\alpha_1} \). This semi-infinite superlattice occupies the half-space \( z \geq 0 \).

In order to make use of the Green function results in § 5.1, we employ the mathematical device of introducing a fictitious semi-infinite superlattice to occupy the half-space \( z \leq -a \). The semi-infinite superlattice under our consideration and this fictitious one together form a new infinite superlattice (see Fig. 5.5). Note that there is no exchange coupling between the two semi-infinite superlattices and exchange constants within the fictitious surface (at \( z = -a \)) are denoted by \( J_{02} \). Apart from the "interface" between \( z = -a \) and 0, this "combined" infinite superlattice is the same as the one
Fig. 5.5 Schematic diagram of a semi-infinite superlattice with 2D translational symmetry (in the $x$ and $y$ directions). The physical superlattice is on the right side (with $z > 0$) and the accompanying fictitious one (with $z < 0$) is employed as a calculational device.
considered in § 5.1.

Following the same algebraic procedure as in § 5.1, we can write the equations of motion for the Green function components \(G(N, \kappa, n; N', \kappa', n')\) for the combined infinite superlattice into a new infinite-dimensional partitioned matrix form:

\[
(A - R)G = -\frac{1}{\hbar} \tag{5.28}
\]

where \(A\) is the same as the partitioned matrix \(A_0 - C\) on the left-hand side of (5.5). According to (5.5) and (5.22), the matrix elements of the inverse of \(A\) in (5.28), denoted by \(B = A^{-1}\), are given explicitly as follows:

\[
B(N, \kappa, n; N', \kappa, n') = \frac{B_\kappa(n; n')}{J_\kappa} \delta_{NN'} - \frac{P_{\kappa\kappa}(n, n')}{J_\kappa} \frac{|N - N'|}{x - x^{-1}} - \frac{P_{\kappa\kappa}(n', n)}{J_\kappa} \frac{|N - N' - 1|}{x - x^{-1}} - \frac{P_{\kappa\kappa}(n', n)}{J_\kappa} \frac{|N - N' + 1|}{x - x^{-1}} \tag{5.29a}
\]

\[
B(N, 1, n; N', 2, n') = -\frac{P_{12}(n, n')}{J_{12}} \frac{|N - N'|}{x - x^{-1}} - \frac{P_{12}(N - n + 1, N', n' + 1)}{J_{12}} \frac{|N - N' - 1|}{x - x^{-1}} \tag{5.29b}
\]

and

\[
B(N, 2, n; N', 1, n') = B(N', 1, n'; N, 2, n) \tag{5.29c}
\]

where the complex parameter \(x\) is the same as defined by (5.19). The expressions for \(B_\kappa(n; n')\), \(P_{\kappa\kappa}(n, n')\), \(P_{\kappa\kappa}(n, n')\), and \(P_{12}(n, n')\) are the same as in § 5.1. The matrix elements of \(R\), which describes the decoupling of the two semi-infinite superlattices, in (5.28) are given by

\[
R(N, \kappa, n; N', \kappa', n') = r_1 \delta_{n_1 n_1'} \delta_{\kappa_1 \kappa_1'} \delta_{\kappa \kappa} \delta_{n_2 n_2'} + r_2 \delta_{n_2 n_2'} \delta_{\kappa \kappa} \delta_{\kappa_2 \kappa_2'} \delta_{n_1 n_1'} \delta_{n' 0}\]

\[- J_{12} \left( \delta_{n_1} \delta_{n'_1} N_{12} \delta_{n_2} \delta_{n'_2} N'_{12} + \delta_{n_1} \delta_{n'_1} N_{12} \delta_{n_2} \delta_{n'_2} N'_{12} \right) \] (5.30)

where

\[ r_1 = 2(J_{s_1} - J_{s_2}) \Lambda_2(q_\parallel) + \frac{J_{12} S_2}{S_1} \] (5.31a)

\[ r_2 = 2(J_{s_2} - J_{s_1}) \Lambda_2(q_\parallel) + \frac{J_{12} S_1}{S_2} \] (5.31b)

Since the two semi-infinite superlattices are completely decoupled, only the Green function components between spins in the same semi-infinite superlattice are non-zero. When \( N > 0 \) and \( N' > 0 \), \( G(N,\kappa,n;N',\kappa',n') \) is the Green function component for the semi-infinite superlattice of our interest. When \( N \leq 0 \) and \( N' \leq 0 \), it is for the fictitious one.

As before, the formal solution of (5.28) can be worked out by means of the Dyson equation

\[ G = - \frac{B}{\pi} + BRG \] (5.32)

By substituting (5.29) and (5.30) into (5.32) and keeping in mind \( N > 0 \) and \( N' > 0 \) for the Green functions of our interest, we get

\[ G(N,\kappa,n;N',\kappa',n') = - \frac{1}{\pi} B(N,\kappa,n;N',\kappa',n') \]

\[ + \left[ r_1 B(N,\kappa,n;1,1,1) - J_{12} B(N,\kappa,n;0,2,N_2) \right] G(1,1,1;N',\kappa',n') \] (5.33)

By setting \( N = 1, \kappa = 1 \), and \( n = 1 \) in (5.33), \( G(1,1,1;N',\kappa',n') \) is easily obtained as

\[ G(1,1,1;N',\kappa',n') = - \frac{B(1,1,1;N',\kappa',n')}{\pi(1-w_1)} \] (5.34)

where

\[ w_1 = r_1 B(1,1,1;1,1,1) - J_{12} B(1,1,1;0,2,N_2) \] (5.35)
The substitution of (5.34) back into (5.33) gives the required Green function result
\[
G(N, \kappa, n; N', \kappa', n') = -\frac{1}{\pi} B(N, \kappa, n; N', \kappa', n')
- \frac{1}{\pi(1-\nu_1)} [r_1 B(N, \kappa, n; 1, 1, 1) - J_{12} B(N, \kappa, n; 0, 2, N'_2)] B(1, 1, 1; N', \kappa', n')
\]
\[(N > 0, N' > 0) \tag{5.36}\]

The dispersion relations of the spin waves in the semi-infinite superlattice under consideration are determined by the poles of the Green function component (5.36). The superlattice surface spin-wave modes (corresponding to real \(x\)), in particular, are given by the solutions of
\[
\nu_1 = 1 \tag{5.37}
\]
while the superlattice bulk spin waves are the same as in § 5.1.

**Numerical results and discussion**

As an example, we solve (5.37) numerically for the case of \(J_{01} = J_1\) (free surface of the semi-infinite superlattice) and for the same parameters as in Fig. 5.3 otherwise. The dispersion relation curves for the surface spin waves in this case are illustrated by the solid lines in Fig. 5.6, where the frequencies are plotted against \(A_2(q_y)\). For comparison, the edges of the bulk bands (labelled by \(B_1\) to \(B_5\)) are also shown in Fig. 5.6 by the dotted lines; these are the same as in Fig. 5.3. As expected, the surface branches exist only outside the bulk bands, although some of them are close in frequency to the bulk bands and terminate at the bulk band edges. The surface spin-wave modes (labelled by \(A_1\) and \(A_2\)) in the stop bands with \(Q = \hbar \xi\) are of the acoustic type (in the sense of \(0 < x \leq 1\)) and those (labelled by \(O_1\) and
Fig. 5.6  The dispersion relation curves for surface spin-wave modes (solid lines) and the edges of the bulk bands (dotted lines) $B_1$ to $B_5$ for a semi-infinite superlattice with 2D translational symmetry. The dimensionless frequency $\omega - \omega_{01}$ is plotted against $\Lambda_2(q_\parallel)$. Two acoustic surface modes ($A_1$ and $A_2$) and two optical surface modes ($O_1$ and $O_2$) are obtained for $J_{01} = J_1$ (free surface of medium 1) and for the same parameters as in Fig. 5.3 otherwise.
in the stop bands with $Q = \frac{x}{D} + i\xi$ are of optical type (in the sense of $-1 \leq x < 0$), as indicated in Fig. 5.6. By recalling that there exists no surface spin wave in semi-infinite homogeneous materials with free surfaces, we can say that the occurrence of surface spin waves in this example (with a free surface) is another consequence of the periodic structure of superlattices.

