TWO MAGNON STATES OF ALTERNATING FERRIMAGNETIC CHAINS

by

Allan Joseph Michael Medved

A Thesis Submitted to the
Faculty of Graduate Studies
in Partial Fulfillment of the
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ABSTRACT

In this thesis, the two-magnon excitation spectra of an alternating ferrimagnetic chain are calculated and then analyzed. Both the spins and bonds of the chain are permitted to alternate in the general formalism. This is followed by intense study of a variety of special cases. A direct analytic approach is used to trace the bound state branches while a real-space rescaling approach is used to calculate the two-magnon densities of states. The latter approach is particularily useful for studying continuum states. The significance of any special features detected in the spectra is discussed.

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Chapter 1

INTRODUCTION

From the time of the ancient Greeks up until early twentieth century, magnetism had long served as a puzzlement to men and women of science. But thanks to the "quantum revolution" of the 1920's, and in particular the work of Heisenberg [HE] and Dirac [DI], we now understand how spontaneous magnetization arises in solids. Spontaneous magnetization is the direct result of interactions between atoms that are quantum mechanical in origin. These interactions are a consequence of the contraints placed on electronic wavefunctions by the Pauli Exclusion principle. The Pauli principle requires that wavefunctions describing systems of electrons (or more generally fermions) are antisymmetric under exchange of both spatial and spin coordinates of any electron pair. As a result, the relative spin orientation of the electrons can influence the electrostatic energy of the system. It is possible to express the effect of the Pauli principle by interactions which can be described by operators of the form

$$\tilde{S}_i \cdot \tilde{S}_j \qquad i \neq j \qquad (1.1)$$

where $\tilde{S}_i$ and $\tilde{S}_j$ are spin operators corresponding to different atomic sites.

To better understand this effect we consider the simple example of a hydrogen molecule or in other words a two-electron system. The Hamiltonian describing this system can be written

$$H = -\frac{1}{2m}\nabla_1^2 - \frac{1}{2m}\nabla_2^2 + V(1) + V(2) + \frac{e^2}{r_{12}} \qquad (1.2)$$

where the indices 1 and 2 label the spatial coordinates of the two electrons and r_{12} is the distance separating the two electrons. (For convenience we have set the fundamental constants $\hbar$ and $4\pi\epsilon_0$ equal to unity.) Clearly (1.2) is invariant under exchange of electron spatial coordinates so the two-electron spatial wavefunction must have definite symmetry. We find a splitting in the energy levels of the system depending on whether this spatial wavefunction is symmetric or antisymmetric under exchange. From the Pauli principle, if the spatial wavefunction is symmetric, then the corresponding two-electron spin wavefunction must be antisymmetric and vice versa. Hence the forementioned splitting can be said to depend on whether the two-electron spin wavefunction is a singlet state (i.e., antisymmetric) or a triplet state (i.e., symmetric).

The singlet and triplet spin states are both eigenstates of the total spin operators $|\tilde{S}_T|^2 = |\tilde{S}_1 + \tilde{S}_2|^2$ with corresponding eigenvalues $S_T^2 = 0$ and $S_T^2 = 2$ respectively. It

therefore follows that the energy splitting can be described in terms of the eigenvalues of this operator. However the operator $2(\tilde{S}_1 \cdot \tilde{S}_2)$ differs from $|\tilde{S}_T|^2$ by only a constant term so it is equally valid to express the energy splitting in terms of eigenvalues of $\tilde{S}_1 \cdot \tilde{S}_2$. It can be explicitly shown (see Smart [SM]) that this energy splitting or "exchange energy" for the hydrogen molecule can be written

$$\Delta H = -J\tilde{S}_1 \cdot \tilde{S}_2 \tag{1.3}$$

where J is a function of electrostatic force between electrons and is often referred to as the "exchange integral". Because of the strength of the electrostatic force relative to magnetic dipole interactions, the latter can be neglected.

Now suppose we extend the previous result to a lattice of atoms, each with magnitude of spin $S_i = \frac{1}{2}$. Then the total energy arising from the effect of the Pauli principle can be described by the following operator which was originally proposed by Dirac [DI] but is commonly referred to as the "Heisenberg exchange Hamiltonian":

$$H_{Heis} = \sum_{i \neq j} J_{ij} \tilde{S}_i \cdot \tilde{S}_j \, . \tag{1.4}$$

We also want to allow for the possibility that $S_i > \frac{1}{2}$ and $S_i \neq S_j$ as would be the case for atoms with greater than one valence electron. However the simple result of (1.3)

depended crucially on the fact $S_1 = S_2 = \frac{1}{2}$. For more general spin magnitudes we expect to obtain a more complicated polynomial in $\tilde{S}_1 \cdot \tilde{S}_2$. In other words, we expect

$$\Delta H = -J^{(0)} (\tilde{S}_1 \cdot \tilde{S}_2)^0 - J^{(1)} (\tilde{S}_1 \cdot \tilde{S}_2)^1 - \ldots - J^{(d)} (\tilde{S}_1 \cdot \tilde{S}_2)^d \tag{1.5}$$

where $d = 2 \text{ minimum } (S_1, S_2)$. The coefficients $J^{(0)}, J^{(1)}, \ldots, J^{(d)}$ can be regarded as being analogous to the coefficients of an electromagnetic multipole expansion. This is because both sets of coefficients are consequences of interactions between extended distributions.

We justify the precise form of (1.5) as follows. If the "exchange Hamiltonian" is to remain rotationally invariant, then so must each individual "exchange operator" describing the interaction between two spins. So if we assume rotational invariance then each exchange operator must be a tensor operator of rank zero or in other words a scalar. From quantum theory of angular momenta (see Watanabe [WA]) any scalar operator acting on the direct product space of two spins $\tilde{S}_1$ and $\tilde{S}_2$ can be written as a linear combination of powers of $\tilde{S}_1 \cdot \tilde{S}_2$. Furthermore, the dimension of the subspace spanned by these operators is equal to the number of possible eigenvalues of $|\tilde{S}_T|$ where $\tilde{S}_T = \tilde{S}_1 + \tilde{S}_2$. Since $S_T = \{(S_1+S_2), (S_1+S_2-1), \ldots, (|S_1-S_2|)\}$ the dimension of this scalar subspace is d+1 where $d = 2 \text{ minimum } (S_1, S_2)$. Hence it is redundant to expand

scalar operators in powers of $\tilde{S}_1 \cdot \tilde{S}_2$ in excess of d.

So a more general version of (1.4) valid for spins of arbitrary magnitude is given by

$$H = - \sum_{i \neq j} \sum_{p} J_{ij}^{(p)} (\tilde{S}_i \cdot \tilde{S}_j)^p \qquad (1.6)$$

where the index p runs from 1 to 2 minimum (S_i, S_j). Note that we have neglected the constant terms $(\tilde{S}_i \cdot \tilde{S}_j)^0$ as we are always free to add or subtract a constant to the Hamiltonian without changing its physical nature.

Reconsider the Heisenberg exchange Hamiltonian (1.4). In order for the exchange interaction to occur, the wavefunctions of the interacting electrons must certainly overlap. Hence the exchange coefficients J_{ij} depend on (among other factors) the degree of overlap of the i^{th} and j^{th} electrons. So it follows that J_{ij} is a function of r_{ij} (the separation between the i^{th} and j^{th} electrons) such that the magnitude of J_{ij} decreases rapidly as r_{ij} increases. So it is not an unrealistic approximation to assume these interactions are significant between nearest neighbours only. With this approximation the Heisenberg exchange Hamiltonian becomes

$$H_{Heis} = - \sum_{i} \sum_{\delta} J_{i,i+\delta} \tilde{S}_i \cdot \tilde{S}_{i+\delta} \qquad (1.7)$$

where for each atom (i) we sum over all nearest-neighbour atoms $(i+\delta)$. For the sake of simplicity we further restrict

ourselves to the case of a one-dimensional lattice or in other words, a linear chain of atoms. Then the Heisenberg exchange Hamiltonian further reduces to

$$H_{Heis} = - \sum_i J_{i,i+1} \tilde{S}_i \cdot \tilde{S}_{i+1} . \qquad (1.8)$$

Note that the extension of subsequent results to two or three dimensional lattices is in most cases straightforward but tedious. The further simplifying case of a uniformly spaced chain of identical atoms gives

$$H_{Heis} = -J \sum_i \tilde{S}_i \cdot \tilde{S}_{i+1} \qquad S_i = S \ \forall \ i . \qquad (1.9)$$

For the case of a uniform chain with nearest neighbour interactions only, the more general exchange Hamiltonian of (1.6) similarily reduces to give

$$H = - \sum_i \sum_{p=1}^{2S} J^{(p)} (\tilde{S}_i \cdot \tilde{S}_{i+1})^p \qquad S_i = S \ \forall \ i . \qquad (1.10)$$

Although most related literature deals with the case of a uniform homogeneous system, in this thesis we allow for the possibility of an "alternating chain". By this we mean a chain composed of two non-identical sublattices, each of which itself is uniform and homogeneous. Generalizing (1.10) for an alternating chain gives

$$H = - \sum_{n=1}^{N/2} \sum_{p=1}^{2S'} J_1^{(p)} (\tilde{S}'_{2n} \cdot \tilde{S}_{2n+1})^p + J_2^{(p)} (\tilde{S}_{2n+1} \cdot \tilde{S}'_{2n+2})^p$$

$$S'_{2n} = S' \text{ and } S_{2n+1} = S \ \forall \ n \quad (1.11)$$

where the total number of atoms N is an even integer and we assume $S' \leq S$ without loss of generality. This is the form of the exchange Hamiltonian which will be studied in the subsequent chapters of this thesis. It can be said to describe an alternating ferrimagnetic chain.

Unless otherwise mentioned we will be considering the limit of an infinite chain. This implies periodic boundary conditions such that for every n,

$$S'_{2n} = S'_{2n+N}, \quad (1.12a)$$

$$S_{2n+1} = S_{2n+1+N}. \quad (1.12b)$$

These boundary conditions insure translational invariance such that the unit cell of repetition contains two atoms.

Before proceeding it should be mentioned that we neglected to consider a number of factors which are often of importance in real materials. These include anisotropic spin exchange, single-ion anisotropies and the effect of an external magnetic field. For instance, if all these factors were taken into account for a nearest-neighbour uniform chain, then the exchange Hamiltonian (1.10) would become

$$H = - \sum_i \sum_{p=1}^{2S} J^{(p)} [\alpha S_i^x S_{i+1}^x + \beta S_i^y S_{i+1}^y + \gamma S_i^z S_{i+1}^z]^p$$

$$- \sum_i \sum_{p=2}^{2S} D^{(p)} (S_i^z)^p - h \sum_i S_i^z \qquad (1.13)$$

where: spin exchange is anisotropic if $\alpha \neq \beta \neq \gamma$

: h is a measure of the external magnetic field which is assumed to be orientated along the z-direction

: $D^{(p)}$ are measures of single-ion anisotropy .

For the sake of simplicity, these factors will not be considered in this thesis. It is however a straightforward process to extend our formalism to include any or all of these effects.

We next examine some general features of the Hamiltonian of interest (1.11) beginning with the ground state. It is instructive to first consider the ground state for the specific case of a uniform chain with $S_i = \frac{1}{2}$ $\forall$ i. For this case we refer to the simpler Heisenberg exchange Hamiltonian of (1.9). If $J > 0$ then clearly the most favourable (lowest energy) state occurs when all spins are parallel. Assuming magnetization is along the z-direction then this is a state with either all spins "flipped up" (i.e., $S_i^z = + \frac{1}{2}$ $\forall$ i) or else all spins "flipped down" (i.e., $S_i^z = - \frac{1}{2}$ $\forall$ i). If $J < 0$ then the corresponding ground state is not so simple.

Anti-parallel spin pairs are obviously favourable but the "intuitive" choice of ground state (spins flipped up alternating with spins flipped down) is not an eigenstate of the Hamiltonian. The actual $J < 0$ ground state (first calculated by Bethe [BE]) turns out to be much more complicated.

In general, for a magnetic material consisting of identical atoms on translationally equivalent sites, we categorize it as either a ferromagnet or an antiferromagnet. This depends on whether parallel or antiparallel alignment of adjacent spins is favoured. So for the previously discussed uniform Heisenberg chain, $J > 0$ and $J < 0$ correspond to ferromagnetic and antiferromagnetic chains respectively.

Now reconsider the alternating chain with general magnitudes of spin. This is an example of a ferrimagnetic system. (A magnetic material is referred to as a ferrimagnet if it is composed of non-equivalent atoms or non-equivalent sublattices or both.) In general, the ground state of such systems cannot be explicitly calculated. For (1.11) the ground state depends on what values are assigned to the set of exchange coefficients $J_i^{(p)}$ ($i = 1,2$, $p = 1,2,\ldots,2S'$). In some cases of (1.11) parallel arrangements of adjacent spins are favoured. Hence the lowest energy state occurs when all spins are aligned along a common direction with maximum projection in that direction. (For

instance, if the direction of magnetization is taken as the negative z-direction, then for such cases the ground state occurs when $S'^{z}_{2n} = -S'$ and $S^{z}_{2n+1} = -S \ \forall \ n.$) This state having maximum alignment of spins is referred to as the "ferromagnetic state" and systems for which this is the ground state are said to exhibit ferromagnetic behaviour.

For other cases of (1.11), the values of the exchange coefficients will be such that antiparallel arrangements of neighbouring spins are favoured. For these cases the ferromagnetic state lies highest in energy and the corresponding systems is said to exhibit antiferromagnetic behaviour. The ground state of such systems is generally incalculable. There will also be cases of (1.11) for which it is unclear whether the chain tends towards ferromagnetic or antiferromagnetic interactions. For these cases the ferromagnetic state lies neither highest or lowest in energy and the corresponding ground state is (generally) incalculable.

If we are to proceed to study the energy spectra of the Hamiltonian (1.11) we require a starting point. In other words, we require an explicit expression for the ground state. Because the ferromagnetic state (all spins aligned with maximum projection) is the simplest eigenstate of (1.11) we have chosen to only consider systems in which this is the ground state. The direction of magnetization is arbitrarily taken as being along the negative z-direction. For the

remainder of this thesis it is to be understood that the parameters of the Hamiltonian (1.11) may only be varied in such a way that all other states have positive energy relative to the ferromagnetic state. In subsequent discussion, the term ferromagnetic chain will imply such cases whereas the term antiferromagnetic chain will imply that the signs of all the exchange coefficients have been reversed so that the ferromagnetic state lies highest in energy (although technically a ferrimagnetic chain is neither a ferromagnet nor antiferromagnet).

Now that we have established the ground state of the exchange Hamiltonian (1.11) as being ferromagnetic the next features to consider are the low-lying excited states. But first note that because of the rotational invariance of the Hamiltonian, S^z_{TOT} is a good quantum number where

$$S^z_{TOT} = \sum_{n=1}^{N/2} (S'^z_{2n} + S^z_{2n+1}) . \qquad (1.14)$$

By good quantum number we mean that H operating on a state of definite S^z_{TOT} gives back a state having the same definite value of S^z_{TOT} associated with it. Consequently, we can partially diagonalize the Hamiltonian by grouping its eigenstates into subspaces labelled by the various values of S^z_{TOT}. These values of S^z_{TOT} range in integral steps from

$-\frac{N}{2}(S+S')$ to 0. (The subspaces with S^z_{TOT} ranging from 1 to $+\frac{N}{2}(S+S')$ are redundant because in this model the positive and negative z-directions are energetically equivalent.) Note that the subspace labelled by $S^z_{TOT} = -\frac{N}{2}(S+S')$ contains only the ferromagnetic ground state.

