

Three Magnon Excitations in Alternating Quantum Spin/Bond Chains

by

José Luis Martínez Cuéllar

A Thesis

Submitted to the Faculty of Graduate Studies

in Partial Fulfillment of the Requirements

for the Degree of

MASTER OF SCIENCE

Department of Physics

The University of Manitoba

Winnipeg, Manitoba

©June, 1997



**National Library
of Canada**

**Acquisitions and
Bibliographic Services**

**395 Wellington Street
Ottawa ON K1A 0N4
Canada**

**Bibliothèque nationale
du Canada**

**Acquisitions et
services bibliographiques**

**395, rue Wellington
Ottawa ON K1A 0N4
Canada**

Your file Votre référence

Our file Notre référence

The author has granted a non-exclusive licence allowing the National Library of Canada to reproduce, loan, distribute or sell copies of this thesis in microform, paper or electronic formats.

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

L'auteur a accordé une licence non exclusive permettant à la Bibliothèque nationale du Canada de reproduire, prêter, distribuer ou vendre des copies de cette thèse sous la forme de microfiche/film, de reproduction sur papier ou sur format électronique.

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

0-612-23412-6

**THE UNIVERSITY OF MANITOBA
FACULTY OF GRADUATE STUDIES
COPYRIGHT PERMISSION**

**THREE MAGNON EXCITATIONS IN ALTERNATING
QUANTUM SPIN/BOND CHAINS**

BY

JOSÉ LUIS MARTÍNEZ CUÉLLAR

**A Thesis submitted to the Faculty of Graduate Studies of the University of Manitoba
in partial fulfillment of the requirements of the degree of**

MASTER OF SCIENCE

Jose Luis Martinez Cuellar © 1997

Permission has been granted to the LIBRARY OF THE UNIVERSITY OF MANITOBA to lend or sell copies of this thesis, to the NATIONAL LIBRARY OF CANADA to microfilm this thesis and to lend or sell copies of the film, and to UNIVERSITY MICROFILMS to publish an abstract of this thesis.

This reproduction or copy of this thesis has been made available by authority of the copyright owner solely for the purpose of private study and research, and may only be reproduced and copied as permitted by copyright laws or with express written authorization from the copyright owner.

A mi madre

Abstract

In this thesis we examine the nature of three magnon excitations in alternating spin/bond ferromagnetic chains. We study a Hamiltonian that describes a chain (composed of two non-identical one-dimensional uniform and homogeneous sublattices) with alternating spin magnitudes, S and S' , and alternating nearest neighbor interactions, J_1 and J_2 . The Recursion Method is used to locate the bound states and their relationship to the three-magnon continuum. The specific cases studied are the $S = S' = 1/2$, $S = 2S' = 1$, and $S = S' = 1$ alternating spin chains. We consider not only the effects of spin alternation but also of varying strengths. For each case, we studied different bond sets, more exactly, $J_1 = 1$ and J_2 equal to 0, $1/4$, $1/2$ and 1.

Acknowledgments

This thesis has matured as a result of the constant suggestions and constructive criticism of Dr. B.W. Southern. I would like to thank him not only for his help, but also for opening the doors to my new life in Canada. I would also like to thank my friends, John Kagan and Glen Radewich, my colleagues, Matilde Bolkovic, Don MacKenzie, Dave Crewson, and the whole team at PBSC Computer Training Centres for their support and understanding. As well, the education that I received at The University of Havana is enormously and gratefully acknowledged.

Contents

Abstract	i
Acknowledgments	ii
1 Introduction	1
2 One and Two-Magnon Excitations	7
2.1 One-magnon Excitations	7
2.2 Two-Magnon Excitations	9
3 Three-Magnon Excitations	18
4 The Recursion Method and the Three-Magnon Problem	28
4.1 Green's Function	28
4.2 The Recursion Method	31
4.3 Tail of the Continued Fraction	33
4.4 Summary	38
5 Results	39
5.1 Uniform Bond Spin $S = S' = \frac{1}{2}$ Case	39
5.1.1 $S = S' = \frac{1}{2}$ Alternating Bond Case	42
5.2 $J_2 \rightarrow 0$ limit	45
5.3 $S = 2S' = 1$ Case	54

5.4	$S = S' = 1$ Case and the Initial Ket Effects	58
6	Summary	65
A	Tail of the Continued Fraction for Multiple Gaps: Mathematica Im- plementation	67

List of Figures

1.1	Graphical representation of an alternating spin/bond chain.	4
2.1	One-magnon excitation energy for an alternating ferromagnetic chain with $S = 2S' = 1$ and $J_1 = 2J_2 = 1$	10
2.2	Two-magnon scattering state continua for an alternating ferromagnetic chain with $S = 2S' = 1$ and $J_1 = 2J_2 = 1$	14
2.3	Two-bound magnon state branches and scattering state continua for an alternating ferromagnetic chain with $S = 2S' = 1$ and $J_1 = 2J_2 = 1$	17
3.1	Three-free magnon scattering state continua for an alternating ferromagnetic chain with $S = 2S' = 1$ and $J_1 = 2J_2 = 1$	22
3.2	The two-bound one-free magnon scattering state continua for an alternating ferromagnetic chain with $S = 2S' = 1$ and $J_1 = 2J_2 = 1$	25
3.3	Three-magnon scattering state continua for an alternating ferromagnetic chain with $S = 2S' = 1$ and $J_1 = 2J_2 = 1$	26
5.1	The two-free magnon continuum and the two-bound state branch of the uniform $S = \frac{1}{2}$ chain.	41
5.2	The three-magnon continuum and the three-bound magnon state branch of the uniform $S = \frac{1}{2}$ chain.	43
5.3	The three-magnon continuum of the uniform $S = \frac{1}{2}$ chain. The star points represent the three-magnon bound states obtained using the Recursion Method.	44

5.4	The three-magnon continuum and the three-magnon bound states of the uniform spin $S = S' = \frac{1}{2}$ chain with alternating bonds ($J_1 = 2J_2 = 1$).	46
5.5	The three-magnon continuum and the three-magnon bound states of the uniform spin $S = S' = \frac{1}{2}$ chain with alternating bonds ($J_1 = 4J_2 = 1$).	47
5.6	Graphical representation of the three-magnon excitation levels in a system of isolated blocks, each block composed of two connected spins, $S = S' = \frac{1}{2}$.	53
5.7	The three-magnon state continuum for the $S = 2S' = 1$ and $J_1 = J_2 = 1$ chain.	55
5.8	The three-magnon state continuum for the $S = 2S' = 1$ and $J_1 = 2J_2 = 1$ chain.	56
5.9	The three-magnon state continuum for the $S = 2S' = 1$ and $J_1 = 4J_2 = 1$ chain.	57
5.10	The three-magnon state continuum for the $S = S' = 1$ and $J_1 = 2J_2 = 1$ chain.	59
5.11	The three-magnon state continuum for the $S = S' = 1$ and $J_1 = 4J_2 = 1$ chain.	60
5.12	Density of states for (a) two magnons on the same site and the third one on the neighboring site, (b) three neighboring magnons on adjacent sites and (c) two neighboring magnons on adjacent sites and the third one on the second-neighboring site for the $S = S' = 1$ and $J_1 = 2J_2 = 1$ chain at $K = 0$.	61
5.13	Density of states for three neighboring magnons on adjacent sites for the $S = S' = 1$ and $J_1 = 2J_2 = 1$ chain at $K = 0$.	63
5.14	Density of states for the first gap region of the $S = S' = 1$ and $J_1 = 2J_2 = 1$ chain at $K = 0$.	64

List of Tables

3.1	Coefficients for each of the terms obtained when the Hamiltonian is applied on a state at an even site with both $x, y \geq 2$	20
3.2	Coefficients for each of the terms obtained when the Hamiltonian is applied on a state at an even site. One of the values of x and y is ≤ 1 while the other is ≥ 2	23
3.3	Coefficients for each of the terms obtained when the Hamiltonian is applied on a state at an even site with both $x, y \leq 1$	24
5.1	Three-magnon excitations for chains of isolated blocks in units of J_1 and where $\Xi = J_1(S + S')$	52

Chapter 1

Introduction

Physics (from the Greek *physika*, meaning nature) is the branch of science dealing with nature at its most fundamental level, the branch searching for the rules that govern the universe. Physicists have always been eager to understand the behavior of atoms, gravity and electromagnetism. They have always wanted to discover the laws of nature. In ancient Greece, some say that natural philosophers like Thales knew that lodestone attracts bits of iron but amber, when rubbed by fur, attracts bits of straw. The similarities between electricity and magnetism have attracted attention for centuries and their investigation resulted in the birth of electrodynamics when Maxwell showed that electricity and magnetism were two aspects of the same phenomenon. But these interests are still alive, especially because the science of electrodynamics underlines much of modern technological civilization. Electrodynamics is brought into play every time a television or lightbulb is turned on, and magnetism with every CD or cassette player used.

Magnetism is the direct result of purely quantum mechanical interactions between atoms, interactions that are a consequence of the constraints placed on electronic wavefunctions by the Pauli Exclusion principle. This principle states that the total wavefunction of a system of fermions must be antisymmetric under a particle interchange. As the spatial and spin parts of the wavefunction cannot have the same

symmetry under exchange, the relative spin orientation of the electrons (as example of fermions) can influence the electrostatic energy of the system.

The study of low-dimensional quantum spin systems has emerged as a central problem in condensed matter physics since the discovery of high T_c superconductivity [1] in lightly doped cuprates with planar structures. Quantum effects are largest for small values of the spin magnitude. These effects are even stronger in one-dimensional quantum spin systems. One-dimensional exchanged-coupled spin systems offer the possibility for describing phenomena that cannot be adequately explained in higher dimensions. Although many exact results are possible in one dimension, (see for example Mattis [2]), these systems still provide a challenge to physicists because they require a many-body solution. One of the first many-body problems which was solved exactly was the spin one-half magnetic chain studied by Bethe [3]. This work has only been recently translated into English and is contained in the book by Mattis [2]. During recent years, mixed quantum spin chains have attracted the interest of theorists [4, 5, 6]. Exactly solvable versions of sophisticated Hamiltonians have been studied using the Bethe Ansatz.

The unusual magnetic behavior of exotic arrays of metal ions have catalyzed our study. For example, a linear chain made up by gadolinium ions bridged by nitronyl nitroxide radicals, $\text{Gd}(\text{hfac})_3\text{NITeT}$, behaves as a one-dimensional material with dominant next-nearest-neighbor (nnn) interactions. Benelli *et al* [7] studied this system using a simple Ising model. A more correct Heisenberg exchange approach would better characterize this system. Some of these systems can be described in terms of isotropic exchange interactions which alternate in strength along a chain. The chains are composed of two sublattices which have unequal spin magnitudes, S and S' .

A review of these systems and the methods for their study has to start with the study of the Pauli principle and the constraints that it imposes on a group of atoms in a lattice. The effect of the Pauli principle can be described by operators of the form $\vec{S}_i \cdot \vec{S}_j$ where $\vec{S}_i$ and $\vec{S}_j$ are spin operators corresponding to different

atomic sites. In the case of two hydrogen-like atoms, there is a splitting in the energy levels of the system depending on the spatial wavefunction symmetry under exchange. If the spatial wavefunction is symmetric, then the corresponding two electron spin wavefunction must be antisymmetric and vice versa. Thus, the splitting depends on the symmetry of the spin wavefunction and can be expressed by a Hamiltonian of the form:

$$\widehat{H}^{spin} = -J\vec{S}_1 \cdot \vec{S}_2 \quad (1.1)$$

where J is a function of electrostatic force between electrons and is known as the exchange integral. When J is positive, it favors alignment of the spins (ferromagnetism) and for J negative, it favors antiparallel alignment of the spins (antiferromagnetism).

The Hamiltonian above can be extended to include the interactions between all pairs of atoms on a lattice:

$$\widehat{H}^{Heis} = -\frac{1}{2} \sum_{ij} J_{ij}(\vec{S}_i \cdot \vec{S}_j) \quad (1.2)$$

This operator was originally proposed by Dirac [8] but it is known as the *Heisenberg exchange Hamiltonian*. It was originally proposed as a model for strongly magnetic systems.

The exchange coefficients J_{ij} depend on many factors but the degree of overlap between the i^{th} and j^{th} electrons is a important one. When r_{ij} increases (the distance between the two electrons), the magnitude of J_{ij} decreases rapidly. If the material is an insulator, the range of the interactions is essentially restricted to nearest and next nearest neighbor spins on the lattice of atoms. Higher order terms are generally much weaker. So, it is very realistic to assume that the interactions are important only between nearest neighbors. The Hamiltonian (1.2) becomes

$$\widehat{H}^{Heis} = -\frac{1}{2} \sum_i \sum_{\delta} J_{i,i+\delta}(\vec{S}_i \cdot \vec{S}_{i+\delta}) \quad (1.3)$$

where δ represents the sum over all nearest-neighbor atoms. We will restrict our analysis to the case of a one-dimensional lattice reducing the Heisenberg Hamiltonian

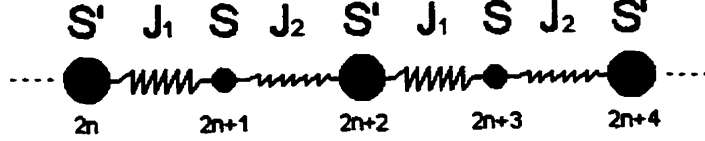


Figure 1.1: Graphical representation of an alternating spin/bond chain.

even further to

$$\widehat{H}^{Heis} = - \sum_i J_{i,i+1} (\vec{S}_i \cdot \vec{S}_{i+1}) \quad (1.4)$$

Our problem will be to consider a chain composed of two non-identical sublattices, each being uniform and homogeneous (Figure (1.1)). The Hamiltonian for these two non-identical one-dimensional sublattices with alternating spin magnitudes, S and S' , and alternating nearest neighbor interactions can be expressed as

$$\widehat{H} = - \sum_{n=1}^{N/2} \left[J_1 (\vec{S}'_{2n} \cdot \vec{S}_{2n+1}) + J_2 (\vec{S}_{2n+1} \cdot \vec{S}'_{2n+2}) \right] \quad (1.5)$$

where the total number of sites of the chain N is even and J_1 and J_2 represent the interactions which alternate in strength along the chain. $\vec{S}'_{2n}$ and $\vec{S}_{2n+1}$ are quantum spin operators at the even and odd sites respectively and they satisfy the commutation relations

$$[S_{i\alpha}, S_{j\beta}] = \delta_{ij} \epsilon_{\alpha\beta\gamma} S_{i\gamma} \quad (1.6)$$

with $\alpha, \beta, \gamma = x, y, z$.

We assume an infinite chain (or a large number of sites N) in which we impose periodic boundary conditions to ensure translational invariance

$$[\hat{\tau}, \widehat{H}] = 0 \quad (1.7)$$

where $\hat{\tau}$ is an operator that performs a translation on each sublattice. This commutation relation indicates that the total wavevector K is a good quantum number. The Hamiltonian (1.5) also satisfies the following commutation relations

$$[\hat{S}_{\text{tot}}^2, \hat{H}] = 0 \quad (1.8)$$

$$[S_{\text{tot}}^z, \hat{H}] = 0 \quad (1.9)$$

with $\hat{S}_{\text{tot}}^2$ denoting the total spin operator and S_{tot}^z the total spin in the z -direction. Thus, $S_{\text{tot}}^z = \sum_{n=1}^{N/2} (S_{2n}^z + S_{2n+1}^z)$ is also a good quantum number.

The ferromagnetic state in which all spins are aligned along some arbitrary direction is an exact eigenstate of $\hat{H}$ with eigenvalue $E_0 = -(N/2)SS'(J_1 + J_2)$. Considering a very weak magnetic field in the z direction, the rotational symmetry (1.8) of our Hamiltonian is broken. We denote the state with spins aligned in this direction by $|0\rangle$ and we assume that this is the lowest energy state, or ground state. The ground state has a z -component of total spin $S_{\text{tot}}^z = \frac{N}{2}(S + S')$.

The excitations relative to the ground state can be classified according to the total amount of reduction in the z -component of the total spin, $S^z = \frac{N}{2}(S + S') - m$, where such a state is called a m -magnon excitation. The general problem is to solve the Schrödinger equation

$$\hat{H}|\psi_m\rangle = E_m(K)|\psi_m\rangle \quad (1.10)$$

for the excitation energies $E_m(K)$ of the m -magnon state as a function of total wavevector K .

These magnon excitations have been observed in real materials. Methods such as inelastic magnetic neutron scattering, infrared absorption, and ESR experiments are used to detect magnons. For example, Hoogerbeets *et al.* [9] used ESR experiments to observe the first 7 bound magnon levels in $(\text{C}_6\text{H}_{11}\text{NH}_3)\text{CuCl}_3$, a quasi-one-dimensional $S = \frac{1}{2}$ nearly Heisenberg ferromagnetic compound. As well, Torrance and Tinkham [10] observed bound magnons in the $S = \frac{1}{2}$ quasi-one-dimensional ferromagnet $\text{CoCl}_2 \cdot 2\text{H}_2\text{O}$ using far-infrared absorption.

The focus of this thesis is on the solution of the three-magnon problem of an alternating ferromagnetic chain described by the Hamiltonian (1.5). The two-magnon excitations of a more general Hamiltonian have been studied previously by Medved *et al* [11]. In Chapter 2, we use their analytic approach to solve both the one and two-magnon problems for the Hamiltonian (1.5). The results of the one-magnon excitation energy will be examined and used to obtain the two-magnon scattering state continuum. We will discuss how to obtain the two-bound magnon state solutions numerically. Chapter 3 discusses the three-magnon problem and the three-magnon scattering state continua will be obtained using the two-magnon results. However, the task of obtaining the three-bound magnon states will require a change in strategy. Chapter 4 will review the concept of Green's functions and, specially, how to obtain the distribution of eigenvalues or the density of states (DOS). This knowledge will provide a way to identify the presence of bound states for different cases of interest. We will also describe the recursion method [12, 13], which will allow us to tridiagonalize the Hamiltonian and obtain a continued fraction representation for the density of states. We will discuss methods of terminating the infinite continued fraction. Chapter 5 applies these methods to different systems in which we try to identify the presence of bound states. Finally, Chapter 6 summarizes the results of the thesis.

Chapter 2

One and Two-Magnon Excitations

We first review the treatment of the one and two-magnon excitations in alternating spin/bond chains [15, 14, 11].

2.1 One-magnon Excitations

A general one-magnon state can be written as

$$|\psi_1\rangle = \sum_{n=1}^{N/2} [a_{2n}|2n\rangle + a_{2n+1}|2n+1\rangle] \quad (2.1)$$

where the ket $|n\rangle$ represents the state with the z-component of the nth spin reduced by one unit relative to the ground state.

Using the commutation relations (1.6) satisfied by the spin operators, we have

$$\vec{S}'_{2n'} \cdot \vec{S}_{2n+1}|2i\rangle = \delta_{in'}\sqrt{SS'}|2n+1\rangle + S(S' - \delta_{in})|2i\rangle \quad (2.2)$$

and

$$\vec{S}'_{2n'} \cdot \vec{S}_{2n+1}|2i+1\rangle = \delta_{in'}\sqrt{SS'}|2n'\rangle + S'(S - \delta_{in})|2i+1\rangle \quad (2.3)$$

The Schrödinger equation $\hat{H}|\psi_1\rangle = E_1|\psi_1\rangle$ results in equations relating the amplitudes a_r

$$\begin{aligned} (E_1 - S(J_1 + J_2)) a_{2n} &= -\sqrt{SS'}(J_1 a_{2n+1} + J_2 a_{2n-1}) \\ (E_1 - S'(J_1 + J_2)) a_{2n+1} &= -\sqrt{SS'}(J_1 a_{2n} + J_2 a_{2n+2}) \end{aligned} \quad (2.4)$$

where E_1 is measured relative to the ground-state energy $E_0 = -(N/2)SS'(J_1 + J_2)$.

These equations are easily solved considering that the solutions are plane waves with different amplitudes on the even and odd sites:

$$\begin{aligned} a_{2n} &= \alpha e^{2ink} \\ a_{2n+1} &= \beta e^{i(2n+1)k} \end{aligned} \quad (2.5)$$

Periodic boundary conditions are assumed and this restricts k to the range $-\pi/2 \leq k \leq \pi/2$.

Substitution into the equations leads to the following 2×2 matrix eigenvalue equation

$$\begin{bmatrix} [E_1 - \varepsilon] & \nu_k \\ \nu_k^* & [E_1 - \varepsilon'] \end{bmatrix} \begin{pmatrix} \alpha \\ \beta \end{pmatrix} = 0 \quad (2.6)$$

where

$$\varepsilon = S(J_1 + J_2) \quad (2.7)$$

$$\varepsilon' = S'(J_1 + J_2) \quad (2.8)$$

$$\nu_k = \sqrt{SS'}(J_1 e^{ik} + J_2 e^{-ik}) \quad (2.9)$$

and ν_k^* is the complex conjugate of ν_k .

The eigenvalue E_1 can be written as

$$E_k^\mu = B + \frac{1}{2}\mu\sqrt{\chi^2 + 4|\nu_k|^2} \quad (2.10)$$

where

$$B = \frac{1}{2}(S + S')(J_1 + J_2) \quad (2.11)$$

and

$$\chi = (S - S')(J_1 + J_2) \quad (2.12)$$

The solutions of the excitations are characterized by real wavevectors. The index $\mu = \pm 1$ labels the two branches which by convention are referred to as optic for the upper branch and acoustic for the lower branch and the dimensionless wave vector

k lies in the range 0 to $\pi/2$. The figure (2.1) displays the general form of the one-magnon excitation energy E_k^μ for an alternating ferromagnetic chain with $S = 2S' = 1$ and exchange coefficients $J_1 = 2J_2 = 1$ (E_k^μ is in units of J_1). In general, there is a non zero gap between the two branches at the Brillouin-zone boundary ($k = \pi/2$):

$$E_{\text{gap}} = 2\sqrt{B^2 - 4SS'J_1J_2} \quad (2.13)$$

This gap vanishes only in the uniform case where $S = S'$ and $J_1 = J_2$. Hence, an important difference between uniform and non-uniform magnetic chains is the presence of gaps in the excitation spectrum.

2.2 Two-Magnon Excitations

The two-magnon states $|\psi_2\rangle$ can be written as

$$\begin{aligned} |\psi_2\rangle = \sum_{n \leq m} [& a_{2n,2m} |2n, 2m\rangle + a_{2n,2m+1} |2n, 2m+1\rangle + \\ & + a_{2n-1,2m} |2n-1, 2m\rangle + a_{2n+1,2m+1} |2n+1, 2m+1\rangle] \end{aligned} \quad (2.14)$$

where the ket $|r, s\rangle$ with $r < s$ represents the state with single deviations on the r th and s th spins relative to the ground state while the ket $|r, r\rangle$ represents the state with two spin deviations on the same (r th) site.

As in the one-magnon problem, we consider the two-magnon Schrödinger equation $\widehat{H}|\psi_2\rangle = E_2|\psi_2\rangle$, where E_2 is the two-magnon excitation energy measured relative to the ground state energy E_0 . The equations relating the various amplitudes are obtained by applying our Hamiltonian (1.5) to the general form of the wavefunction (2.14) and then equating the coefficients of each basis ket. The resulting equations can be artificially grouped into two sets. One set involves amplitudes with spin deviations separated by at least two sites ($m > n$) that we will refer as the “noninteracting equations”. The other set will be called the “interacting equations” and will involve amplitudes with spin deviations on the same or neighboring sites.