From (5.36), we can calculate the imaginary part of the analytically continued Green function $G(N, \kappa; n; N', \kappa', n'; E+i\nu, q_\parallel)$ to examine the spectral intensity of the surface spin wave modes as well as the bulk modes in the semi-infinite superlattice. A notation similar to (5.27) is introduced for convenience as follows:

$$Y(N, \kappa, n; \omega_1 - \omega_{01}, \Lambda_2) = \text{Im}[G(N, \kappa; n; N, \kappa, n; E+i\nu, q_\parallel)] \bigg|_{\nu \to 0} \quad (5.38)$$

For consistency and comparison, we take the surface branches and bulk bands shown in Fig. 5.6 as an example to investigate the spin wave intensities. With the same parameters as assumed there, we plot $Y(N, 1, n; \omega_1 - \omega_{01}, 2)$ as a function of $\omega_1 - \omega_{01}$ for $n = 1$ and $N_1$ (representing the two different "surfaces" of film 1) and for three different values of $N$ (representing three different distances from the external surface in units of the periodic length $D$). At $N = 1$, the surface spin-wave modes have dominantly strong intensities and the bulk modes are relatively weak (see Fig. 5.7). As we move one period farther into the superlattice ($N = 2$), the intensities of the surface modes decrease sharply and the bulk modes gain dominant strength (see Fig. 5.8). At considerably large distances (e.g., $N = 5$) from the external surface, the surface modes have essentially decayed away (see Fig. 5.9) and the bulk modes tend to resume the intensities shown in Fig. 5.4(a).
Fig. 5.7  The intensities of the bulk and surface spin-waves modes shown in Fig. 5.6 at $\Lambda_2(q_0) = 2$. The site is chosen to be in: (a) the outmost surface ($n = 1$), (b) the interior "surface" ($n = 3$) of film 1 in the outmost unit cell $N = 1$. The spin-wave modes with noticeable intensity are indicated by the same symbols as in Fig. 5.6.
Fig. 5.8 As in Fig. 5.7 but for the unit cell \( N = 2 \) next to the outmost one.
Fig. 5.9  As in Fig. 5.7 but for the unit cell $N = 5$ farther from the outmost surface. Only the spin-wave modes in the bulk bands $B_1$ to $B_5$ have noticeable intensity in this case.
We note also that the spin wave intensities show little difference between Fig. 5.9(a) for one "surface" and Fig. 5.9(b) for the other. As one could expect, the physical properties (such as spectral intensities) of the spin waves in the interior region far enough away from the surface of the semi-infinite superlattice eventually become the same as those in the corresponding infinite superlattice. This is strongly indicated by Fig. 5.9 and confirmed by our other numerical calculations for even larger values of $N$. Again, our calculations of the spectral intensities of the surface spin waves complement the previous study of semi-infinite ferromagnetic superlattices by Dobrzynski et al (1986) with the Green function method.

§ 5.3 Perpendicularly Cleaved Infinite Superlattices

From the last two sections we have acquired a good understanding of the spin wave behavior in ferromagnetic superlattices with 2D translational symmetry. In this and the next sections we shall study the spin wave behavior in perpendicularly cleaved (or truncated) ferromagnetic superlattices.

Let us begin by considering a new type of infinite ferromagnetic superlattice that has a pair of cleaved surfaces (located at $y = 0$ and $y = (N-1)a$) perpendicular to the interfaces (see Fig. 5.10). The structure is periodic in the $z$ direction (as in § 5.1) and extends indefinitely as $z \to \pm \infty$. In the region between the cleaved surfaces, this perpendicularly cleaved superlattice is assumed to be described by the same physical parameters (e.g., lattice structures, exchange constants, spin quantum numbers) as the uncleaved superlattice in §
Fig. 5.10 Schematic diagram of a perpendicularly cleaved infinite superlattice, showing the exchange interactions.
5.1. Hence, the same notations (such as $J_{\kappa}$, $J_{\text{sk}}$, $J_{12}$, and $S_{\kappa}$) continue to be used in this section. There are $M$ atomic layers in the $y$ direction. For simplicity, the cleaved (010) surfaces are considered to be free surfaces, by which we mean that the nearest-neighbor exchange constants within each cleaved surface remain the same as in the interior layers (i.e., $J_{\text{sk}}$ if the nearest neighbors are both in the same "surface" of film $\kappa$, $J_{\kappa}$ if they are any other pair of sites in film $\kappa$, and $J_{12}$ if they are adjacent sites across the interfaces between films 1 and 2). The spin of any atom in material $\kappa$ in the $N$th unit cell has the position vector

$$r = \left( x, (m-1)a, (N-1)D + (N_1 \delta_{\kappa_2} + n - 1)a \right)$$

$$(-\infty < N < \infty, 1 \leq m \leq N, 1 \leq n \leq N_\kappa) \quad (5.39)$$

where $D$ is the superlattice period given by (5.1).

The Hamiltonian of this cleaved superlattice and the equation of motion for the spin-spin Green functions are given again by (2.3) and (2.14), respectively. Since this cleaved superlattice possesses translational symmetry only in the $x$ direction, we can only make the 1D Fourier transformations (by analogy with (3.2) and (3.3))

$$\langle \langle S^+_r ; S^-_{r'} \rangle \rangle_E = \frac{1}{Q_1} \sum_{q_x} G(N, \kappa, n, m; N', \kappa', n', m' \mid E, q_x) \exp[i q_x (x-x')] \quad (5.40)$$

$$\langle \langle S^-_r S^+_r \rangle \rangle_E = \frac{1}{Q_1} \sum_{q_x} F(N, \kappa, n, m; N', \kappa', n', m' \mid E, q_x) \exp[i q_x (x-x')] \quad (5.41)$$

where $Q_1$ is the number (macroscopically large) of spins in any crystalline axis in the $x$ direction. For brevity, the dependence of the Fourier components of the Green functions and the correlation functions on $E$ and $q_x$ will not be written down explicitly where it is obvious.
We note that this cleaved superlattice is built up alternately of two different types of truncated films considered in § 3.3 and that its interfaces are taken to be of the same type as considered in § 4.2. There is a minor notational difference in that the axis perpendicular to the free surfaces (original or cleaved) changes from the z axis in Chapters 3 and 4 to the y axis here. However, due to the above-mentioned connections with the previous ferromagnetic structures, we can combine the procedures used in § 3.3, § 4.2, and § 5.1 to rewrite the equations of motion for the Green function components \( G(N, \kappa, n, m; N', \kappa', n', m') \) in a partitioned matrix form, i.e.,

\[
(A_0 - C)G = - \frac{1}{\pi} \tag{5.42}
\]

Here the matrix elements of \( A_0 \) are given by (generalizing (5.6))

\[
A_0(N, \kappa, n, m; N', \kappa', n', m') = J_{\kappa} A_\kappa(n, m; n', m') \delta_{\kappa \kappa'} \delta_{NN'} \tag{5.43}
\]

where \( A_\kappa(n, m; n', m') \) is the element of the partitioned matrix \( A_\kappa \):

\[
A_\kappa(n, m; n', m') = \left[ (d_{\kappa} \delta_{m1} - c_{\kappa} \delta_{m2}) \delta_{nn'} - \delta_{nn'} - \delta_{mm'} \right] \delta_{nn'} - \delta_{mm'} \delta_{nn'} \delta_{nn'} + \delta_{nn'} \delta_{nn'} + \delta_{nn'} \delta_{nn'} \tag{5.45}
\]

The \( M \times M \) matrices \( D_\kappa \) and \( C_\kappa \) are defined to have the following elements (similar to (3.38) and (3.39)):

\[
(D_{\kappa})_{mm'} = (d_{\kappa} \delta_{m1} - c_{\kappa} \delta_{m2}) \delta_{mm'} - \delta_{mm'} - \delta_{m+1,m'} \tag{5.46}
\]

\[
(C_{\kappa})_{mm'} = c_{\kappa} \delta_{mm'} - (1 - c_{\kappa})[(\delta_{m1} + \delta_{m2}) \delta_{mm'} + \delta_{m-1,m'} + \delta_{m+1,m'}] \tag{5.47}
\]

where \( d_{\kappa}, c_{\kappa}, \) and \( e_{\kappa} \) are given by (4.8), (4.9), and (4.12) respectively. The parameter \( \Lambda_1(q_\kappa) \) and dimensionless frequencies \( \omega_\kappa \) and \( \omega_{\kappa} \) involved therein are defined by (3.42), (4.10), and (4.12) respectively. The matrix \( C \) in (5.42) again describes the exchange coupling across the interfaces between the two materials, and its
matrix elements are given by

\[ C(N, \kappa, n, m; N', \kappa', n', m') = J_{12} \delta_{mm'} \left[ \left( \delta_{nN} \delta_{n'1} \delta_{1\kappa} \delta_{2\kappa'} + \delta_{n'N} \delta_{nl} \delta_{1\kappa'} \delta_{2\kappa} \right) \delta_{NN'} + \delta_{n1} \delta_{n'N} \delta_{l\kappa} \delta_{2\kappa'} \delta_{N-1, N'} + \delta_{n'1} \delta_{nl} \delta_{2\kappa'} \delta_{3\kappa} \delta_{N+1, N'} \right] \]  

(5.47)

Finally, the partitioned matrix \( G \) has \( G(N, \kappa, n, m; N', \kappa', n', m') \) as its matrix elements, representing the Green function components between one spin in the atomic layer labelled by \( n \) and \( m \) of film \( \kappa \) in the \( N \)th unit cell and the other in the atomic layer labelled by \( n' \) and \( m' \) of film \( \kappa' \) in the \( N' \)th unit cell. Our aim is to work out \( G(N, \kappa, n, m; N', \kappa', n', m') \) from (5.42) and hence to deduce the spin wave behavior.