Again it is instructive to first consider the states of the uniform Heisenberg chain (1.9) with $S_i = \frac{1}{2}\ \forall\ i$. Since the ground state (all spins flipped down) has the most negative value of S^z_{TOT} associated with it ($S^z_{TOT} = -\frac{N}{2}$) we first consider the subspace of eigenstates labelled by $S^z_{TOT} = -\frac{N}{2}+1$. Any state in this subspace can be written as a linear combination of states having all but one spin parallel. In other words, if $|0\rangle$ represents the ground state then the excited states in this particular subspace can be written as linear combinations of the states $|1\rangle, |2\rangle,\ldots,|N\rangle$ where $|j\rangle = S^+_j|0\rangle$. ($S^+_j = S^x_j + iS^y_j$ is the quantum raising operator corresponding to the j^{th} site.) Because of the translational invariance of the Hamiltonian we can be even more explicit. By way of Bloch theorem [AM] we can write

$$H_{Heis}|\psi_K\rangle = E(K)|\psi_K\rangle$$

$$\text{where:}\quad |\psi_K\rangle = \frac{1}{\sqrt{N}}\sum_m e^{iKm}|m\rangle\ . \tag{1.15}$$

By using the explicit form of the Hamiltonian (1.9) and

applying the well-known properties of quantum spin operators [SAK] we obtain the result

$$E(K) = E_0 + 2J\sin^2(\frac{K}{2}) \tag{1.16}$$

where E_0 is the ground state energy. A plot of this dispersion is given in Figure (1.1). Note that the periodic boundary conditions (1.12) restrict unique values of the wavevector K to those in the first Brillouin zone ($|K| \leq \pi$). Hence we obtain a "band" of energies with minimum energy at K = 0 coinciding with the ground state. Because of the plane wave nature of these excitations they are referred to as spin waves. They are also referred to as magnons, this latter name reflecting that they represent quanta of magnetic excitation.

Next consider the subspace of excited states labelled by $S^z_{TOT} = -\frac{N}{2} + 2$. Any state in this subspace can be written as a linear combination of states having all but two spins parallel. Alternatively, such states can be regarded as a pair of interacting spin waves and hence are referred to as two-magnon excitations. The corresponding dispersion relation (as derived Mattis [M]) is shown in Figure (1.2). K is now the sum of the wavevectors describing the two individual magnons or in other words the "total wavevector". Along with the continuous spectrum of states there is an isolated curve in Figure (1.2) corresponding to a bound state (that is a

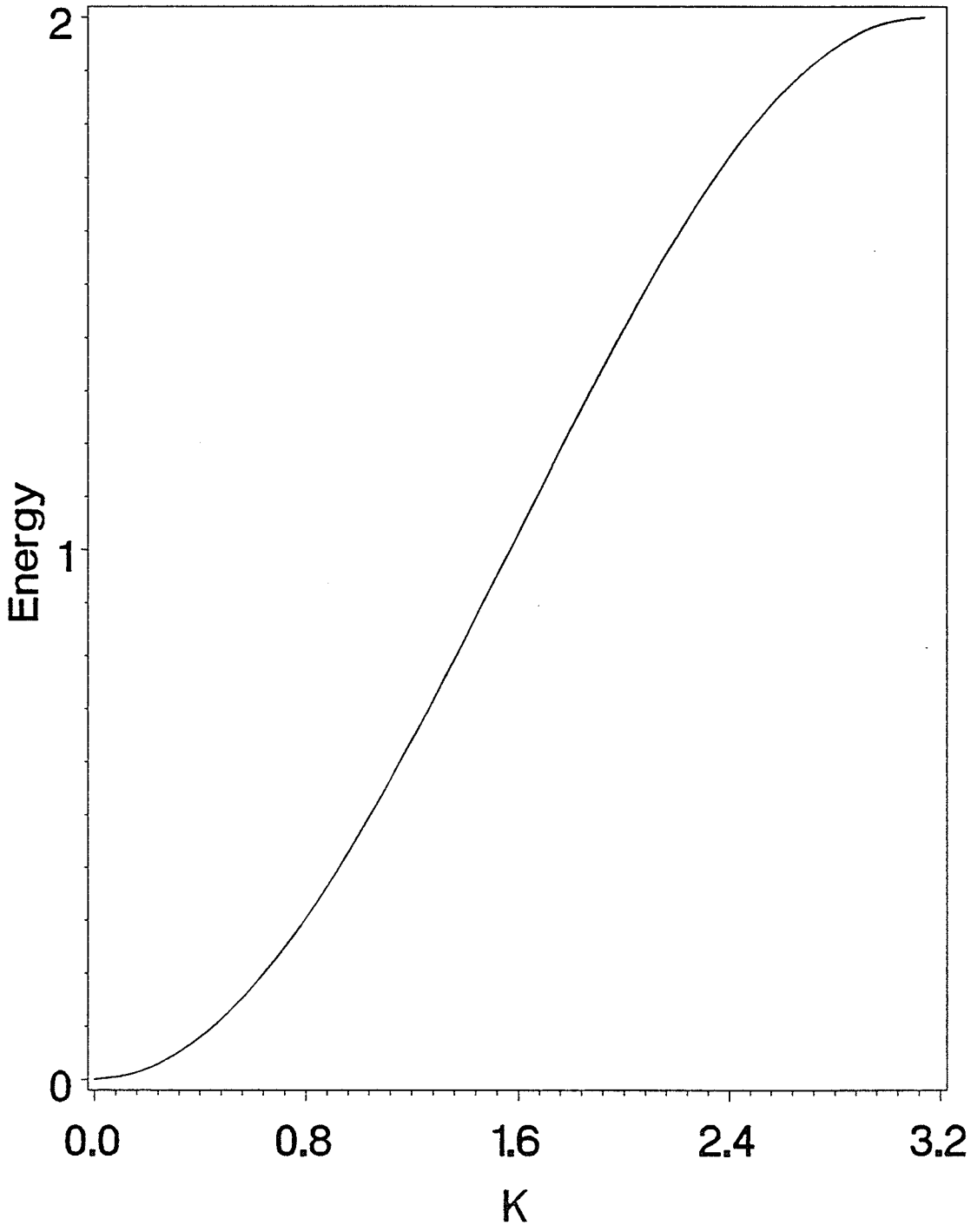

FIGURE 1.1 : One–magnon dispersion relation for a uniform Heisenberg chain (S=1/2). Energy is in units of exchange integral J .

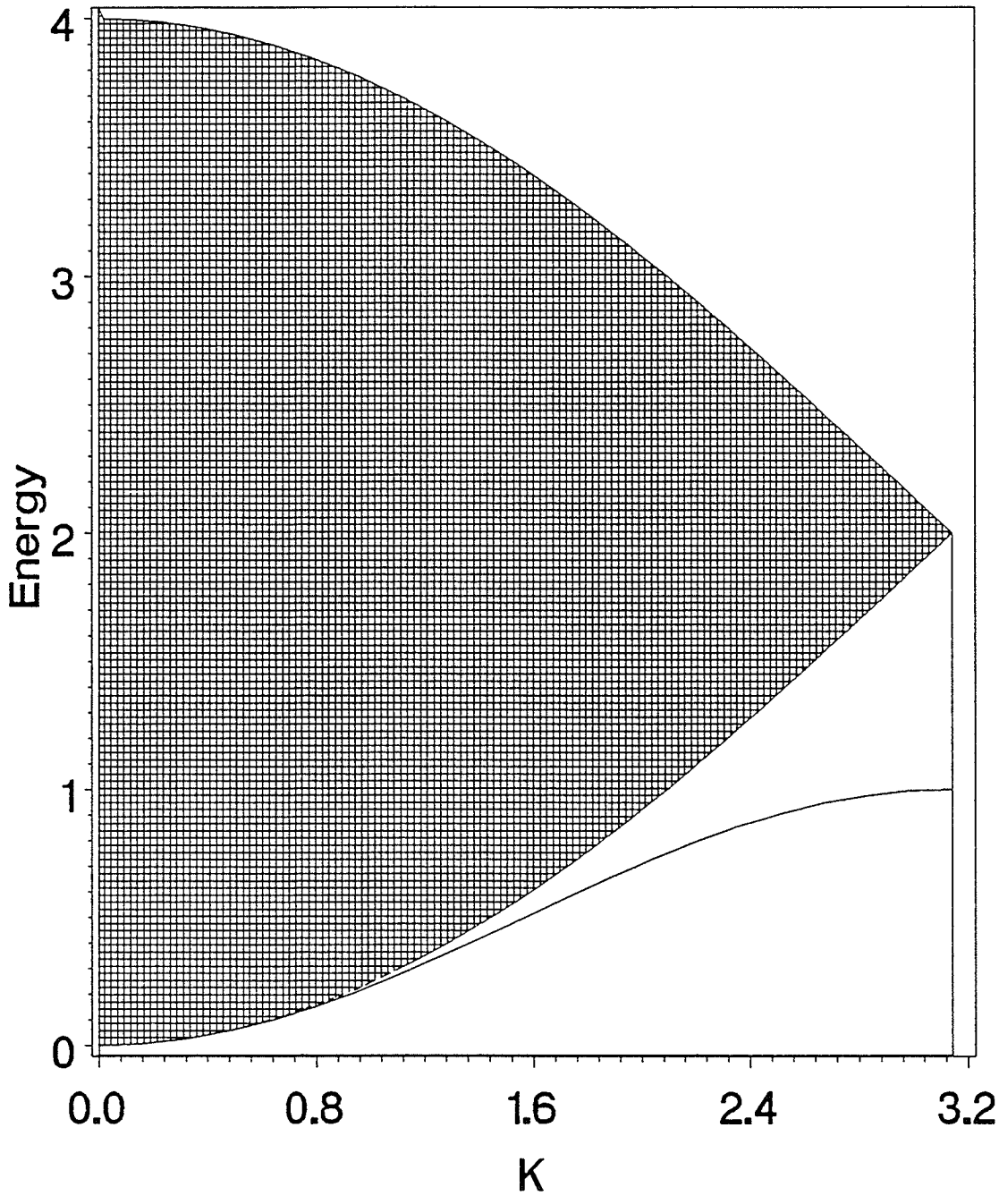

FIGURE 1.2 : Two-magnon dispersion relation for a uniform Heisenberg chain (S=1/2). Energy is in units of exchange integral J . Shaded region indicates the continuum. The bound state is indicated by a solid curve.

state localized in the neighbourhood of an attractive interaction).

The subspace of states labelled by $S^z_{TOT} = -\frac{N}{2}+3$ corresponds to three-magnon excited states, the subspace of states labelled by $S^z_{TOT} = -\frac{N}{2}+4$ corresponds to four-magnon excited states, and so on. The $\frac{N}{2}$- magnon excitations include the highest lying excited state which is the ground state of the corresponding antiferromagnetic chain ($J < 0$). It is expected that the dispersion relations get increasingly complicated as the number of magnons increases.

Now reconsider the exchange Hamiltonian of interest (1.11) describing the alternating ferrimagnetic chain with ferromagnetic ground state. As in the previous example the various excited states can be categorized as being one-magnon excitations, two-magnon excitations, three-magnon excitations, etc...., depending on the value of S^z_{TOT} associated with the states in question. For an m-magnon excitation the corresponding eigenvalue is $S^z_{TOT} = -\frac{N}{2}(S+S') + m$. The m-magnon dispersion relation or spectrum is generally much more complicated than it would be for the previously discussed uniform Heisenberg chain. For instance, the one-magnon spectrum of the alternating chain contains a two branch dispersion curve. The second branch arises as a result of having two atoms in the unit cell of repetition. The two-magnon spectrum generally has three isolated energy

continua and as many as six bound state branches (as will be shown in the chapters ahead).

Both the one and two-magnon spectra of a ferrimagnetic chain with ferromagnetic ground state can be solved for exactly, regardless of how otherwise general the model is. However, the m-magnon spectra for $m \geq 3$ are generally insoluble, as these correspond to many body problems. Unfortunately, it is the arbitrary m-magnon problem that is of greatest interest because solving this leads directly to the ground state and low-lying excitations of the more interesting antiferromagnetic model. However, there are special cases of (1.11) for which the arbitrary m-magnon problem can be solved exactly and hence the complete excitation spectra can be obtained. Such cases are referred to as completely integrable models [SU2]. The previously discussed uniform Heisenberg chain with $S = \frac{1}{2}$ is a completely integrable model [BE].

The focus of this thesis is on solving the two-magnon problem of an alternating ferrimagnetic chain with ferromagnetic ground state. Yet most real life magnetic materials possess antiferromagnetic interactions, so as mentioned above it is the arbitrary m-magnon problem which is of primary interest. So why do we bother to study the two-magnon excitations with such diligence? Because by examining the features of the two-magnon spectra for a wide variety of

cases it may be possible to identify special cases corresponding to completely integrable models. It has been shown that such models typically have special features in their m-magnon spectra [CK].

For instance, consider the uniform chain exchange Hamiltonian (1.10). It has been conjectured by Haldane [HAL] that the corresponding m-magnon spectra have bound state branches with range over ρ = minimum (m,2S) consecutive Brillouin zones in the extended zone scheme. In general, these branches enter the energy continua (where they are no longer true bound states) and are discontinuous at Brillouin zone boundaries. Haldane further conjectured that for integrable models only, these branches are both real and continuous across ρ Brillouin zones. This implies that completely integrable models of (1.10) can be identified by studying the two-magnon spectra for cases in which the bound state branches stay completely outside the continua and have no gaps at the first Brillouin zone boundary. Such studies were made successfully by Chubukov and Kveschenko [CK] and by Southern et al [SLL]. Similar studies of two-magnon spectra for alternating chains may lead to the identification of additional integrable cases, hence motivating our research.

In this thesis we will try to identify possible candi-

dates for complete integrability. This will be done by studying the spectral nature of two-magnon excitations of an alternating ferrimagnetic chain. Hence we require a method (or methods) for rigorously solving the two-magnon problem of an exchange interaction system. A rather well-known technique, commonly used in solving multi-magnon (and analagous) problems is the "Bethe ansatz" approach, originated by Bethe in 1931 [BE]. This approach was first applied to the uniform Heisenberg exchange Hamiltonian (1.9) with $S = \frac{1}{2}$. By assuming periodic boundary conditions and then making use of translational invariance, Bethe was able to make an "educated guess" to the form of the m-magnon wave-function. As a result, he succeeded in completely diagonal-izing the Hamiltonian. As it turns out, the Bethe ansatz (or suitable generalization) can be used to solve for the complete set of states for essentially any Hamiltonian repre-senting a completely integrable system [SU2]. (Such systems occur not only in magnetism but a wide range of physical problems. But virtually all known integrable cases correspond to systems confined to one dimension in space or time.) Consequently, the Bethe ansatz can be used to solve the arbitrary m-magnon spectra (and hence the complete anti-ferromagnetic problem) of any spin exchange system which corresponds to a completely integrable model. However the Bethe ansatz is not applicable to systems of limited inte-

grability and therefore not suitable for studying general models such as (1.11).