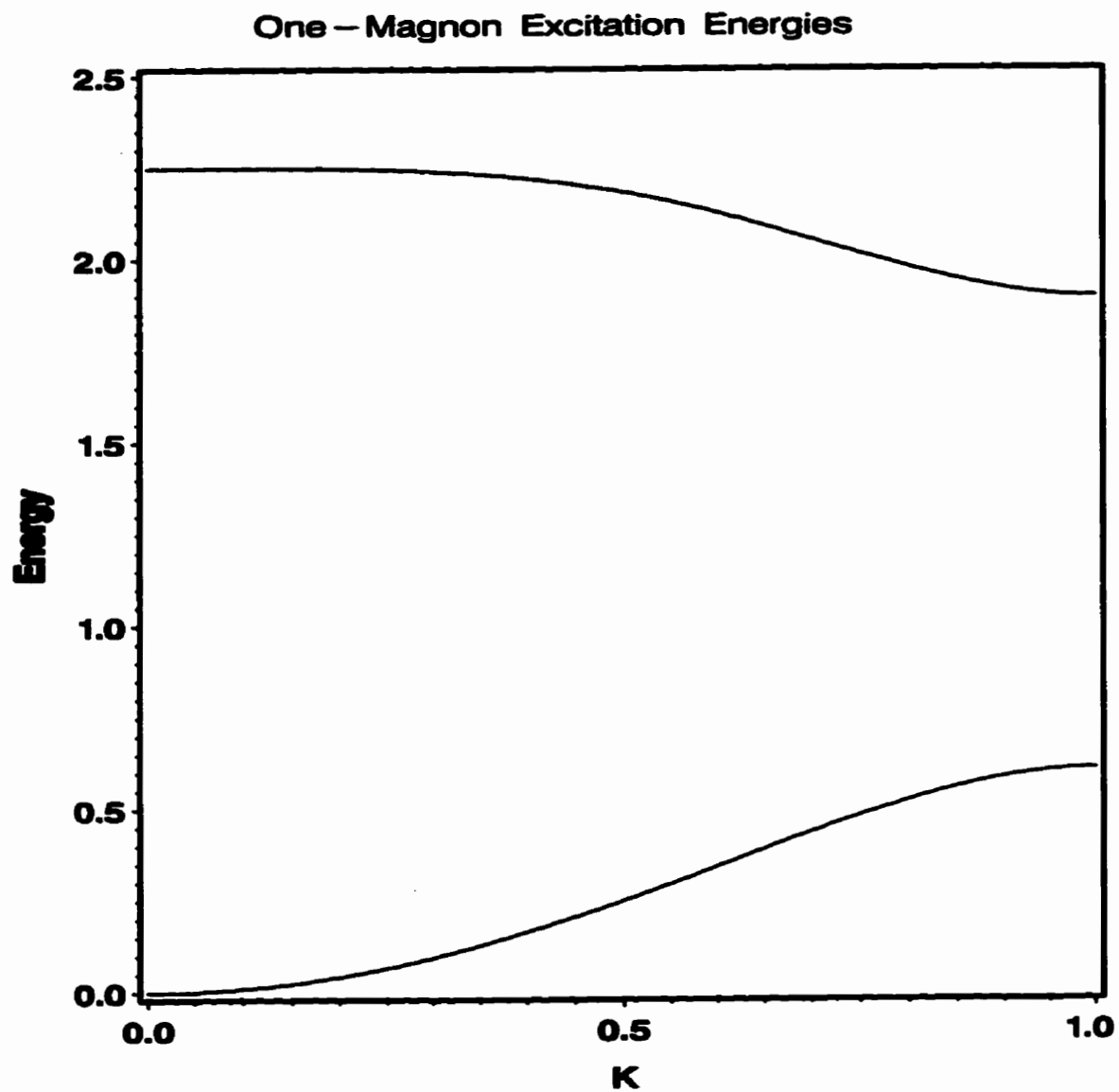


Figure 2.1: One-magnon excitation energy for an alternating ferromagnetic chain with $S = 2S' = 1$ and $J_1 = 2J_2 = 1$. The energy is in units of J_1 and the wavevector k is in units of $\frac{\pi}{2}$.

The noninteracting equations ($m > n$) are

$$\begin{aligned}
(\Omega - \chi)a_{2n,2m} &= -v_0 [J_1(a_{2n,2m+1} + a_{2n+1,2m}) + J_2(a_{2n,2m-1} + a_{2n-1,2m})] \\
\Omega a_{2n-1,2m} &= -v_0 [J_1(a_{2n-2,2m} + a_{2n-1,2m+1}) + J_2(a_{2n,2m} + a_{2n-1,2m-1})] \\
\Omega a_{2n,2m+1} &= -v_0 [J_1(a_{2n,2m} + a_{2n+1,2m+1}) + J_2(a_{2n-1,2m+1} + a_{2n,2m+2})] \\
(\Omega + \chi)a_{2n+1,2m+1} &= -v_0 [J_1(a_{2n,2m+1} + a_{2n+1,2m}) + J_2(a_{2n+2,2m+1} + a_{2n+1,2m+2})]
\end{aligned} \tag{2.15}$$

where $\Omega = E_2 - 2B$, E_2 is measured with respect to E_0 and $v_0 = \sqrt{SS'}$. The interacting equations are

$$\begin{aligned}
(\Omega - \chi)a_{2n,2n} &= -v_1 [J_1 a_{2n,2n+1} + J_2 a_{2n-1,2n}] \\
(\Omega + J_2)a_{2n-1,2n} &= -J_1 v_0 (a_{2n-2,2n} + a_{2n-1,2n+1}) - J_2 (v_1 a_{2n,2n} + v'_1 a_{2n-1,2n-1}) \\
(\Omega + J_1)a_{2n,2n+1} &= -J_1 (v_1 a_{2n,2n} + v'_1 a_{2n+1,2n+1}) + J_2 v_0 (a_{2n-1,2n+1} + a_{2n,2n+2}) \\
(\Omega + \chi)a_{2n+1,2n+1} &= -v'_1 [J_1 a_{2n,2n+1} + J_2 a_{2n+1,2n+2}]
\end{aligned} \tag{2.16}$$

where

$$v_1 = \sqrt{S(2S' - 1)} \tag{2.17}$$

$$v'_1 = \sqrt{S'(2S - 1)} \tag{2.18}$$

The noninteracting equations (2.15) are satisfied by solutions in the form of products of one-magnon solutions having wave vectors k_1 and k_2 , respectively, as follows:

$$\begin{aligned}
a_{2n,2m} &= \alpha e^{i2nk_1} e^{2imk_2} \\
a_{2n-1,2m} &= \beta e^{i(2n-1)k_1} e^{2imk_2} \\
a_{2n,2m+1} &= \gamma e^{2ink_1} e^{i(2m+1)k_2} \\
a_{2n+1,2m+1} &= \delta e^{i(2n+1)k_1} e^{i(2m+1)k_2}
\end{aligned} \tag{2.19}$$

where α , β , γ and δ are generally non-equal complex coefficients corresponding to the four possible configurations of spin deviation pairs.

Substituting into the noninteracting equations (2.15), it leads to the following 4×4 matrix eigenvalue equation

$$\begin{bmatrix} [\Omega - \chi] & \nu_{k_1} & \nu_{k_2} & 0 \\ \nu_{k_1}^* & \Omega & 0 & \nu_{k_2} \\ \nu_{k_2}^* & 0 & \Omega & \nu_{k_1} \\ 0 & \nu_{k_2}^* & \nu_{k_1}^* & [\Omega + \chi] \end{bmatrix} \begin{pmatrix} \alpha \\ \beta \\ \gamma \\ \delta \end{pmatrix} = 0 \quad (2.20)$$

where $\nu_{k_1}^*$ and $\nu_{k_2}^*$ are the complex conjugates of ν_{k_1} and ν_{k_2} defined in (2.9) respectively.

The secular determinant for this eigenvalue problem is given by

$$\Omega^4 - \Omega^2 \chi^2 - 2\Omega^2[\nu_{k_1}^2 + \nu_{k_2}^2] + [\nu_{k_1}^2 - \nu_{k_2}^2] = 0 \quad (2.21)$$

By solving for Ω^2 and then substituting $\Omega = E_2 - 2B$, it can be shown that the energy eigenvalues are simply the sum of the energy of two noninteracting magnons:

$$E_2(k_1, k_2) = E_{K,q}^{\mu_1, \mu_2} = E_{k_1}^{\mu_1} + E_{k_2}^{\mu_2} \quad (2.22)$$

where k_1 and k_2 are the wave vectors of the individual magnons, μ_1 and μ_2 label the branches of the single magnon dispersion curves. The total wave vector $K = k_1 + k_2$ and the relative wave vector $q = (k_1 - k_2)/2$ can also be used to label the energies. Translational invariance requires K to be real but k_1 and k_2 can be complex. Also, the components of the corresponding eigenvectors are

$$\begin{aligned} \frac{\alpha}{\delta} &= \frac{\Omega^2 + \Omega\chi - \nu_{k_1}^2 - \nu_{k_2}^2}{2\nu_{k_1}^* \nu_{k_2}^*} \\ \frac{\beta}{\delta} &= \frac{\nu_{k_1}^2 - \nu_{k_2}^2 - \Omega^2 - \Omega\chi}{2\Omega\nu_{k_2}^*} \\ \frac{\gamma}{\delta} &= \frac{\nu_{k_2}^2 - \nu_{k_1}^2 - \Omega^2 - \Omega\chi}{2\Omega\nu_{k_1}^*} \end{aligned} \quad (2.23)$$

with $|\alpha|^2 + |\beta|^2 + |\gamma|^2 + |\delta|^2 = 1$.

For real values of k_1 and k_2 , or equivalently, for real values of K and q , there are three energy regions which form three different energy continua due to the gap in the

one magnon dispersion curve. Depending on the values used for μ_1 and μ_2 , they can be identified as “acoustic-acoustic,” ($\mu_1 = \mu_2 = -1$) “optic-optic,” ($\mu_1 = \mu_2 = +1$) or “mixed-mode” ($\mu_1 = -\mu_2 = \pm 1$). The figure (2.2) represents these continua for an alternating ferromagnetic chain with $S = 2S' = 1$ and $J_1 = 2J_2 = 1$.

We can use the equation (2.22) for the two-magnon dispersion relation to solve for q with fixed values of K and E_2 (or Ω). Although K and E_2 are real, q can be complex.

The expression for q as a function of K and Ω is

$$\cos(2q) = \frac{-\Omega^2 \cos K \pm \sqrt{\Pi - (\Omega \chi \sin K)^2}}{4SS'J_1J_2 \sin^2 K} \quad (2.24)$$

where

$$\Pi = [\Omega^2 - 4SS'(J_1 \sin K)^2][\Omega^2 - 4SS'(J_2 \sin K)^2] \quad (2.25)$$

In general, there are four complex solutions for q occurring in complex conjugate pairs for each value of Ω and K . For each value of q there is a corresponding eigenvector defined by (2.23), and any linear combination of these four eigenvectors is a solution of the noninteracting two-magnon problem. However, only certain combinations will also satisfy the interacting equations as well. There will always be a nontrivial solution for the wave function for values of K and E_2 inside the energy continua and these solutions are referred to as “scattering states.” Nonetheless, a nonvanishing solution for the wave function only exists for certain values of K and E_2 outside of the energy continua and such solutions are referred to as “bound states.” These solutions correspond to complex values of q and are localized states. When we consider points outside the energy continua, we will obtain four complex values of q . They will form two pairs with equal and opposite imaginary parts.

From the equations (2.16) and as we are working with an infinite chain, only decaying solutions for the wave function are acceptable. Only two solutions of q will give the appropriate decaying eigenvectors. Then, expressing the amplitudes as a

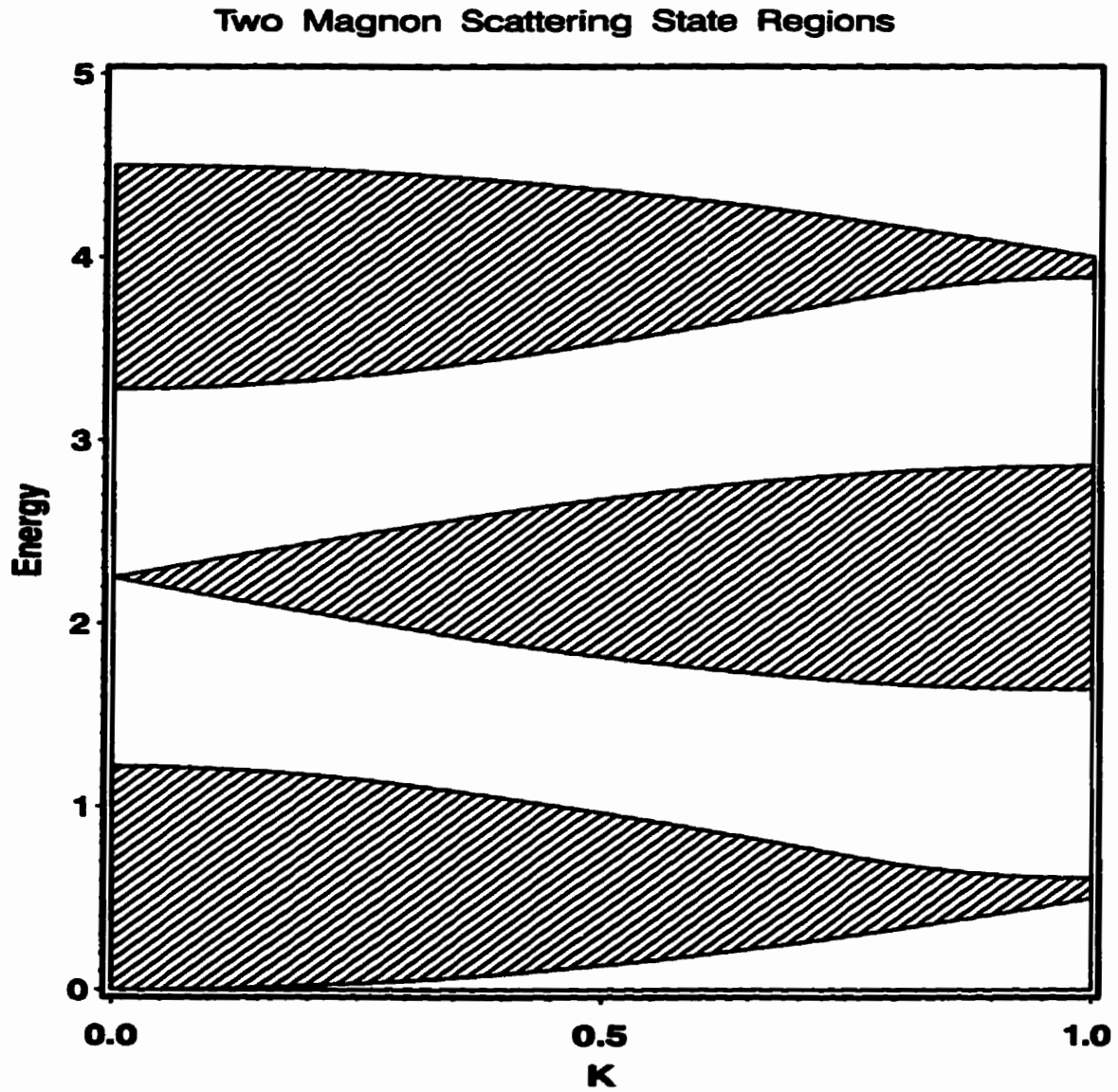


Figure 2.2: Two-magnon scattering state continua for an alternating ferromagnetic chain with $S = 2S' = 1$ and $J_1 = 2J_2 = 1$. The energy is in units of J_1 and the total wavevector K is in units of $\frac{\pi}{2}$.

combination of this two eigenvectors

$$\begin{aligned}
a_{2n,2n} &= e^{2inK}(C_0\alpha + D_0\bar{\alpha}) \\
a_{2n,2m} &= e^{iK(n+m)}(C\alpha e^{-iq(2m-2n)} + D\bar{\alpha}e^{-i\bar{q}(2m-2n)}) \\
a_{2n-1,2m} &= e^{iK(n+m-\frac{1}{2})}(C\beta e^{-iq(2m-2n+1)} + D\bar{\beta}e^{-i\bar{q}(2m-2n+1)}) \\
a_{2n,2m+1} &= e^{iK(n+m+\frac{1}{2})}(C\gamma e^{-iq(2m-2n+1)} + D\bar{\gamma}e^{-i\bar{q}(2m-2n+1)}) \\
a_{2n+1,2n+1} &= e^{iK(2n+1)}(C_0\delta + D_0\bar{\delta}) \\
a_{2n+1,2m+1} &= e^{iK(n+m+1)}(C\delta e^{-iq(2m-2n)} + D\bar{\delta}e^{-i\bar{q}(2m-2n)})
\end{aligned} \tag{2.26}$$

where $m > n$ and the sets $\alpha, \beta, \gamma, \delta$ and $\bar{\alpha}, \bar{\beta}, \bar{\gamma}, \bar{\delta}$ are the components of the “noninteracting” eigenvectors corresponding to q and $\bar{q}$, respectively.

Substituting these expressions into the interacting equations (2.16), we obtain the following 4×4 matrix eigenvalue problem which nonvanishing solutions of its secular determinant correspond to the “bound states”.

$$\mathbf{M} \begin{pmatrix} C_0 \\ D_0 \\ C \\ D \end{pmatrix} = 0 \tag{2.27}$$

where

$$\begin{aligned}
M_{11} &= \alpha(\Omega - \chi) \\
M_{13} &= v_1 e^{-iq}(J_1 e^{iK/2}\gamma + J_2 e^{-iK/2}\beta) \\
M_{21} &= J_2(v_1 e^{iK/2}\alpha + v'_1 e^{-iK/2}\delta) \\
M_{23} &= (\Omega + J_2)e^{-iq}\beta + J_1 v_0 e^{-2iq}(e^{-iK/2}\alpha + e^{iK/2}\delta) \\
M_{31} &= J_1(v_1 e^{-iK/2}\alpha + v'_1 e^{iK/2}\delta) \\
M_{33} &= (\Omega + J_1)e^{-iq}\gamma + J_2 v_0 e^{-2iq}(e^{iK/2}\alpha + e^{-iK/2}\delta) \\
M_{41} &= \delta(\Omega + \chi) \\
M_{43} &= v'_1 e^{-iq}(J_1 e^{-iK/2}\gamma + J_2 e^{iK/2}\beta)
\end{aligned}$$

The remaining elements can be obtained from those above by replacing the set $(q, \alpha, \beta, \gamma, \delta)$ by $(\bar{q}, \bar{\alpha}, \bar{\beta}, \bar{\gamma}, \bar{\delta})$ and are given by

$$\begin{array}{ll} M_{12} = \bar{M}_{11} & M_{14} = \bar{M}_{13} \\ M_{22} = \bar{M}_{21} & M_{24} = \bar{M}_{23} \\ M_{32} = \bar{M}_{31} & M_{34} = \bar{M}_{33} \\ M_{42} = \bar{M}_{41} & M_{44} = \bar{M}_{43} \end{array}$$

where the bar over the matrix elements indicates that the set $q, \alpha, \beta, \gamma, \delta$ has to be substituted by their corresponding bar set.

This eigenvalue equation is resolved numerically and the solutions are the bound states of the problem. Figure (2.3) shows a typical two-magnon spectrum in the $E_2(K)$ versus K plane.

The knowledge of the solution of the one-magnon problem allows us to determine the regions in the $E_2(K)$ versus K plane where scattering state solutions corresponding to two free magnons can occur. These continua correspond to solutions in which both individual wave vectors k_1 and k_2 are real, or equivalently, both the total wave vector K and the relative wave vector q are real.

However, by considering the possibility of solutions with q complex, we also find the existence of solutions ("bound states") outside these continua. Hence, the energy regions where the scattering states are located are determined by the one-magnon spectrum. Similarly, the two-magnon spectrum will determine the location of the scattering states in the three-magnon problem.

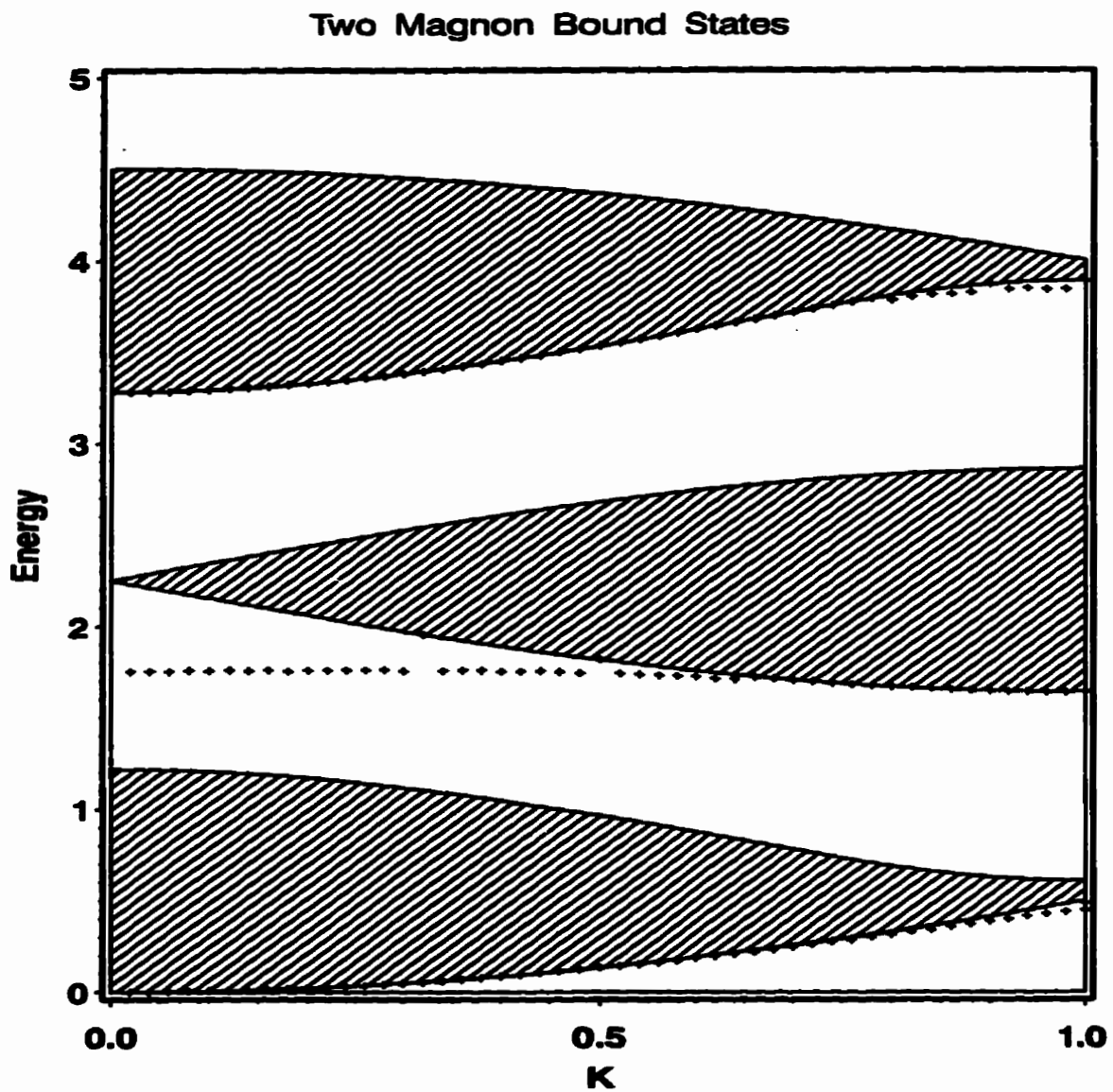


Figure 2.3: Two-bound magnon state branches and scattering state continua for an alternating ferromagnetic chain with $S = 2S' = 1$ and $J_1 = 2J_2 = 1$. The energy is in units of J_1 and the total wavevector K is in units of $\frac{\pi}{2}$.