By applying the matrix "subdiagonalization" procedure used in Chapter 3 and 4 to this cleaved superlattice, we next show how to extend algebraic results in § 5.1 to the superlattice geometry in this section (analogous to the extension of § 3.1 to § 3.3). We notice that all the \( M \times M \) submatrices (at the lowest level) of \( A \) and \( C \) (such as \( D'_{\kappa} \) and \( C'_{\kappa} \)) can be simultaneously diagonalized by similarity transformations (involving the same orthogonal matrix \( V \)) such as

\[ D'_{\kappa} = V^{-1} D_{\kappa} V \]  

(5.48)

\[ C'_{\kappa} = V^{-1} C_{\kappa} V \]  

(5.49)

where the \( M \times M \) orthogonal matrix \( V \) has the following elements (analogous to (3.47)):

\[ (V)_{mm'} = \left( \frac{2-\delta_{m'1}}{M} \right)^{1/2} \cos \frac{(2m-1)(m'-1)\pi}{2M} \]  

(5.50)

In what follows we denote the "(sub)diagonalized" matrices by the same symbols with a prime. The matrices \( D'_{\kappa} \) and \( C'_{\kappa} \) have the following
elements:

\[
\begin{align*}
(D')_{\kappa\lambda\mu} &= d_{\kappa\mu} \delta_{\lambda\nu}, \\
(C')_{\kappa\lambda\mu} &= c_{\kappa\lambda\mu} \delta_{\nu\mu},
\end{align*}
\] (5.51)

where

\[
\begin{align*}
d_{\kappa\mu} &= d_{\kappa} - 2\cos\left(\frac{(m-1)\pi}{N}\right), \\
c_{\kappa\mu} &= c_{\kappa} - 2(1-\xi_{\kappa})\cos\left(\frac{(m-1)\pi}{N}\right)
\end{align*}
\] (5.53)

(5.54)

Now we can construct a partitioned matrix \(U\) with elements

\[
U(N, \kappa, n, m; N', \kappa', n', m') = (V)_{\mu\nu} \delta_{\eta\nu} \delta_{\kappa\kappa'} \delta_{NN'}
\] (5.55)

and transform \(A, C,\) and \(G\) into a representation in which all the \(M\times N\) submatrices are diagonal. In this "subdiagonal" representation, (5.42) remains formally the same, i.e., we have

\[
(A'_0 - C')G' = -\frac{1}{\pi}
\] (5.56)

where

\[
\begin{align*}
A'_0 &= U^{-1} A_0 U, \\
C' &= U^{-1} C U, \\
G' &= U^{-1} G U
\end{align*}
\] (5.57) (5.58) (5.59)

Next, we work out the partitioned matrix \(G'\) from (5.56). In the "subdiagonal" representation (in which all the \(M\times N\) submatrices can be treated as ordinary \(c\)-numbers), this can be done by translating the algebraic results in § 5.1 to the present geometry. As an extension of (5.11), the expression for the matrix elements of \(B' = A'^{-1}_\kappa\) is given by

\[
B'_{\kappa}(n, m; n', m') = \begin{cases} 
    P_{\kappa\eta}(n, m') \delta_{\eta\eta}, & (n = n') \\
    P_{\kappa\eta}(n', m) \delta_{\eta\eta}, & (n' > n)
\end{cases}
\] (5.60)

and the function \(P_{\kappa\eta}(n, m')\) is defined by
\( P_{k,a}(n,n') = \frac{\{\sin((N_k - n + 1)k_{1a}) - c_{k-1a}\sin((N_k - n)k_{1a})\}\{\sin(n'k_{2a}) - c_{k-1a}\sin((n' - 1)k_{2a})\}}{\sin(k_{2a})}(5.61) \)

where

\( v_{k,a} = \sin((N_k + 1)k_{1a}) - 2c_{k-1a}\sin(N_k k_{1a}) + c_{k-1a}^2\sin((N_k - 1)k_{1a}) \quad (5.62) \)

By analogy with the previous chapters, the parameter \( k_{k,a} \) is defined by

\[
2\cos(k_{k,a}) = d_{k,a} = \omega_{kk} - \omega_k + 2\left[2 - \cos\left(\frac{m-1}{N}\right) + \Lambda_1(q)\right]
\]

\[
\text{[Im}(k_{k,a}) > 0]\]

(5.63)

Noting the diagonal structure of \( A_0 \) in (5.43), we immediately obtain the matrix elements of \( B'_0 = A_0^{-1} \) as follows:

\[
B'_0(N,k,n,m;N',k',n',m') = \frac{B'_k(n,m;n',m')}{J_k} \delta_{kk'} \delta_{NN'} \quad (5.64)
\]

The Green-function expression (5.56) can be rewritten in the form of a Dyson equation as

\[
\mathcal{S}' = -\frac{B'_0}{\mathcal{K}} + B'\mathcal{G}'\mathcal{G}' \quad (5.65)
\]

In the "subdiagonal" representation, we can now repeat the algebraic derivations outlined in Appendix B to obtain the matrix elements of \( G' \) for a fixed value of \( m \) (= 1, 2, ..., \( N \)) from those of \( B'_k \). This will result in a complex parameter \( x_m \) (analogous to \( x \) in (5.19)) defined by

\[
x_m + x_m^{-1} = d_m \quad (|x_m| \leq 1) \quad (5.66)
\]

where

\[
d_m = \rho^{-1}\nu_{1a}w_{2a} - 2u_{1a}v_{2a}(N_1) + \rho\sin((N_1 - 1)k_{1a})\sin((N_2 - 1)k_{2a})
\]

\[
\sin(k_{1a})\sin(k_{2a}) \quad (5.67)
\]
Here the function \( u_{K,n}(n) \) is defined by

\[
u_{n,n}(n) = \sin(nk_{n,n}) - c_{n,n}\sin((n-1)k_{n,n})
\]

and \( \rho \) is defined in (4.39). Without presenting the straightforward but lengthy algebraic calculations of \( G'(N,\kappa,n,m;N',\kappa',n',m) \), we only quote the final results here:

\[
G'(N,\kappa,n,m;N',\kappa,n',m) = -\frac{B'(n,m;\kappa',m)}{\pi J_n^{\kappa}} \delta_{NN'} + \frac{P_{0Kn}(n,m)}{\pi J_n^{K_n}} \frac{|N-N'|}{x_m - x_m^{-1}}
\]

\[
\cdot \frac{P_{K,n}(n,m) x_m^{-|N-N'-1|}}{\pi J_n^{K_n}} + \frac{P_{K,n}(n',m) x_m^{-|N-N'+1|}}{\pi J_n^{K_n}}
\]

(5.69a)

\[
G'(N,1,n,m;N',2,n',m) = \frac{P_{12n}(n,m) x_m^{-|N-N'|}}{\pi J_{12}} + \frac{P_{12n}(N-\kappa,1,2-n',1) x_m^{-|N-N'-1|}}{\pi J_{12}}
\]

(5.69b)

\[
G'(N,2,n,m;N',1,n',m) = G'(N',1,n',m;N,2,n,m)
\]

(5.69c)

where

\[
P_{01n}(n,m)
\]

\[
= \frac{1}{\sin(k_{1m})\sin(k_{1m}')} \left((u_{1m}(N-\kappa,1)u_{1m}(N',1)+u_{1m}(N)u_{1m}(N'))u_{2m}(N,2)\right) \\
- \rho(u_{1m}(N-\kappa,1)\sin((N-\kappa)k_{1m})+u_{1m}(N)\sin((N-\kappa-1)k_{1m})\sin((N-1)k_{2m})) \\
\]

(5.70)

and \( P_{02n}(n,n') \) can be obtained from \( P_{01n}(n,n') \) by interchanging the subscripts 1 and 2. Also we have
\[ p_{1\alpha}(n,n') = \frac{u_{1\alpha}(n)u_{2\alpha}(N_2-n'+1) - \rho \sin((n-1)k_{1\alpha})\sin((N_2-n')k_{2\alpha})}{\sin(k_{1\alpha})\sin(k_{2\alpha})} \]  

(5.71)

Finally, we transform \( G'(N, \kappa, n, s; N', \kappa', n', s) \) back to the original representation by using (5.59) to get the required Green function components in the form

\[ G(N, \kappa, n, s; N', \kappa', n', s' \mid E, q_x) = \sum_{s''} \langle \psi_{s''} | \psi_{s'} \rangle G'(N, \kappa, n, s; N', \kappa', n', s') \]  

(5.72)

By analogy with \( \S \) 5.1, the dispersion relations of the bulk spin wave modes in this cleaved superlattice are determined by the following \( M \) equations involving the same wavevector component \( Q \) (in the \( z \) direction) and the superlattice period \( D \):

\[ d_{s''} = 2\cos(QD) \quad (s'' = 1, 2, \ldots, M) \]  

(5.73)

With real \( Q \) ranging from 0 to \( \frac{\pi}{D} \), the bulk modes fill up a series of bulk bands. As before, the stop bands (the frequency regions where no bulk modes exist) would correspond to complex \( Q \) in the forms of \( Q = i\xi \) or \( Q = \frac{\pi}{D} + i\xi \) (with \( \xi > 0 \)).