Since a system is integrable only if it can be solved using the Bethe ansatz, this approach can also be used as a means of identifying integrable models. Another technique which can be used for the purpose of identifying such models is the quantum inverse scattering method, as has been done by Takhtujan [T] and Babujian [BAB]. However, using such tedious methods for the purpose of identifying integrable cases of a general system is a massive undertaking. It is much preferable to have criteria to apply beforehand which indicates which particular cases are the most likely candidates for solvability by these methods. Special features of the two-magnon spectra is one such criteria.

We now focus on methods for solving the two-magnon problem which can be used independent of the integrability of the system. One such method which we refer to as the "analytic approach" (for lack of a better name) entails solving the one-magnon problem beforehand and then describing the two-magnon problem as an interaction between pairs of one-magnon states or spin waves. Such an approach has been used previously by Fukuda and Wortis [FW] and Hanus [HAN]. An approach with a similar philosophy but formalized in terms of Green's functions was initiated by Dyson [DY] and later developed by Wortis [WO]. Approaches such as these are advantageous in their easy applicability to a wide range of

magnetic systems. The dimensionality of the lattice, presence of anisotropies, and the range of interaction are of little concern when applying such methods. The Green's function formalism is generally favourable because a system's spectral properties are easily extractable once these functions are known. However using the "Green's function approach" usually requires performing a cumbersome fourier transform so that the results are expressed in real-space (rather than reciprocal-space) coordinates.

An alternative technique, which we refer to as the "scaling approach", is based upon the ideas of real-space rescaling methods. Such methods were used originally in the study of critical phenomena [NL] but are applicable to a wide range of problems. Such an approach was shown to be effective in the study of exchange Hamiltonians (and more generally tight-binding Hamiltonians) by Southern et al. [SKL], [SKA]. This approach entails constructing a transformation on a system of equations which eliminates a fraction of the variables while leaving the form invariant. This technique has the advantages that the one-magnon problem need not be solved beforehand and the real-space Green's functions can be calculated directly. Unfortunately, the scaling approach is limited to systems describing one-dimensional lattices.

In our study of the alternating ferrimagnetic chain we have chosen to use two of the previously discussed approaches, analytic and scaling, in solving for the two-magnon excitation spectra. The two methods complement one another in that the former provides an efficient process for cataloguing bound states while the latter provides a more detailed account of the two-magnon spectra. This includes the relative contribution of states both inside the energy continua (i.e., scattering states) and the bound states outside. Chapter 2 of this thesis develops the general formalism of the one- and two-magnon problems and discusses how the analytic approach leads to the bound state solutions. Chapter 3 discusses the scaling approach and then develops the formalism necessary for applying this method to the two-magnon problem. Chapter 4 of this thesis uses the formalism and calculations of the previous two chapters to study the two-magnon spectral results for a number of interesting cases. Chapter 5 summarizes the results of the thesis. Particular attention is paid to what spectral features (if any) may lead to the indentification of previously unknown cases of completely integrable systems.

We conclude this introductory chapter by noting the existence of an alternate viewpoint to the two-magnon problem. This viewpoint stems from experimental studies

of two-magnon Raman scattering. Such light scattering experiments are most appropriate in the study of three-dimensional antiferromagnets. Although a detailed understanding of such systems has not been possible, quite good agreement with experimental results has been achieved by using rather approximate calculations. Raman scattering has been a motivating factor in previous two-magnon research at the University of Manitoba. Loly et al. have intensively studied ferromagnets in one, two, and three dimensions [LO] including single-ion anisotropy [LS] and next-nearest-neighbour effects [BL]. Fundamental to the Raman scattering concern has been the profile of the two-magnon continuum (i.e., densities of states) with the bound states being of secondary concern compared with studies of integrable one-dimensional models.

Chapter 2

GENERAL FORMALISM

In this chapter we will develop the formalism necessary in solving the two-magnon problem of an alternating ferrimagnetic chain as described by the spin exchange Hamiltonian of (1.11). A direct analytic approach will be used to first solve the one-magnon problem and then expand the interacting two-magnon states in terms of non-interacting spin waves. A method for locating bound state solutions will be discussed in detail.

2.1 One-Magnon Formalism

Recall the Hamiltonian (1.11) under study:

$$H = -\sum_{n=1}^{N/2}\sum_{p=1}^{2S'}\left[J_1^{(p)}(\tilde{S}'_{2n}\cdot\tilde{S}_{2n+1})^p + J_2^{(p)}(\tilde{S}_{2n+1}\cdot\tilde{S}'_{2n+2})^p\right] \tag{2.1}$$

where: N is a large even integer

: $\tilde{S}'_{2n}$ and $\tilde{S}_{2n+1}$ are spin operators such that $S'_{2n} = S'$ and $S_{2n+1} = S \quad \forall\, n$

: $S' \leq S$

: $J_1^{(p)}$ and $J_2^{(p)}$ $(p = 1,2,\ldots,2S')$ represent the interactions between neighbouring spins that alternate in strength along the chain.

Also recall that we assume periodic boundary conditions (1.12) and that the ground state $|0\rangle$ of this Hamiltonian is the ferromagnetic state with all spins aligned along the negative z-direction. Consequently, we can write

$$H|0\rangle = E_0|0\rangle \tag{2.2}$$

where the ground state energy E_0 is given by

$$E_0 = -\frac{N}{2}\sum_{p=1}^{2S'}(J_1^{(p)} + J_2^{(p)})(SS')^p \tag{2.3}$$

since $S'^z_{2n} = -S'$ and $S^z_{2n+1} = -S \quad \forall\, n$.

Alternatively, the Hamiltonian (2.1) can be described in terms of parameters related to eigenvalues of the operator $\tilde{S}\cdot\tilde{S}'$. If $\tilde{J} = \tilde{S} + \tilde{S}'$, then

$$\begin{aligned}\tilde{S}\cdot\tilde{S}' &= \frac{1}{2}\left[|\tilde{J}|^2 - |\tilde{S}|^2 - |\tilde{S}'|^2\right] \\ &= \frac{1}{2}\left[J(J+1) - S(S+1) - S'(S'+1)\right].\end{aligned} \tag{2.4}$$

The various eigenvalues for $\tilde{S}\cdot\tilde{S}'$ are given by substituting for the possible quantum numbers of $\tilde{J}$ which range from $(S+S')$ to $|S-S'|$ in integral steps. If we let λ_m $(m = 0,1,\ldots,2S')$ denote the eigenvalues of $\tilde{S}\cdot\tilde{S}'$ in descending order, then

$$\begin{aligned}\lambda_m &= \frac{1}{2}\left[(S+S'-m)(S+S'-m+1) - S(S+1) - S'(S'+1)\right] \\ &= SS' - m(S+S') + \frac{1}{2}m(m-1).\end{aligned} \tag{2.5}$$

We further define

$$g_m^{(i)} = \sum_{p=1}^{2S'} J_i^{(p)} \lambda_m^p \qquad i = 1,2;\ m = 0,1,\ldots,2S' \quad (2.6a)$$

$$G_m^{(i)} = \frac{g_0^{(i)} - g_m^{(i)}}{\lambda_0 - \lambda_m} \qquad i = 1,2;\ m = 1,2,\ldots,2S' \quad (2.6b)$$

The n-magnon problem involves only the $G_m^{(i)}$ with $m = 1,2,\ldots,n$. This is regardless of what values are assigned to the generally larger number of $J_i^{(p)}$ parameters. Actually, the n-magnon problem can be described by exactly 2n' exchange parameters where n' is the minimum of n and 2S'. Furthermore, if we restrict all relevant $G_m^{(i)}$ to non-negative values only then we are assured of a ferromagnetic ground state. Because of these conveniences we will use the $G_m^{(i)}$ parameters whenever possible in describing our subsequent results. Note that the ground state energy (2.3) is given by

$$E_0 = -\frac{N}{2}\left(g_0^{(1)} + g_0^{(2)}\right). \quad (2.7)$$

We now consider the one-magnon excited states. That is, the simultaneous eigenstates of the Hamiltonian (2.1) and the total spin operator S_{TOT}^z (1.14) such that the corresponding eigenvalue of S_{TOT}^z has been incremented by exactly one unit from its minimal ferromagnetic value of $-\frac{N}{2}(S+S')$. First note that states with all but one spin

parallel are not eigenstates of the Hamiltonian and hence are not one-magnon states. (This can be shown explicitly by applying the well-known properties of quantum spin operators [SAK]. For further discussion, refer to Appendix A.) Instead we find that the deviation in spin resulting in a one-magnon state must be shared by all spin sites. In other words, a one-magnon state is a "collective excitation".

The set of states having all but one spin parallel do however span the eigenspace of S_z^{TOT} corresponding to eigenvalue $-\frac{N}{2}(S+S')+1$. So it follows that any one-magnon state can be written as a linear combination of all such single spin deviation states. Therefore a general expression for the one-magnon wavefunction $|\psi_1>$ can be written as follows:

$$|\psi_1> = \sum_{n=1}^{N/2} [a_{2n}|2n> + a_{2n+1}|2n+1>] \qquad (2.8)$$

where: $|j>$ is the state in which all spins are alligned with maximum projection along the negative z-direction except at the j^{th} site where if j is even $S_j'^z = -S'+1$ and if j is odd, $S_j^z = -S+1$;

: a_j is some yet unknown amplitude measuring the contribution of the state $|j>$ to the total one-magnon wavefunction.

Next, consider the Schrödinger equation:

$$H|\psi_1\rangle = (E_1 + E_0)|\psi_1\rangle \tag{2.9}$$

where: E_1 is the one-magnon excitation energy measured relative to the ground state energy.

Since the states $|1\rangle$, $|2\rangle,\ldots,|N\rangle$ form a complete (and hence orthonormal) set we can obtain equations relating the various amplitudes $a_1, a_2, \ldots, a_N$ by substituting (2.8) and (2.1) into (2.9) and then equating the coefficients of each given state. The details of this procedure are given in Appendix A. The resulting equations relating the "one-magnon amplitudes" are as follows:

$$[E_1 - S(G_1^{(1)} + G_1^{(2)})]a_{2n} = -\sqrt{SS'}\,[G_1^{(1)} a_{2n+1} + G_1^{(2)} a_{2n-1}] \tag{2.10a}$$

$$[E_1 - S'(G_1^{(1)} + G_1^{(2)})]a_{2n+1} = -\sqrt{SS'}\,[G_1^{(1)} a_{2n} + G_1^{(2)} a_{2n+2}]\,. \tag{2.10b}$$

Notice that both of these equations involve $G_m^{(i)}$ for $m = 1$ only, as expected.

Because of the similarity of these equations (2.10) to those obtained for phonons on a diatomic chaim [AM] we can predict plane wave solutions of the form

$$a_{2n} = \alpha e^{2ink} \tag{2.11a}$$

$$a_{2n+1} = \beta e^{i(2n+1)k} \tag{2.11b}$$

where k is a real number referred to as the wavevector. Because of the periodic boundary conditions, all unique values of k are restricted to the range $[-\frac{\pi}{2}, \frac{\pi}{2}]$ which is

referred to as the first Brillouin zone. Substituting (2.11) into (2.10) leads to a pair of homogeneous equations with unknowns α and β. Satisfying the secular determinant leads to a quadratic expression for the single-magnon excitation energy E_1. Solving this expression for the dispersion relation gives

$$E_1(K) = \frac{1}{2}(S+S')(G_1^{(1)}+G_1^{(2)}) \pm \frac{1}{2}\sqrt{(S+S')^2(G_1^{(1)}+G_1^{(2)})^2-16SS'G_1^{(1)}G_1^{(2)}\sin^2(k)} \tag{2.12}$$

or alternatively

$$E_1(k,\mu) = B + \frac{\mu}{2}\sqrt{4A^+A^-+D^2} \tag{2.13}$$

where μ takes on the values ± 1 and where we have defined

$$A^{\pm} = \sqrt{SS'}\,[G_1^{(1)}e^{\pm ik} + G_1^{(2)}e^{\mp ik}] \tag{2.14a}$$

$$B = \frac{1}{2}(S+S')(G_1^{(1)}+G_1^{(2)}) \tag{2.14b}$$

$$D = (S-S')(G_1^{(1)}+G_1^{(2)})\,. \tag{2.14c}$$

The index μ labels the two branches of the one-magnon dispersion curve as shown in Figure (2.1). In analogy with phonons on a diatomic chain the upper branch is referred to as "optic" and the lower branch is referred to as "acoustic".

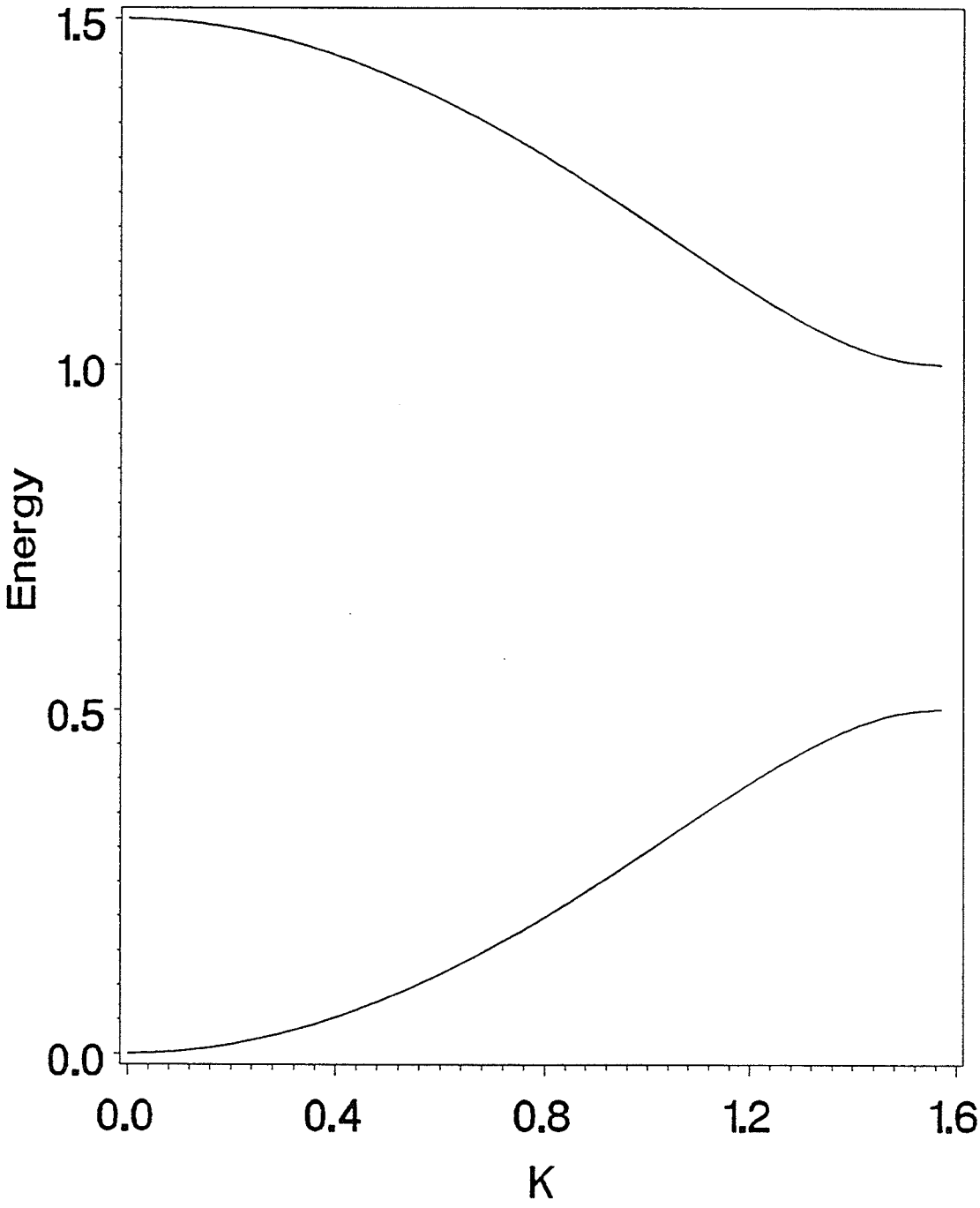

FIGURE 2.1 : One-magnon dispersion relation for an alternating ferrimagnetic chain ($S=S'=1/2$; bonds alternate in strength by factor of 2). Energy is in units of stronger exchange coefficent.