Chapter 3

Three-Magnon Excitations

A general three-magnon state can be written as

$$|\psi_3\rangle = \sum_{i<j<k} a_{ijk} |ijk\rangle \quad (3.1)$$

where we define an orthonormal set of three spin deviation states

$$|i, j, k\rangle = C_{ijk} S_i^- S_j^- S_k^- |0\rangle \quad (3.2)$$

with C_{ijk} being the coefficients normalizing these states and satisfying

$$C_{2i,2j,2k} = \begin{cases} \frac{1}{\sqrt{8S'^3}}, & i \neq j \neq k \\ \frac{1}{\sqrt{8S'^2(2S'-1)}}, & 2 \text{ of } i, j, k \text{ equal} \\ \frac{1}{\sqrt{24S'(2S'-1)(S'-1)}}, & i = j = k \end{cases} \quad (3.3)$$

$$C_{2i,2j,2k+1} = \begin{cases} \frac{1}{\sqrt{8S'^2S}}, & i \neq j \\ \frac{1}{\sqrt{8SS'(2S'-1)}}, & i = j \end{cases} \quad (3.4)$$

In order to obtain the coefficients with two odd indices and one even index or with three odd indices, we need only to exchange S with S' .

We study the effect of the Hamiltonian on the complete set of states in coordinate space in the same way as was done for $m = 1$ and $m = 2$. The translational invariance

property of the Hamiltonian can be taken into account by the following transformation of the states $|i, j, k\rangle$:

$$|i, j, k\rangle \equiv |j; x, y\rangle \quad (3.5)$$

with $i \leq j \leq k$ and

$$\begin{aligned} x &= j - i \geq 0 \\ y &= k - j \geq 0 \end{aligned} \quad (3.6)$$

In this transformation, there are two types of ket $|m; x, y\rangle$ for any pair of values (x, y) where m is odd or even. Now, we define the following Fourier transforms with respect to the center of mass of each ket

$$\begin{aligned} |e, K; x, y\rangle &= \sqrt{\frac{2}{N}} \sum_{m=0}^{N/2-1} e^{-iK(2m-x/3+y/3)} |2m; x, y\rangle \\ |o, K; x, y\rangle &= \sqrt{\frac{2}{N}} \sum_{m=0}^{N/2-1} e^{-iK(2m+1-x/3+y/3)} |2m+1; x, y\rangle \end{aligned} \quad (3.7)$$

where e and o stand for “even” and “odd” respectively.

The effect of the Hamiltonian on these states can be summarized by the following two equations

$$\begin{aligned} (E_3 - \varepsilon_{x,y}^{K,e})|e, K; x, y\rangle + \kappa_{x,y}^e|e, K; x, y+1\rangle + \rho_{x,y}^e|e, K; x+1, y\rangle + \vartheta_{x,y}^e|e, K; x-1, y\rangle + \\ + \sigma_{x,y}^e|e, K; x, y-1\rangle + \tau_{x,y}^e|o, K; x-1, y+1\rangle + \lambda_{x,y}^e|o, K; x+1, y-1\rangle = 0 \end{aligned} \quad (3.8)$$

$$\begin{aligned} (E_3 - \varepsilon_{x,y}^{K,o})|o, K; x, y\rangle + \kappa_{x,y}^o|o, K; x, y+1\rangle + \rho_{x,y}^o|o, K; x+1, y\rangle + \vartheta_{x,y}^o|o, K; x-1, y\rangle + \\ + \sigma_{x,y}^o|o, K; x, y-1\rangle + \tau_{x,y}^o|e, K; x-1, y+1\rangle + \lambda_{x,y}^o|e, K; x+1, y-1\rangle = 0 \end{aligned} \quad (3.9)$$

where the first equation represents the action of the Hamiltonian on a state at an even site and the second equation corresponds to an odd site. These equations can be divided into three groups depending on whether both $x, y \geq 2$, one is ≥ 2 while the other is ≤ 1 and, the last group when both $x, y \leq 1$.

When both $x, y \geq 2$, we have a set of three non-interacting magnons and the coefficients in (3.8) have the form shown in Table 3.1. The notation used for the coefficients in this table and for those that will follow, allow for a straightforward

Non-interacting coefficients							
x, y	$\varepsilon_{x,y}^{K,e}$	$\kappa_{x,y}^e$	$\rho_{x,y}^e$	$\vartheta_{x,y}^e$	$\sigma_{x,y}^e$	$\tau_{x,y}^e$	$\lambda_{x,y}^e$
$2l, 2m$	ε_6	w	$\bar{w}^*$	w	$\bar{w}^*$	$\bar{w}^*$	w
$2l, 2m + 1$	ε_4	$\bar{w}$	$\bar{w}^*$	w	w^*	$\bar{w}^*$	w
$2l + 1, 2m$	ε_4	w	w^*	$\bar{w}$	$\bar{w}^*$	$\bar{w}^*$	w
$2l + 1, 2m + 1$	ε_4'	$\bar{w}$	w^*	$\bar{w}$	w^*	$\bar{w}^*$	w

Table 3.1: Coefficients for each of the terms obtained when the Hamiltonian is applied on a state at an even site with both $x, y \geq 2$. The group of equations associated with these coefficients is referred to as the non-interacting group.

transfer of an equation for an even site (with general form (3.8)) to an equation for an odd site (with general form (3.9)). The coefficients are defined as follows:

$$\begin{aligned}
\varepsilon &= S(J_1 + J_2) && \text{from equation (2.7)} \\
\varepsilon' &= S'(J_1 + J_2) && \text{from equation (2.8)} \\
\varepsilon_0 &= \varepsilon_3 = \varepsilon_6 = 3\varepsilon \\
\varepsilon_1 &= 2\varepsilon + \varepsilon' - 2J_1 \\
\varepsilon_2 &= \varepsilon + 2\varepsilon' - J_1 - J_2 \\
\varepsilon_4 &= 2\varepsilon + \varepsilon' \\
\varepsilon_5 &= 2\varepsilon + \varepsilon' - J_2 \\
w_0 &= -\kappa J_1 \sqrt{3S(S' - 1)} \\
w_2 &= -\kappa J_1 \sqrt{S(2S' - 1)} \\
w_4 &= -\kappa J_1 \sqrt{(2S - 1)(2S' - 1)} \\
w &= -\kappa J_1 \sqrt{SS'}
\end{aligned}$$

and $\kappa = e^{iK/3}$. The presence of a prime indicates that S should be replaced by S' and vice versa, while the presence of a bar indicates that J_1 should be replaced by J_2 and

vice versa in relation to the corresponding coefficient without the bar or the prime. As usual, an asterisk (*) indicates that the complex conjugate of the coefficient should be taken. For example, the coefficient ε'_4 (appearing in Table 3.1) is equal to $2\varepsilon' + \varepsilon$ once the proper replacements of S and S' are made in the definition of ε_4 . Similarly, $\bar{w} = -\kappa J_2 \sqrt{SS'}$ once J_1 is replaced by J_2 in the definition for w .

The coefficients obtained by the action of the Hamiltonian on the odd states are easily obtained by taking the corresponding even coefficients and putting or taking away their primes or bars depending whether they are present or not. This is a direct acknowledgment that one sublattice has the same equations as the other, only with exchanged spins S and S' and interactions J_1 and J_2 . As an example of the above statement, the coefficients obtained when the Hamiltonian acts on an odd site $|o, K; 2l, 2m\rangle$ are $(\bar{\varepsilon}'_6, \bar{w}', w'^*, \bar{w}', w'^*, w'^*, \bar{w}')$, where the above procedure was applied to the first row of coefficients in Table 3.1.

Returning to the first group of equations when both $x, y \geq 2$, the energy eigenvalues are given by the sum of the energy of three non-interacting magnons:

$$E_3 = E_{K, q_1, q_2}^{\mu_1, \mu_2, \mu_3} = E_{k_1}^{\mu_1} + E_{k_2}^{\mu_2} + E_{k_3}^{\mu_3} \quad (3.10)$$

For k_1, k_2, k_3 real, the solutions are scattering states as encountered in the two-magnon problem and fall into four continua as shown in Figure (3.1). These continua are a consequence of the three-magnon excitation energy being the sum of one-magnon excitations and of the presence of the energy gap in the one-magnon dispersion curve for all values of wavevector. Each of these continua arises from the different pairing of one-magnon branches. The lowest continuum is due to the pairing of three acoustic (A) branches ($\mu_1 = \mu_2 = \mu_3 = -1$) and is referred to as “A-A-A”; the highest continuum is due to the pairing of three optic (O) branches ($\mu_1 = \mu_2 = \mu_3 = +1$) and is referred to as “O-O-O”. The other two continua are labelled by “A-A-O” and “A-O-O” and they both are three-fold degenerate.

When one of the values of x and y is ≤ 1 while the other is ≥ 2 , the coefficients in (3.8) are given in Table 3.2.

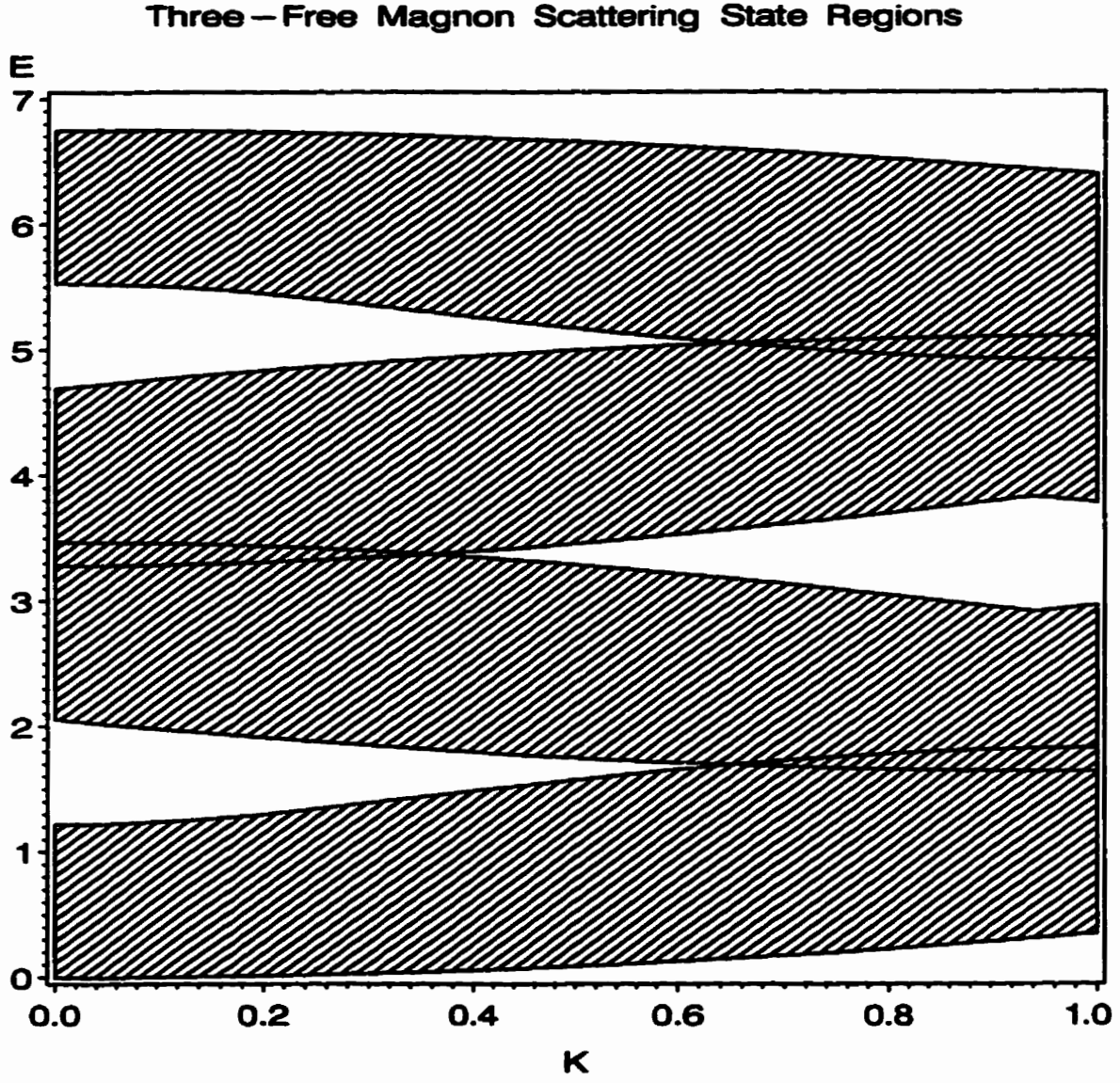


Figure 3.1: Three-free magnon scattering state continua for an alternating ferromagnetic chain with $S = 2S' = 1$ and $J_1 = 2J_2 = 1$. The energy is in units of J_1 and the total wavevector K is in units of $\frac{\pi}{2}$.

Two-bound and one-free magnon coefficients							
x, y	$\varepsilon_{x,y}^{K,e}$	$\kappa_{x,y}^e$	$\rho_{x,y}^e$	$\vartheta_{x,y}^e$	$\sigma_{x,y}^e$	$\tau_{x,y}^e$	$\lambda_{x,y}^e$
$0, 2m$	ε_3	w	$\bar{w}_2^*$		$\bar{w}^*$		w_2
$0, 2m + 1$	ε_4	$\bar{w}$	$\bar{w}_2^*$		w^*		w_2
$2l, 0$	ε_3	w_2	$\bar{w}^*$	w		$\bar{w}_2^*$	
$2l + 1, 0$	ε_4	w_2	w^*	$\bar{w}$		$\bar{w}_2^*$	
$1, 2m$	ε_5	w	w^*	$\bar{w}_2$	$\bar{w}^*$	$\bar{w}_2'^*$	w
$1, 2m + 1$	ε_5'	$\bar{w}$	w^*	$\bar{w}_2$	w^*	$\bar{w}_2'^*$	w
$2l, 1$	$\bar{\varepsilon}_5$	$\bar{w}$	$\bar{w}^*$	w	w_2^*	$\bar{w}^*$	w_2'
$2l + 1, 1$	$\bar{\varepsilon}_5'$	$\bar{w}$	w^*	$\bar{w}$	w_2^*	$\bar{w}^*$	w_2'

Table 3.2: Coefficients for each of the terms obtained when the Hamiltonian is applied on a state at an even site. One of the values of x and y is ≤ 1 while the other is ≥ 2 . The group of equations associated with these coefficients is referred to as the two-bound and one-free magnon group.

Three-bound magnon coefficients							
x, y	$\varepsilon_{x,y}^{K,e}$	$\kappa_{x,y}^e$	$\rho_{x,y}^e$	$\vartheta_{x,y}^e$	$\sigma_{x,y}^e$	$\tau_{x,y}^e$	$\lambda_{x,y}^e$
0, 0	ε_0	w_0	$\bar{w}_0^*$				
0, 1	ε_1	$\bar{w}$	$\bar{w}_2^*$		w_0^*		w_4
1, 0	$\bar{\varepsilon}_1$	w_2	w^*	$\bar{w}_0$		$\bar{w}_4^*$	
1, 1	ε_2	$\bar{w}$	w^*	$\bar{w}_2$	w_2^*	$\bar{w}_2'^*$	w_2'

Table 3.3: Coefficients for each of the terms obtained when the Hamiltonian is applied on a state at an even site with both $x, y \leq 1$. The group of equations associated with these coefficients is referred to as the three-bound magnon group.

We can express the eigenvalue solution of these equations as $E_3 = E_2(k_1, k_2) + E_{k_3}^{\mu_3}$. The term $E_2(k_1, k_2)$ corresponds to two bound magnons; and both terms are the result of complex values of k_1 and k_2 and a real value of k_3 . Still, these eigenstates correspond to scattering states in which one magnon is free and two are bound. They form a continuum which overlap with the three-free magnon scattering state continua, discussed previously. Figure (3.2) shows an example of the two-bound one-free scattering state continuum. Figure (3.3) shows a superposition of the three-free with the two-bound one-free scattering state continua.

Table 3.3 gives the coefficients obtained when the Hamiltonian is applied to a ket $|e, K; x, y\rangle$ with both $x, y \leq 1$, i.e. for the case of three magnons on the same sites or on nearest neighbor sites.

The complete solution of the three-magnon problem involves finding the solution of this last group together with the two previous groups. With the two-magnon problem, the combined problem of solving the non-interacting set of equations with the interacting set reduced to a numeric implementation of a 4×4 matrix eigenvalue problem. A similar approach to resolving the three-magnon problem is almost numerically impossible, as we would have to find the eigenvalues of an infinite matrix

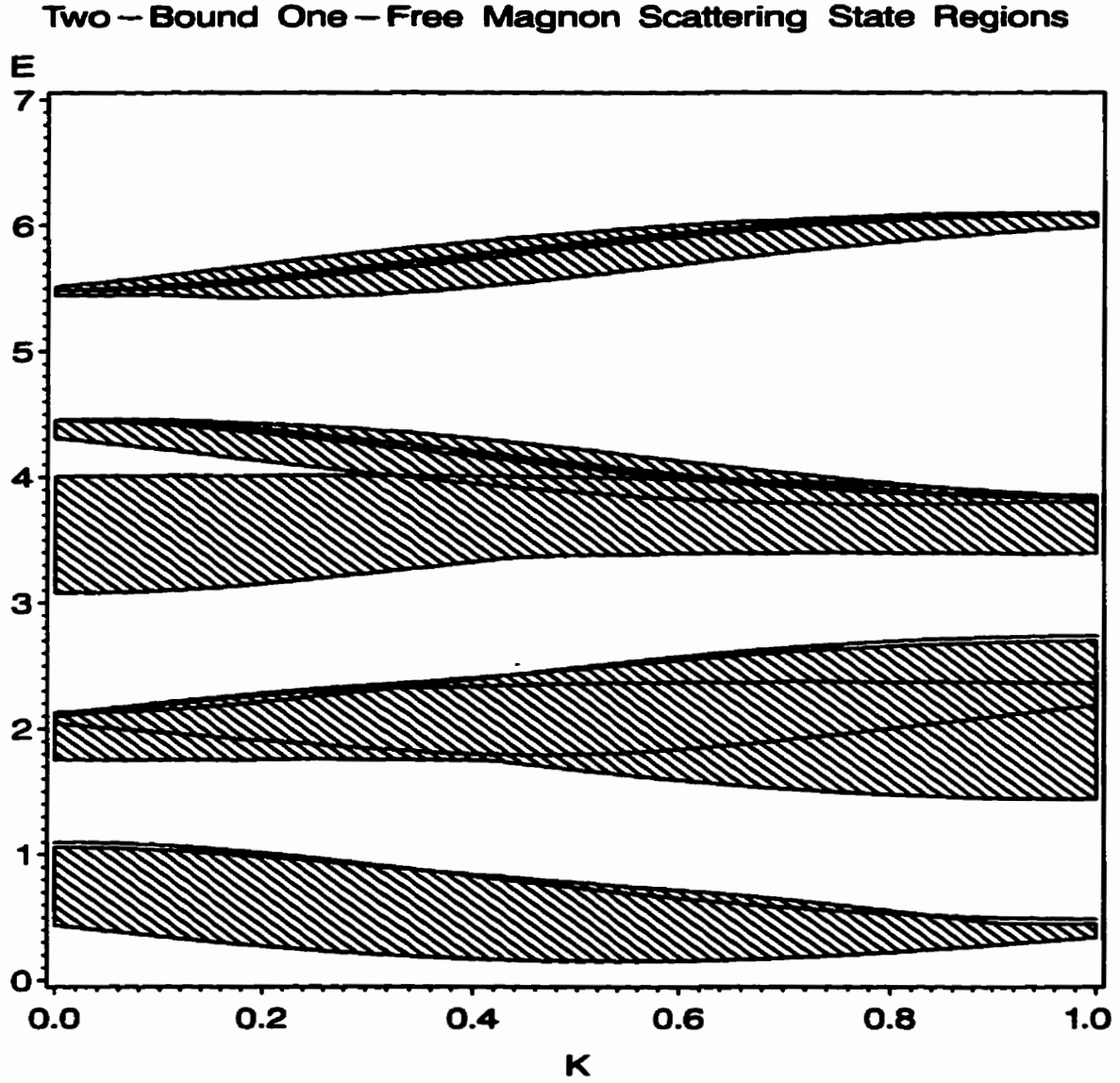


Figure 3.2: The two-bound one-free magnon scattering state continua for an alternating ferromagnetic chain with $S = 2S' = 1$ and $J_1 = 2J_2 = 1$. The energy is in units of J_1 and the total wavevector K is in units of $\frac{\pi}{2}$.