**Numerical results and discussion**

To illustrate the dispersion relations for the bulk spin waves in a cleaved infinite superlattice, we first plot \( \omega_1 - \omega_{01} \) against \( QD \) at \( \lambda_1(q_x) = 0.25 \) for \( M = 4, N_1 = 3, N_2 = 2 \), and for the same spin quantum numbers and exchange constants as in Fig. 5.2(b). In Fig. 5.11 we get four times (corresponding to \( M = 4 \)) as many dispersion relation curves as in Fig. 5.2(b) and these curves are again "folded" back at the reduced Brillouin-zone boundary, leaving narrow frequency gaps inside an intermediate frequency range and broad frequency gaps outside.
Fig. 5.11 The dispersion relation curves for bulk spin-wave modes in a perpendicularly cleaved infinite superlattice. The dimensionless frequency $\omega_1 - \omega_{01}$ is plotted against $QD$. The assumed parameters are $N = 4$, $N_1 = 3$, $N_2 = 2$, $S_z/S_1 = 2$, $J_z/J_1 = 0.25$, $J_{s1}/J_1 = 0.9$, $J_{s2}/J_1 = 0.3$, $J_{12}/J_1 = 0.6$, and $\Lambda_s(q_z) = 0.25$. The number of curves is $N(N_1+N_2) = 20$. 
this frequency range.

Following § 5.1 we then illustrate the dispersion relations in a conventional way by plotting frequency versus \( q_x \) for the same parameters as in Fig. 5.11. In this case the number of bulk bands is \( MN_1 + N_2 \) = 20, and in Fig. 5.12 only the edges of these bulk bands are shown. Many bulk bands overlap in frequency. To show the finite-size (i.e., finite \( M \)) effects on the bulk bands more clearly, we restrict our attention, for example, to the bulk bands \( B_{3m} (m = 1, 2, \ldots, M) \) that would become equivalent to the bulk band labelled as \( B_3 \) in Fig. 5.3 for the corresponding uncleaved infinite superlattice. In Fig. 5.13 the edges of these four bulk bands are distinguished from the others by the solid lines where their edges in the overlapping area are shown distinctly by the dashed lines. It is interesting to note that the bulk spin-wave modes in \( B_3 \) for a uncleaved superlattice have "split" into a series of bulk bands \( B_{3m} (m = 1, 2, \ldots, M) \) due to the finite-size effect. To show this effect further, we plot in Fig. 5.14 exclusively the bulk bands \( B_{3m} (m = 1, 2, \ldots, M) \) for \( M = 6 \), taking the same parameters as in Fig. 5.13 otherwise.

If \( N_1 \) and \( N_2 \) are kept fixed while \( M \) is increased without limit, the \( MN_1 + N_2 \) bulk bands would ultimately group together to form \( N_1 + N_2 \) continua. This trend is apparent, taking the above example of the bulk bands \( B_{3m} (m = 1, 2, \ldots, M) \) and comparing Fig. 5.13 for \( M = 4 \) to Fig. 5.14 for \( M = 6 \). In the limit of \( M \rightarrow \infty \), a continuum would be formed between the lower edge of \( B_{31} \) and the dotted line in Fig. 5.14, and this continuum would converge to reproduce the bulk band \( B_3 \) in Fig. 5.3 (for the corresponding uncleaved superlattice) if the frequencies were
Fig. 5.12 The bulk bands (shown shaded) and their edges (solid lines) for a perpendicularly cleaved infinite superlattice. The dimensionless frequency $\omega_1 - \omega_{01}$ is plotted against $\Lambda_1(q_z)$. The assumed parameters are $M = 4$, $N_1 = 3$, $N_2 = 2$, $S_z/S_1 = 2$, $J_2/J_1 = 0.25$, $J_{s1}/J_1 = 0.9$, $J_{s2}/J_1 = 0.3$, and $J_{12}/J_1 = 0.6$. 
Fig. 5.13 A further illustration of the effects of the perpendicular cleavages on the bulk bands in Fig. 5.12. The four bulk bands $B_{3m}$ ($m = 1, 2, 3, 4$) are distinguished by the solid lines from the others.
Fig. 5.14  A particular series of bulk bands for a perpendicularly cleaved infinite superlattice with the same parameters as in Fig. 5.12 except that $M$ is increased from 4 to 6. The dotted line indicates the upper boundary for these bulk bands in the limit of $M \rightarrow \infty$. 
plotted against $\Lambda_2(q_x,q_y)$ instead of $\Lambda_1(q_x)$. Physically, this means that, when the distance between the two cleaved surfaces becomes effectively infinite, the superlattice regains the translational symmetry in the $y$ direction and an additional Fourier transformation can be made from the lattice space to the wavevector space in the $y$ direction. Indeed, it can be algebraically verified (by analogy with the argument that leads to (3.66) from (3.63) in § 3.2) that our results for the cleaved infinite superlattices will recover the results of § 5.1 in the limit of $M \to \infty$.

As before, the spin wave intensities for this cleaved infinite superlattice can be obtained by calculating the imaginary part of the corresponding Green functions (5.69) and (5.72). We omit these numerical calculations here because they are straightforward in principle but complicated in practice due to the multiplicity of bulk-mode branches.

§ 5.4 Perpendicularly Cleaved Semi-Infinite Superlattices

Based on our knowledge of spin waves in perpendicularly cleaved infinite superlattice, we finally consider in this section a perpendicularly cleaved semi-infinite superlattice (see the right side of Fig. 5.15) as a generalization of § 5.3. For simplicity, the two cleaved (010) surfaces (located respectively at $y = 0$ and $y = (M-1)a$) perpendicular to the interfaces are assumed, again, to be free surfaces as in § 5.3. In the interior region (corresponding to $0 \leq y \leq (M-1)a$ and $0 < z < \omega$), this perpendicularly cleaved semi-infinite superlattice is assumed to be the same as the cleaved superlattice described in §
Fig. 5.15  Schematic diagram of a perpendicularly cleaved semi-infinite superlattice. The physical superlattice is on the right side (with $z \geq 0$) and the accompanying fictitious one (with $z < 0$) is employed as a calculational device.
5.3 in all its physical attributes (e.g., lattice structures, exchange constants, spin quantum numbers). Hence, the same notations continue to be used in this section. Only the exchange constants within the outermost surface (at \( z = 0 \)) are taken to be different, in general, from those within the corresponding "surfaces" of material 1 in the interior region and denoted by \( J_{01} \).

In order to make use of the Green function results in § 5.3, we employ the same mathematical device as used in generalizing from § 5.1 to § 5.2. Specifically, we imagine placing a perpendicularly cleaved semi-infinite fictitious superlattice in the space limited by \( 0 \leq y \leq (N-1)a \) and \(-\infty < z \leq -a\). The exchange constants within the fictitious surface (at \( z = -a \)) are denoted by \( J_{02} \). These two perpendicularly cleaved semi-infinite superlattices form a new perpendicularly cleaved infinite superlattice, which is different from the one considered in § 5.3 only in the "interface" region between \( z = -a \) and 0.

Following the same method as in § 5.3, we can write the equations of motion for the Green function components \( G(N,k,n,m;N',k',n',m') \) for this new perpendicularly cleaved infinite superlattice in a partitioned matrix form, i.e.,

\[
(A - R)G = -\frac{1}{\pi}
\]  

(5.74)

where \( A \) is the same as the partitioned matrix \( A_{0} - \mathbf{C} \) in (5.42). The matrix elements of \( R \) in (5.74) are given by
\[ R(N, \kappa, n, m; N', \kappa', n', m') \]

\[ = (R_1)_{mm'} \delta_{n1} \delta_{n'1} \kappa_1 \kappa_1' \delta_{N1} \delta_{N'1} + (R_2)_{mm'} \delta_{nN_2} \delta_{n'N_1} \kappa_2 \kappa_2' \delta_{N0} \delta_{N'0} \]

\[ - J_{12} \delta_{mm'} \left( \delta_{n1} \delta_{n'N_2} \kappa_1 \kappa_2' \delta_{N1} \delta_{N'0} + \delta_{nN_2} \delta_{n'1} \kappa_2 \kappa_1' \delta_{N0} \delta_{N'1} \right) \]  

(5.75)

The \(M \times M\) matrix \(R\) has the following elements

\[ (R)_{mm'} = r_{kk} \delta_{mm'} - (J_{sk} - J_{ok})[(\delta_{m1} + \delta_{mN}) \delta_{mm'} + \delta_{m-1, m'} + \delta_{m+1, m'}] \]  

(5.76)

where

\[ r_1 = 2(J_{s1} - J_{o1})[1 + \Lambda_1(q_x)] + \frac{J_{12} S_2}{S_1} \]  

(5.77a)

\[ r_2 = 2(J_{s2} - J_{o2})[1 + \Lambda_1(q_x)] + \frac{J_{12} S_1}{S_2} \]  

(5.77b)

Note that the first terms on the right-hand sides of (5.77) are due to the variations of exchange constants in the two face-to-face surfaces (at \(z = -a\) and 0) and the second terms describe the complete decoupling of the two cleaved semi-infinite superlattices. As before, \(G(N, \kappa, n, m; N', \kappa', n', m')\) is the Green function component for the cleaved semi-infinite superlattice under our study when \(N > 0\) and \(N' > 0\), the Green function component for the fictitious one when \(N \leq 0\) and \(N' \leq 0\), and zero otherwise.