Note that in general there is a non-zero gap between the two branches at the Brillouin zone boundary ($k = \pi/2$). This gap vanishes only if both $S = S'$ and $G_1^{(1)} = G_1^{(2)}$ are satisfied. These two conditions do not necessarily describe a uniform chain since $G_m^{(1)}$ and $G_m^{(2)}$ ($m = 2,3,\ldots,2S'$) are yet unspecified.

2.2 Two-Magnon Formalism

The next level in the "hierarchy" of excited states corresponds to the subspace of two-magnon excitations. These are the simultaneous eigenstates of the Hamiltonian (2.1) and the total spin operator S^z_{TOT} (1.14) such that the eigenvalue of S^z_{TOT} has been incremented by exactly two units from the ground state value. By explicit calculation (refer to Appendix A for more details) we see that neither states with single spin deviations on two separate sites nor states with two spin deviations on a single site are eigenstates of the Hamiltonian. Hence, such "two spin deviation states" do not correspond to two-magnon excitations.

However, the states that are two spin deviations away from the ferromagnetic ground state do form a set which spans the eigenspace of S_z^{TOT} corresponding to eigenvalue $-\frac{N}{2}(S+S') + 2$. So it follows that we can expand the two-magnon wavefunction $|\psi_2\rangle$ in the basis of two spin deviation states. Doing so gives the following general expression:

$$|\psi_2\rangle = \sum_{\substack{n=1 \\ n\leq m}}^{N/2} \sum_{m=1}^{N/2} [a_{2n,2m}|2n,2m\rangle + a_{2n,2m+1}|2n,2m+1\rangle + a_{2n-1,2m}|2n-1,2m\rangle + a_{2n+1,2m+1}|2n+1,2m+1\rangle] \tag{2.15}$$

where: $|i,j\rangle$ $(i < j)$ is the state differing from the ground state $|0\rangle$ by single spin deviations at both the i^{th} and j^{th} sites

: $|j,j\rangle$ is the state differing from $|0\rangle$ by two spin deviations at the j^{th} site only

: $a_{i,j}$ $(i \leq j)$ is some yet unknown amplitude measuring the contribution of the state $|i,j\rangle$ to the total two-magnon wavefunction.

and where the four possible configurations of spin excitation pairs (even-even, even-odd, odd-even, odd-odd) have been segregated to insure complete generality. Note that sites with magnitude of spin S' (or S) = $\frac{1}{2}$ can support at most a single spin deviation. As a result, states such as $|2n,2n\rangle$ if S' = $\frac{1}{2}$ and $|2n+1,2n+1\rangle$ if S = $\frac{1}{2}$ are unphysical. Technically these unphysical states should be omitted from the summation but we will soon see that including them does not create a problem.

Now consider the two-magnon Schrödinger equation:

$$H|\psi_2\rangle = (E_2 + E_0)|\psi_2\rangle \tag{2.16}$$

where: E_2 is the two-magnon excitation energy measured relative to the ground state energy E_0 .

As in the one-magnon problem we derive equations relating the various amplitudes by explicitly substituting for the Hamiltonian and general form of wavefunction and then equating the coefficients of each basis ket. The details of this derivation are given in Appendix A while only the results are presented here.

The equations for the "two-magnon amplitudes" can be grouped into two sets. One set involves only amplitudes with spin deviations separated by at least two sites while the other set involves amplitudes with spin deviations on same or neighbouring sites. Since the range of interaction is limited to nearest-neighbours we refer to the former set as the "non-interacting equations" and the latter set as the "interacting equations". The non-interacting equations are as follows:

$$(\Omega-D)a_{2n,2m} = -\sqrt{SS'}\,[G_1^{(1)}(a_{2n,2m+1} + a_{2n+1,2m} + G_1^{(2)}(a_{2n,2m-1} + a_{2n-1,2m})] \qquad (2.17a)$$

$$\Omega a_{2n-1,2m} = -\sqrt{SS'}\,[G_1^{(1)}(a_{2n-2,2m} + a_{2n-1,2m+1}) + G_1^{(2)}(a_{2n,2m} + a_{2n-1,2m-1})] \qquad (2.17b)$$

$$\Omega a_{2n,2m+1} = -\sqrt{SS'}\,[G_1^{(1)}(a_{2n,2m} + a_{2n+1,2m+1}) + G_1^{(2)}(a_{2n-1,2m+1} + a_{2n,2m+2})] \quad (2.17c)$$

$$(\Omega+D)a_{2n+1,2m+1} = -\sqrt{SS'}\,[G_1^{(1)}(a_{2n,2m+1} + a_{2n+1,2m}) + G_1^{(2)}(a_{2n+2,2m+1} + a_{2n+1,2m+2})] \quad (2.17d)$$

where $m > n$, D is given by (2.14c), and where we have defined

$$\Omega = E_2 - 2B\,. \quad (2.18)$$

Meanwhile the interacting equations are as follows:

$$[E_2-\theta_S]a_{2n,2n} = -\Phi_{S'}^{(1)}a_{2n,2n+1} - \Phi_{S'}^{(2)}a_{2n-1,2n} - \Delta^{(1)}a_{2n+1,2n+1} - \Delta^{(2)}a_{2n-1,2n-1} \quad (2.19a)$$

$$[E_2-\tau^{(1)}]a_{2n-1,2n} = -\Phi_S^{(2)}a_{2n-1,2n-1} - \Phi_{S'}^{(2)}a_{2n,2n} - \sqrt{SS'}\,G_1^{(1)}[a_{2n-1,2n+1} + a_{2n-2,2n}] \quad (2.19b)$$

$$[E_2-\tau^{(2)}]a_{2n,2n+1} = -\Phi_S^{(1)}a_{2n+1,2n+1} - \Phi_{S'}^{(1)}a_{2n,2n} - \sqrt{SS'}\,G_1^{(2)}[a_{2n,2n+2} + a_{2n-1,2n+1}] \quad (2.19c)$$

$$[E_2-\theta_{S'}]a_{2n+1,2n+1} = -\Phi_S^{(1)}a_{2n,2n+1} - \Phi_S^{(2)}a_{2n+1,2n+2} - \Delta^{(2)}a_{2n+2,2n+2} - \Delta^{(1)}a_{2n,2n} \quad (2.19d)$$

where we have defined

$$\theta_S = \frac{S}{S+S'-1}\left[(2S'-1)\left(G_1^{(1)}+G_1^{(2)}\right)+(2S-1)\left(G_2^{(1)}+G_2^{(2)}\right)\right] \quad (2.20a)$$

$$\tau^{(1)} = (S+S')G_1^{(1)} + \frac{1}{S+S'-1}\left[(S-S')^2 G_1^{(2)} + (2S-1)(2S'-1)G_2^{(2)}\right] \quad (2.20b)$$

$$\Phi_S^{(i)} = \frac{\sqrt{(2S-1)S'}}{S+S'-1}\left[(S-S')G_1^{(i)} + (2S'-1)G_2^{(i)}\right], \quad i = 1,2 \quad (2.20c)$$

$$\Delta^{(i)} = \frac{\sqrt{SS'(2S-1)(2S'-1)}}{S+S'-1}\left[G_1^{(i)} - G_2^{(i)}\right] \quad i = 1,2 \quad (2.20d)$$

and where $\theta_{S'}$ and $\Phi_{S'}^{(i)}$ are obtained by interchanging S and S' while $\tau^{(2)}$ is obtained by interchanging superscripts $^{(1)}$ and $^{(2)}$. As expected, the non-interacting equations involve only $G_1^{(1)}$ and $G_1^{(2)}$ while the interacting equations involve $G_2^{(1)}$ and $G_2^{(2)}$ as well. However, $G_m^{(i)}$ with $m > 2$ are not required anywhere in the two-magnon problem. Note that if $S' = \frac{1}{2}$, then the amplitude $a_{2n,2n}$ represents an unphysical state (and similarily for $a_{2n+1,2n+1}$ if $S = \frac{1}{2}$). However, we see from the interacting equations that the unphysical amplitude $a_{2n,2n}$ completely decouples from all other two-magnon amplitudes since $\Phi_{S'}^{(1)}$, $\Phi_{S'}^{(2)}$, $\Delta^{(1)}$, and $\Delta^{(2)}$ all vanish if $S' = \frac{1}{2}$. Because of this complete decoupling, unphysical amplitudes are not a concern in the subsequent formalism.

We proceed by first attempting to solve the set of non-interacting equations (2.17). Since this set of equations describes a system of two non-interacting spin waves, it should be possible to solve these equations with a simple product of one-magnon plane waves. Hence we choose to write the two-magnon amplitudes as follows:

$$a_{2n,2m} = \alpha e^{2ink_1} e^{2imk_2} \tag{2.21a}$$

$$a_{2n-1,2m} = \beta e^{i(2n-1)k_1} e^{2imk_2} \tag{2.21b}$$

$$a_{2n,2m+1} = \gamma e^{2ink_1} e^{i(2m+1)k_2} \tag{2.21c}$$

$$a_{2n+1,2m+1} = \delta e^{i(2n+1)k_1} e^{i(2m+1)k_2} \tag{2.21d}$$

where: k_1 and k_2 are the wavevectors of the two individual one-magnon states which form the non-interacting two-magnon state

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

Substituting (2.21) into the non-interacting equations (2.17) results in the following 4×4 matrix eigenvalue equation:

$$\begin{bmatrix} \Omega-D & A_1^+ & A_2^+ & 0 \\ A_1^- & \Omega & 0 & A_2^+ \\ A_2^- & 0 & \Omega & A_1^+ \\ 0 & A_2^- & A_1^- & \Omega+D \end{bmatrix} \begin{bmatrix} \alpha \\ \beta \\ \gamma \\ \delta \end{bmatrix} = 0 \qquad (2.22)$$

where $A_1^{\pm}$ and $A_2^{\pm}$ are defined by (2.14a) with wavevector k replaced by k_1 and k_2 respectively. The secular determinant for this matrix equation is quartic in energy (E_2 or equivalently Ω) and is as follows:

$$\Omega^4 - \Omega^2 D^2 - 2\Omega^2[|A_1|^2 + |A_2|^2] + [|A_1|^2 - |A_2|^2]^2 = 0 \qquad (2.23)$$

where: $|A_j|^2 = A_j^+ A_j^-$ $\quad (j = 1,2)$.

By solving for Ω^2 (via quadratic formula) and then substituting $\Omega = E_2 - 2B$ it can be shown that

$$E_2 = E_1(k_1,\mu_1) + E_2(k_2,\mu_2) \qquad (2.24)$$

where $E_1(k_j,\mu_j)$ is the one-magnon excitation energy as specified by (2.13). Consequently, the two-magnon excitation energy is simply equal to the sum of the excitation energies for two non-interacting magnons. The two indices μ_1, μ_2 which label the branches of the single magnon dispersion curves take on the values ±1 independently. Next, we will see that these indices also serve as labels for the two-magnon energy spectrum.

The two-magnon energy spectrum is taken as the E_2 versus K plane where $K = k_1+k_2$ is the total wavevector. Because of periodic boundary conditions (1.12) all unique values of K can be confined to the first Brillouin zone ($|K| \leq \pi/2$). If we restrict ourselves (for the time being) to real values of k_1 and k_2, then all spectral points fall within three distinct "energy continua" as shown in Figure (2.2). These continua are a direct consequence of (1) the two-magnon excitation energy being the sum of one-magnon excitations and (2) the energy gap that separates the two branches of the one-magnon dispersion curve for all values of wavevector.

A different continuum arises for each possible pairing of one-magnon dispersion branches. For instance, the lowest of the three continua is due to the pairing of two acoustic branches. By this we mean all spectral points inside this particular continuum satisfy $E_2 = E_1(k_1,-1) + E_1(k_2,-1)$ for real values of k_1 and k_2. Hence this continuum is referred to as "acoustic-acoustic" (A-A) and is labelled by $\mu_1 = \mu_2 = -1$. The uppermost continuum is due to the pairing of two optic branches and therefore is designated as "optic-optic" (O-O) and labelled by $\mu_1 = \mu_2 = +1$. The middle continuum results from the pairing of an optic branch with an acoustic. Hence this continuum is two-fold degenerate,

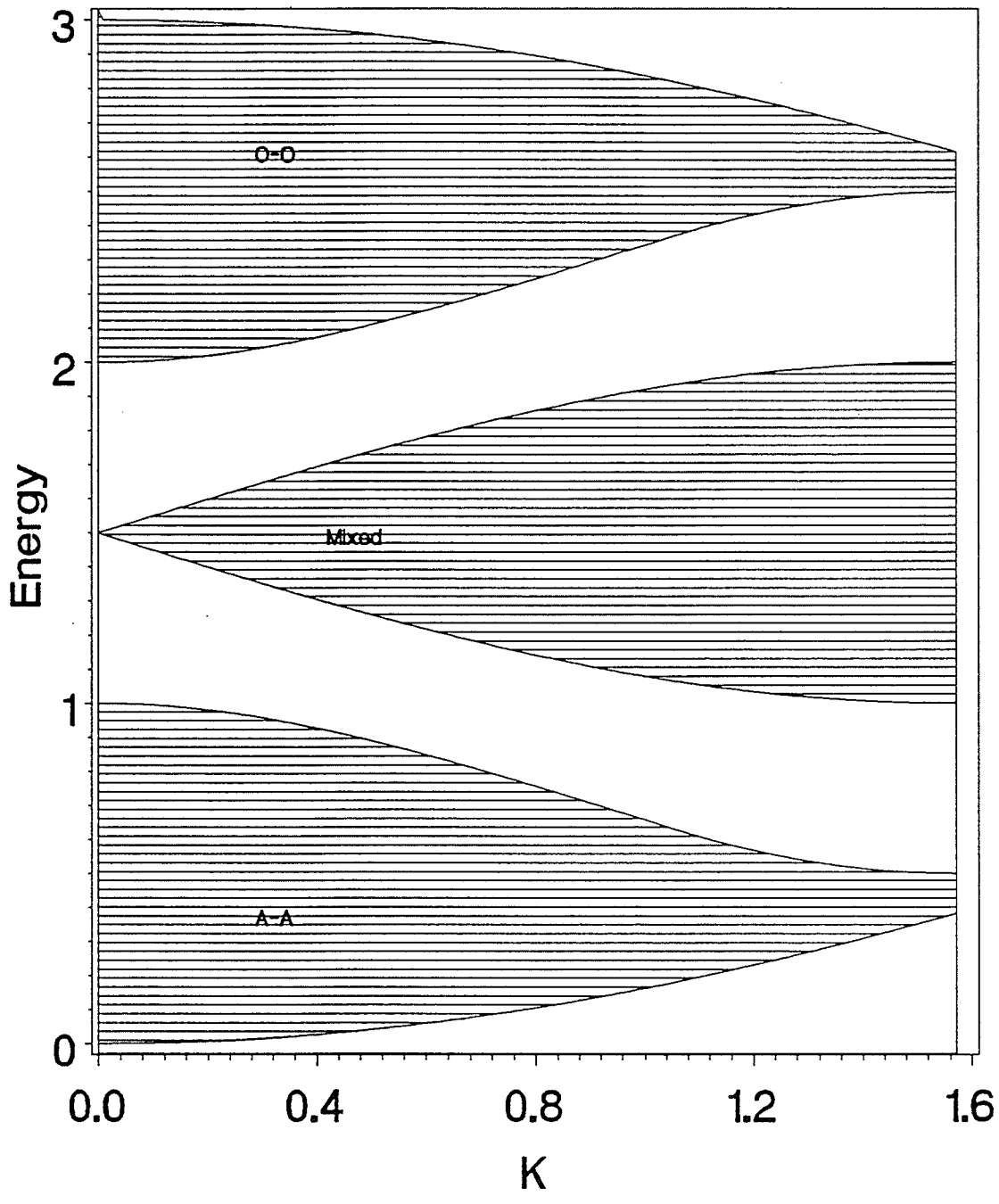

FIGURE 2.2 : Two-magnon energy continua for an alternating ferrimagnetic chain (S=S'=1/2 ; bonds alternate in strength by factor of 2). Energy is in units of stronger exchange coefficent. Shaded regions indicate the three continua.

being labelled by either $\mu_1 = +1$, $\mu_2 = -1$ or $\mu_1 = -1$, $\mu_2 = +1$. It is referred to as the "mixed-mode" continuum. We will see a little later that these continua boundaries can be solved for explicitly.