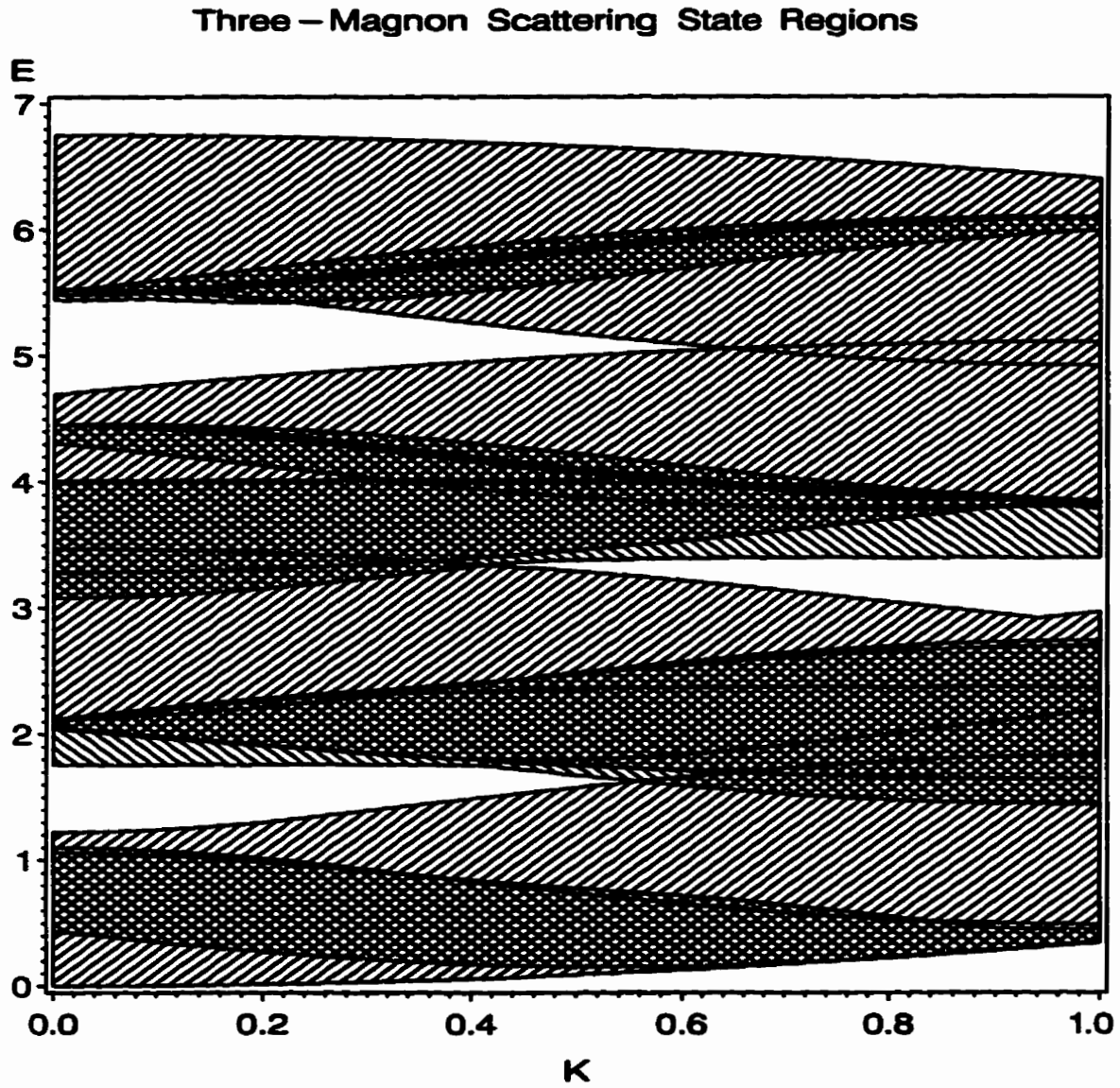


Figure 3.3: Three-magnon scattering state continua for an alternating ferromagnetic chain with $S = 2S' = 1$ and $J_1 = 2J_2 = 1$. The results of the three-free and two-bound one-free are superimposed. The energy is in units of J_1 and the total wavevector K is in units of $\frac{\pi}{2}$.

that correspond to the set of three-magnon equations. In the next chapter, we will present a different method that will give us the possibility of identifying bound states for the three-magnon problem.

Chapter 4

The Recursion Method and the Three-Magnon Problem

The Recursion Method [13, 12, 16] can be used to obtain spectral information about any Hamiltonian. The basic idea is to transform the Hamiltonian to a tridiagonal form so that a continued fraction representation of the Green's function can be obtained. We first review the definition of the Green's function.

4.1 Green's Function

The local Green's function is defined by

$$G_j(E + i\varepsilon) = \langle j | (E - \hat{H} + i\varepsilon)^{-1} | j \rangle \quad (4.1)$$

where $\varepsilon \ll 1$ and $|j\rangle$ is an arbitrary ket in the three-magnon basis.

Writing $|j\rangle$ as a linear combination of the eigenstates of the Hamiltonian ($\hat{H}|\lambda\rangle = E_\lambda|\lambda\rangle$)

$$|j\rangle = \sum_{\lambda} c_{\lambda}^j |\lambda\rangle \quad (4.2)$$

and substituting in (4.1), the local Green's function becomes

$$G_j(E + i\varepsilon) = \sum_{\lambda} \frac{|c_{\lambda}^j|^2}{E - E_{\lambda} + i\varepsilon} \quad (4.3)$$

The imaginary part of $G_j(E + i\varepsilon)$ is given by

$$\text{Im}(G_j(E + i\varepsilon)) = - \sum_{\lambda} |c_{\lambda}^j|^2 \frac{\varepsilon}{(E - E_{\lambda})^2 + \varepsilon^2} \quad (4.4)$$

which in the limit $\varepsilon \rightarrow 0^+$ is proportional to the sum of delta functions at the exact eigenvalues, i.e.

$$\lim_{\varepsilon \rightarrow 0} [\text{Im}(G_j(E + i\varepsilon))] = -\pi \sum_{\lambda} |c_{\lambda}^j|^2 \delta(E - E_{\lambda}) \quad (4.5)$$

Then, the local density of states can be defined as

$$\eta_j(E) = \lim_{\varepsilon \rightarrow 0} \frac{-1}{\pi} \text{Im}[G_j(E + i\varepsilon)] \quad (4.6)$$

and the total density of states is obtained by summing over all the kets in the basis

$$\eta(E) = \sum_j \eta_j(E) = \sum_{\lambda} \delta(E - E_{\lambda}) \quad (4.7)$$

since $\sum_j |c_{\lambda}^j|^2 = 1$.

Using the definition in (4.1) and a matrix representation for the operator $(E - \hat{H})^{-1}$, a single matrix element of this operator can be taken as the local Green's function, without loss of generality:

$$G_0(E) = \frac{D_1([E - \hat{H}])}{D_0([E - \hat{H}])} \quad (4.8)$$

where $D_n([E - \hat{H}])$ is the determinant of the matrix $[E - \hat{H}]$ with the first n rows and n columns deleted.

If the local Green's function were difficult to calculate, its definition would be of little value. Only for some sets of bases is its calculation trivial as in the case where a basis diagonalizes the Hamiltonian. Usually it is almost impossible or extremely difficult to find a basis that diagonalizes the Hamiltonian, but it is always feasible to find a basis which transforms the Hamiltonian to a tridiagonal and symmetric matrix

form

$$\hat{H} = \begin{pmatrix} h_{00} & h_{01} & & 0 \\ h_{01} & h_{11} & h_{12} & \\ & h_{12} & h_{22} & h_{23} \\ & 0 & & \ddots \\ & & h_{n-1n} & h_{nn} \end{pmatrix} \quad (4.9)$$

Expanding (4.8) using the Hamiltonian in the form (4.9), the local Green's function for the ket $|0\rangle$ is

$$G_0(E) = \frac{1}{E - h_{00} - h_{01}^2 \frac{D_2(E-\hat{H})}{D_1(E-\hat{H})}} \quad (4.10)$$

The factor $\frac{D_1(E-\hat{H})}{D_0(E-\hat{H})}$ has the same form as (4.8) and the local Green's function can be represented by the continued fraction

$$G_0(E) = \frac{1}{E - h_{00} - \frac{h_{01}^2}{E - h_{11} - \frac{h_{12}^2}{E - h_{22} - \frac{h_{23}^2}{\ddots}}}} \quad (4.11)$$

With a procedure to transform the Hamiltonian into a tridiagonal, symmetric matrix, we would be able to find the local Green's function and thus the density of states. The Recursion method, described in the next section, is a procedure to tridiagonalize the Hamiltonian.

4.2 The Recursion Method

The recursion method will give us the tool to transform our Hamiltonian into a tridiagonal matrix. We will build a new basis $\{\mathbf{v}_n\}$ in which the Hamiltonian assumes a tridiagonal form, as opposed to our actual basis $\{|p, K; x, y\rangle$ where it is not tridiagonal.

The main assumption of this method is that there exists a complete orthonormal set of states ($\{\mathbf{v}_n\}$ being the n^{th} state) that under the action of the Hamiltonian produces a three-term recursion relation of the form

$$\hat{H}\mathbf{v}_n = a_n\mathbf{v}_n + b_{n+1}\mathbf{v}_{n+1} + b_n\mathbf{v}_{n-1} \quad (4.12)$$

where $a_i, b_i \in \mathbb{R}$

• Recursion Method First Step

1. For this step, $\mathbf{v}_{-1}$ is taken as zero and $\mathbf{v}_0$ is some arbitrary state in the three-magnon basis, consequently equation (4.12) becomes

$$\hat{H}\mathbf{v}_0 = a_0\mathbf{v}_0 + b_1\mathbf{v}_1 \quad (4.13)$$

where $\mathbf{v}_0$ and $\hat{H}\mathbf{v}_0$ are known and a_0, b_1 and $\mathbf{v}_1$ are to be determined.

2. As $\{\mathbf{v}_n\}$ is an orthonormal basis, the scalar product $\mathbf{v}_0^\dagger \mathbf{v}_1 = 0$ and a_0 can be determined by

$$a_0 = \mathbf{v}_0^\dagger \hat{H}\mathbf{v}_0 \quad (4.14)$$

- 3.

$$b_1\mathbf{v}_1 = \hat{H}\mathbf{v}_0 - a_0\mathbf{v}_0 \quad (4.15)$$

4. b_1 is taken as the normalization factor for $\mathbf{v}_1$:

$$b_1 = \sqrt{[\hat{H}\mathbf{v}_0 - a_0\mathbf{v}_0]^\dagger [\hat{H}\mathbf{v}_0 - a_0\mathbf{v}_0]} \quad (4.16)$$

5. Finally for this step,

$$\mathbf{v}_1 = \frac{\hat{H}\mathbf{v}_0 - a_0\mathbf{v}_0}{b_1} \quad (4.17)$$

which is orthonormal to $\mathbf{v}_0$ and normalized to unity.

• Recursion Method General Step

By iterating this procedure, the orthonormal states $\{\mathbf{v}_i\}$ with $i = 0, 1, \dots, n$ can be found together with the parameters $\{a_0, \dots, a_{n-1}\}$ and $\{b_1, \dots, b_n\}$, so that

1.

$$\hat{H}\mathbf{v}_n = a_n\mathbf{v}_n + b_{n+1}\mathbf{v}_{n+1} + b_n\mathbf{v}_{n-1} \quad (4.18)$$

where $\mathbf{v}_n$, $b_n\mathbf{v}_{n-1}$ and $\hat{H}\mathbf{v}_n$ are known and a_n , b_{n+1} and $\mathbf{v}_{n+1}$ are to be determined.

2. The scalar products $\mathbf{v}_n^\dagger \mathbf{v}_{n-1} = \mathbf{v}_n^\dagger \mathbf{v}_{n+1} = 0$ and a_n can be determined by

$$a_n = \mathbf{v}_n^\dagger \hat{H}\mathbf{v}_n \quad (4.19)$$

3.

$$b_{n+1}\mathbf{v}_{n+1} = \hat{H}\mathbf{v}_n - a_n\mathbf{v}_n - b_n\mathbf{v}_{n-1} \quad (4.20)$$

4. b_{n+1} is taken as the normalization factor for $\mathbf{v}_{n+1}$:

$$b_{n+1} = \sqrt{[\hat{H}\mathbf{v}_n - a_n\mathbf{v}_n - b_n\mathbf{v}_{n-1}]^\dagger [\hat{H}\mathbf{v}_n - a_n\mathbf{v}_n - b_n\mathbf{v}_{n-1}]} \quad (4.21)$$

5. Having determined b_{n+1} , $\mathbf{v}_{n+1}$ can be determined by

$$\mathbf{v}_{n+1} = \frac{\hat{H}\mathbf{v}_n - a_n\mathbf{v}_n - b_n\mathbf{v}_{n-1}}{b_{n+1}} \quad (4.22)$$

which is orthonormal to $\mathbf{v}_i$ with $i = 0, 1, \dots, n$ and it is normalized to one.

The new matrix representation of the Hamiltonian under the basis $\{\mathbf{v}_n\}$ is

$$\hat{H} = \begin{pmatrix} a_0 & b_1 & & & \\ b_1 & a_1 & b_2 & & 0 \\ & b_2 & a_2 & b_3 & \\ & & 0 & & \ddots \end{pmatrix} \quad (4.23)$$

and the Green's function for the initial ket in the three-magnon basis could be found from

$$G_0(E) = \frac{1}{E - a_0 - \frac{b_1^2}{E - a_1 - \frac{b_2^2}{E - a_2 - \frac{b_3^2}{\ddots}}}}} \quad (4.24)$$

4.3 Tail of the Continued Fraction

In carrying on the procedure described above, we chose an initial ket in the three-magnon basis and generate the coefficients a_i, b_{i+1} up to some maximum value of $i = i_{max}$. The asymptotic behavior of these coefficients as function of i depends upon the scattering state spectrum. If at a particular value of total wavevector K , there are no gaps, then the coefficients will approach constant values asymptotically. However, if there are one or more gaps present, then the asymptotic behavior is oscillatory. In practice, we need only to calculate the coefficients up to some suitable value of i_{max} and terminate the continued fraction using our knowledge of the scattering state spectrum,

$$G_0(E) = \frac{1}{E - a_0 - \frac{b_1^2}{E - a_1 - \frac{b_2^2}{\ddots \frac{b_{i_{max}}^2}{E - a_{i_{max}} - b_{i_{max}+1}^2 G_0^\infty(E)}}}}} \quad (4.25)$$

In the case of no gaps in the scattering state continuum, the coefficients a_i and b_i converge to constant values,

$$\left. \begin{array}{l} a_i = a \\ b_{i+1} = b \end{array} \right\} \quad \text{for } i > i_{max} \quad (4.26)$$

and the tail of the continued fraction will be given by

$$\begin{aligned}
 G_0^\infty(E) &= \frac{1}{E - a - \frac{b^2}{E - a - \frac{b^2}{\ddots}}} \\
 &= \frac{1}{E - a - b^2 G_0^\infty(E)}
 \end{aligned} \tag{4.27}$$

Solving for G_0^∞ , we have

$$G_0^\infty(E) = \frac{E - a \pm \sqrt{(E - a)^2 - 4b^2}}{2b^2} \tag{4.28}$$

This is known as the square root terminator and the choice of the positive or negative square root depends on whether E is less than or greater than a . The terminator determines the analytic properties of G_0 . For example, G_0 is complex in the region of E where the argument of the square root is negative and this corresponds to the scattering state continuum. However, G_0 can also have isolated poles outside this region.

In the case of the square root terminator, this condition is satisfied when:

$$(E - a)^2 - 4b^2 < 0 \tag{4.29}$$

or equivalently when,

$$E_1 = a - 2b \leq E \leq a + 2b = E_2 \tag{4.30}$$

It is straightforward to conclude that the asymptotic values of a_i and b_i (a and b respectively) are related to the minimum energy E_1 and maximum energy E_2 by

$$\begin{aligned}
 a &= \frac{1}{2}(E_1 + E_2) \\
 b &= \frac{1}{4}(E_2 - E_1)
 \end{aligned} \tag{4.31}$$

Hence, if at a particular value of K , the three-magnon continuum has no gaps, we can terminate the continued fraction using equation (4.28). Using the Recursion Method, we generate a large set of coefficients a_i and b_i assuming that it is reached

the asymptotic behavior (4.26) in which the coefficients are constant. Then, with a last pair (a_i, b_{i+1}) we calculate G_0^∞ and using equation (4.25) we are able to evaluate the Green's function.

As was demonstrated in the work of Turchi *et al* [13], the coefficients (a_i, b_{i+1}) of the continued fraction exhibit undamped oscillations if gaps are present. Consider the case in which the coefficients oscillate between two pairs, (a_1, b_1) and (a_2, b_2) , in the asymptotic region in the continued fraction, i.e.:

$$\left. \begin{array}{l} a_{2i} = a_1 \\ b_{2i} = b_1 \end{array} \right\} \quad \text{for} \quad 2i > i_{max}$$

$$\left. \begin{array}{l} a_{2i+1} = a_2 \\ b_{2i+1} = b_2 \end{array} \right\} \quad \text{for} \quad 2i + 1 > i_{max} \quad (4.32)$$

and the terminator of the continued fraction is equal to

$$G_0^\infty(E) = \frac{1}{E - a_1 - \frac{b_2^2}{E - a_2 - \frac{b_1^2}{\ddots}}}$$

$$= \frac{1}{E - a_1 - \frac{b_2^2}{E - a_2 - b_1^2 G_0^\infty(E)}} \quad (4.33)$$

Solving the previous equation, we obtain

$$G_0^\infty(E) = \frac{1}{2b_1^2(E - a_1)} \left\{ (E - a_1)(E - a_2) + b_1^2 - b_2^2 \pm \sqrt{F} \right\} \quad (4.34)$$

where the square root term F can be factored the following way

$$F = [(E - a_1)(E - a_2) + b_1^2 - b_2^2]^2 - 4b_1^2(E - a_1)(E - a_2)$$

$$= (E - \lambda_1)(E - \lambda_2)(E - \lambda_3)(E - \lambda_4) \quad (4.35)$$

and here

$$\lambda_1 = \frac{1}{2} \left[a_1 + a_2 - \sqrt{(a_1 - a_2)^2 + 4(b_1 + b_2)^2} \right] \quad (4.36)$$

$$\lambda_2 = \frac{1}{2} \left[a_1 + a_2 - \sqrt{(a_1 - a_2)^2 + 4(b_1 - b_2)^2} \right] \quad (4.37)$$

$$\lambda_3 = \frac{1}{2} \left[a_1 + a_2 + \sqrt{(a_1 - a_2)^2 + 4(b_1 - b_2)^2} \right] \quad (4.38)$$

$$\lambda_4 = \frac{1}{2} \left[a_1 + a_2 + \sqrt{(a_1 - a_2)^2 + 4(b_1 + b_2)^2} \right] \quad (4.39)$$

with $\lambda_1 \leq \lambda_2 \leq \lambda_3 \leq \lambda_4$

Now, we take the imaginary part of G_0 with $E = E + i\varepsilon$ to find the regions of non-zero density of states in the limit of $\varepsilon \rightarrow 0^+$. F is negative when $\lambda_1 \leq E \leq \lambda_2$ and $\lambda_3 \leq E \leq \lambda_4$ are the only ones with non-zero density of states. The limits of these regions constitute the edges of two bands extending from $(E_1, E_2) = (\lambda_1, \lambda_2)$ and $(E_3, E_4) = (\lambda_3, \lambda_4)$ and hence these are the regions corresponding to the scattering states continua.

With the presence of one gap, the coefficients oscillate in the form a_1, b_2, a_2, b_1 and with these two pairs we can calculate the tail of the continued fraction using equation (4.34).

Turchi *et al* [13] generalized this procedure for the calculation of the tail of the continued fraction in the presence of multiple gaps. Generalizing equations (4.28) and (4.34), the tail of the continued fraction for the case of q gaps is given by,

$$G_0^\infty(E) = \frac{\nu_{n-1}(E) - \sqrt{X(E)}}{2b_{n-1}^2 \alpha_{n-1}(E)} \quad (4.40)$$

where

$$X(E) = \prod_{i=0}^{2q+1} (E - E_i) = \sum_{i=0}^{2q+2} s_i E^{2q+2-i} \quad (4.41)$$

where the s_i are symmetric functions of the E_i with $s_0 = 1$.

The tail of the continued fraction corresponds to a periodic chain of period $q + 1$. The polynomials $\alpha_n(E)$ and $\nu_{n-1}(E)$ can be determined using the exact Green's functions for an infinite ring with periodicity $q + 1$. The Green's functions for an infinite periodic ring have the form (Turchi *et al* [13])

$$G_{nn}(E) = \langle n | \frac{1}{E - \hat{H}} | n \rangle = \frac{\alpha_n(E)}{\sqrt{X(E)}} \quad (4.42)$$

$$G_{n-1,n}(E) = \langle n-1 | \frac{1}{E - \hat{H}} | n \rangle = \frac{\nu_{n-1}(E) - \sqrt{X(E)}}{2b_{n-1}\sqrt{X(E)}} \quad (4.43)$$

Expanding both sides of these equations in powers of $\frac{1}{E}$ provides the necessary relationships between the coefficients $\{a_n, b_n\}$ describing $\hat{H}$ and the polynomials.

The corresponding coefficients in the left hand side of (4.42) are the moments of the local density of states at site n , i.e:

$$G_{nn}(E) \xrightarrow{E \rightarrow \infty} \frac{1}{E} + \frac{a_n}{E^2} + \frac{a_n^2 + b_{n-1}^2 + b_n^2}{E^3} + \dots \quad (4.44)$$

For the right hand side, since we will frequently have to expand $\sqrt{X(E)}$, we introduce the following notation:

$$\sqrt{X(E)} \xrightarrow{E \rightarrow \infty} E^2(1 + A_1/E + \dots + A_m/E^m + \dots) \quad (4.45)$$

where A_m will be related to the s_i defined in (4.41).

In the same way, we expand in powers of $1/E$ the off-diagonal Green's function (4.43) where the left hand side of $G_{n-1,n}$ behaves as

$$G_{n-1,n}(E) \xrightarrow{E \rightarrow \infty} \frac{b_{n-1}}{E^2} + \frac{b_{n-1}(a_{n-1} + a_n)}{E^3} + \dots \quad (4.46)$$

Finally, we can determine:

$$\alpha_n(E) = (E - \alpha_n^1) \dots (E - \alpha_n^q) \quad (4.47)$$

$$\nu_{n-1}(E) = E^{q+1} + A_1 E^q + \rho_{n-1}(E) \quad (4.48)$$

$$\rho_{n-1}(E) = (A_2 + 2b_{n-1}^2)E^{q-1} + \dots \quad (4.49)$$

In the present work, as we encounter a maximum of five gaps for the spin chains that we studied, we have derived the previous expressions considering up to five gaps. Appendix A presents a Mathematica program that implements this procedure. We also list the results for the cases of one to four gaps.

4.4 Summary

Summarizing our procedure to this point, for given values of S , S' , J_1 and J_2 :

- We use the one-magnon results to determine the three-free continua in the energy (E) versus wave vector (K) plane.
- We use the two-bound magnon state results and the one-magnon excitation energy to determine the two-bound one-free continua in the E - K plane.
- We superimpose all these continua to determine the number of gaps in the energy continua at any value of the total wavevector K .
- We use the appropriate terminator to study the density of states for the three-magnon problem.

Chapter 5

Results

The procedures described in the previous chapters allow us to investigate the presence of bound-state solutions for a system with alternating bonds, alternating spins or both. Medved, Southern and Lavis [11] have previously examined the two-magnon excitations for these systems. The three-magnon excitations were also studied for ferromagnetic spin- S chains by Southern, Lee and Lavis [17]; but no alternation was included in the analysis. We extend their work by studying the three-magnon problem for various cases of spin chains using the Recursion method.

5.1 Uniform Bond Spin $S = S' = \frac{1}{2}$ Case

Before we discuss the results for either alternating spin or bond chains, we will first consider the $S = \frac{1}{2}$ uniform Heisenberg chain. This case was solved exactly by Bethe [3, 2] for an arbitrary number of spin deviations using the Bethe Ansatz method. The three-magnon spectrum consists of a three-free continuum, a two-bound one-free continuum and a single bound state branch which lies below the continua throughout the Brillouin zone. If alternation is introduced, a basis of two atoms per unit cell must be used and this corresponds to a reduction in size of the first Brillouin zone by a factor of two. In the alternating case, the wavevector K is restricted to the range

$-\pi/2 \leq K \leq \pi/2$ and corresponds to a folding of the zone at $K = \pm\pi/2$. In order to make clear the relationship of the known exact results of Bethe with those to be described here, we will first discuss Bethe's results for the $m = 1, 2, 3$ magnon spectra in the folded zone.