On comparing the tridiagonal matrix structures of \(R\), \(D\), and \(C\) (given in (5.76), (5.45), and (5.46) respectively), we find that partitioned matrices \(A\) and \(R\) can be simultaneously "subdiagonalized" by the similarity transformations (involving the same orthogonal matrix \(U\) as in (5.55)):

\[ A' = U^{-1} A U \]  

(5.78)
\[ R' = U^{-1} R U \]  
(5.79)

In the above representation, the matrix elements of \( R' \) are

\[
R'(N, \kappa, n, m; N', \kappa', n', m') = r_{1m} \delta_{mm'} \delta_{n1} \delta_{n1'} \delta_{\kappa1} \delta_{\kappa1'} \delta_{N1} \delta_{N1'} + r_{2m} \delta_{mm'} \delta_{nN2} \delta_{nN2'} \delta_{\kappa2} \delta_{\kappa2'} \delta_{N0} \delta_{N0'}
\]

\[
- J_{12} \delta_{mm'} \left( \delta_{n1} \delta_{n1'} \delta_{\kappa1} \delta_{\kappa1'} \delta_{N1} \delta_{N1'} + \delta_{nN2} \delta_{nN2'} \delta_{\kappa2} \delta_{\kappa2'} \delta_{N0} \delta_{N0'} \right)
\]

(5.80)

where

\[
r_{km} = r_{k} - 2(J_{sk} - J_{ok}) \cos \left( \frac{(a-1)\pi}{N} \right)
\]

(5.81)

Also, (5.74) remains formally the same in this new representation:

\[
(A' - R')G' = - \frac{I}{\pi}
\]

(5.82)

where

\[
G' = U^{-1} G U
\]

(5.83)

Obviously, \( A' \) is the same as the partitioned matrix \( A_0' - C' \) on the left-hand side of (5.56). According to (5.56) and (5.69), the matrix elements of the inverse of \( A' \) in (5.82), denoted by \( B' \) (\( = A'^{-1} \)), are given explicitly as follows:

\[
B'(N, \kappa, n, m; N', \kappa', n', m) = \frac{B_k'(n, m; n', m)}{J_{kk'}} \delta_{NN'} - \frac{P_{okm}(n, n')}{J_{kk'}} \frac{x_m |N-N'|}{x_m - x_m^{-1}}
\]

\[
- \frac{P_{km}(n, n')}{J_{kk'}} \frac{x_m |N-N'-1|}{x_m - x_m^{-1}} - \frac{P_{k'm}(n', n)}{J_{kk'}} \frac{x_m |N-N'+1|}{x_m - x_m^{-1}}
\]

(5.84a)
\[ B'(N, 1, n, m; N', 2, n', m) = \frac{P_{12}(n, n')}{J_{12}} \frac{x_1^{-|N-N'|}}{x_1 - x_1^{-1}} - \frac{P_{12}(N_1 - n + 1, N_2, -n' + 1)}{J_{12}} \frac{x_1^{-|N-N'|-1}}{x_1 - x_1^{-1}} \] (5.84b)

\[ B'(N, 2, n, m; N', 1, n', m) = B'(N', 1, n', m; N, 2, n, m) \] (5.84c)

where the complex parameters \( x_1 \) are the same as defined by (5.66).

Also, the expressions for \( B'_K(n, m; n', m) \), \( P_{KmA}(n, n') \), and \( P_{12mA}(n, n') \) are the same as in § 5.3.

We now work out the partitioned matrix \( G' \) from (5.82) in the "subdiagonal" representation. As before, this can be done by means of the Dyson equation:

\[ G' = -\frac{B'}{\pi} + B'C'G' \] (5.85)

By substituting (5.80) and (5.84) into (5.85) and keeping in mind \( \gamma > 0 \) and \( N' > 0 \) for the Green functions of our interest, we get

\[ G'(N, \kappa, n, m; N', \kappa, n', m) = -\frac{1}{\pi} B'(N, \kappa, n, m; N', \kappa, n', m) \]

\[ + [r_{1\mathbb{M}} B'(N, \kappa, n, m; 1, 1, 1, m) - J_{12} B'(N, \kappa, n, m; 0, 2, N_2, m)] G'(1, 1, 1, m; N', \kappa, n', m) \] (5.86)

By setting \( N = 1 \), \( \kappa = 1 \), and \( n = 1 \) in (5.86), \( G'(1, 1, 1, m; N', \kappa, n', m) \) is easily obtained as follows:

\[ G'(1, 1, 1, m; N', \kappa, n', m) = -\frac{B'(1, 1, 1, m; N', \kappa, n', m)}{\pi(1 - z_{1\mathbb{M}})} \] (5.87)

where

\[ z_{1\mathbb{M}} = r_{1\mathbb{M}} B'(1, 1, 1, m; 1, 1, 1, m) - J_{12} B'(1, 1, 1, m; 0, 2, N_2, m) \] (5.88)

Next, by substituting (5.87) back into (5.86), we have
\[ G'(N, \kappa, n, m; N', \kappa, n', m) = -\frac{1}{\pi} B'(N, \kappa, n, m; N', \kappa, n', m) \]

\[ + \frac{[r_1 B'(N, \kappa, n, m; 1, 1, 1, m) - J_{12} B'(N, \kappa, n, m; 0, 2, 2, m)] B'(1, 1, 1, 1; N', \kappa, n', m)}{\pi(1 - z_{1,m})} \]

\[(N > 0, \; N' > 0) \quad (5.89)\]

Finally, we transform \( G'(N, \kappa, n, m; N', \kappa', n', m) \) back to the original representation by using (5.83) to get the required Green function components in the form

\[ G(N, \kappa, n, m; N', \kappa', n', m' \mid E, q_x) = \sum_{m''} \langle V \rangle_{m,n} \langle V \rangle_{m',n'} G'(N, \kappa, n, m''; N', \kappa', n', m'') \]

\[(N > 0, \; N' > 0) \quad (5.90)\]

where the elements of the \( M \times M \) matrix \( V \) are the same as in (5.50).

The dispersion relations of the spin waves in the cleaved semi-infinite superlattice under our study are determined by the poles of the Green function components (5.90). From (5.89) and (5.90), we immediately find that the superlattice surface spin-wave modes (corresponding to real \( z_{m} \) between -1 and 1), in particular, are given by the solutions of the following \( M \) equations:

\[ z_{1,m''} = 1 \quad (m'' = 1, 2, \ldots, M) \quad (5.91)\]

The superlattice bulk spin waves are the same as in § 5.3.

**Numerical results and discussion**

As an example, we solve (5.91) numerically for \( j_{01} = j_1 \) (free surface) and for the same parameters as in Fig. 5.12 otherwise. The dispersion relation curves for the acoustic and optical surface spin waves in this case are illustrated by various types of lines other than the dotted lines in Fig. 5.16, where the edges of the bulk bands are also shown, for comparison, by the dotted lines. By recalling that
Fig. 5.16  The dispersion relation curves for acoustic and optical surface spin-wave modes and the bulk-band edges (the dotted lines) for a perpendicularly cleaved semi-infinite superlattice with a free surface ($J_{01} = J_1$). The assumed parameters are the same as in Fig. 5.12. The surface branches obtained are: $O_{11}$ and $O_{12}$ (the dash-dot-dotted lines), $A_{1m}$ (the solid lines), $O_{2m}$ (the dash-dotted lines), and $A_{2m}$ (the dashed lines) with $m = 1, 2, 3, 4$. 
there exists no surface spin wave in truncated homogeneous films with free surfaces, we can say that the occurrence of the surface spin waves in this example (with a free surface at \( z = 0 \)) is due to the periodic structure of this multilayer system. Compared with the surface spin-wave modes in an uncleaved semi-infinite superlattice (see curves \( O_1, A_1, O_2, \) and \( A_2 \) in Fig. 5.6), the surface modes \( O_{11}', O_{12}', A_{1m}', O_{22m}', \) and \( A_{2m} \) (\( m = 1, \ldots, 4 \)) shown in Fig. 5.16 can be regarded as being "quantized" due to the finite size (\( N = 4 \)), corresponding to the surface modes \( O_1, A_1, O_2, \) and \( A_2 \). As one could expect, these surface modes would form four continua as \( M \) is increased without limit. Again, these four continua would converge back to the surface modes \( O_1, A_1, O_2, \) and \( A_2 \) as \( M \to M \). In fact, this recovery to the results of § 5.2 in the limit of \( M \to M \) can be easily verified algebraically by analogy with the argument that leads to (3.66) from (3.63) in § 3.2.