Once we have specified E_2, k_1, and k_2, we can solve for the non-interacting wavefunction (to within an arbitrary phase factor) as follows. From (2.22) we have a linear homogeneous system with unknowns α, β, γ, and δ. Any three of these coefficients can be solved in terms of the fourth and the magnitude of the fourth is fixed by normalization. Choosing to solve in terms of δ leads to the following relations:

$$\alpha = \left(\frac{\Omega^2 + D\Omega - |A_1|^2 - |A_2|^2}{2\bar{A_1}\bar{A_2}} \right) \delta \tag{2.25a}$$

$$\beta = \left(\frac{-\Omega^2 - D\Omega + |A_1|^2 - |A_2|^2}{2\bar{A_2}\Omega} \right) \delta \tag{2.25b}$$

$$\gamma = \left(\frac{-\Omega^2 - D\Omega - |A_1|^2 + |A_2|^2}{2\bar{A_1}\Omega} \right) \delta \tag{2.25c}$$

Since we now know α, β, γ, δ (to within a phase) we can explicitly solve for the amplitudes (2.21) and hence we can solve the complete non-interacting wavefunction.

We can label this wavefunction by the individual magnon wavevectors k_1 and k_2 or alternatively we can label with total wavevector K and relative wavevector q where $q = (k_1-k_2)/2$. Total wavevector K describes the center of mass motion and hence is restricted to being a real quantity. However relative wavevector q is free to be real or complex valued. So in general, k_1 and k_2 are complex quantities with imaginary parts that are equal in magnitude and opposite in sign.

We can rewrite the secular determinant equation (2.2) in terms of K and q by sutstituting for $A_1^{\pm}$ and $A_2^{\pm}$ (2.14a) and then using $k_1 = K/2+q$ and $k_2 = K/2-q$. The result is as follows:

$$\Omega^4 - D^2\Omega^2 - 4SS'\Omega^2[(G_1^{(1)})^2 + (G_1^{(2)})^2 + 2G_1^{(1)}G_1^{(2)}\cos(K)\cos(2q)] - [4SS'G_1^{(1)}G_1^{(2)}\sin(K)\sin(2q)]^2 = 0 . \qquad (2.26)$$

This equation can be re-expressed as a quadratic polynomial with respect to cos(2q). Solving this quadratic yields:

$$\cos(2q) = \frac{1}{4SS'G_1^{(1)}G_1^{(2)}\sin^2(K)}\left[-\Omega^2\cos(K) \pm \sqrt{[\Omega^2-4SS'(G_1^{(1)}\sin(K))^2][\Omega^2-4SS'(G_1^{(2)}\sin(K))^2]-(D\Omega\sin(K))^2}\right] \qquad (2.27)$$

Careful examination of this result reveals that for a given spectral point (K,E_2) there are four allowed values of relative wavevector q. These four values are generally complex and non-degenerate. For each of the four allowed q values there is a corresponding "eigenvector" as specified by (2.21) and (2.25). Once we have specified K and E_2 then any linear combination of these four corresponding eigenvectors is a solution of the non-interacting equations (2.17).

As previously discussed, the real values of k_1 and k_2 and hence the real values of q occur in three distinct regions of the two-magnon spectral plane which are referred to as energy continua. (Since $K = k_1+k_2$ is real, $q = (k_1-k_2)/2$ is real if and only if both k_1 and k_2 are real.) So it follows that the boundaries of these continua can be solved for explicitly by examining the preceding equation (2.27) for conditions that allow q to be real. A detailed discussion on calculating these boundaries is fully documented in Appendix B. Also from this appendix, we find that the spectral plane can be divided into a set of regions such that the nature of the allowed values of q varies from region to region. The various spectral regions are identified in Figure (2.3). In regions I, III, and V all four allowed values of q must be complex whereas in regions II, IV, and VI at least two of the four values must be real. These even numbered regions are of course the energy continua. Note that regions II and

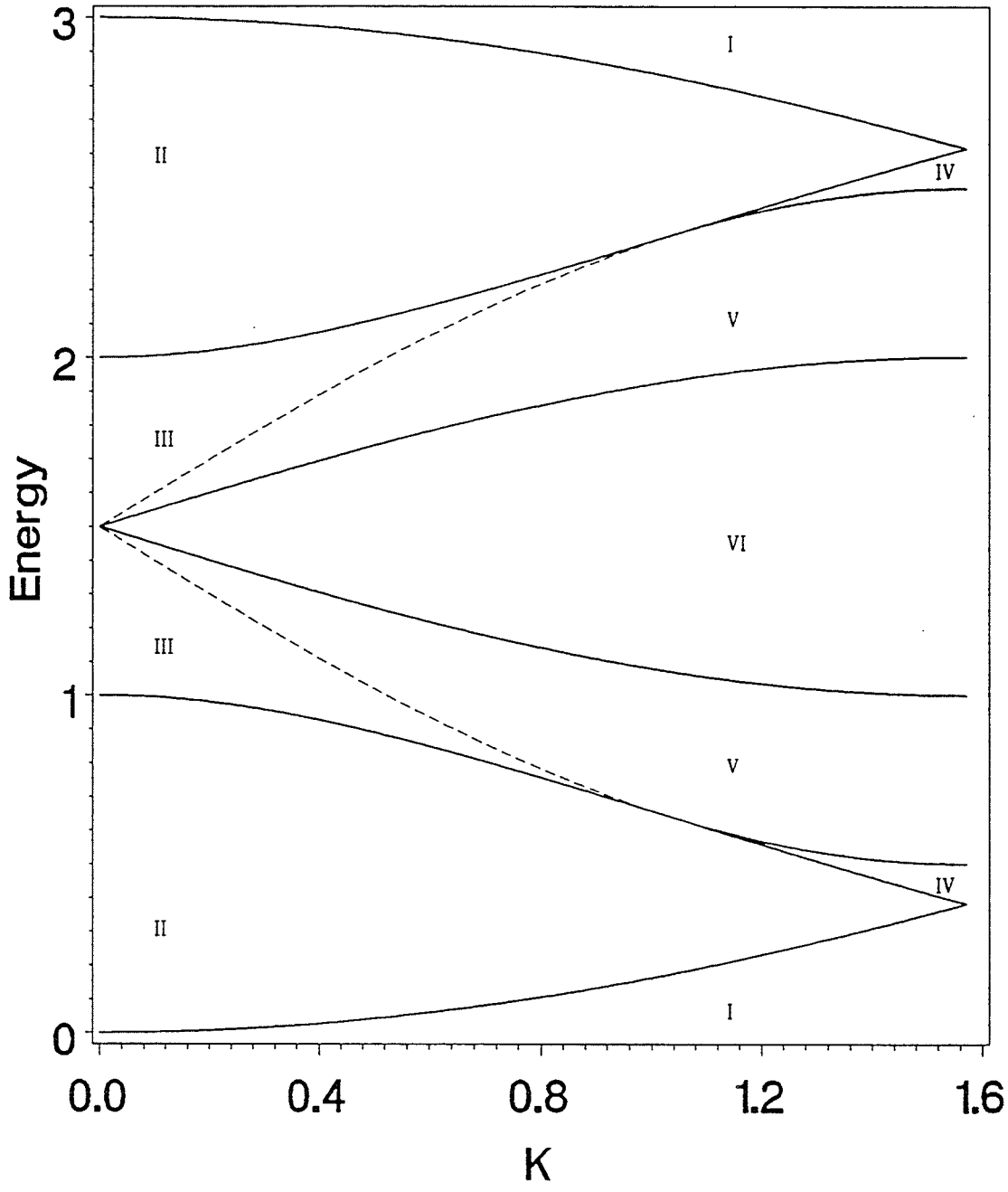

FIGURE 2.3 : Two-magnon spectral regions for an alternating ferrimagnetic chain ($S=S'=1/2$; bonds alternate in strength by factor of 2). Energy is in units of stronger exchange coefficent. Solid lines indicate both continua boundaries and internal singularities. Dashed lines separate regions III and V.

IV are separated by an internal van Hove singularity which occurs in the O-O and A-A continua. These singularities do not occur at small values of K but originate at a special value of wavevector which we denote by K_c (see Appendix B for details).

Consider solutions of the non-interacting equations corresponding to spectral points (K,E_2) in the odd numbered spectral regions (i.e., outside the energy continua). As previously mentioned, all four allowed values of relative wavevector must be complex valued. In fact, the four allowed values always occur in two pairs such that each pair has equal and opposite imaginary parts. The two pairs are degenerate if and only if the spectral point lies on the curve separating regions III and V (again refer to Appendix B). Suppose we rewrite the amplitudes in (2.21) by substituting $k_1 = \frac{K}{2} \pm q$. For instance (2.21a) becomes $a_{2n,2m} = \alpha e^{i(n+m)K_e - 2i(m-n)q}$ It is now apparent that Imag(q) > 0 results in an exponentially increasing solution while Imag(q) < 0 results in an exponentially decreasing solution (since m > n).

Recall that we are only considering the limit of an infinite chain as implied by the periodic boundary conditions. In this limit, exponentially growing solutions are unphysical and hence must be rejected. Consequently, we must always reject two of the four allowed values of relative wavevector

q in regions outside the energy continua. Both surviving values of q have Imag(q) < 0 and therefore the corresponding eigenvectors are exponentially decaying. That is, the corresponding two-magnon amplitudes must decay exponentially in magnitude as the separation between spin deviations increases. Therefore, solutions outside of the energy continua are always localized (in relative real coordinate space). In the complete interacting problem, such localized solutions outside of the energy continua are referred to as bound states.

Next consider solutions of the non-interacting equations corresponding to even numbered spectral regions or in other words inside the energy continua. Here we find that at least two of the four allowed values of relative wavevector are real valued while the remaining two values of q are either both real or both complex. Real values of q occur in pairs with equal magnitudes and opposite signs while complex values of q occur in pairs with equal and opposite imaginary parts. As previously discussed, the complex values of q with positive imaginary parts must be rejected. This is to avoid unphysical, exponentially growing solutions. The real values of q will have corresponding eigenvectors that are strictly plane wave solutions while the surviving complex value of q (if there is one) will have a corresponding eigenvector that is exponentially decaying.

Recall that any linear combination of eigenvectors corresponding to allowed values of relative wavevector is an acceptable solution of the non-interacting problem. Therefore, solutions inside the energy continua generally have both plane wave and exponentially decaying components. In the complete interacting problem, these solutions can be regarded as pairs of plane waves whose amplitdues are distorted by the interaction between one-magnon states. Hence solutions inside the energy continua are referred to as scattering states. Note that it is possible to have spectral points inside the continua where the exponentially decaying component dominates over the plane wave components of the two-magnon wavefunction. For such points the solution is effectively localized (in relative real coordinate space). Such localized solutions inside of the energy continua are referred to as resonant states.

Up until now, our study of the two-magnon problem has focussed on the non-interacting equations (2.17) while neglecting the interacting equations (2.19). To summarize, for each given spectral point there are two to four allowed values of relative wavevector which correspond to physically allowed solutions. Any linear combination of the eigenvectors corresponding to these allowed values is a valid solution of the non-interacting problem. However, the actual solution of the complete two-magnon problem must satisfy

both the interacting and non-interacting sets of equations. One way of determining the actual two-magnon wavefunction is to express the non-interacting solution in its most general form and then determine what particular combination of eigenvectors (if any) satisfies the complete set of interacting equations (2.19). In other words, we treat the interacting equations as "constraints", similar in philosophy to Lagrange multiplier problems.

As one might expect, there is always a non-trivial solution for any spectral point inside an energy continua (although nodes are possible). Meanwhile, outside of the continua there are non-vanishing solutions occuring only for special combinations of K and E_2. So the "typical" two-magnon spectra consists of three distinct scattering state continua along with a few isolated bound state branches.

2.3 Bound State Solutions

In principle, we can use the formalism of the preceding sections to evaluate all of the various two-magnon amplitudes at any given spectral point. Consequently, the preceding formalism can be used to calculate the complete two-magnon wavefunction. Such calculations would entail using (2.21), (2.25), and (2.27) to obtain the most general solution of the non-interacting problem and then using the set of interacting equations (2.19) as constraints. This turns out to

be a rather cumbersome process whereas the same information can be obtained in much more elegant fashion by using the scaling approach (as will be discussed in the chapter to follow). On the other hand, the preceding formalism does provide a very useful and convenient method for analytically locating the bound state solutions throughout the spectral plane.