Bethe's analytic result for the one-magnon case has the familiar form

$$E_1(k) = J(1 - \cos(k)) \quad (5.1)$$

in the unfolded zone. In our case this would be described by two branches which meet at the zone boundary with no gap

$$E_1^\pm = J(1 \pm \cos(k)) \quad (5.2)$$

where k is now restricted to the range $-\pi/2 \leq k \leq \pi/2$. This corresponds to equation (2.10) when $J_2 = J_1 = J$ and $S = S' = \frac{1}{2}$.

The two-magnon spectrum of the uniform model consists of a continuum with a single bound state below whose energy is half the one-magnon energy

$$E_2 = \frac{J}{2}(1 - \cos(K)) \quad (5.3)$$

in the unfolded zone. However, in the folded zone, the bound state lies below the continuum but folds back at $K = \pi/2$ and enters the same region of energy occupied by the continuum as shown in Figure (5.1). However, the bound state character is not changed provided $J_1 = J_2$ and these contributions to the spectrum can be separated by using different initial kets in our recursion procedure. This point will be discussed later in this chapter. When the bonds alternate, we expect this upper branch of the bound state to become a true resonance when it enters the continuum and a gap to appear at the zone boundary.

Also, the uniform chain has a three-magnon bound state whose energy is equal to one third of the one-magnon state and lies below a single continuum formed by the three-free magnon scattering states and the two-bound one-free magnon scattering states. Figure (5.2) shows the unfolded and the folded representations. As for the

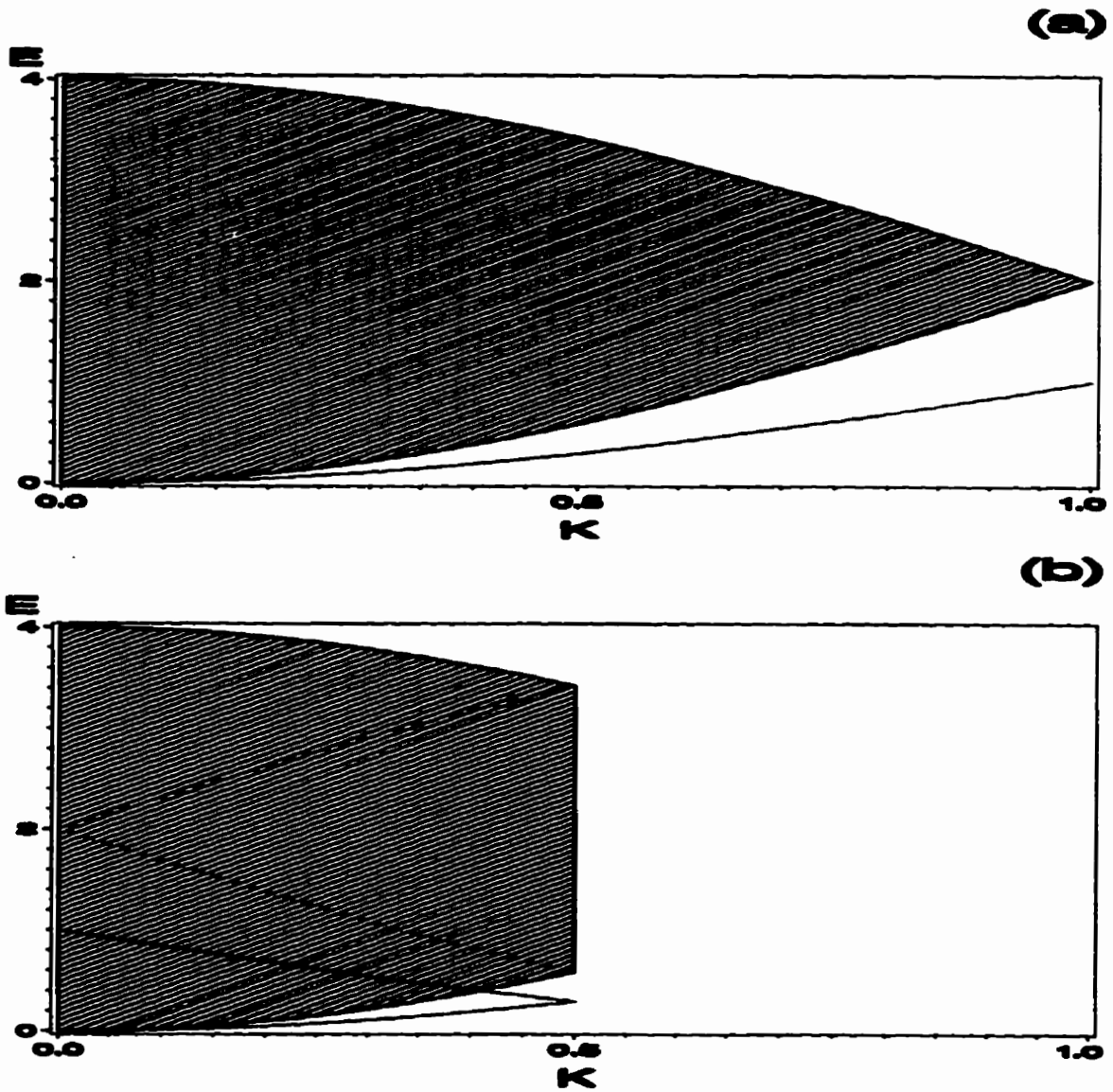


Figure 5.1: The two-free magnon continuum (shaded region) and the two-bound state branch (curve) of the uniform $S = \frac{1}{2}$ chain. Representation resulting from considering (a) one site per cell and (b) two sites per cell. The energy is in units of J_1 and the total wavevector K is in units of π .

two-magnon spectrum in the folded representation, the optic branch of the three-magnon bound state enters the continuum and can only be separated using different initial conditions in the recursion method. But near $K = \pi/2$, the two states appear below the scattering continua with no gap at the zone boundary.

Using the Recursion Method, we reproduce these results for the Heisenberg spin chain. In Figure (5.3), we show our three-magnon bound states obtained using the numerical approach. The star symbols correspond to the bound state which evidently agree with the exact results just described. The lines inside the continuum are an artifact of the numerical approach and arise due to the fact that the termination procedure uses the one and two-magnon results to determine where gaps may occur in the continua. In this case there are no gaps.

5.1.1 $S = S' = \frac{1}{2}$ Alternating Bond Case

S. C. Bell *et al* [15] studied the two-magnon spectrum of the alternating bond $S = \frac{1}{2}$ ferromagnetic Heisenberg chain, finding three two-bound magnon state branches which represents two additional to those appearing in the uniform chain. We extend their study by resolving the three-magnon problem for alternating bond or spin chains. Once an alternation of the spins or the bonds is introduced, the folded representation becomes the natural one, as it corresponds to two sites per primitive cell. Then, the optic branch of the three-magnon bound state is expected to become a resonant state inside the continuum region unless it emerges again inside a continuum gap.

Only near the Brillouin boundary will the two bound state branches be easily visible, showing a gap at the boundary. In Figures (5.4) and (5.5), we show the effects of varying the bond strengths. First, as J_2/J_1 varies from 1.0 to 0.0, it is clear that gaps open up and broaden, simultaneously with the decrease in the width of each band. As expected from the uniform case, the lower three-magnon bound state is still present below the continua. But as $J_2/J_1 \rightarrow 0$, additional three-magnon bound state branches show up in the first and second gap. This behavior is similar to

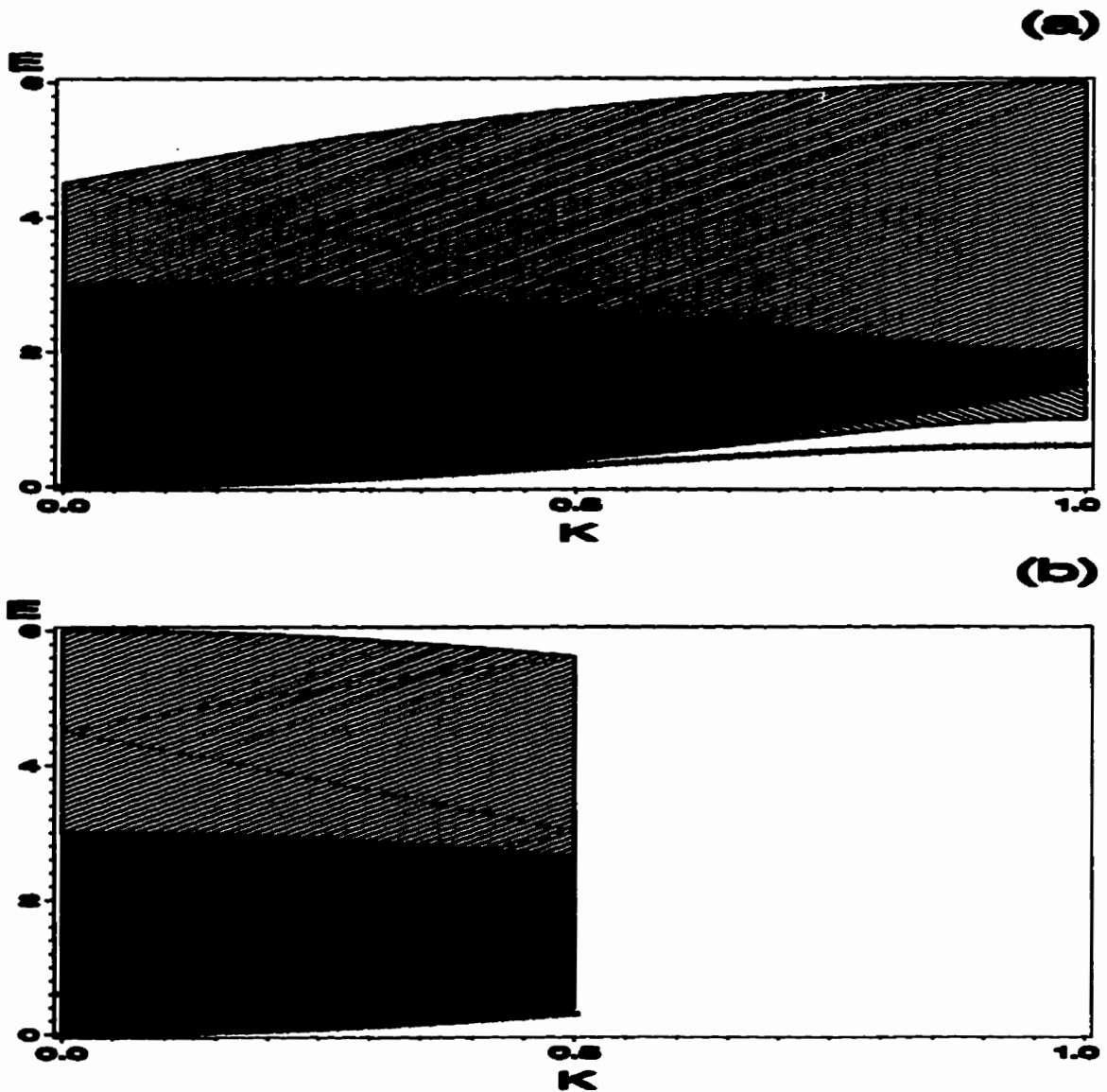


Figure 5.2: The three-magnon continuum (shaded region) and the three-bound magnon state branch (curve) of the uniform $S = \frac{1}{2}$ chain. Representation resulting from considering (a) one site per cell (the primitive cell), and (b) two sites per cell. The energy is in units of J_1 and the total wavevector K is in units of π .

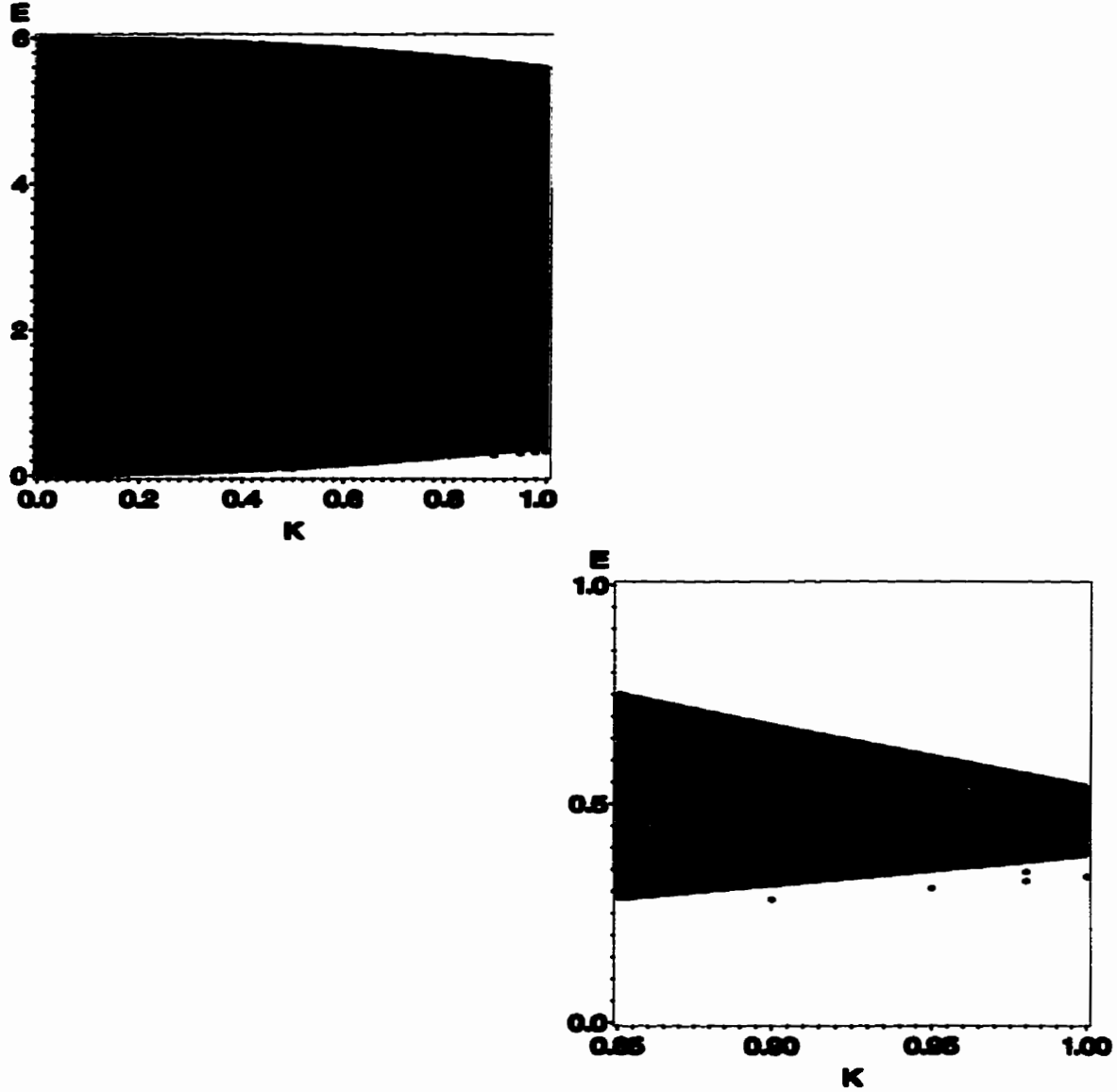


Figure 5.3: The three-magnon continuum (shaded region) of the uniform $S = \frac{1}{2}$ chain. The star points represent the three-magnon bound states obtained using the Recursion Method. Representation resulting from considering two sites per cell. The energy is in units of J_1 and the total wavevector K is in units of $\frac{\pi}{2}$.

the two-magnon case studied by Bell *et al* [15] where additional bound states appear within the gaps of the two-magnon continuum. However, there do not seem to be any bound states in the third gap.

Exact results can be obtained in the case where either J_1 or J_2 is zero. We will discuss this case next as it provides a useful reference for comparing our results with both J_1 and J_2 non-zero. This limit will help understand why there are no bound states in the highest gap for the case $S = S' = \frac{1}{2}$.

5.2 $J_2 \rightarrow 0$ limit

In the $J_2 \rightarrow 0$ limit, the Hamiltonian (1.5) becomes

$$\widehat{H} = \sum_{n=1}^{N/2} \widehat{H}_{2n}^b \quad (5.4)$$

where

$$\widehat{H}_{2n}^b = -J_1 \vec{S}_{2n-1} \cdot \vec{S}_{2n}' \quad (5.5)$$

This constitutes an exactly solvable problem of isolated blocks. Let $\vec{J} = \vec{S} + \vec{S}'$ be the total spin of a block. Considering the expression

$$\vec{S} \cdot \vec{S}' = \frac{1}{2}[(\vec{S} + \vec{S}')^2 - \vec{S} \cdot \vec{S} - \vec{S}' \cdot \vec{S}'] \quad (5.6)$$

and since S and S' are quantum spins, the energy per block is given by

$$E = \langle \widehat{H}_{2n}^b \rangle = -\frac{J_1}{2}[J(J+1) - S(S+1) - S'(S'+1)] \quad (5.7)$$

where $J = |S - S'|, |S - S'| + 1, \dots, S + S'$.

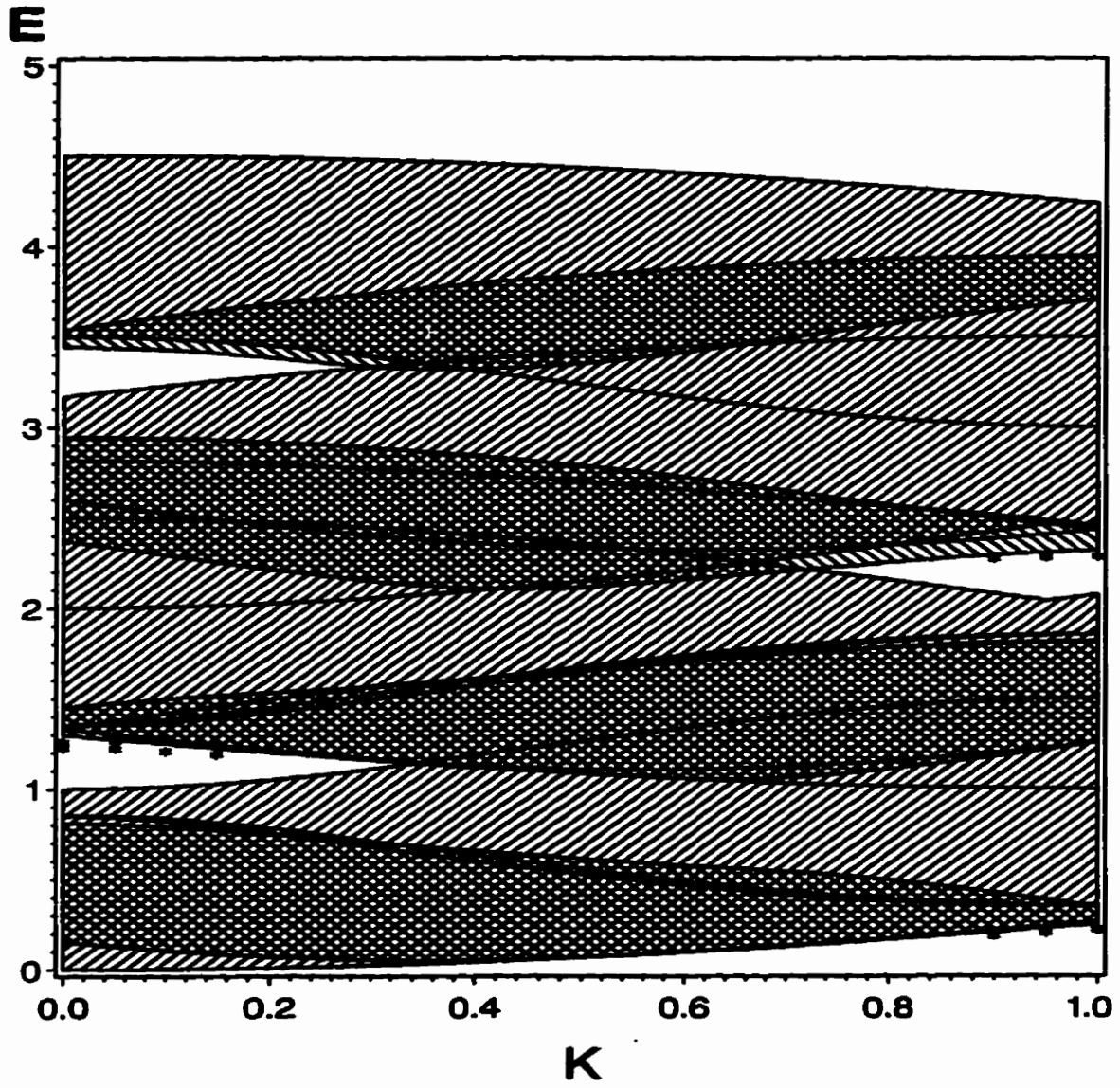


Figure 5.4: The three-magnon continuum and the three-magnon bound states (star points) of the uniform spin $S = S' = \frac{1}{2}$ chain with alternating bonds ($J_1 = 2J_2 = 1$). The energy is in units of J_1 and the total wavevector K is in units of $\frac{\pi}{2}$.

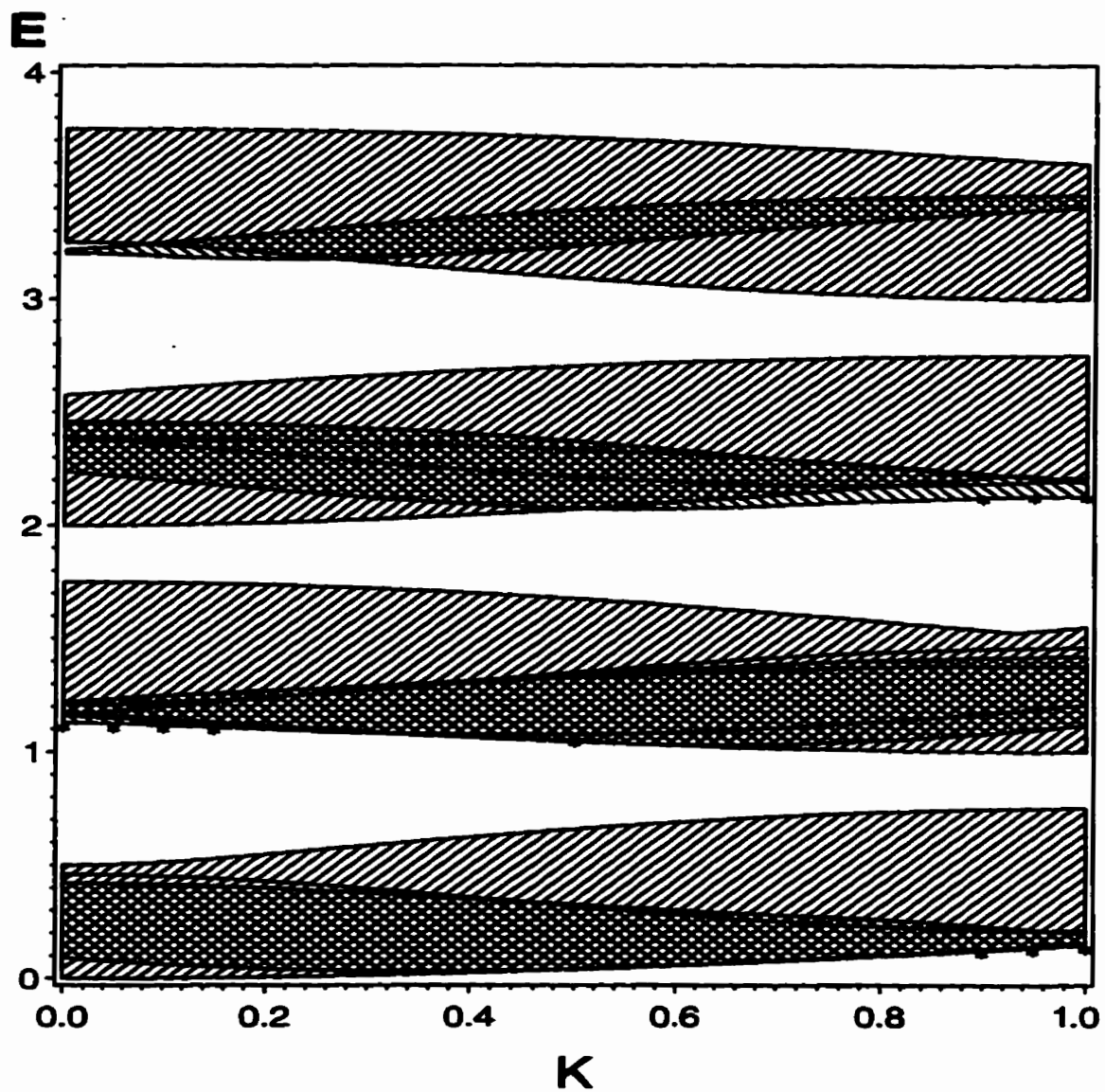


Figure 5.5: The three-magnon continuum (shaded region) and the three-magnon bound states (star points) of the uniform spin $S = S' = \frac{1}{2}$ chain with alternating bonds ($J_1 = 4J_2 = 1$). The energy is in units of J_1 and the total wavevector K is in units of $\frac{\pi}{2}$.