Since we have obtained the Green function expressions (5.89) and (5.90) for this cleaved semi-infinite superlattice, the spectral intensities of the bulk and surface spin waves can be calculated straightforwardly from the imaginary part of the corresponding Green functions.
CHAPTER 6
CONCLUSIONS

In the preceding chapters we have studied, by means of the quantum-mechanical Green functions, the collective behavior of exchange-dominated spin waves in a variety of ferromagnetic layered structures. In this concluding chapter we shall summarize the results obtained and briefly discuss some possibilities of extending these results to other low-dimensional magnetic layered structures.

§ 6.1 Summary of Results

After presenting a general review of the theoretical studies of spin-wave excitations in magnetic materials, we have set up the quantum-mechanical spin-spin Green function formalism in a microscopic approach that is particularly suitable for the study of the exchange-dominated spin waves in ferromagnets at $T < T_c$. followed by a simple example of the bulk spin waves in infinite ferromagnets.

For completeness, we have re-derived the spin-spin Green functions for complete ferromagnetic films (see Fig. 1.1(b)) and reproduced the standard spin-wave spectra. We have complemented these calculations with results for the spectral intensities, which were not sufficiently investigated in the past. Then we have derived the Green functions for perpendicularly truncated ferromagnetic films (see Figs. 1.3(a) and (b)) by the so-called "subdiagonalization" matrix technique. From these Green function results we have deduced the dispersion relations of particularly the surface spin waves due to the perpendicular
truncation(s) and calculated the intensities of spin-wave modes. Also by the "subdiagonalization" technique, we have established a general scheme for deriving the appropriate Green functions and henceforth deducing the spin wave behavior in a geometrically more complicated ferromagnetic structure (see Fig. 1.3(c)). The spin-wave spectra and spectral intensities have been calculated explicitly for two special cases of particular interest: a perpendicular interface in a "binary" film with uniform thickness (see Fig. 4.2) and a surface step on a homogeneous thin film (see Fig. 4.7).

For all the ferromagnetic single-layered structures examined, we have discussed the finite-size effects on the behavior of the bulk and surface (interface) spin waves. Specifically, we have examined the asymptotic behavior of spin waves in these single-layered structures in two types of geometrical limits: semi-infinite media (see Figs. 1.1(a) and (c)) and complete film (see Fig. 1.1(b)). As expected, the standard results have been recovered from our new results in these limits.

As for ferromagnetic multilayer structures, we have derived the Green functions for infinite and semi-infinite superlattices either with 2D translational symmetry (see Figs. 1.2(a) and (b)) or with a pair of truncations or cleavages (see Figs. 1.4(a) and (b)). In the latter case (with perpendicular cleavages), the "subdiagonalization" technique has been extended and used appropriately. Accordingly, the superlattice spin-wave spectra and spectral intensities have been calculated in detail. In the case of uncleaved superlattices, our general results have reduced to the previously-derived results in appropriate simplifications. In the case of perpendicularly cleaved
superlattices, we have discussed the finite-size effects on the behavior of the superlattice bulk and surface spin waves and examined the limiting case where the distance between the cleavages becomes effectively infinite.

The Green function expressions obtained in this thesis can be straightforwardly applied to calculate many other experimentally observable quantities (such as cross sections in light scattering and absorption strengths in spin wave resonance) in addition to the spin-wave spectra and intensities. In these applications we need to calculate various spin-spin correlation functions such as \( \langle S^-(t)S^+, (t') \rangle \) and \( \langle S^+(t)S^-, (t') \rangle \) (which can be deduced straightforwardly from the imaginary part of the Green functions). The theory developed in this thesis can also be extended in a variety of aspects as summarized below.

§ 6.2 Some Possible Extensions

As the first study of its type, our theoretical analysis in this thesis was restricted to certain particular physical situations of low-dimensional structures. Many of these structures have recently been fabricated in laboratories (e.g., see Fig. 6.1) for experimental studies. However, the physical conditions and geometries of the layered structures that we have considered are not the only possibilities allowed by the experimental conditions and by the technology of nanostructure materials fabrication. Here we briefly discuss some aspects in which our studies could be extended.

First, our results could be extended to other lattice structures
Fig. 6.1  A schematic sketch of an array of NiFe ferromagnetic wires fabricated for Brillouin light scattering experiments [after Gurney et al 1991].
(e.g., b.c.c. and f.c.c.) and other surface (interface) orientations (e.g., (110) and (111)). The treatment of these lattice structures and surface orientations is entirely straightforward following the same methods; in many cases it involves making only minor redefinitions of structural factors \( \Lambda_1(q_z) \) or \( \Lambda_2(q_y) \) and Brillouin zone parameters, by analogy with previous calculations for spin-wave dispersion relations (e.g., see Kontos 1985). The qualitative features of the spin waves would remain generally similar to those obtained for the simple cubic lattice structure and the (001) surfaces (interfaces). But detailed results, such as the existence conditions for surface modes, would be modified. Another extension would be to other magnetically-ordered materials, such as antiferromagnetic layered structures. This would require some more significant algebraic modifications to our previous treatment for ferromagnets, and the spin wave behavior in antiferromagnets would be quite different (e.g., because there are two sublattices of spins in antiferromagnets).

Second, our present analysis of layered structures could be extended from symmetric surfaces to asymmetric surfaces, from free surfaces to perturbed surfaces, and from ferromagnetically coupled interfaces to antiferromagnetically coupled interfaces. The extensions from symmetric surfaces to asymmetric surfaces would be straightforward. For example, the spin-wave spectra in an \( N \)-layer complete film with asymmetric surface parameters \( J_{sk} \) and \( H_{ask} \) (\( \kappa = 1 \) for one surface and \( \kappa = 2 \) for the other) would be given by

\[
W = \sin((N+1)ka) - (c_1 + c_2)\sin(Nka) + c_1 c_2 \sin((N-1)ka) = 0 \quad (6.1)
\]

with
\[ c_\kappa = 1 - \frac{g_{\mu \nu} H_{\text{ASK}}}{J_S} \left( 1 - \frac{J_{\text{SK}}}{J} \right) \Lambda_2(q_{\kappa}) \quad (\kappa = 1, 2) \]  

(6.2)

However, the extensions from free surfaces to perturbed surfaces would require some methodological modifications except for structures with 2D translational symmetry. In case of perturbed surfaces, all the \( N \times N \) submatrices of \( A \) and \( R \) in (3.35) for a truncated \( N \)-layer film, for instance, can no longer be simultaneously diagonalized. We expect that this type of extension would rely largely upon numerical analysis.

Third, for superlattices, we could straightforwardly extend the mathematical device of introducing a fictitious superlattice (as used in § 5.2 and § 5.4 for semi-infinite superlattices) and apply it to finite superlattices (with an arbitrary finite number \( N_0 \) of unit cells). Let us take the case of finite superlattices with 2D translational symmetry as an example. We could introduce two semi-infinite fictitious superlattices situated on both sides of a finite superlattice and let them form an infinite superlattice with one decoupled "interface" (identical to the one shown in Fig. 5.5) between the 0th and 1st unit cells and another similar decoupled "interface" between the \( N_0 \)th and \((N_0 + 1)\)th unit cells. Then the matrix form of the equation of motion for the Green functions remains formally the same as (5.28) with the partitioned matrix \( R \) being modified as follows:

\[
R(N, \kappa, n; N', \kappa', n') = r_1 n_1 \delta_{n_1 n'} \delta_{\kappa_1 \kappa'} \left( \delta_{N_1 N'} + \delta_{N, N_0 + 1} \delta_{N', N_0} \right) \\
+ r_2 n_2 \delta_{n_2 n'} \delta_{\kappa_2 \kappa'} \left( \delta_{N_0 N'} + \delta_{N_0 N_0} \delta_{N', N_0} \right) \\
- J_1 n_1 \delta_{n_1 n'} \delta_{\kappa_1 \kappa'} \left( \delta_{N_1 N'} + \delta_{N, N_0 + 1} \delta_{N', N_0} \right) \\
- J_2 n_2 \delta_{n_2 n'} \delta_{\kappa_2 \kappa'} \left( \delta_{N_0 N'} + \delta_{N_0 N_0} \delta_{N', N_0} \right) 
\]  

(6.3)
where \( r_k \) remains the same as (5.31). By analogy with the algebraic procedures in § 3.1 and § 5.2, we could derive the required Green functions and accordingly calculate the dispersion relations and spectral intensities of spin waves in the finite superlattice. We could imagine that the bulk spin-wave modes in finite superlattices would be discrete (with "quantized" frequencies) and finite in number (rather than forming bulk continuum bands as in the case of infinite and semi-infinite superlattices) due to the finite-size effects.