The procedure used in detecting bound state solutions is as follows. For any spectral point (K,E_2) outside of the energy continua we know there are exactly two allowed values of relative wavevector which correspond to physically acceptable solutions. These are the two solutions of (2.27) with negative imaginary parts. (Recall that the other two solutions must have positive imaginary parts and hence result in unphysical exponentially growing solutions.) We will denote these two physically allowed values of relative wavevector as q and $\bar{q}$. We know that for either one of these values (say q) that the non-interacting equations (2.17) are solved by

$$a_{2n,2m} = \alpha e^{i(n+m)K_e - iq(2m-2n)} \tag{2.28a}$$

$$a_{2n-1,2m} = \beta e^{i(n+m-\frac{1}{2})K_e - iq(2m-2n+1)} \tag{2.28b}$$

$$a_{2n,2m+1} = \gamma e^{i(n+m+\frac{1}{2})K_e - iq(2m-2n+1)} \tag{2.28c}$$

$$a_{2n+1,2m+1} = \delta e^{i(n+m+1)K_e - iq(2m-2n)} \tag{2.28d}$$

where the relative values of the coefficients α, β, γ, δ are given explicitly by (2.25). Now suppose we generalize these expressions for the two-magnon amplitudes to include both q and $\bar{q}$. In other words we now express the wavefunction as a linear combination of non-interacting eigenvectors corresponding to q and $\bar{q}$ respectively. If $\bar{\alpha}$, $\bar{\beta}$, $\bar{\gamma}$, and $\bar{\delta}$ are the coefficients corresponding to $\bar{q}$ then we can write

$$a_{2n,2m} = e^{i(n+m)K}[C\alpha e^{-iq(2m-2n)} + D\bar{\alpha}e^{-i\bar{q}(2m-2n)}] \quad (2.29a)$$

$$a_{2n-1,2m} = e^{i(n+m-\frac{1}{2})K}[C\beta e^{iq(2m-2n+1)} + D\bar{\beta}e^{i\bar{q}(2m-2n+1)}] \quad (2.29b)$$

$$a_{2n,2m+1} = e^{i(n+m+\frac{1}{2})K}[C\gamma e^{-iq(2m-2n+1)} + D\bar{\gamma}e^{-i\bar{q}(2m-2n+1)}] \quad (2.29c)$$

$$a_{2n+1,2m+1} = e^{i(n+m+1)K}[C\delta e^{-iq(2m-2n)} + D\bar{\delta}e^{-i\bar{q}(2m-2n)}] \quad (2.29d)$$

where C and D are arbitrary complex constants. However these expressions (2.29) are still not sufficiently general. We must allow for the possibility that amplitudes with two spin deviations on the same site are unphysical and hence can vanish independently of the other amplitudes. So (2.29a) and (2.29d) are restricted to the cases $m > n$ only and when $m = n$ these then become

$$a_{2n,2n} = e^{i2nK}[C_0\alpha + D_0\bar{\alpha}] \quad (2.30a)$$

$$a_{2n+1,2n+1} = e^{i(2n+1)K}[C_0\delta + D_0\bar{\delta}] \quad (2.30b)$$

where C_0 and D_0 are arbitrary constants that are generally different from C and D. (One could argue that these expressions are still not sufficiently general. For instance, one might write $a_{2n-1,2n}$ and $a_{2n,2n+1}$ in terms of C_1 and D_1 generally different from C and D. However there is no obvious motivation for doing so. Furthermore, the results obtained using the amplitudes as given by (2.29) and (2.30) agree conclusively with the results of the scaling approach, in all cases. And the scaling approach makes no assumptions regarding the form of solution.)

Direct substitution of the amplitudes given by (2.29) and (2.30) into the interacting or constraint equations (2.19) results in the following 4×4 matrix equation:

$$W\begin{bmatrix} C_0 \\ D_0 \\ C \\ D \end{bmatrix} = 0 \tag{2.31}$$

where

$$W_{11} = \alpha(E_2-\theta_S) + \delta(\Delta^{(1)}e^{+iK} + \Delta^{(2)}e^{-iK}) \tag{2.32a}$$

$$W_{12} = \bar{\alpha}(E_2-\theta_S) + \bar{\delta}(\Delta^{(1)}e^{+iK} + \Delta^{(2)}e^{-iK}) \tag{2.32b}$$

$$W_{13} = \beta\Phi^{(2)}_{S'}e^{-iK/2}e^{-iq} + \gamma\Phi^{(1)}_{S'}e^{+iK/2}e^{-iq} \tag{2.32c}$$

$$W_{14} = \bar{\beta}\Phi^{(2)}_{S'}e^{-iK/2}e^{-i\bar{q}} + \bar{\gamma}\Phi^{(1)}_{S'}e^{+iK/2}e^{-i\bar{q}} \qquad (2.32d)$$

$$W_{21} = \alpha\Phi^{(2)}_{S'}e^{+iK/2} + \delta\Phi^{(2)}_{S}e^{-iK/2} \qquad (2.32e)$$

$$W_{22} = \bar{\alpha}\Phi^{(2)}_{S'}e^{+iK/2} + \bar{\delta}\Phi^{(2)}_{S}e^{-iK/2} \qquad (2.32f)$$

$$W_{23} = \alpha\sqrt{SS'}\,G^{(1)}_{1}e^{-iK/2}e^{-2iq} + \beta(E_2-\tau^{(1)})e^{-iq} + \delta\sqrt{SS'}\,G^{(1)}_{1}e^{+iK/2}e^{-2iq} \qquad (2.32g)$$

$$W_{24} = \bar{\alpha}\sqrt{SS'}\,G^{(1)}_{1}e^{-iK/2}e^{-2i\bar{q}} + \bar{\beta}(E_2-\tau^{(1)})e^{-i\bar{q}} + \bar{\delta}\sqrt{SS'}\,G^{(1)}_{1}e^{+iK/2}e^{-2i\bar{q}} \qquad (2.32h)$$

$$W_{31} = \alpha\Phi^{(1)}_{S'}e^{-iK/2} + \delta\Phi^{(1)}_{S}e^{+iK/2} \qquad (2.32i)$$

$$W_{32} = \bar{\alpha}\Phi^{(1)}_{S'}e^{-iK/2} + \bar{\delta}\Phi^{(1)}_{S}e^{+iK/2} \qquad (3.32j)$$

$$W_{33} = \alpha\sqrt{SS'}\,G^{(2)}_{1}e^{+iK/2}e^{-2iq} + \gamma(E_2-\tau^{(1)})e^{-iq} + \delta\sqrt{SS'}\,G^{(2)}_{1}e^{-iK/2}e^{-2iq} \qquad (2.32k)$$

$$W_{34} = \bar{\alpha}\sqrt{SS'}\,G^{(2)}_{1}e^{+iK/2}e^{-2i\bar{q}} + \bar{\gamma}(E_2-\tau^{(2)})e^{-i\bar{q}} + \bar{\delta}\sqrt{SS'}\,G^{(2)}_{1}e^{-iK/2}e^{-2i\bar{q}} \qquad (2.32\,l)$$

$$W_{41} = \alpha(\Delta^{(1)}e^{-iK} + \Delta^{(2)}e^{+iK}) + \delta(E_2-\theta_{S'}) \qquad (2.32m)$$

$$W_{42} = \bar{\alpha}(\Delta^{(1)}e^{iK} + \Delta^{(2)}e^{+iK}) + \bar{\delta}(E_2 - \theta_{S'}) \qquad (2.32n)$$

$$W_{43} = \beta\Phi_S^{(2)}e^{+iK/2}e^{-iq} + \gamma\Phi_S^{(1)}e^{-iK/2}e^{-iq} \qquad (2.32o)$$

$$W_{44} = \bar{\beta}\Phi_S^{(2)}e^{+iK/2}e^{-i\bar{q}} + \bar{\gamma}\Phi_S^{(1)}e^{-iK/2}e^{-i\bar{q}} . \qquad (2.32p)$$

Clearly a non-trivial solution of the wavefunction requires that the secular determinant of this matrix equation vanishes. Therefore locating bound state solutions for a given system requires a numerical scanning of regions I, III, and V of the spectral plane for points satisfying det[W] = 0.

In our research, we used the above method to locate the complete set of two-magnon bound states for a number of special cases of the Hamiltonian (2.1). These results will be presented and discussed in Chapter 4 of this thesis. As hinted earlier, analysis of scattering state solutions will be left to the real-space rescaling approach discussed in the following chapter.

Chapter 3

REAL-SPACE RESCALING FORMALISM

In this chapter we will consider a real-space rescaling treating of the two-magnon problem of an alternating ferrimagnetic chain. We will begin by discussing the scaling approach with respect to a more general problem. We will then consider the system of interest. In particular, we show how the scaling approach leads to the two-magnon Green's functions and consequently the two-magnon local densities of states.

3.1 General Method

The basic concept underlying the scaling approach is as follows. Given a system of linear equations with a large (and possibly infinite) number of degrees of freedom, then a special transformation is constructed. This transformation must eliminate a fraction of the degrees of freedom while leaving the form of the equations invariant. The so-called "scaling transformation" is then iterated until only a single degree of freedom remains. The "final" equation can be used to describe the properties of the system local to the remaining degree of freedom. It should be noted that the original equations generally require a high degree of symmetry for such an approach to be feasible.

The scaling transformation is essentially a three step procedure. If we regard each degree of freedom as a site on a lattice then these steps are as follows:

(1) elimination of some fraction of the sites

(2) renormalization of the parameters in the new equations so that these equations have the same form as the originals

(3) rescaling of the distance between sites (and relabelling sites if necessary) so that the transformation may be reapplied to the reduced system.

If the original equations describe the mutual interactions of the various lattice sites, then the renormalized parameters are essentially the "effective" interactions between the remaining sites.

We choose one site never to be eliminated and identify this one as the origin. If we eliminate a fraction $(f-1)/f$ of the sites for any one transformation then the overall process is said to have a scaling factor of f. For a one-dimensional lattice in which the origin is labelled as the 0^{th} site then a scaling transformation of factor f would eliminate the sites labelled by $\pm 1, \pm 2, \ldots, \pm(f-1), \pm(f+1), \ldots$. After elimination the distance between remaining sites would be rescaled by a factor $1/f$. Figure (3.1) depicts a schematic illustration of this procedure for scaling factor $f = 2$.

The elimination process can be (perhaps) better understood by considering the Schrödinger equation of an arbi-

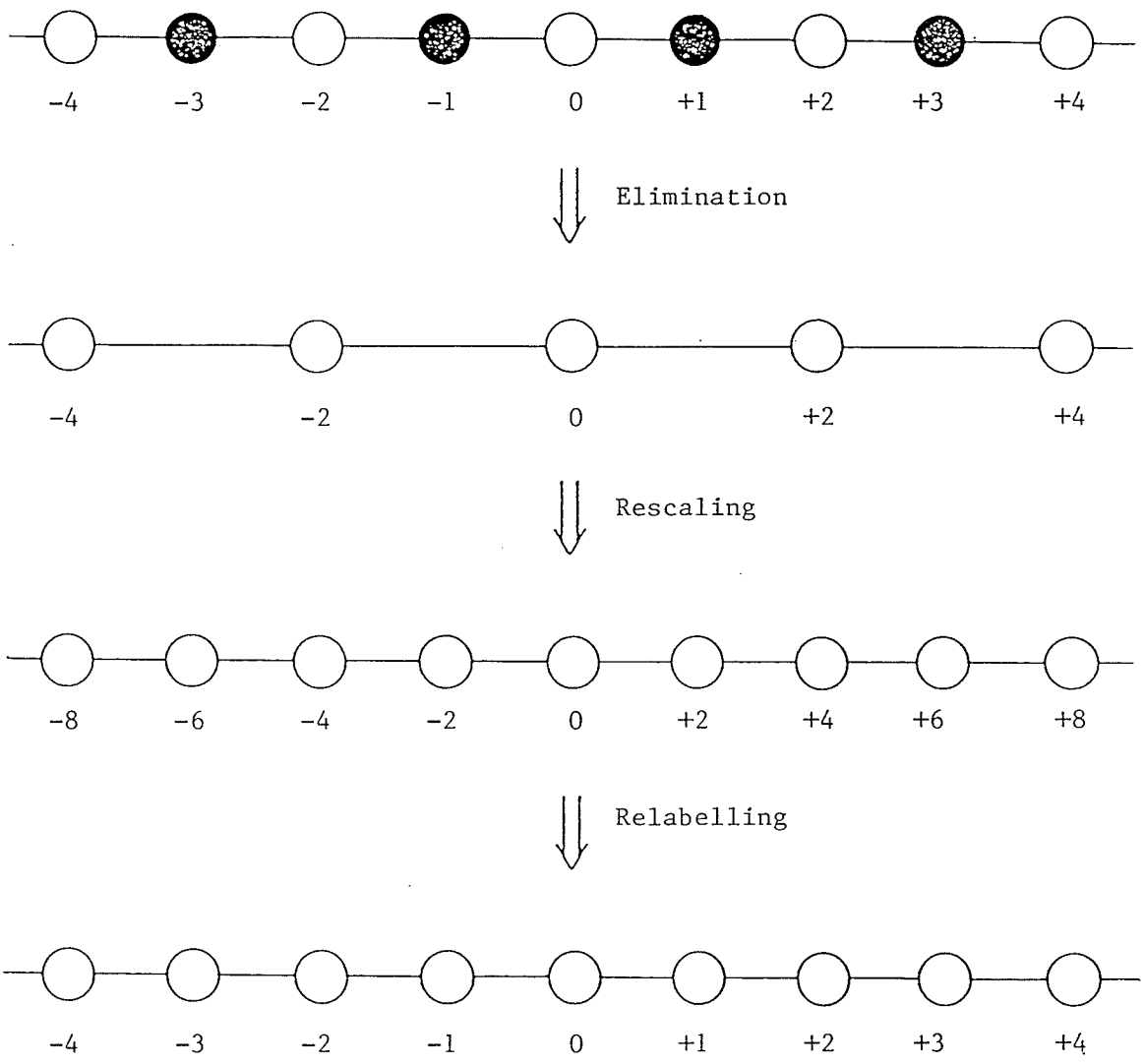

FIGURE 3.1: Schematic illustration of the scaling procedure (f=2). The first step eliminates the odd sites. The second step rescales all distances by a factor 1/2. The third step relabels the surviving sites.

trary system:

$$H\psi = E\psi \tag{3.1}$$

where: H is a known N×N matrix (typically $N \to \infty$)

: E is a scalar

: ψ is an N-dimensional column vector whose elements are that which satisfy the equation.

Suppose after arranging the elements of ψ in some appropriate order (and re-arranging the rows and columns of H accordingly) that we partition ψ into two "subvectors" ψ_1 and ψ_2 of dimensions n_1 and $N-n_1$ respectively. Then we can write

$$H_{11}\psi_1 + H_{12}\psi_2 = E\psi_1 \tag{3.2a}$$

$$H_{21}\psi_1 + H_{22}\psi_2 = E\psi_2 \tag{3.2b}$$

where H_{ij} are the submatrices of the appropriately partitioned matrix H (H_{ij} has dimensions $n_i \times n_j$). Eliminating ψ_2 from (3.2) gives

$$H_{11}\psi_1 + H_{12}[(E-H_{22})^{-1}H_{21}\psi_1] = E\psi_1 \tag{3.3}$$

or alternatively

$$H'_{11}\psi_1 = E\psi_1 \tag{3.4}$$

where $H'_{11} = H_{11} + H_{12}(E-H_{22})^{-1}H_{21}$.

Notice that we have succeeded in eliminating a fraction

n_2/N of the variables without changing the form (only the dimensionality) of the original equations. Once we have appropriately relabelled the elements of ψ_1 we can repartition and eliminate the same fraction of varibles and continue in this manner indefinitely. Note that the f = 2 scaling transformation depicted in Figure (3.1) would correspond to having all even sites in ψ_1 and all odd sites in ψ_2.