Assuming that $S \geq S'$, the values for the total spin J are $S + S', S + S' - 1, S + S' - 2, \dots, S - S'$; and from (5.7), the energy levels present for each block are:

$$\begin{aligned}
E(J = S + S') &= -J_1 S S' \\
E(J = S + S' - 1) &= -J_1 [S S' - (S + S')] \\
E(J = S + S' - 2) &= -J_1 [S S' - 2(S + S') + 1] \text{ if } S' \geq 1 \\
E(J = S + S' - 3) &= -J_1 [S S' - 3(S + S') + 3] \text{ if } S' \geq 3/2 \\
&\vdots \\
E(J = S - S') &= J_1 S'(S + 1)
\end{aligned} \tag{5.8}$$

The ground state of each block has maximum $J = S + S'$ and energy $-J_1 S S'$. The excitations from this state within a block are given by:

$$\begin{aligned}
\Delta E_{J=S+S' \rightarrow J=S+S'-1} &= J_1 (S + S') \\
\Delta E_{J=S+S' \rightarrow J=S+S'-2} &= 2J_1 (S + S') - J_1 \text{ if } S' \geq 1 \\
\Delta E_{J=S+S' \rightarrow J=S+S'-3} &= 3J_1 (S + S') - 3J_1 \text{ if } S' \geq 3/2 \\
&\vdots \\
\Delta E_{J=S+S' \rightarrow J=S-S'} &= 2J_1 S S' + J_1
\end{aligned} \tag{5.9}$$

When the system is in the ground state, all the blocks have a total spin of $J = S + S'$ and the total energy is $E_0 = -J_1 S S' N/2$. One-magnon excitations correspond to having a single deviation in any block with the z-component of the total spin, J_z , jumping from $+J$ to $+J - 1$. This excited state with $J_z = +J - 1$ can correspond only to states with total spin equal to J or $J - 1$. Hence, the energy transitions for the one-magnon excitations are

$$\begin{aligned}
\Delta E_{J, J_z=+J \rightarrow J-1, J_z=+J-1} &= J_1 (S + S') \\
\Delta E_{J, J_z=+J \rightarrow J, J_z=+J-1} &= 0
\end{aligned} \tag{5.10}$$

which are in complete agreement with equation (2.10) when evaluated for $J_2 = 0$.

The two-magnon case corresponds to two single deviations which can be in two different blocks or in the same block of the system. When in different blocks, the energy is the sum of two single excitations, i.e.:

$$\begin{aligned}\Delta E &= \{0 \text{ or } J_1(S + S')\} + \{0 \text{ or } J_1(S + S')\} \\ &= \{0, J_1(S + S'), 2J_1(S + S')\}\end{aligned}$$

which correspond to the excitations for the two-free magnon problem.

Two deviations in the same block correspond to a transition $J_z = +J \rightarrow J_z = +J - 2$. A state with $J_z = +J - 2$ could correspond to states with total spin equal to J , $J - 1$ or $J - 2$, and the excitation energies are given by:

$$\Delta E = \begin{cases} 0 \\ J_1(S + S') \\ 2J_1(S + S') - J_1 \quad \text{if } S' \geq 1 \end{cases} \quad (5.11)$$

The combination of the transitions for the two deviations in different blocks or in the same block, gives the two-magnon states of the system.

$$\Delta E = \begin{cases} 0 \\ J_1(S + S') \\ 2J_1(S + S') - J_1 \quad \text{if } S' \geq 1 \\ 2J_1(S + S') \end{cases} \quad (5.12)$$

Similarly, the three-magnon states are the result of combining three deviations that could be in three separate blocks, two in one block and the other in a different block, or the three in the same block. When the three deviations are all in different blocks, and considering the one-magnon excitations (5.10), the possible transitions are the result of the following logical expression:

$$\begin{aligned}\Delta E &= \{0 \text{ or } J_1(S + S')\} + \{0 \text{ or } J_1(S + S')\} + \{0 \text{ or } J_1(S + S')\} \\ &= \{0, J_1(S + S'), 2J_1(S + S'), 3J_1(S + S')\}\end{aligned}$$

and correspond to the three-free magnon states.

When two deviations are in the same block and the other in a different block, and using the two-magnon excitation and the one-magnon excitation results above, the possible transitions are given by:

$$\begin{aligned}\Delta E &= \begin{cases} 0 \\ J_1(S + S') \end{cases} + \begin{cases} 0 \\ J_1(S + S') \\ 2J_1(S + S') - J_1 & \text{if } S' \geq 1 \\ 2J_1(S + S') \end{cases} \\ &= \begin{cases} 0 \\ J_1(S + S') \\ 2J_1(S + S') - J_1 & \text{if } S' \geq 1 \\ 2J_1(S + S') \\ 3J_1(S + S') - J_1 & \text{if } S' \geq 1 \\ 3J_1(S + S') \end{cases} \end{aligned} \quad (5.13)$$

and corresponds to the two-bound one-free continua.

For the condition where the three deviations are in the same block, a transition $J_z = +J \rightarrow J_z = +J - 3$ occurs. A state with $J_z = +J - 3$ corresponds to states with total spin equal to $J, J - 1, J - 2$ or $J - 3$, with excitation energies:

$$\Delta E = \begin{cases} 0 \\ J_1(S + S') \\ 2J_1(S + S') - J_1 & \text{if } S' \geq 1 \\ 3J_1(S + S') - 3J_1 & \text{if } S' \geq 3/2 \end{cases} \quad (5.14)$$

which correspond to the three-magnon bound states.

Summarizing, the three-magnon excitations will be given by:

$$\Delta E = \begin{cases} 0 \\ J_1(S + S') \\ 2J_1(S + S') - J_1 & \text{if } S' \geq 1 \\ 2J_1(S + S') \\ 3J_1(S + S') - 3J_1 & \text{if } S' \geq 3/2 \\ 3J_1(S + S') - J_1 & \text{if } S' \geq 1 \\ 3J_1(S + S') \end{cases} \quad (5.15)$$

In Table 5.1, we have grouped the three-magnon excitations derived from the $J_2 \rightarrow 0$ limit for different S, S' chains. The first observation that we can derived from Table 5.1 is that the number of levels (not considering degeneracy) that the chain will have for the three-magnon excitations will change from 4 to 6 and then to 7 as the smaller spin in the chain takes the values $\frac{1}{2}$, 1 or $3/2$. Also, these levels separate as the total spin increases, augmenting the possibility that gaps will appear even in the case of homogeneous bonds.

The degeneracy of each three-magnon level in the $J_2 \rightarrow 0$ limit allows us to predict where three-magnon bound states could be found in non-limit cases. We expect to find three-magnon bound states in the bands associated with the levels 0, Ξ , $2\Xi - J_1$ and $3\Xi - 3J_1$, where $\Xi = J_1(S + S')$ (see equation 5.14). Depending on the degeneracy of their corresponding energies, these bound states could split from the rest of the levels, 3ϵ and 2ϵ , once J_2 is different from zero. It is clear that the $2\Xi - J_1$ level will only appear for chains with both spins greater or equal to 1; and the $3\Xi - 3J_1$ level, for chains with both spins greater or equal to $3/2$.

For example, returning to our previous discussion on the $S = S' = \frac{1}{2}$ alternating bond case, when considering the $J_2 \rightarrow 0$ limit, the three-magnon excitations occur at 0, J_1 , $2J_1$ and $3J_1$. And, as we can see in Figure (5.6), the three-magnon continua for the $S = S' = \frac{1}{2}$, $J_1 = 1$, $J_2 = \frac{1}{10}$ chain is quite collapsed into the predicted discrete theoretical states, clearly manifesting this tendency as J_2 goes from 1 to 0

Three-magnon excitations in the $J_2 \rightarrow 0$ limit							
S, S'	0	Ξ	$2\Xi - J_1$	2Ξ	$3\Xi - 3J_1$	$3\Xi - J_1$	3Ξ
degeneracy	3f, 2b1f, 3b	3f, 2b1f, 3b	2b1f, 3b	3f, 2b1f	3b	2b1f	3f, 2b1f
1/2, 1/2	0	1		2			3
1, 1/2	0	1.5		3			4.5
3/2, 1/2	0	2		4			6
1, 1	0	2	3	4		5	6
3/2, 1	0	2.5	4	5		6.5	7.5
3/2, 3/2	0	3	5	6	6	8	9
2, 3/2	0	3.5	6	7	7.5	9.5	10.5

Table 5.1: Three-magnon excitations for chains of isolated blocks in units of J_1 and where $\Xi = J_1(S + S')$. The degeneracy of the levels due to the three-free (3f), two-free one-bound (2b1f) and three-bound (3b) states has been explicitly tabulated.

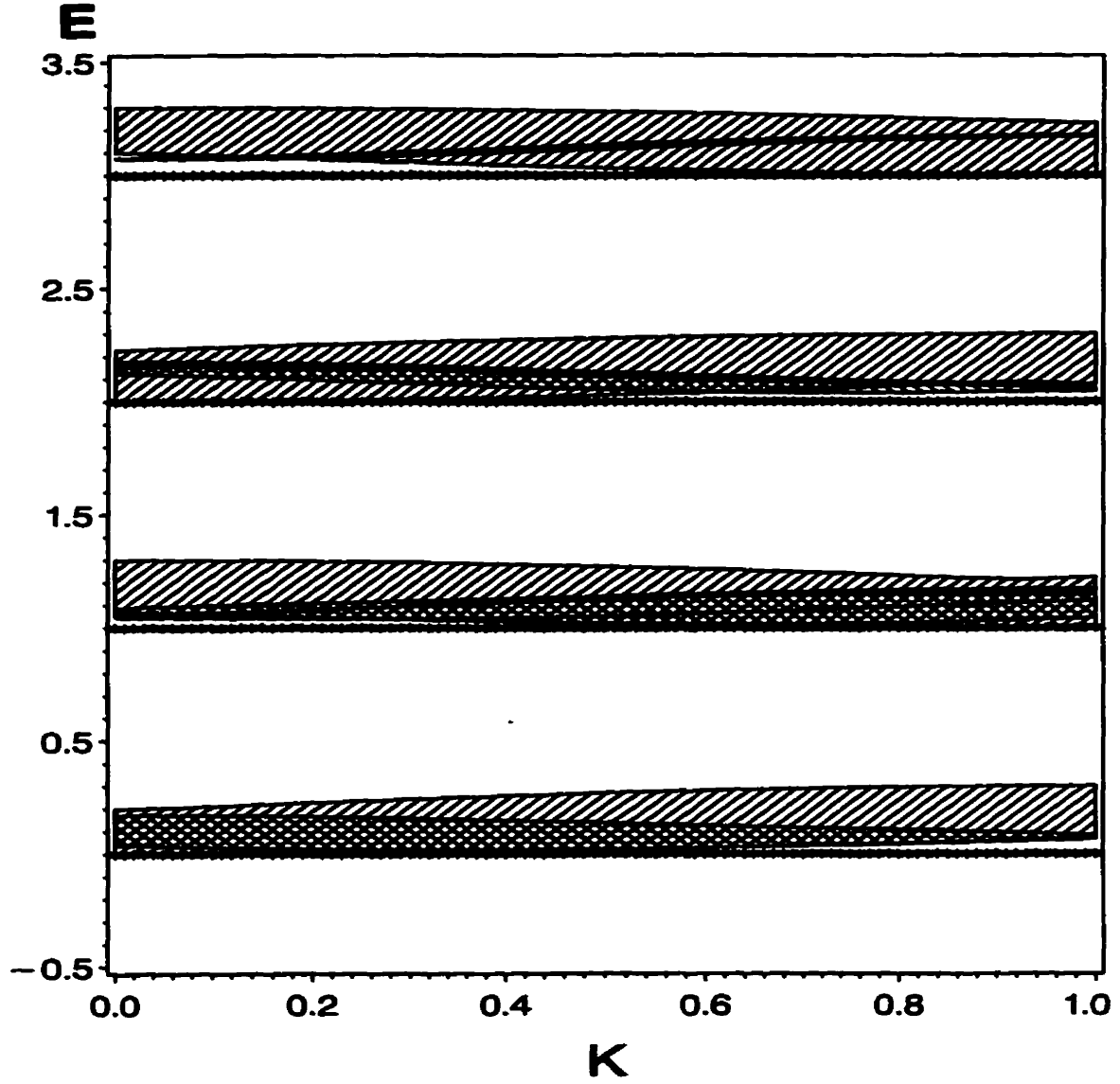


Figure 5.6: Graphical representation of the three-magnon excitation levels (star points) in a system of isolated blocks, each block composed of two connected spins, $S = S' = \frac{1}{2}$. The shaded continua correspond to the three-magnon continuum of a very weakly bond $S = S' = \frac{1}{2}$, $J_1 = 1$, $J_2 = \frac{1}{10}$ chain. The energy is in units of J_1 and the total wavevector K is in units of $\frac{\pi}{2}$.

in figures (5.3), (5.4) and (5.5). Also, we did not find bound states in the third gap. Theoretically, we predict that a bound state would not exist in the last gap as the last band will be formed from three-free and two-bound one-free states. Figures (5.4) and (5.5) show the absence of bound states in the last gap which corroborate this conclusion. Following the same theoretical analysis, the middle gap should not present bound states as its upper band is also formed by three-free and two-bound one-free states. Nonetheless, they are present for both the $J_2 = \frac{1}{2}$ and the $J_2 = \frac{1}{4}$ cases. We estimate that these bound states are due to three-bound magnons in three adjacent sites which can not be predicted in the $J_2 \rightarrow 0$ limit. The three sites are disconnected as they belong to two different isolated blocks.

5.3 $S = 2S' = 1$ Case

This section will briefly present the results for a $S = 2S' = 1$ chain. In the previous $J_2 = 0$ limit section, we predicted that gaps could appear due to the fact that the levels separate as the total spin of a block increases, even in the case of no bond alternation,. As can be seen in Figure (5.7) and comparing with Figure (5.3), one gap is present as a simple consequence of the increase of the total spin. When $J_2 \rightarrow 0$, more gaps start to appear and widen as shown in Figures (5.8) and (5.9).

Figures (5.7), (5.8) and (5.9) summarize our results for the $S = 2S' = 1$ case. We found bound states below the lower edge of the three-magnon continuum for chains with J_2 equal to $\frac{1}{4}$, $\frac{1}{2}$ and 1. Also, when gaps were present, there were bound states below the third band associated with the $3J_1$ limit level. For $J_2 = \frac{1}{4}$, we found bound states in the first gap as expected from the $J_2 \rightarrow 0$ analysis. Nonetheless, for $J_2 = \frac{1}{2}$, we searched the same first gap for total wavevector $K = 0, 0.05, 0.1$ and 0.15 and we did not find any. In general, the results for a $S = 2S' = 1$ chain look quite similar to the $S = S' = \frac{1}{2}$ ones: wider spectrum and gaps, and bound states located in similar regions.

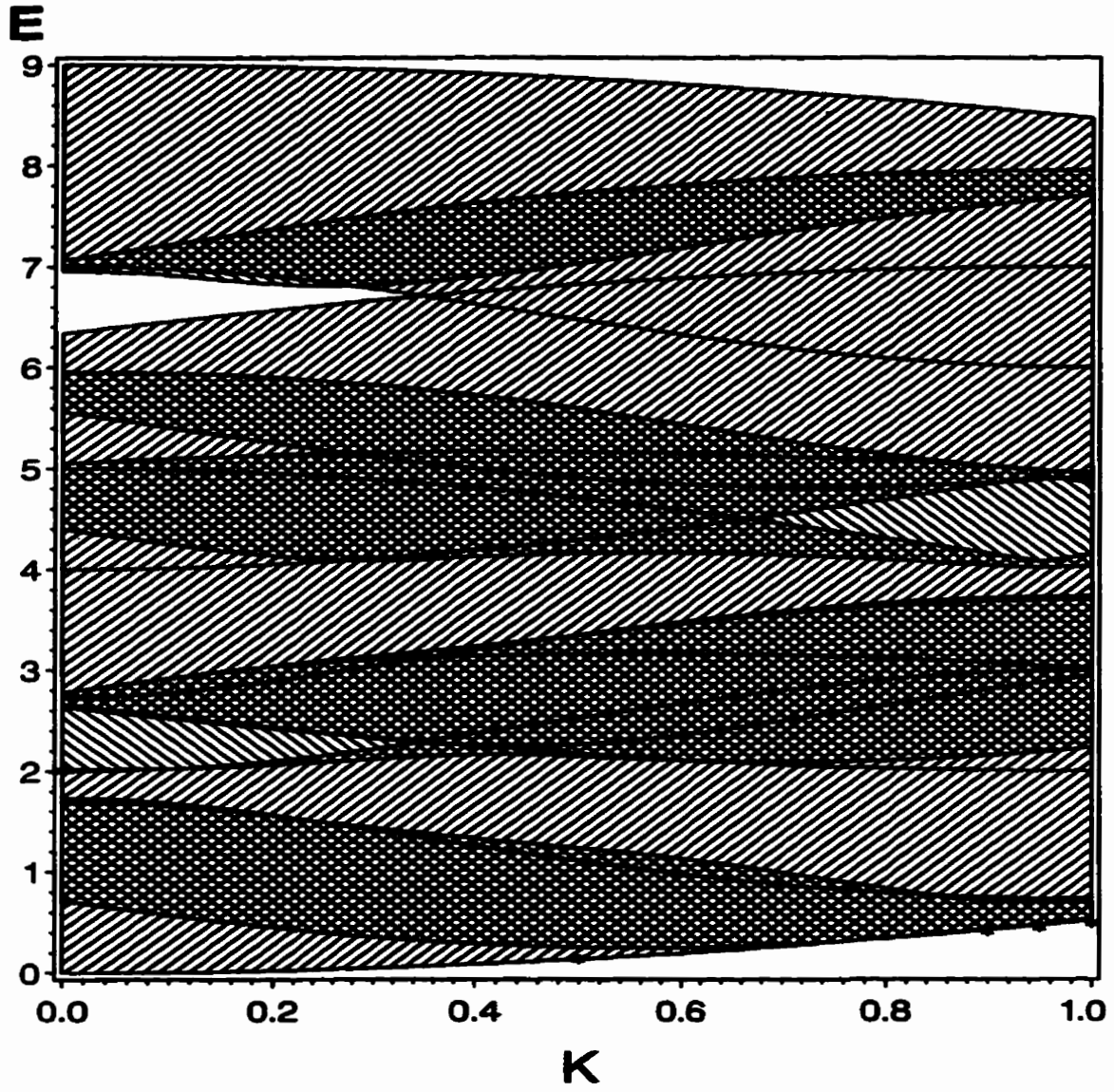


Figure 5.7: The three-magnon state continuum for the $S = 2S' = 1$ and $J_1 = J_2 = 1$ chain. The isolated points represent the bound states found through the Recursion Method. The energy is in units of J_1 and the total wavevector K is in units of $\frac{\pi}{2}$.

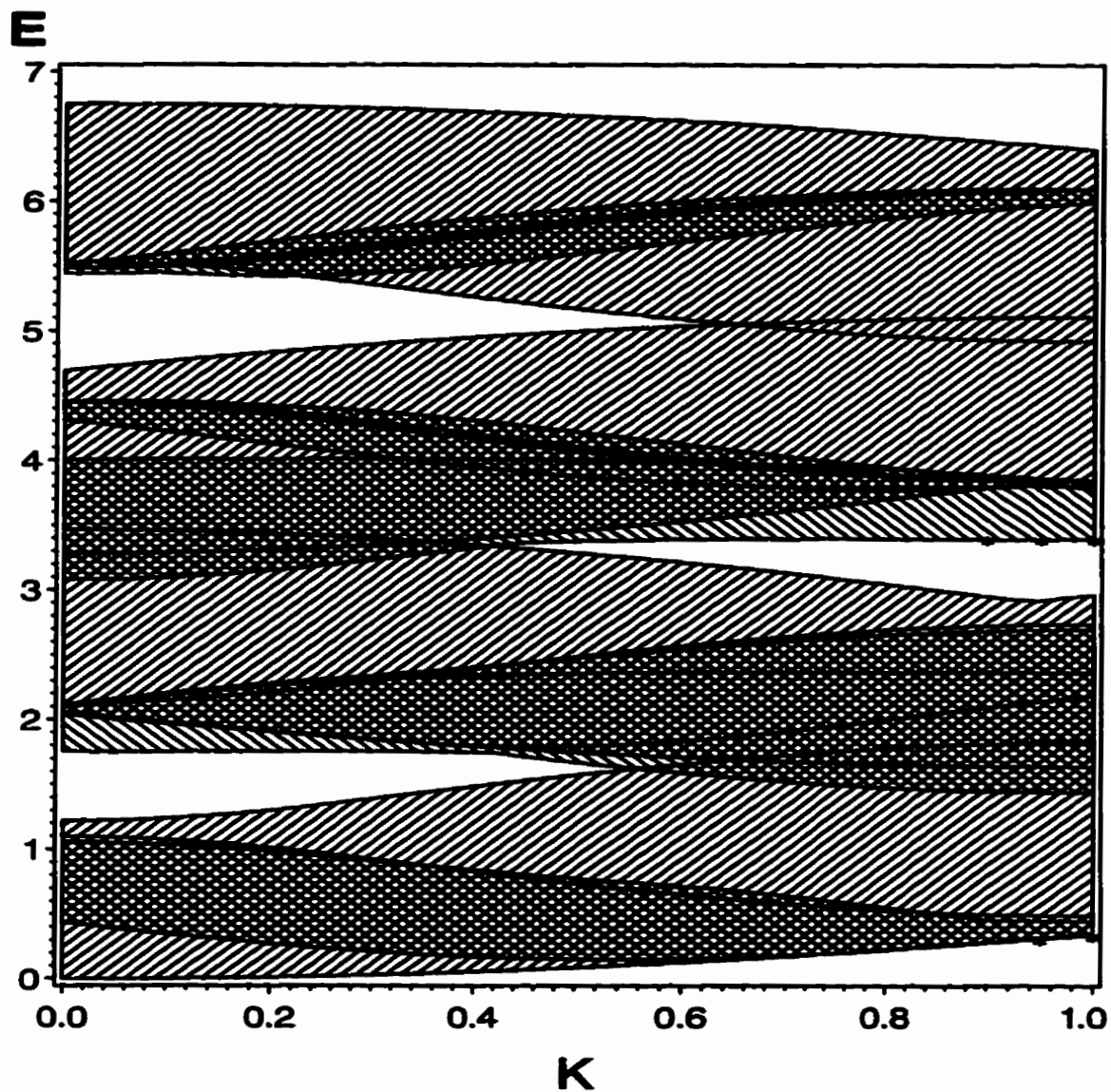


Figure 5.8: The three-magnon state continuum for the $S = 2S' = 1$ and $J_1 = 2J_2 = 1$ chain. The isolated points represent the bound states found through the Recursion Method. The energy is in units of J_1 and the total wavevector K is in units of $\frac{\pi}{2}$.