Finally, we believe that the particular submatrix diagonalization technique developed in this thesis could be applied to theoretical studies of ordered magnetic systems without translational symmetry. The simplest example in this category might be a ferromagnetic solid box (i.e., the analogy of the study of quantum "dots" in semiconductors).
APPENDIX A

INVERTING SOME PARTITIONED MATRICES

In this appendix, we present a general procedure (required in Chapter 4) for inverting a partitioned matrix and we demonstrate its applications to various special cases in Chapter 4.

Let us consider a partitioned matrix $\mathbf{M}$ in the following form:

$$
\mathbf{M} = \begin{pmatrix}
\mathbf{M}_1 & \mathbf{T} \\
\mathbf{T}' & \mathbf{M}_2
\end{pmatrix}
$$

(A.1)

where $\mathbf{M}_k$ ($k = 1, 2$), $\mathbf{T}$, and $\mathbf{T}'$ may be ordinary matrices (with elements being c-numbers) or other partitioned matrices (with elements being matrices again). The inverse of $\mathbf{M}_k$ is denoted by $\mathbf{N}_k = \mathbf{M}_k^{-1}$. Note that the dimension of $\mathbf{M}_1$ is not necessarily the same as the dimension of $\mathbf{M}_2$. It can be easily checked (e.g., by direct matrix multiplication) that the inverse of $\mathbf{M}$ is

$$
\mathbf{N} = \mathbf{M}^{-1} = \begin{pmatrix}
\mathbf{Z}_1^{-1} & -\mathbf{N}_1 \mathbf{T} \mathbf{Z}_2^{-1} \\
-\mathbf{N}_2 \mathbf{T}' \mathbf{Z}_1^{-1} & \mathbf{Z}_2^{-1}
\end{pmatrix}
$$

(A.2)

where

$$
\mathbf{Z}_1 = \mathbf{M}_1^{-1} - \mathbf{T} \mathbf{N}_2 \mathbf{T}'
$$

(A.3)

$$
\mathbf{Z}_2 = \mathbf{M}_2^{-1} - \mathbf{T}' \mathbf{N}_1 \mathbf{T}
$$

(A.4)

If we take $\mathbf{M}_1 = \mathbf{I}$, then $\mathbf{N}_1 = \mathbf{I}$ and (A.2) becomes

$$
\begin{pmatrix}
\mathbf{I} & \mathbf{T} \\
\mathbf{T}' & \mathbf{M}_2
\end{pmatrix}^{-1} = \begin{pmatrix}
\mathbf{I} + \mathbf{T} \mathbf{Z}_2^{-1} \mathbf{T}' & -\mathbf{T} \mathbf{Z}_2^{-1} \\
-\mathbf{Z}_2^{-1} \mathbf{T}' & \mathbf{Z}_2^{-1}
\end{pmatrix}
$$

(A.5)

where

$$
\mathbf{Z}_2 = \mathbf{M}_2^{-1} - \mathbf{T}' \mathbf{T}
$$

(A.6)
Due to the following matrix identity:

\[
\begin{pmatrix}
I & T \\ T' & M_2
\end{pmatrix} = 
\begin{pmatrix}
I & 0 \\ T' & I
\end{pmatrix}
\begin{pmatrix}
I & 0 \\ 0 & M_2 - T'T
\end{pmatrix}
\begin{pmatrix}
I & T \\ 0 & I
\end{pmatrix}
\]  

(A.7)

we have

\[
\text{det}
\begin{pmatrix}
I & T \\ T' & M_2
\end{pmatrix} = \text{det}(M_2 - T'T)
\]  

(A.8)

If we take \( T' = 0 \) in (A.5), it becomes

\[
\begin{pmatrix}
I & T \\ 0 & M_2
\end{pmatrix}^{-1} = 
\begin{pmatrix}
I & -TN_2 \\ 0 & N_2
\end{pmatrix}
\]  

(A.9)

A similar matrix identity can also be obtained

\[
\begin{pmatrix}
M_1 & 0 \\ T' & I
\end{pmatrix}^{-1} = 
\begin{pmatrix}
M_1 & 0 \\ -T'N_1 & I
\end{pmatrix}
\]  

(A.10)

Now we discuss the applications of the above matrix identities to some special cases in the relevant sections of the text. When the identity (A.10) is used to invert the partitioned matrix \( W = W_2 \) expressed by (4.58) in § 4.3, we have

\[
M_1 = W = I - X_2P - X_2L^TX_1L, \quad \text{and} \quad T' = - \begin{pmatrix}
X_2^2 \\
X_2^2 \\
\vdots
\end{pmatrix}
(P + L^TX_1L)
\]

Once \( M_1 = W^{-1} \) in this case) is obtained, we immediately get \( W_2^{-1} \) in terms of \( W^{-1} \) from (A.10).

When we use (A.2) to invert the partitioned matrix \( I - B'R' \) on the right-hand side of (4.34) in § 4.2, we have...
\[ M_1 = \begin{pmatrix}
1 & \cdots & -x_1^3c_1' \\
-\frac{x_1^2c_1'}{J_1} & 1 & \cdots \\
0 & 1-x_1'c_1' & 1
\end{pmatrix}, \quad T = -\frac{J_{12}}{J_1} \begin{pmatrix}
\cdots & \cdots & \cdots \\
x_1^3 & 0 & \cdots \\
x_1^2 & 0 & \cdots \\
x_1' & 0 & \cdots
\end{pmatrix} \]

\[ T' = -\frac{J_{12}}{J_2} \begin{pmatrix}
0 & x_2' \\
\cdots & \cdots \\
0 & x_2^2 \\
0 & x_2^3 \\
\cdots & \cdots
\end{pmatrix}, \quad \text{and} \quad M_2 = \begin{pmatrix}
1-x_2'c_2' & 0 & \cdots \\
-x_2'^2c_2' & 0 & \cdots \\
-x_2'^3c_2' & 0 & \cdots \\
\cdots & \cdots & \cdots
\end{pmatrix} \]

Obviously, the matrices \( M_1 \) and \( M_2 \) here can be inverted by using (A.9) and (A.10) respectively. We then substitute \( N_\kappa = M_\kappa^{-1} (\kappa = 1, 2) \) into (A.3) and (A.4) to calculate \( Z_1 \) and \( Z_2 \) in this case. When we use the matrix identities (A.9) and (A.10) once again to invert the partitioned matrices \( Z_1 \) and \( Z_2 \), a matrix expressed by (4.38) in § 4.2 must be inverted first. Finally, (A.2) gives the result for \( (I-B'R')^{-1} \).
APPENDIX B
DERIVATION OF THE GREEN FUNCTIONS FOR AN INFINITE SUPERLATTICE

In this appendix we give the algebraic details in obtaining the
Green functions for an infinite superlattice with 2D translational
symmetry (quoted in § 5.1) from those for complete films by using a
Dyson equation approach. For brevity of notation, the dependence of the
Green functions on $E$ and $q_{||}$ is not written down explicitly.

On substituting (5.10) and (5.17) into the Dyson equation (5.18),
we get (taking $\kappa = 1$ and $\kappa = 2$ in turn)

$$
G(N, 1, n; N', k', n') = -\frac{B_1(n; n')}{\pi J_1} \delta_{k_1} \delta_{NN'}
+ \frac{J_1}{\pi} [G(N-1, 2, N_2; N', k', n') + B_1(n; N_1)G(N, 2, 1; N', k', n')]
$$

(B.1)

$$
G(N, 2, n; N', k', n') = -\frac{B_2(n; n')}{\pi J_2} \delta_{k_2} \delta_{NN'}
+ \frac{J_2}{\pi} [G(N, 1, N_1; N', k', n') + B_2(n; N_2)G(N+1, 1, 1; N', k', n')]
$$

(B.2)

Next, substituting (B.1) into the right-hand side of (B.2) and putting
$n = 1$ and $N_2$ in turn, we get

$$(a_1 a_2^{-1})g(N; N') + b_1 b_2 g(N+1; N') + a_1 b_2 h(N; N') + b_1 a_2 h(N-1; N')$$

$$= \frac{1}{\pi J_1} [a_{1 B}(n; n') \delta_{NN'} + b_{1 B}(1; n') \delta_{N+1, N'}] \delta_{k_1} + \frac{J_1}{\pi J_2} B_2(1; n') \delta_{k_2} \delta_{NN'}$$

(B.3)
a_1 b_2 g(N; N') + b_1 a_2 g(N+1; N') + (a_1 a_2 - \rho^{-1}) h(N; N') + b_1 b_2 h(N-1; N')

= \frac{1}{\pi J^2} \left[ b_1 B_1(N_1; n') \delta_{NN'} + a_2 B_1(1; n') \delta_{N+1, N'} \right] \delta_{\kappa_1} + \frac{1}{\pi J^2} B_2(N_2; n') \delta_{NN'} \delta_{\kappa_2} \delta_{NN'}