We can also use the arbitrary system to illustrate how the scaling approach leads to the Green's functions of the system under study. If we add an inhomogeneous term to the Schrödinger equation then we can write

$$[E-H]G = Z \tag{3.5}$$

where: Z is a normalized N-dimensional column vector with only one non-zero entry

: G is an N-dimensional column vector whose elements satisfy the inhomogeneous equation.

If we partition the vector G into two subvectors G_1 and G_2 such that the "element of interest" coincides with G_1 then we can write

$$[E-H_{11}]G_1 - H_{12}G_2 = Z_1 \tag{3.6a}$$

$$[E-H_{22}]G_2 - H_{21}G_1 = Z_2 \tag{3.6b}$$

where H_{ij} and Z_j (i,j = 1,2) are obtained by appropriately partitioning H and Z. Eliminating G_2 from these equations gives

$$[E-H'_{11}]G_1 = Z'_1 \tag{3.7}$$

$$\text{where: } H'_{11} = H_{11} + H_{12}(E-H_{22})^{-1}H_{21}$$

$$: \quad Z'_1 = Z_1 + H_{12}(E-H_{22})^{-1}Z_2 .$$

Suppose this transformation is iterated (always keeping the element of interest in the subvector of surviving elements) until the limit $H_{12} \to 0$ is attained. Then in this limit

$$H'_{11} = H_{11} \equiv H_{11}^{(\infty)} \tag{3.8a}$$

$$Z'_1 = Z_1 \equiv Z_1^{(\infty)} \tag{3.8b}$$

and so

$$G_1 = [E - H_{11}^{(\infty)}]^{-1}Z_1^{(\infty)} . \tag{3.9}$$

If the element of interest is the i^{th} element of G and the non-zero element of the inhomogeneous term is the j^{th} element of Z (these labels are with respect to the original equations (3.5)) then it follows that

$$[E - H_{11}^{(\infty)} + iO^+]^{-1}Z_1^{(\infty)} = \langle i \left| \frac{1}{E-H+iO^+} \right| j \rangle \tag{3.10}$$

where the right-hand side is defined as the i,j^{th} element of the Green's function $G(E+iO^+)$ (see Economou [E]). As is

convention, a small imaginary part ($i0^+$) has been added to the energy E to insure that the inverse of E-H is well defined (H is assumed to be Hermitian and hence has only real eigenvalues). It is to be understood by our choice of notation that we are considering the limiting case in which the imaginary part goes to zero from the positive side. To summarize:

$$G_{ij}(E-H+i0^+) = [E-H^{(\infty)}(i)+i0^+]^{-1}Z^{(\infty)}(i,j) \qquad (3.11)$$

where: $H^{(\infty)}(i)$ is the limit of the partitioned Hamiltonian if the element of interest is the i^{th} element

: $Z^{(\infty)}(i,j)$ is the limit of the partitioned column vector Z if the corresponding non-zero entry is the j^{th} element.

Before proceeding to discuss the two-magnon problem a technical point should be mentioned. If the dimensionality of the "degree of freedom" lattice is greater than one then the elimination procedure causes the effective range of interaction to increase under iteration [SKL]. Hence, for such systems the scaling transformation must be made valid for an arbitrary range of interaction. Consequently, the analytic construction of the scaling transformation becomes an extremely tedious problem. Fortunately, the two-magnon problem for a quantum spin chain maps to a one-dimensional degree of freedom

lattice or in this case relative coordinate lattice. (It is relative coordinates between excited spin sites which label the degrees of freedom in multi-magnon problems.) However, for the arbitrary m-magnon problem of a quantum spin chain the dimensionality of this relative coordinate lattice is m-1. Hence, there are immediate difficulties in extending the subsequent formalism to the m-magnon problem for any $m \geq 3$.

3.2 Two-Magnon Analysis

We now proceed to apply the scaling approach specifically to the two-magnon problem of an alternating ferrimagnetic chain. Recall (2.16), the two-magnon Schrödinger equation. This can be rewritten as

$$H'|\psi_2\rangle = E_2|\psi_2\rangle \tag{3.12}$$

where: $H' = H - E_0$

and where the Hamiltonian H and the ground state energy E_0 are as defined in (2.1) and (2.3) respectively. Also recall (2.15) the general expression for the two-magnon wavefunction:

$$|\psi_2\rangle = \sum_{n=1}^{N/2} \sum_{m=1}^{N/2} [a_{2n,2m}|2n,2m\rangle + a_{2n-1,2m}|2n-1,2m\rangle + a_{2n,2m+1}|2n,2m+1\rangle + a_{2n+1,2m+1}|2n+1,2m+1\rangle] . \tag{3.13}$$

In Chapter 2 we derived two sets of coupled equations relating the various two-magnon amplitudes $a_{i,j}$. These were referred to as the non-interacting equations (2.17) and the interacting equations (2.19). These two sets effectively describe the complete interacting two-magnon problem for our system of interest.

Each two-magnon amplitude $a_{i,j}$ is labelled by two different coordinates corresponding to sites along the chain where the spins are excited. Because of the alternation in both bond and spin along the chain, there are four possible "configurations" of these coordinate pairs; even-even, odd-even, even-odd, and odd-odd. Hence there are four different categories of amplitudes. Each of these can be expressed in terms of a center of mass coordiate (i+j)/2 and a relative coordinate j-i as follows:

$$a_{2n,2m} = U^{(1)}_{2(m-n)} V^{(1)}_{2n+2m} \tag{3.14a}$$

$$a_{2n-1,2m} = U^{(2)}_{2(m-n)+1} V^{(2)}_{2n+2m-1} \tag{3.14b}$$

$$a_{2n,2m+1} = U^{(3)}_{2(m-n)+1} V^{(3)}_{2n+2m+1} \tag{3.14c}$$

$$a_{2n+1,2m+1} = U^{(4)}_{2(m-n)} V^{(4)}_{2n+2m+2} \tag{3.14d}$$

Because of translational invariance it follows from Bloch

theorem [AM] that the center of mass components can be expressed as plane waves. Hence (3.14) becomes

$$a_{2n,2m} = U^{(1)}_{2(m-n)} e^{iK(2n+2m)/2} \tag{3.15a}$$

$$a_{2n-1,2m} = U^{(2)}_{2(m-n)+1} e^{iK(2n+2m-1)/2} \tag{3.15b}$$

$$a_{2n,2m+1} = U^{(3)}_{2(m-n)+1} e^{iK(2n+2m+1)/2} \tag{3.15c}$$

$$a_{2n+1,2m+1} = U^{(4)}_{2(m-n)} e^{iK(2n+2m+2)/2} \tag{3.15d}$$

which is actually a generalization of formalism used originally by Fukuda and Wortis [FW] as well as by Boyd and Callaway [BC]. Note that K is the total wavevector as defined in Chapter 2.

Using the notation of (3.15), both the non-interacting and the interacting sets of two-magnon equations can be re-expressed in terms of the "relative coordinate amplitudes" $U^{(j)}_r$ ($r = 0,1,2,\ldots$; $j = 1,2,3,4$). Furthermore, if we define the four-component vector:

$$U_{2r} = \begin{bmatrix} U^{(1)}_{2r} \\ U^{(2)}_{2r+1} \\ U^{(3)}_{2r+1} \\ U^{(4)}_{2r} \end{bmatrix} \qquad r = 0,1,2,\ldots \tag{3.16}$$

then both sets of equations can be expressed in very concise

4×4 matrix form. The non-interacting equations (2.17) can be written as follows:

$$MU_{2r} = V_p U_{2r+2} + V_m U_{2r-2} \qquad r > 0 \qquad (3.17)$$

where:

$$M = \begin{bmatrix} \Omega - D & \sqrt{SS'}\, G_1^{(2)} e^{-iK/2} & \sqrt{SS'}\, G_1^{(1)} e^{+iK/2} & 0 \\ \sqrt{SS'}\, G_1^{(2)} e^{+iK/2} & \Omega & 0 & \sqrt{SS'}\, G_1^{(2)} e^{-iK/2} \\ \sqrt{SS'}\, G_1^{(1)} e^{-iK/2} & 0 & \Omega & \sqrt{SS'}\, G_1^{(1)} e^{+iK/2} \\ 0 & \sqrt{SS'}\, G_1^{(2)} e^{+iK/2} & \sqrt{SS'}\, G_1^{(1)} e^{-iK/2} & \Omega + D \end{bmatrix} \qquad (3.18)$$

$$V_p = -\sqrt{SS'} \begin{bmatrix} 0 & 0 & 0 & 0 \\ G_1^{(1)} e^{-iK/2} & 0 & 0 & G_1^{(1)} e^{+iK/2} \\ G_1^{(2)} e^{+iK/2} & 0 & 0 & G_1^{(2)} e^{-iK/2} \\ 0 & 0 & 0 & 0 \end{bmatrix} \qquad (3.19)$$

$$V_m = -\sqrt{SS'} \begin{bmatrix} 0 & G_1^{(1)} e^{+iK/2} & G_1^{(2)} e^{-iK/2} & 0 \\ 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \\ 0 & G_1^{(1)} e^{-iK/2} & G_1^{(2)} e^{+iK/2} & 0 \end{bmatrix} . \qquad (3.20)$$

And the interacting equations (2.19) are now given by the following:

$$M_0 U_0 = V_p U_2 \qquad (3.21)$$

where:

$$(M_0)_{11} = E_2 - \theta_S \tag{3.22a}$$

$$(M_0)_{12} = \Phi_{S'}^{(2)} e^{-iK/2} \tag{3.22b}$$

$$(M_0)_{13} = \Phi_{S'}^{(1)} e^{+iK/2} \tag{3.22c}$$

$$(M_0)_{14} = \Delta^{(1)} e^{+iK} + \Delta^{(2)} e^{-iK} \tag{3.22d}$$

$$(M_0)_{21} = \Phi_{S'}^{(2)} e^{+iK/2} \tag{3.22e}$$

$$(M_0)_{22} = E_2 - \tau^{(1)} \tag{3.22f}$$

$$(M_0)_{23} = 0 \tag{3.22g}$$

$$(M_0)_{24} = \Phi_{S}^{(2)} e^{-iK/2} \tag{3.22h}$$

$$(M_0)_{31} = \Phi_{S'}^{(1)} e^{-iK/2} \tag{3.22i}$$

$$(M_0)_{32} = 0 \tag{3.22j}$$

$$(M_0)_{33} = E_2 - \tau^{(2)} \tag{3.22k}$$

$$(M_0)_{34} = \Phi_{S}^{(1)} e^{+iK/2} \tag{3.22 l}$$

$$(M_0)_{41} = \Delta^{(1)} e^{-iK} + \Delta^{(2)} e^{+iK} \tag{3.22m}$$

$$(M_0)_{42} = \Phi_S^{(2)} e^{+iK/2} \tag{3.22n}$$

$$(M_0)_{43} = \Phi_S^{(1)} e^{-iK/2} \tag{3.22o}$$

$$(M_0)_{44} = E_2 - \theta_S, \tag{3.22p}$$

where all parameters in the preceding matrices are as defined in Chapter 2 (see (2.6), (2.14), (2.18), (2.20)). So summarizing:

$$M_0 U_0 = V_p U_2 \tag{3.23a}$$

$$MU_{2r} = V_p U_{2r+2} + V_m U_{2r-2} \qquad r = 1,2,3,... \tag{3.23b}$$

Each vector or unit cell U_{2r} can be regarded as the r^{th} site on a semi-infinite linear lattice. Note that interactions only exist between nearest-neighbour lattice sites. If we eliminate alternate sites starting with U_2 from (3.23) then we obtain the following set of "transformed" equations:

$$M_0 U_0 = V_p M^{-1}[V_p U_4 + V_m U_0] \tag{3.24a}$$

$$MU_{2r} = V_p M^{-1}[V_p U_{2r+4} + V_m U_{2r}] + V_m M^{-1}[V_p U_{2r} + V_m U_{2r-4}] \qquad r = 2,4,6,... \tag{3.24b}$$

or alternatively:

$$M_0' U_0 = V_p' U_4 \tag{3.25a}$$

$$M' U_{4r} = V_p' U_{4r+4} + V_m' U_{4r-4} \qquad r = 1,2,3,... \tag{3.25b}$$

where we have defined

$$M_0' = M_0 - V_p M^{-1} V_m \tag{3.26a}$$

$$M' = M - V_p M^{-1} V_m - V_m M^{-1} V_p \tag{3.26b}$$

$$V_p' = V_p M^{-1} V_p \tag{3.26c}$$

$$V_m' = V_m M^{-1} V_m . \tag{3.26d}$$

Notice that the primed parameters in (3.25) describe the effective interaction between next-nearest-neighbours.

Now suppose we relabel the surviving vectors in (3.25) such that $U_{4r} \to U_{2r}$. Then in terms of the renormalized (primed) parameters the new set of equations (3.25) have exactly the same form as the originals (3.23). However, in (3.25) exactly one half of the degrees of freedom (i.e., vectors) have been eliminated. Hence, this elimination corresponds to a $f = 2$ scaling transformation. If we add a small imaginary part to the energy E_2 (so that all inverses are well defined) and iterate this transformation then we find that V_p' and V_m' both approach zero. So we eventually obtain the limiting result

$$M_0^{(\infty)} U_0 = 0 . \tag{3.27}$$

In this limit the "motion" of the vector or unit cell U_0 has been completely decoupled from the motion of all other vectors.

We can obtain a similarily decoupled equation for the vector U_2 as follows. First, eliminate alternate sites starting with U_0 from (3.23) to give the following:

$$MU_2 = V_p M^{-1}[V_p U_6 + V_m U_2] + V_m M_0^{-1}[V_p U_2] \tag{3.28a}$$

$$MU_{2s} = V_p M^{-1}[V_p U_{2s+4} + V_m U_{2s}] + V_m M^{-1}[V_p U_{2s} + V_m U_{2s-4}], \quad s = 3,5,7,... \tag{3.28b}$$

If we relabel the surviving vectors in (3.28) such that $U_{2s} \to U_{(2s-2)/2}$ then we can write

$$\bar{M}_0 U_0 = \bar{V}_p U_2 \tag{3.29a}$$

$$\bar{M} U_{2r} = \bar{V}_p U_{2r+2} + \bar{V}_m U_{2r-2} \qquad r = 1,2,3,... \tag{3.29b}$$

where we have defined

$$\bar{M}_0 = M - V_p M^{-1} V_m - V_m M_0^{-1} V_p \tag{3.30a}$$

$$\bar{M} = M - V_p M^{-1} V_m - V_m M^{-1} V_p \tag{3.30b}$$

$$\bar{V}_p = V_p M^{-1} V_p \tag{3.30c}$$

$$\bar{V}_m = V_m M^{-1} V_m . \qquad (3.30d)$$

The newly transformed set of equations (3.29) has exactly the same form as the original set (3.23) so we can now iterate with the "original" transformation described by (3.26). The limiting result will be a decoupled equation analagous to (3.27) except now it is the motion of the unit cell U_2 which has been decoupled.

A decoupled equation can similarily be obtained for any of the unit cells U_{2r} (r = 0,1,2,...) by using some appropriate combination of the previous two scaling transformations (described by (3.26) and (3.30)). To avoid confusion, we let $M_0^{(\infty)}(2r)$ denote the limiting matrix obtained when decoupling the unit cell labelled by r. Note that each such matrix is the projection of the operator E_2-H' in the subspace spanned by $\{|U_{2r}^{(1)}>, |U_{2r+1}^{(2)}>, |U_{2r+1}^{(3)}>, |U_{2r}^{(4)}>\}$.