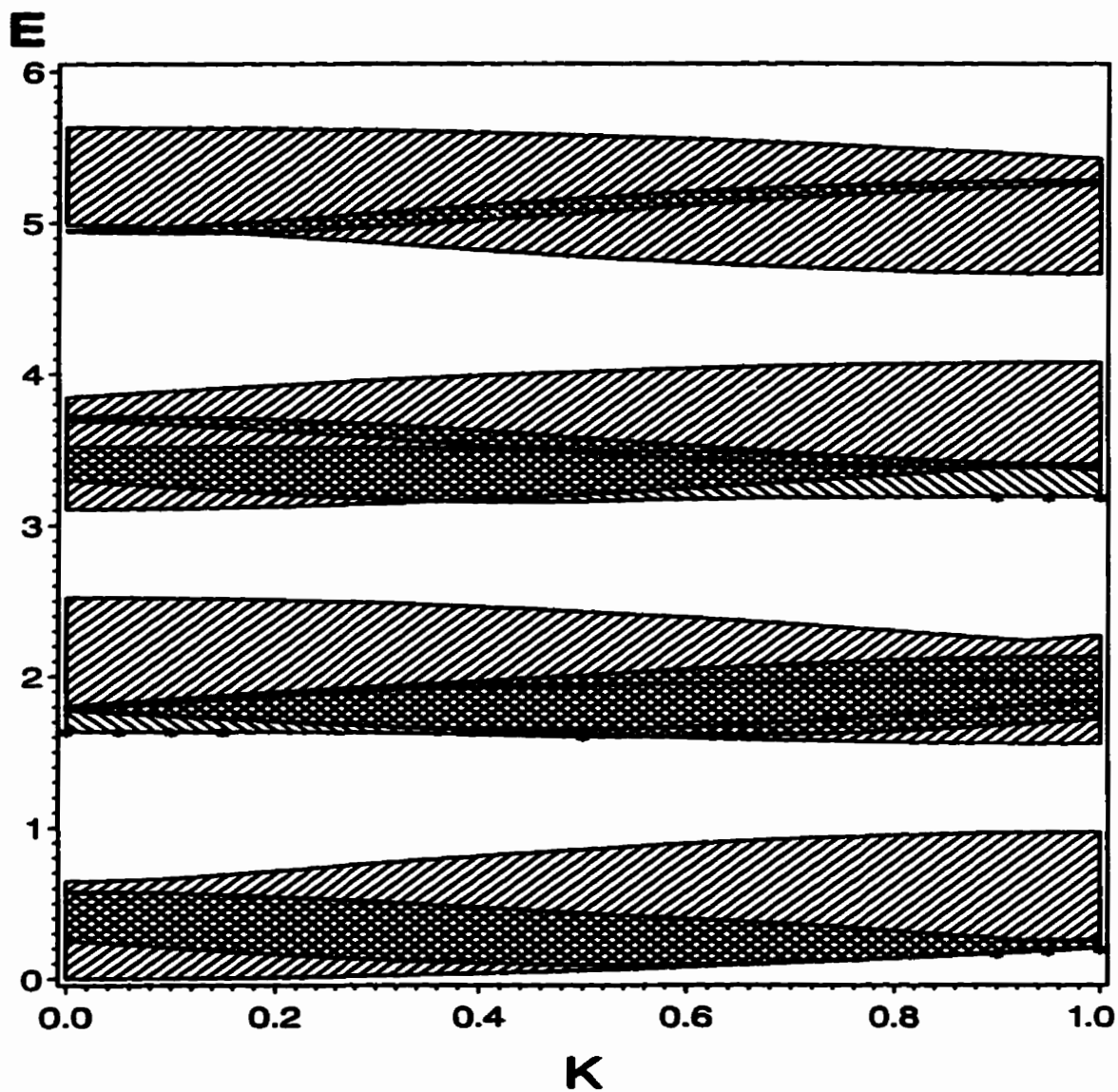


Figure 5.9: The three-magnon state continuum for the $S = 2S' = 1$ and $J_1 = 4J_2 = 1$ chain. The isolated points represent the bound states found through the Recursion Method. The energy is in units of J_1 and the total wavevector K is in units of $\frac{\pi}{2}$.

5.4 $S = S' = 1$ Case and the Initial Ket Effects

Figures (5.10) and (5.11) show that the $S = S' = 1$ spin chain does provide different results compared to the $S = 2S' = 1$ case. The spectrum is broader as the bands increase in width due to a larger spin value. As predicted in the $J_2 \rightarrow 0$ analysis, we see that the spectrum collapse to six levels instead of the four levels seen in the previous two cases. But in general, the same behavior can be observed.

Now, we want to discuss the influence of the chosen initial ket on the numerical three-magnon density of states. The contributions that can be identified from both bound states and scattering states will depend on the values chosen for the the initial states $|e, K; x, y\rangle$ and $|o, K; x, y\rangle$, as defined in equations (3.7). One first consideration would be the effect of different choices of $\{x, y\}$ on the results. In Figure (5.12) the local density of states is presented for three different cases:

- (a) Two magnons on the same site and the third one on the neighboring site; i.e., $\{x, y\} = \{1, 0\}$.
- (b) Three neighboring magnons on adjacent sites; i.e., $\{x, y\} = \{1, 1\}$.
- (c) Two neighboring magnons on adjacent sites and the third one on the second-neighbor site; i.e., $\{x, y\} = \{2, 1\}$.

As can easily been seen from these plots, there is a stronger contribution to optical states (higher energies) from the more widely distributed magnons than from tightly bound magnons. This behavior is consistent with the fact that bound states usually have lower energies than the scattering states.

Another important consideration is the symmetry of the initial ket with respect to interchange of the spins on even and odd sites. This information is described in terms of the weight for the initial even ket $|e, K; x, y\rangle$ in comparison to the initial odd ket $|o, K; x, y\rangle$. In Figure (5.13) the local density of states is presented for four different cases:

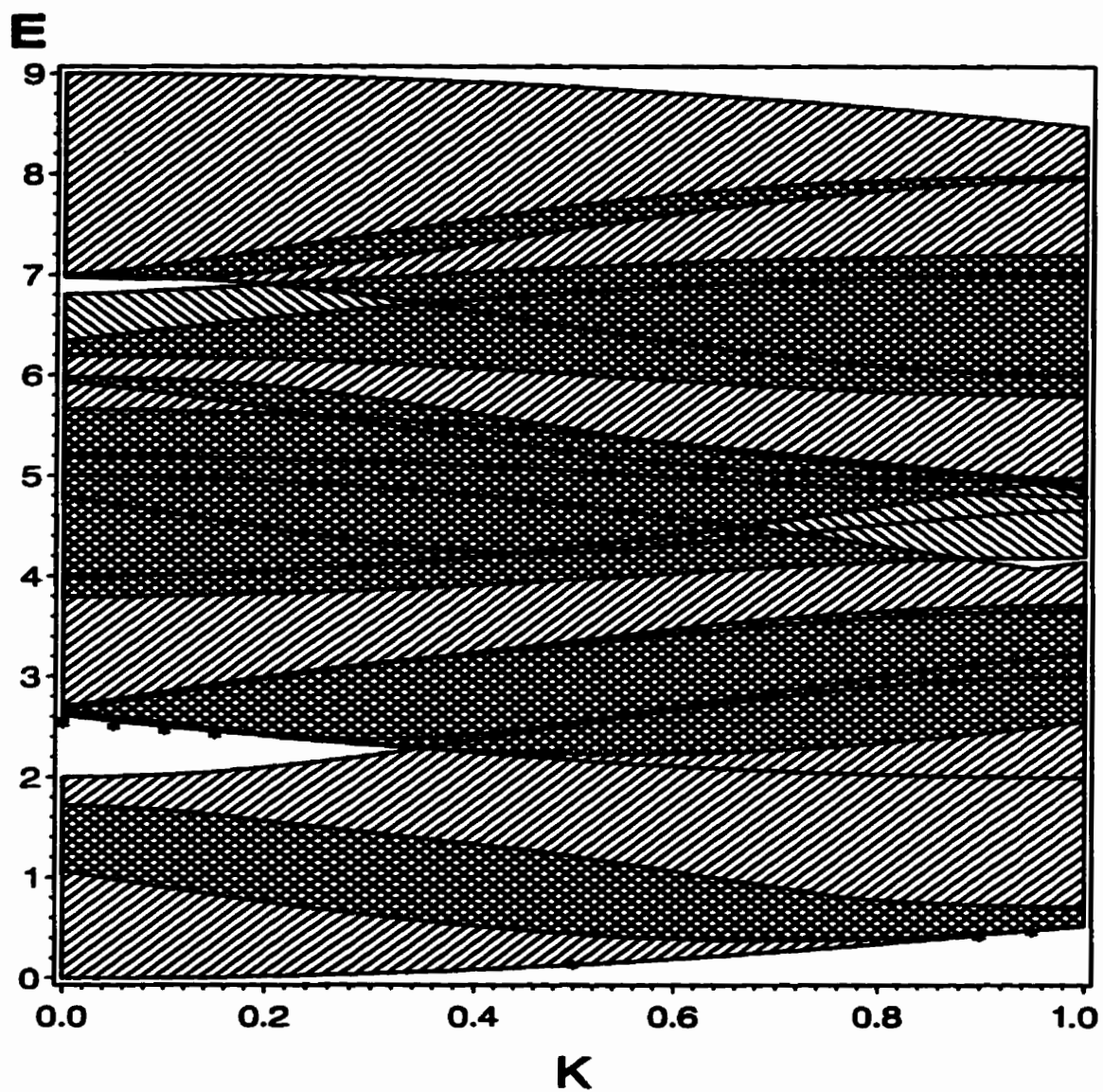


Figure 5.10: The three-magnon state continuum for the $S = S' = 1$ and $J_1 = 2J_2 = 1$ chain. The isolated points represent the bound states found through the Recursion Method. The energy is in units of J_1 and the total wavevector K is in units of $\frac{\pi}{2}$.

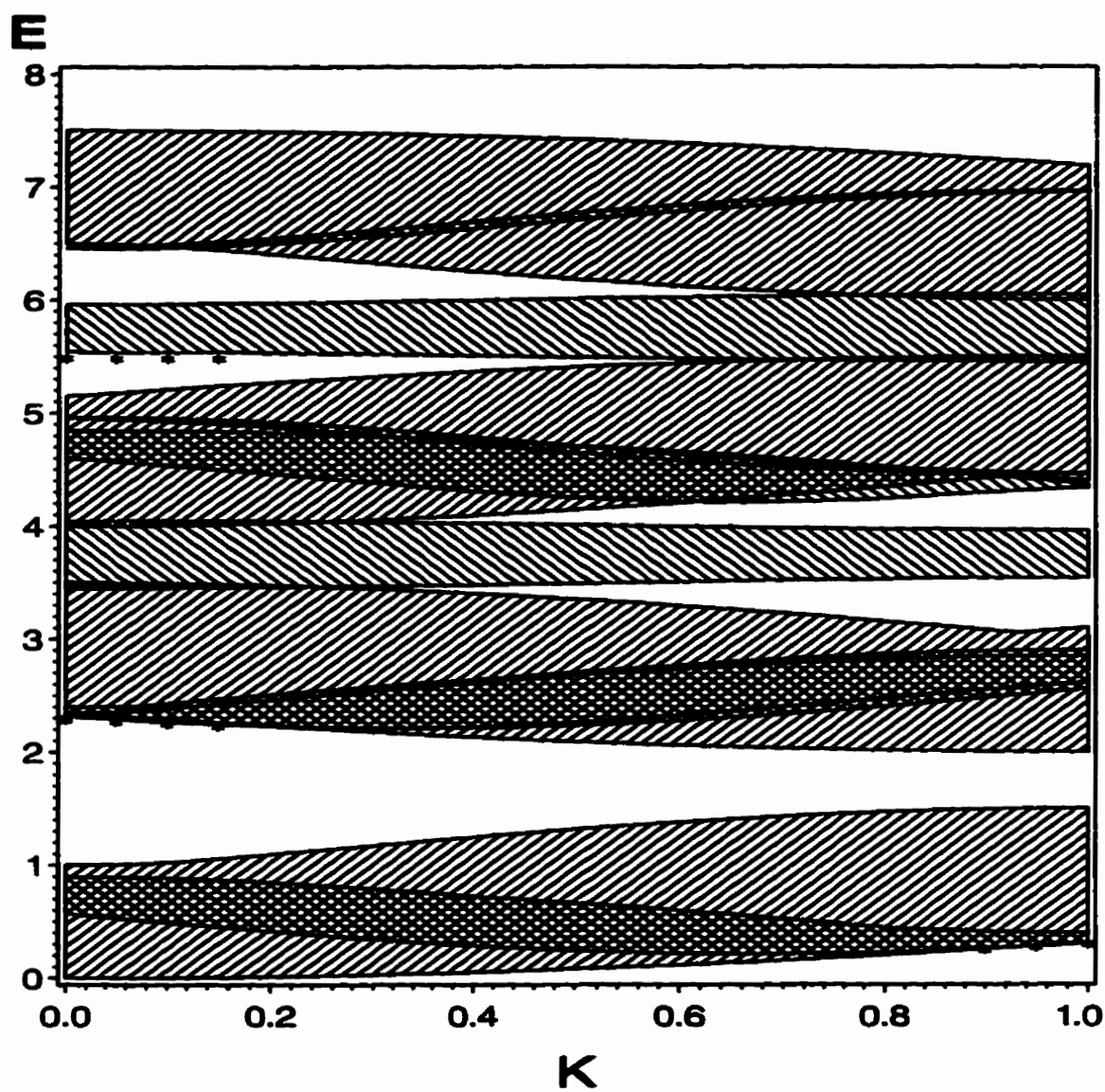


Figure 5.11: The three-magnon state continuum for the $S = S' = 1$ and $J_1 = 4J_2 = 1$ chain. The isolated points represent the bound states found through the Recursion Method. The energy is in units of J_1 and the total wavevector K is in units of $\frac{\pi}{2}$.

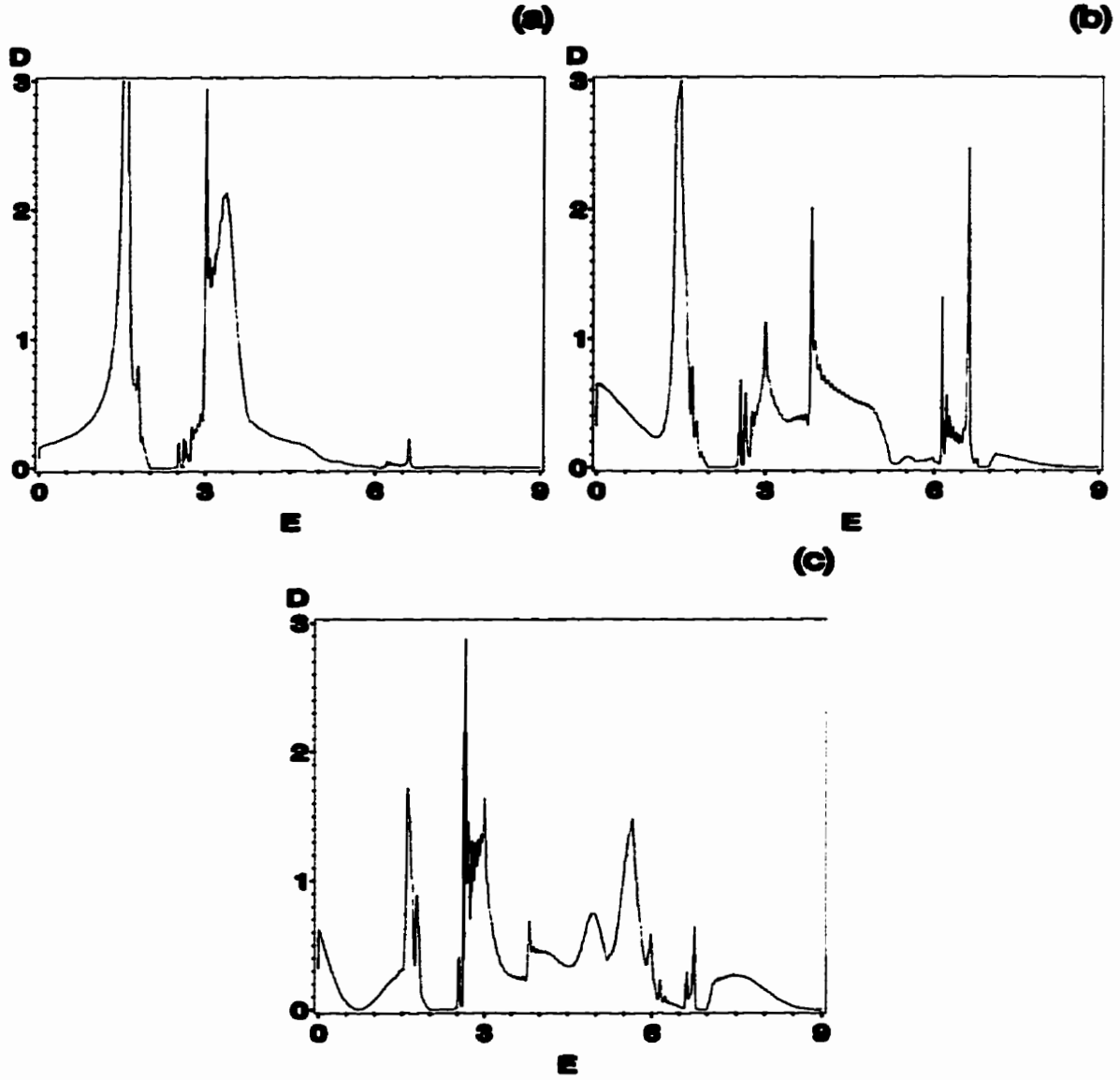


Figure 5.12: Density of states for (a) two magnons on the same site and the third one on the neighboring site, (b) three neighboring magnons on adjacent sites and (c) two neighboring magnons on adjacent sites and the third one on the second-neighboring site for the $S = S' = 1$ and $J_1 = 2J_2 = 1$ chain at $K = 0$. The energy is in units of J_1 .

- (a) no initial odd ket contribution; i.e., $\{|e, K; x, y\rangle, |o, K; x, y\rangle\} = \{1, 0\}$.
- (b) no initial even ket contribution; i.e., $\{|e, K; x, y\rangle, |o, K; x, y\rangle\} = \{0, 1\}$.
- (c) an initial symmetric contribution from both an even ket and odd ket; i.e., $\{|e, K; x, y\rangle, |o, K; x, y\rangle\} = \{\frac{1}{\sqrt{2}}, \frac{1}{\sqrt{2}}\}$.
- (d) an initial antisymmetric contribution from both an even ket and odd ket; i.e., $\{|e, K; x, y\rangle, |o, K; x, y\rangle\} = \{\frac{1}{\sqrt{2}}, -\frac{1}{\sqrt{2}}\}$.

Although the difference is quite evident in each of the cases presented, it is important to emphasize the influence that has over the search for bound states. One clear example occurs for the alternating bond chain ($S = S' = 1$ and $J_1 = 2J_2 = 1$) when $K = 0$ and in the first gap. Depending on the initial ket chosen, either two bound states or only one of them is observed. In Figure (5.14) we present the density of states near the energy gap located between $[2.00, 2.61]$. We found two bound states in this region at the energies 2.53 and 2.56. When the initial state is taken as $\{|e, K; 2, 1\rangle, |o, K; 2, 1\rangle\} = \{1, 0\}$, only the bound state at 2.53 appears as can be seen in Figure (5.14)(a). In contrast, when chosen the initial state as $\{|e, K; 1, 1\rangle, |o, K; 1, 1\rangle\} = \{\frac{1}{\sqrt{2}}, \frac{1}{\sqrt{2}}\}$, only the second bound state at 2.56 appears as shown in Figure (5.14)(b). Figures (5.14)(c) and (5.14)(d) show both bound states when the initial states correspond to $\{|e, K; 1, 1\rangle, |o, K; 1, 1\rangle\} = \{1, 0\}$ and $\{|e, K; 1, 0\rangle, |o, K; 1, 0\rangle\} = \{\frac{1}{\sqrt{2}}, \frac{1}{\sqrt{2}}\}$, respectively.