(B.4)

where the shorthand notations

\rho = \frac{J^2}{J_1 J_2}, \ a_\kappa = B_\kappa(1; 1) = B_\kappa(N_1; N), \ b_\kappa = B_\kappa(N_2; 1) = B_\kappa(1; N_2)

g(N; N') = G(N, 2, 1; N', \kappa', n'), \text{ and } h(N; N') = G(N, 2, N; N', \kappa', n')

are used in (B.3) and (B.4). By eliminating \( g(N+1; N') \) and \( h(N-1; N') \) from (B.3) and (B.4), we can express \( g \) in terms of \( h \) and vice versa as follows:

\[
g(N; N') = \frac{1}{(a_1^2 - b_2^2) a_1 - \rho^{-1} a_2} \left\{ -\rho^{-1} b_2 h(N; N') - (a_1^2 - b_2^2) b_1 h(N-1; N') \right. \\
+ \frac{1}{\pi J^2} (a_2^2 - b_2^2) B_1(N_1; n') \delta_{N_1 N_1'} + \frac{1}{\pi J^2} \left[ a_2 B_2(1; n') - b_2 B_2(N_2; n') \right] \delta_{\kappa_2} \delta_{NN'} \right. \\
+ \left. \frac{1}{\pi J^2} \left[ a_2 B_2(N_2; n') - b_2 B_2(1; n') \right] \delta_{NN'} \delta_{\kappa_2} \delta_{NN'} \right\}
\]

(B.5)

\[
h(N; N') = \frac{1}{(a_1^2 - b_2^2) a_1 - \rho^{-1} a_2} \left\{ -\rho^{-1} b_2 g(N; N') - (a_1^2 - b_2^2) b_1 g(N+1; N') \right. \\
+ \frac{1}{\pi J^2} (a_2^2 - b_2^2) B_1(1; n') \delta_{\kappa_1} \delta_{N+1, N'} + \frac{1}{\pi J^2} \left[ a_2 B_2(N_2; n') - b_2 B_2(1; n') \right] \delta_{\kappa_2} \delta_{NN'} \right. \\
+ \left. \frac{1}{\pi J^2} \left[ a_2 B_2(N_2; n') - b_2 B_2(1; n') \right] \delta_{NN'} \delta_{\kappa_2} \delta_{NN'} \right\}
\]

(B.6)

The substitution of (B.5) into the left-hand side of (B.4) yields a finite-difference equation for \( h \)

\[
h(N-1; N') - d h(N; N') + h(N+1; N') = \nu \delta_{NN'} + \nu' \delta_{N+1, N'}
\]

(B.7)

where we denote
\[ d = \frac{\rho^{-1}a_1a_2 + \rho(a_2^2 - b_2^2)(a_2^2 - b_2^2)}{b_1b_2} \]  

\[ v = \frac{1}{\pi J_{12}} \frac{B_1(N_1; n')}{b_1} \delta_{\kappa, 1} + \frac{1}{\pi J_{12}^2} \left[ \rho \frac{a_1}{b_1} B_2(1; n') + \frac{\rho a_2 - 1}{b_1b_2} B_2(N_2; n') \right] \delta_{\kappa, 2} \] 

\[ v' = \frac{1}{\pi J_{12}} \left[ \rho \frac{a_2^2 - b_2^2}{b_2} B_1(N_1; n') + \frac{\rho(a_2^2 - b_2^2)a_1 - a_2}{b_1b_2} B_1(1; n') \right] \delta_{\kappa, 1} \]

\[ + \frac{J_1}{\pi J_{12}^2} \rho \left[ \frac{a_2}{b_2} B_2(1; n') - B_2(N_2; n') \right] \delta_{\kappa, 2} \]

Likewise, the substitution of (B.6) into the left-hand side of (B.3) yields a finite-difference equation for \( g \):

\[ g(N-1; N') - d g(N; N') + g(N+1; N') = u \delta_{NN'} + u' \delta_{N+1, N} + u'' \delta_{N-1, N'} \]

\[ (B.10) \]

where

\[ u = \frac{1}{\pi J_{12}} \left[ \rho \frac{a_2^2 - b_2^2}{b_2} B_1(1; n') + \frac{\rho(a_2^2 - b_2^2)a_1 - a_2}{b_1b_2} B_1(N_1; n') \right] \delta_{\kappa, 1} \]

\[ + \frac{J_1}{\pi J_{12}^2} \left[ \rho \frac{a_1}{b_1} B_2(N_2; n') + \frac{\rho a_2 - 1}{b_1b_2} B_2(1; n') \right] \delta_{\kappa, 2} \] 

\[ u' = \frac{1}{\pi J_{12}} \frac{B_1(1; n')}{b_1} \delta_{\kappa, 1} \] 

\[ u'' = \frac{J_1}{\pi J_{12}^2} \rho \left[ \frac{a_2}{b_2} B_2(N_2; n') - B_2(1; n') \right] \delta_{\kappa, 2} \]

Next, noting that the solution of the following standard finite-difference equation:
\[ f(N-1; N') = (x + x^{-1})f(N; N') + f(N+1; N') = \delta_{NN'} \]  
\hspace{1cm} \text{(B.14)}

is \(\text{e.g., see Wax 1954} \)

\[ f(N; N') = \frac{x^{N-N'}}{x - x^{-1}} \]  
\hspace{1cm} \text{(B.15)}

we immediately get the solutions of (B.7) and (B.10) as follows:

\[ h(N; N') = v \frac{x^{N-N'}}{x - x^{-1}} + v' \frac{x^{N-N'+1}}{x - x^{-1}} \]  
\hspace{1cm} \text{(B.16)}

\[ g(N; N') = u \frac{x^{N-N'}}{x - x^{-1}} + u' \frac{x^{N-N'+1}}{x - x^{-1}} + u'' \frac{x^{N-N'-1}}{x - x^{-1}} \]  
\hspace{1cm} \text{(B.17)}

where \( x \) is here defined by

\[ x + x^{-1} = d \quad (|x| \leq 1) \]  
\hspace{1cm} \text{(5.19)}

Finally, we can substitute (B.16) and (B.17) back into the right-hand side of (B.1) to get \( G(N,1,n; N', \kappa', n') \) for \( \kappa' = 1 \) and \( \kappa' = 2 \) in turn. In the same manner we can derive \( G(N,2,n; N', \kappa', n') \). By inspection of our algebraic results, we find that \( G(N,\kappa,n; N', \kappa', n') \) satisfies the following symmetry properties (for any integer values of \( N, N', N'' \)):

\[ G(N,\kappa,n; N', \kappa', n') = G(N+N'', \kappa, n; N' + N'', \kappa', n'') \]  
\hspace{1cm} \text{(B.18)}

\[ G(N,\kappa,n; N', \kappa', n') = G(N', \kappa', n'; N, \kappa, n) \]  
\hspace{1cm} \text{(B.19)}

as expected. In particular, (B.19) is consistent with the fact that the partitioned matrices \( A \) in (5.6) and \( C \) in (5.10) are symmetric.

As an algebraically straightforward extension of the above derivations, the Green functions for a perpendicularly cleaved infinite superlattice can be similarly obtained in the "subdiagonal" representation.
REFERENCES


Bloch F. (1930), *Z.Phys.* 61, 206


V.M. Agranovich and R. Loudon, (North-Holland: Amsterdam), p. 1


Dyson F.J. (1956), Phys. Rev. 102, 1217


Fallot M. (1936), Ann. Phys. 6, 305


Fillipov B.N. (1967), Sov. Phys. 9, 1048


Griffith J.H.E. (1946), Nature 158, 670

*J.Appl.Phys.* 53, 2078
Gurney B.A., Baumgart P., Speriosu V., Fontana R., Patlac A., Logan T.,
and Humbert P. (1991), *Proc.Intl.Conf. on Magnetic Films and
Surfaces* (Glasgow, 1991), p. 474
(Academic: New York)
Holstein T. and Primakoff H. (1940), *Phys.Rev.* 58, 1098
New York)
B29, 2879
Magnan H., Chandiesris D., Villette B., Heckmann O., and Lecante J.
4490
Meada A., Kume M., Ogura T., Kuroki K., Yamada T., Nishikawa M., and
Mills D.L. (1984), in Surface Excitations, ed. V.M. Agranovich and
R. Loudon, (North-Holland: Amsterdam), p. 379
Puszkarski H. (1979), Prog. Surf. Sci. 9, 191
Rickayzen G. (1980), Green's Functions and Condensed Matter (Academic:
London)
Phys. Rev. B52, 350


Weiss P. (1907), *J. Phys.* 6, 661

Weiss P. (1937), *Ext. Actes VII Congr. intern. froid* 1, 508


Zubarev D.N. (1960), *Usp. Fiz. Nauk* 71, 71