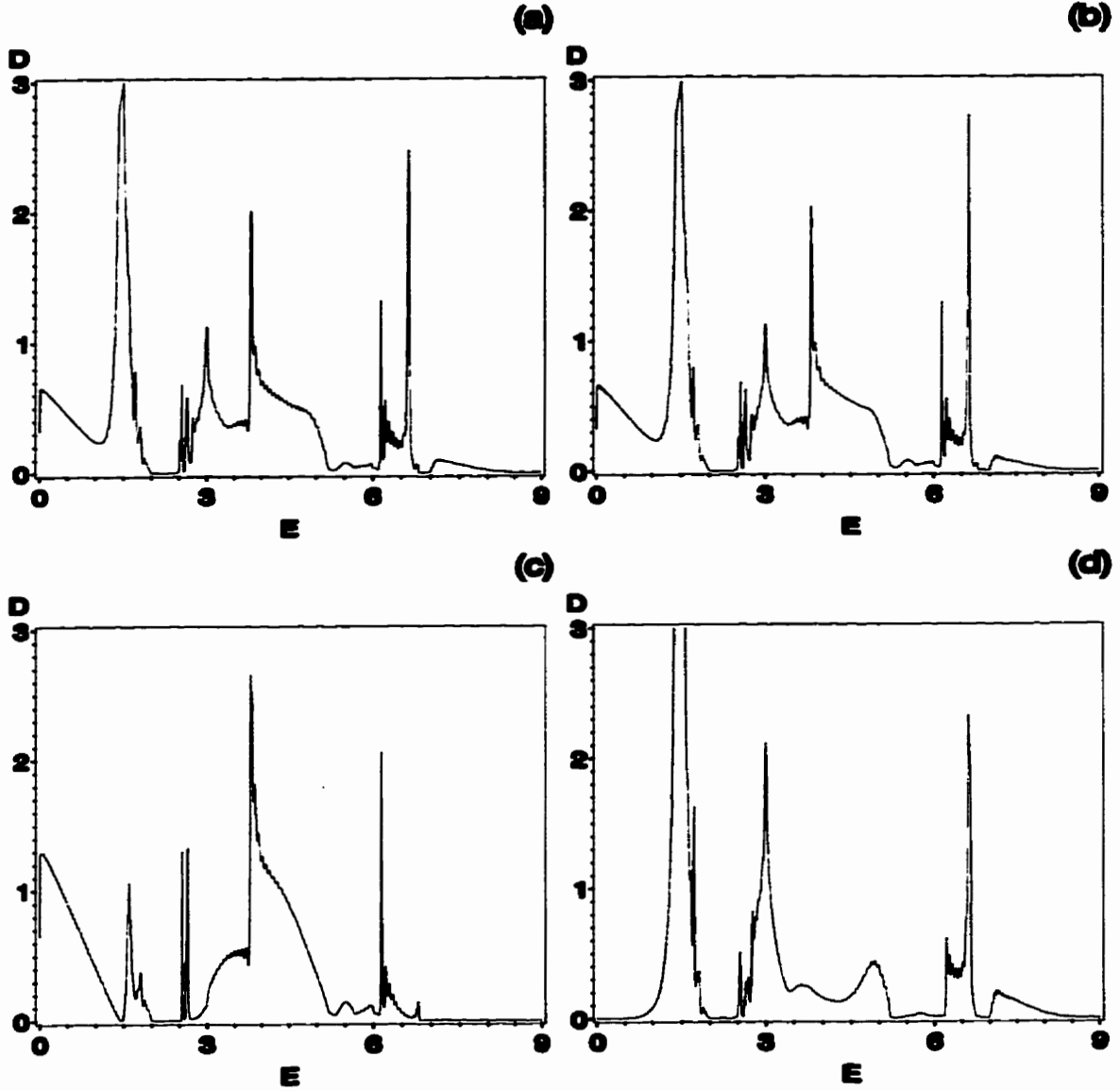


Figure 5.13: Density of states for three neighboring magnons on adjacent sites for the $S = S' = 1$ and $J_1 = 2J_2 = 1$ chain at $K = 0$. For case (a) there is no initial odd ket contribution ($\{|e, K; x, y\rangle, |o, K; x, y\rangle\} = \{1, 0\}$); for case (b), there is no initial even ket contribution ($\{|e, K; x, y\rangle, |o, K; x, y\rangle\} = \{0, 1\}$). Case (c) shows an initial symmetric contribution from both an even ket and an odd ket ($\{|e, K; x, y\rangle, |o, K; x, y\rangle\} = \{\frac{1}{\sqrt{2}}, \frac{1}{\sqrt{2}}\}$); and case (d), an initial antisymmetric contribution from both an even ket and an odd ket ($\{|e, K; x, y\rangle, |o, K; x, y\rangle\} = \{\frac{1}{\sqrt{2}}, -\frac{1}{\sqrt{2}}\}$). The energy is in units of J_1 .

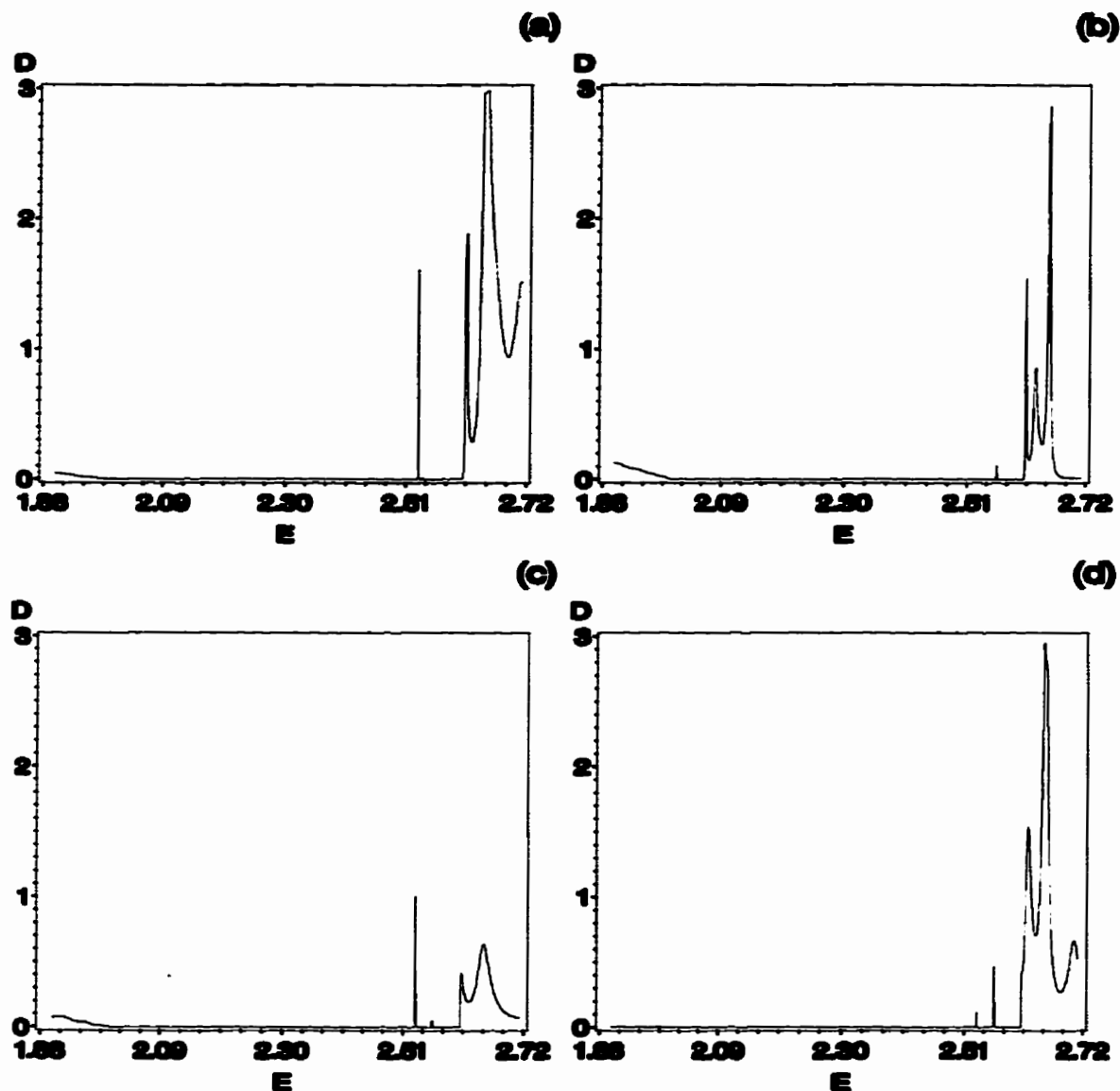


Figure 5.14: Density of states for the first gap region of the $S = S' = 1$ and $J_1 = 2J_2 = 1$ chain at $K = 0$. The presence of two bound states near the higher edge of the gap is observed depending on the initial kets chosen. For case (a), $\{|e, K; 2, 1\rangle, |o, K; 2, 1\rangle\} = \{1, 0\}$, only the lower bound state is observed. In case (b), $\{|e, K; 1, 1\rangle, |o, K; 1, 1\rangle\} = \{\frac{1}{\sqrt{2}}, \frac{1}{\sqrt{2}}\}$, only the higher bound state appears. Cases (c) and (d) correspond to $\{|e, K; 1, 1\rangle, |o, K; 1, 1\rangle\} = \{1, 0\}$ and $\{|e, K; 1, 0\rangle, |o, K; 1, 0\rangle\} = \{\frac{1}{\sqrt{2}}, \frac{1}{\sqrt{2}}\}$, respectively, and both bound states appear. The energy is in units of J_1 .

Chapter 6

Summary

We have studied the three-magnon excitations for one-dimensional Heisenberg spin chains, paying close attention to the effect of alternation for either spins and/or bonds. We only considered systems with ferromagnetic ground states and described by the Hamiltonian (1.5):

$$\widehat{H} = - \sum_{n=1}^{N/2} \left[J_1(\vec{S}'_{2n} \cdot \vec{S}_{2n+1}) + J_2(\vec{S}_{2n+1} \cdot \vec{S}'_{2n+2}) \right] \quad (6.1)$$

which describes a one-dimensional lattice with alternating spins/bonds. We successfully applied the Recursion Method to solve the three-magnon problem. First, we obtained the two-magnon states numerically and then combined the three-free continuum and the two-bound one-free continuum to find the entire three-magnon continuum, allowing us to determine where any gaps occur. Once the edges of the three-magnon continuum are known, we were able to terminate the continued fraction of the three-magnon density of states using a generalized procedure developed by Turchi *et al* [13] that allows to obtain the tail of the continued fraction (4.40) in the presence of multiple gaps. Using the three-magnon density of states, we were able to determine the location of the bound states in different systems.

In general, we found the usual bound state branch below the lower edge of the three-magnon continuum for every case studied. We compared our results to previous

analytical results, such as those of Bethe in the $S = S' = 1/2$ chain with homogeneous bonds. We were able to reproduce his exact results. Also, we extended the study of S. C. Bell *et al* [15] from the two-magnon spectrum of the alternating bond $S = 1/2$ ferromagnetic Heisenberg chain, to the three-magnon problem. When a bond alternation is introduced for this chain, gaps immediately appear and additional bound states are found. As J_2 decreases, the continuum start to collapse into very predictable levels and the different bands of the spectrum become narrower.

In order to predict these levels and the location of bound states, as it was evident that the higher gap never had bound states, we studied a $J_2 \rightarrow 0$ limit case of isolated S, S' spin blocks. We derived from this limit analysis that the number of levels (not considering degeneracy) for the three-magnon excitations changes from 4 to 6 and then to 7 as the smaller spin in the chain takes the values $1/2$, 1 or $3/2$. Also, these levels separate as the total spin increases, with gaps appearing even in the case of homogeneous bonds as can be seen in the results for $S = 2S' = 1$ and $S = S' = 1$ spin chains. The $J_2 \rightarrow 0$ limit analysis also provided another way of checking the numerical results obtained through the Recursion Method.

In conclusion, with this work, we have presented a direct and relatively simple procedure to search for bound states in alternating spin/bond chains. The Recursion Method was used very effectively to achieve this purpose and the generalization to an m -magnon problem would be straight forward, specially with the implemented termination of the continued fraction using a Mathematica program.

Appendix A

Tail of the Continued Fraction for Multiple Gaps: Mathematica Implementation

In this appendix, we explain how we implement the procedure to obtain the termination of the continued fraction as described in Section 4.3 for the case of several gaps. To obtain the density of states for the specific cases of spin chains that we studied, we had to consider a maximum of five gaps.

The following Mathematica program listing provides the coefficients needed to obtain the tail of the continued fraction for cases of up to five gaps. Nonetheless, this program can be easily generalized.

```
1. FstEq[ns_,q_,x_] :=  
   CoefficientList[Glhs[ns,x],x]==CoefficientList[Grhs[ns,q,x],x]  
  
2. Glhs[ns_,x_] :=1+Sum[ph[i,0,0]*x^i,{i,1,ns}]  
  
3. ph[1,i_,j_] :=h[i,j]  
  
4. ph[n_,i_,j_] :=Sum[h[i,1]*ph[n-1,1,j],{1,i-1,i+1}]
```

```

5. h[i_,j_] := Which[i==j, a[i], i==j-1, b[i], j==i-1, b[j], True, 0]

6. Grhs[ns_, q_, x_] := Normal[Series[gnn[q, x], {x, 0, ns}]]

7. gnn[q_, x_] := num[q, x] / den[q, x]

8. num[q_, x_] := 1 + Sum[bx[i] * (-x)^i, {i, 1, q}]

9. den[q_, x_] := Sqrt[1 + Sum[2*s[i] * x^i, {i, 1, 2*q+2}]]

10. ScndEq[ns_, q_, x_] :=
    CoefficientList[ndGlhs[ns, x], x] == CoefficientList[ndGrhs[ns, q, x], x]

11. ndGlhs[ns_, x_] := Sum[ph[i, -1, 0] * x^(i+1), {i, 1, ns-1}]

12. ndGrhs[ns_, q_, x_] := Normal[Series[ndg[q, x], {x, 0, ns}]]

13. ndg[q_, x_] := arr[q, x] / (2*b[-1] * den[q, x])

14. arr[q_, x_] := 1 + Sum[cx[i] * x^i, {i, 1, q+1}] - den[q, x]

15. eb1 = Simplify[FstEq[1, 1, x]]

16. eb2 = Simplify[FstEq[2, 2, x]]

17. eb3 = Simplify[FstEq[3, 3, x]]

18. eb4 = Simplify[FstEq[4, 4, x]]

19. eb5 = Simplify[FstEq[5, 5, x]]

20. sb1 = Solve[eb1, {bx[1]}]

21. sb2 = Solve[eb2, {bx[1], bx[2]}]

22. sb3 = Solve[eb3, {bx[1], bx[2], bx[3]}]

23. sb4 = Solve[eb4, {bx[1], bx[2], bx[3], bx[4]}]

```

```

24. sb5=Solve[eb5,{bx[1],bx[2],bx[3],bx[4],bx[5]}]

25. FortranForm[Simplify[sb1]]>>>bxcoef.tex

26. FortranForm[Simplify[sb2]]>>>bxcoef.tex

27. FortranForm[Simplify[sb3]]>>>bxcoef.tex

28. FortranForm[Simplify[sb4]]>>>bxcoef.tex

29. FortranForm[Simplify[sb5]]>>>bxcoef.tex

30. ec1=Simplify[ScndEq[2,1,x]]

31. ec2=Simplify[ScndEq[3,2,x]]

32. ec3=Simplify[ScndEq[4,3,x]]

33. ec4=Simplify[ScndEq[5,4,x]]

34. ec5=Simplify[ScndEq[6,5,x]]

35. sc1=Solve[ec1,{cx[1],cx[2]}]

36. sc2=Solve[ec2,{cx[1],cx[2],cx[3]}]

37. sc3=Solve[ec3,{cx[1],cx[2],cx[3],cx[4]}]

38. sc4=Solve[ec4,{cx[1],cx[2],cx[3],cx[4],cx[5]}]

39. sc5=Solve[ec5,{cx[1],cx[2],cx[3],cx[4],cx[5],cx[6]}]

40. FortranForm[Simplify[sc1]]>>>cxcoef.tex

41. FortranForm[Simplify[sc2]]>>>cxcoef.tex

42. FortranForm[Simplify[sc3]]>>>cxcoef.tex

43. FortranForm[Simplify[sc4]]>>>cxcoef.tex

```


44. FortranForm[Simplify[sc5]]>>>cxcoef.tex

Line 1 represents the diagonal Green's function of equation (4.42). Lines 2 and 6 are the series expansions for the left and right hand side of this Green's function, which are compared to determine the recurrence relations between the coefficients. The definitions for $\text{ph}[n,i,j]$ and $\text{h}[i,j]$ give the moments for the local density of states at site n as defined in equation (4.44). The $\text{s}[i]$ coefficients defined in line 9 are the coefficients s_i in equation (4.41).

The off-diagonal Green's function of equation (4.43) is defined in line 10 with line 11 and 12 representing the series expansion of each side.

When $\alpha_n(E)$ (4.47) is expanded, the coefficients of its series are represented by $\text{bx}[i]$ in line 8. Also, the expansion of $\nu_{n-1}(E)$ (4.48) gives the $\text{cx}[i]$ coefficients of line 14.

Line 15 and forward resolve the first and second equations for the diagonal and off-diagonal Green's functions. Then, the program prints the coefficients $\text{bx}[i]$ and $\text{cx}[i]$ in files "bxcoef.tex" and "cxcoef.tex", which once substituted in expression (4.40), the tail of the continued fraction $G_0^\infty(E)$ is obtained.

The followings are the coefficients needed to compute a case of up to four gaps.

$$\begin{aligned}
\text{cx}(0) &= 1 \\
\text{cx}(1) &= s(1) \\
\text{cx}(2) &= 2b_{n-2}^2 - s(1)^2/2 + s(2) \\
\text{cx}(3) &= 2a_{n-2}b_{n-2}^2 + 2a_{n-1}b_{n-2}^2 + 2b_{n-2}^2s(1) + s(1)^3/2 - s(1)s(2) + s(3) \\
\text{cx}(4) &= 2a_{n-2}^2b_{n-2}^2 + 2a_{n-2}a_{n-1}b_{n-2}^2 + 2a_{n-1}^2b_{n-2}^2 + 2b_{n-3}^2b_{n-2}^2 + 2b_{n-2}^2b_{n-1}^2 \\
&\quad + 2a_{n-2}b_{n-2}^2s(1) + 2a_{n-1}b_{n-2}^2s(1) - b_{n-2}^2s(1)^2 + 2b_{n-2}^2s(2) \\
&\quad + 3s(1)^2s(2)/2 - s(2)^2/2 - s(1)s(3) + s(4) + 2b_{n-2}^4 - 5s(1)^4/8 \\
\text{cx}(5) &= 2a_{n-2}^3b_{n-2}^2 + 2a_{n-2}^2a_{n-1}b_{n-2}^2 + 2a_{n-2}a_{n-1}^2b_{n-2}^2 + 2a_{n-1}^3b_{n-2}^2 \\
&\quad + 2a_{n-3}b_{n-3}^2b_{n-2}^2 + 4a_{n-2}b_{n-3}^2b_{n-2}^2 + 2a_{n-1}b_{n-3}^2b_{n-2}^2 + 4a_{n-2}b_{n-2}^4
\end{aligned}$$

$$\begin{aligned}
& +4a_{n-1}b_{n-2}^4 + 2a_{n-2}b_{n-2}^2b_{n-1}^2 + 4a_{n-1}b_{n-2}^2b_{n-1}^2 + 2a_nb_{n-2}^2b_{n-1}^2 \\
& +2a_{n-2}^2b_{n-2}^2s(1) + 2a_{n-2}a_{n-1}b_{n-2}^2s(1) + 2a_{n-1}^2b_{n-2}^2s(1) + 2b_{n-3}^2b_{n-2}^2s(1) \\
& +2b_{n-2}^4s(1) + 2b_{n-2}^2b_{n-1}^2s(1) - a_{n-2}b_{n-2}^2s(1)^2 - a_{n-1}b_{n-2}^2s(1)^2 \\
& +b_{n-2}^2s(1)^3 + 7s(1)^5/8 + 2a_{n-2}b_{n-2}^2s(2) + 2a_{n-1}b_{n-2}^2s(2) - 2b_{n-2}^2s(1)s(2) \\
& -5s(1)^3s(2)/20 + 3s(1)s(2)^2/20 + 2b_{n-2}^2s(3) + 3s(1)^2s(3)/20 \\
& -s(2)s(3) - s(1)s(4) + s(5)
\end{aligned}$$

$$\text{bx}(0) = 1$$

$$\text{bx}(1) = a_{n-1} + s(1)$$

$$\text{bx}(2) = a_{n-1}^2 + b_{n-2}^2 + b_{n-1}^2 + a_{n-1}s(1) - s(1)^2/2 + s(2)$$

$$\begin{aligned}
\text{bx}(3) = & a_{n-1}^3 + a_{n-2}b_{n-2}^2 + 2a_{n-1}b_{n-2}^2 + a_nb_{n-1}^2 + a_{n-1}^2s(1) + b_{n-2}^2s(1) - a_{n-1}s(1)^2/2 \\
& +s(1)^3/2 + a_{n-1}s(2) - s(1)s(2) + 2a_{n-1}b_{n-1}^2 + b_{n-1}^2s(1) + s(3)
\end{aligned}$$

$$\begin{aligned}
\text{bx}(4) = & a_{n-1}^4 + a_{n-2}^2b_{n-2}^2 + 2a_{n-2}a_{n-1}b_{n-2}^2 + 3a_{n-1}^2b_{n-2}^2 + b_{n-3}^2b_{n-2}^2 + b_{n-2}^4 \\
& +3a_{n-1}^2b_{n-1}^2 + 2a_{n-1}a_nb_{n-1}^2 + a_n^2b_{n-1}^2 + 2b_{n-2}^2b_{n-1}^2 + b_{n-1}^4 + b_{n-1}^2b_n^2 \\
& +a_{n-1}^3s(1) + a_{n-2}b_{n-2}^2s(1) + 2a_{n-1}b_{n-2}^2s(1) + 2a_{n-1}b_{n-1}^2s(1) \\
& +a_nb_{n-1}^2s(1) - a_{n-1}^2s(1)^2/2 - b_{n-2}^2s(1)^2/2 - b_{n-1}^2s(1)^2/2 \\
& +a_{n-1}s(1)^3/2 - 5s(1)^4/8 + a_{n-1}^2s(2) + b_{n-2}^2s(2) + b_{n-1}^2s(2) \\
& -a_{n-1}s(1)s(2) + 3s(1)^2s(2)/2 - s(2)^2/2 + a_{n-1}s(3) - s(1)s(3) + s(4)
\end{aligned}$$

Bibliography

- [1] J.G. Bednorz and K.A. Müller, Z. Phys. B **64**, 188 (1986).
- [2] D.C. Mattis *The Many-Body Problem*, World Scientific Publishing Co. Ltd., Singapore (1993).
- [3] H.A. Bethe, Z. Phys. **71**, 205 (1931).
- [4] S.R. Aladim and M.J. Martins, J. Phys. A: Math. Gen. **26**, L529 (1993).
- [5] B.D. Dörfel and St. Meißner, J. Phys. A: Math. Gen. **29**, 6471 (1996).
- [6] H.J. de Vega and F. Woyanrovich, J. Phys. A **25**, 4499 (1992).
- [7] C. Benelli, A. Caneschi, D. Gatteschi, L. Pardi and P. Rey, Inorg. Chem. **29**, 4223 (1990).
- [8] P.A.M. Dirac, Proc. Roy. Soc. **112A**, 661 (1926).
- [9] R. Hoogerbeets, A.J. van Duyneveldt, A.C. Phaff, C.H.W. Swüste and W.J.M. de Jonge, J. Phys. C **17**, 2595 (1984).
- [10] J.B. Torrance, Jr., and M. Tinkham, Phys. Rev. Series 2 **187**, 595 (1969).
- [11] A.J.M. Medved, B.W. Southern and D.A. Lavis, Phys. Rev. B **43**, 816 (1991).
- [12] R. Haydock, *The Recursive Solution of the Schrödinger equation*, Solid State Physics **35**, 216-94 (New York: Academic Press 1980).

- [13] P. Turchi, F. Ducastelle and G. Tréglià, J. Phys. C: Solid State Phys. **15**, 2891 (1982).
- [14] A.J.M. Medved *Two Magnon States of Alternating Ferrimagnetic Chains*, M.Sc. Thesis, University of Manitoba (1990).
- [15] S.C. Bell, P.D. Loly and B.W. Southern, J. Phys.: Condens. Matter **1**, 9899 (1989).
- [16] V.S. Viswanath and G. Müller *The Recursion Method: Application to Many-Body Dynamics* **m23** Springer-Verlag (1994).
- [17] B.W. Southern, R.J. Lee, and D.A. Lavis, J. Phys.: Condens. Matter **6**, 10075 (1994).