It follows from the formalism in Section 3.1 that we can use these transformations to evaluate the two-magnon Green's functions. We define the i,j^{th} element of the local two-magnon Green's functions as follows:

$$G_{2r}^{i,j}(E_2 + i0^+,K) = \langle U_{2r}^{(i)} \left| \frac{1}{E_2+i0^+-H'} \right| U_{2r}^{(j)} \rangle ,$$

$$i,j = 1,2,3,4;\ r = 0,1,2,\ldots . \qquad (3.31)$$

The evaluation of the elements of $G_{2r}(E_2+i0^+,K)$ requires

adding an appropriate inhomogeneous term to each of the equations in the set (3.23) and then iterating the transformation(s) so that the motion of the corresponding unit cell U_{2r} has been decoupled.

For instance, suppose we want to evaluate $G_0^{i,j}(E_2+i0^+,K)$ $(i,j = 1,2,3,4)$. First consider the inhomogeneous version of (3.23) in its most general form

$$M_0U_0 = V_pU_2 + Z_0 \tag{3.32a}$$

$$MU_{2r} = V_pU_{2r+2} + V_mU_{2r-2} + Z_{2r}, \quad r = 1,2,3,... \tag{3.32b}$$

where each Z_{2r} is a four-component column vector. Under the scaling transformation described by (3.26) (i.e., that which eliminates alternate sites starting with U_2) the form of (3.32) remains invariant provided the inhomogeneous terms are renormalized as follows:

$$Z_0' = Z_0 + V_pM^{-1}Z_2 \tag{3.33a}$$

$$Z_{2r}' = Z_{2r} + V_pM^{-1}Z_{2r+2} + V_mM^{-1}Z_{2r-2} \quad r = 2,4,6,... \tag{3.33b}$$

To calculate the particular element $G_0^{i,j}$ we must set all $Z_{2r} = 0$ except for Z_0. Meanwhile Z_0 must have a non-zero entry in the j^{th} row only. We then iterate the scaling transformation which yields the limiting result

$$M_0^{(\infty)}(0)\begin{bmatrix} G_0^{1,j} \\ G_0^{2,j} \\ G_0^{3,j} \\ G_0^{4,j} \end{bmatrix} = Z_0^{(\infty)} . \tag{3.34}$$

Since all $Z_{2r} = 0$ except Z_0 it follows from (3.33) that the inhomogeneous terms are invariant under this scaling transformation for any number of iterations. Consequently

$$Z_0^{(\infty)} = Z_0 = \begin{bmatrix} \delta_{1j} \\ \delta_{2j} \\ \delta_{3j} \\ \delta_{4j} \end{bmatrix} \tag{3.35}$$

where: δ_{ij} is the Kronecker delta.

(This invariance is actually a direct consequence of the range of interaction between unit cells being limited to nearest neighbours only [SKL]. If the unit cells separated by two or more sites could directly interact then we would have to calculate $Z_0^{(\infty)}$ explicitly.) From (3.34) and (3.35) we can solve for any element of $G_0(E_2+i0^+,K)$ by simply inverting the limiting matrix $M_0^{(\infty)}(0)$. In other words,

$$G_0^{i,j}(E_2 + i0^+,K) = [M_0^{(\infty)}(0)]^{-1}_{i,j} \tag{3.36}$$

In similar fashion we can obtain the more general result

$$G_{2r}^{i,j}(E_2 + i0^+,K) = [M_0^{(\infty)}(2r)]^{-1}_{i,j} \qquad r = 0,1,2,... \qquad (3.37)$$

Recall that each matrix $M_0^{(\infty)}(2r)$ is a representation of E_2-H' where H' = H-E_0. Since the Hamiltonian H' is hermitian, adding a small imaginary part $i0^+$ to the excitation energy insures that the inverse of any such matrix is well defined. Therefore, the two-magnon Green's functions are well defined quantities.

3.3 Local Densities of States

Various spectral and thermodynamic information about a system can be extracted from that system's Green's functions. The two-magnon Green's functions, as described in the previous section, will be used to extract the local densities of states.

For an arbitrary system we define the local densities of states $\rho_n(E)$ as follows

$$\rho_n(E) = \delta(E - E_n) \qquad (3.38)$$

where: E_n is the energy eigenvalue of the n^{th} state

: $\delta(X)$ is the one-dimensional Dirac delta function

The local densities of states can be shown to be related to the diagonal elements of the system's Green's functions (see Economou [E]). This relation is as follows:

$$\rho_n(E) = -\frac{1}{\pi}\,\mathrm{Imag}[\langle n|G(E + i0^+)|n\rangle]\,. \qquad (3.39)$$

Now consider the two-magnon problem for an alternating ferrimagnetic chain. It follows from (3.39) that the imaginary part of each diagonal Green's function element $G_{2r}^{jj}(E_2+i0^+,K)$ $(r = 0,1,2,\ldots;\ j = 1,2,3,4)$ measures the local densities of states corresponding to a specific configuration of spin excitations. For instance, $\mathrm{Imag}[G_2^{44}]$ measures the local densities of states for a pair of spin excitations separated by two sites such that both occur at odd sites along the chain. Similarily we can obtain measures of the local densities of states for any of the four categories of configurations (even-even, odd-even, even-odd, odd-odd) and for any number of sites separating the excitations. All we require is knowing $\mathrm{Imag}[G_{2r}^{jj}]$ which can be calculated for all r and j using the formulism of Section 3.2.

The significance of the two-magnon local densities of states is that such calculations provide a direct measure of the relative contribution of any two spin deviation state to the complete two-magnon wavefunction. For instance, $\mathrm{Imag}[G_2^{44}]$ directly measures $|U_2^{(4)}|$, the magnitude of the corresponding relative coordinate amplitude. In other words, $\mathrm{Imag}[G_2^{44}]$ directly measures $|a_{i,j}|$ for any i and j which satisfy j-i = 2 such that both i and j are odd. And recall that the two-magnon amplitude $a_{i,j}$ is a measure of the contribution of the two spin deviation state $|i,j\rangle$ to the two-magnon

wavefunction. So Imag[G_2^{44}] directly measures the contribution of any state $|i,j\rangle$ such that $j-i = 2$ and both i and j are odd.

In Chapter 2 we distinguished between two very different types of solutions to the two-magnon problem. These were bound states and scattering (i.e., continuum) states. We find that this difference in solutions is manifested in the local densities of states. First consider the bound state solutions. Such states are spectrally isolated from all other non-trivial states and hence make a simple delta function contribution to the densities of states. These delta functions can also be regarded as corresponding to real-valued poles in the Green's functions. That is, poles which coincide with the real-axis in the complex energy plane. Actually, because of the small imaginary part added to the energy to insure convergence, these poles occur slightly off the real axis. Consequently, these bound state contributions are not true delta functions but rather have a finite width proportional to ϵ (magnitude of imaginary part) and a finite height proportional to $1/\epsilon$.

Meanwhile the scattering state solutions are not spectrally isolated but instead lie inside a continuum of states. Because of the infinitesimally close proximity of neighbouring continuum states, the various delta function contributions to the densities of states must overlap. So the overall contribution of a continuum of scattering states is not a

series of delta functions but rather a "band" of finite height which extends over the entire spectral region corresponding to the continuum. (This is analagous to a wavepacket which spreads and flattens as more and more waves are added so that any one wave gradually loses its identity while inside the packet.) This effective spreading of density of state contributions inside the continuum can also be attributed to poles in the Green's functions moving off the real axis. That is, for a spectral point (K,E_2) inside of a continua the corresponding pole in the Green's functions will occur at a complex energy value $E_2 + i\Gamma$ where $\Gamma \neq 0$.

Suppose a complex valued pole in the Green's function has a relatively small imaginary part (i.e., $|\Gamma| << E_2$ but Γ is finite). Such an occurrence manifests itself as a Lorentzian shaped "bump" in a continuum region of the local densities of states [WH]. Such bump or peak-like structures have a width proportional to Γ and a height proportional to $1/\Gamma$ and are commonly referred to as resonant peaks. The corresponding "resonant states" are expected to be related to our previous definition of a resonant state (Chapter 2). This was a state localized in relative coordinate space due to an exponentially decaying factor but (unlike bound states) falls inside a continuum region where the states are generally plane wave in nature. Resonant states can often be regarded as bound

states that have lost their "identity" upon entering a scattering continuum.

Recall that both bound state solutions and continuum boundaries are easily solved for by way of the analytic approach of Chapter 2. Hence, we are most interested in using calculations of the two-magnon densities of states for the purpose of identifying resonant states inside the continua. We expect that resonant states (like bound states) decay exponentially as relative coordinate between spin excitations increases. This is because we expect resonant states to be dominated by a factor exp[-iqr] where r is the relative coordinate and q is the relative wavevector for which we know Im(q) < 0. Therefore, resonant state (as well as bound state) contributions to the local densities of states are most prominent in cases where relative coordinate between spin excitations is small. As a result, it is most informative to calculate the Green's function elements G_0^{jj} (j = 1,2,3,4) which describe the states with spin excitations on same or neighbouring sites. The results of such calculations are discussed in Chapter 4.

We conclude this chapter by discussing a technical but pertinent point, the size of the imaginary part added to the two-magnon excitation energy. Recall that this imaginary component is added to insure that all inverted matrices are

well defined. This in turn insures that the overall limiting process of iterating the scaling transformation is convergent. In the preceding formal treatment we have denoted this imaginary component by $i0^+$ and in doing so have implied an infinitesimally small magnitude. Formally, this is sufficient for convergence to occur; however, in practice the number of iterations allowed is restricted by the computing facilities available. So in practice, the size of this imaginary component is not such a trivial consideration.

The actual computing procedure for calculating G_0^{jj} ($j = 1,2,3,4$) entails adding a small imaginary $i\epsilon$ to the excitation energy and then iterating the scaling transformation (3.26) until the matrices V_p' and V_m' effectively vanish. By effectively vanish we mean that the sum of the absolute values of their entries drops below some preselected tolerance level. Once this level is reached the resulting matrix M_0' is inverted to give the elements of the desired Green's function. We found that for spectral points outside the energy continua that no more than six iterations were required for convergence and the number of iterations was independent of ϵ. However for spectral points inside of the energy continua, the smaller the value of ϵ the greater the number of iterations required.

To understand this relation between the number of iterations required and the magnitude of the imaginary component (ϵ) first note that convergence occurs only if $V_p' \to 0$. What

is significant is that the matrix V_p' describes the effective interaction between the 0^{th} unit cell and the $(2^x)^{th}$ unit cell where x is the corresponding number of iterations. Equivalently it can be said that V_p' describes the extent of the solution in relative coordinate space. Consider solutions inside the continua. If $\epsilon = 0$ then such solutions always have a pure plane wave component (since at least two values of relative wavevector q are real). Since plane waves have infinite extent, V_p' cannot vanish even in the limit $x \to \infty$. However, for $\epsilon \neq 0$, then each plane wave component is effetively multiplied by an exponentially decaying factor since complex energy implies complex wavevector. This decaying factor limits the extent of the solution in relative coordinate space thereby insuring that V_p' vanishes after a sufficient number of iterations. Furthermore, the larger the value of ϵ, the stronger the decaying factor and hence the fewer iterations required for convergence. Meanwhile, solutions outside the energy continua must already have a strong exponentially decaying factor (since all values of q are complex) and therefore convergence occurs irrespective of ϵ.

Rapid convergence inside the energy continua is the motivation for making ϵ large; however, there is a conflicting motivation for ϵ to be made small. If we plot local densities of states versus E_2 then the resolution of these plots gets

worse as ϵ increases. This can be understood by considering a typical resonant peak. As previously discussed the width of such a peak depends on Γ where $E_2 + i\Gamma$ is the corresponding complex pole in the two-magnon Green's functions. However if $\epsilon \neq 0$, then this pole is actually given by $E_2 + i\Gamma(\epsilon)$ (that is, Γ is no longer a fixed value but instead varies as a function of the imaginary part added to energy). Typically we choose ϵ to be small enough so that $\Gamma(\epsilon) \simeq \Gamma$ and hence the pole remains close to its "true" location. However if ϵ is allowed to become too large, then it is easy to see how the resonant structure in the local densities of states can become distorted. Note that for bound states $\Gamma = 0$, so the width of bound state peaks is directly proportional to ϵ.

To summarize, we must adjust the value of ϵ (magnitude of the imaginary energy component) until a satisfactory compromise is found between resolution of densities of states and rate of convergence inside the continua. We eventually decided upon $\epsilon = 1\times10^{-5}$. For this value we found that 20-25 iterations were needed to achieve convergence inside the continua regions. Alternatively, we can decrease the number of iterations required by increasing the scaling factor of the transformation. Recall that we use a scaling factor $f = 2$. However any increase in f would require analytic construction of a new and more complicated set of transformation equations.

Chapter 4

RESULTS

In this chapter we will use the techniques formulated in Chapters 2 and 3 to study the two-magnon spectra for a variety of special cases of the alternating ferrimagnetic chain. Section 4.1 of this chapter focuses on the bound state solutions of the two-magnon problem. This section uses the direct analytic approach of Chapter 2 to determine the complete set of bound states for each special case of interest. Section 4.2 of this chapter applies the real-space rescaling approach of Chapter 3 to obtain additional information regarding scattering states inside the continua. Such information is obtained via local densities of states calculated for fixed values of total wavevector. Section 4.3 displays the various spectra referred to in the prior sections.

The number of different systems we are potentially able to examine is endless as we are free to independently vary six parameters of the Hamiltonian (2.1). These parameters are S, S', $G_1^{(1)}$, $G_1^{(2)}$, $G_2^{(1)}$, and $G_2^{(2)}$. To help in classification of the various cases to be studied we define the following "relative" parameters:

$$r^{(i)} = G_2^{(i)}/G_1^{(i)} \qquad i = 1,2 \qquad (4.1a)$$

$$b = G_1^{(2)}/G_1^{(1)} \qquad (4.1b)$$

$$\Delta S = S - S' \geq 0 \tag{4.1c}$$

$$\xi_2 = E_2/G_1^{(1)} . \tag{4.1d}$$

The ratios $r^{(i)}$ describe the form of the interactions between neighbouring spins. (But note that unless $S' \leq 1$ then $r^{(1)}$ and $r^{(2)}$ do not completely specify these interactions. These require specification of $G_m^{(i)}$ for all $m = 1,2,\ldots,2S'$.) The ratio b measures the degree of bond alternation while the difference ΔS measures the degree of spin alternation. The ratio ξ_2, which we refer to as the reduced energy, reflects that the parameter $G_1^{(1)}$ can be used to scale the excitation energy. In fact all energy scales in Section 4.3 will be in units of $G_1^{(1)}$ or "reduced energy units". Note that we only consider cases in which b, $r^{(1)}$, and $r^{(2)}$ are greater than or equal to zero to insure a ferromagnetic ground state.

Before proceeding we note that if $S' = \frac{1}{2}$, then the unphysical amplitudes $a_{2n,2n}$ decouple completely from all other amplitudes in the interacting equations (2.19). Furthermore, the equations involving the physical amplitudes and hence all physical results are independent of $G_2^{(1)}$ and $G_2^{(2)}$. This is expected because setting $S' = \frac{1}{2}$ restricts the form of the Hamiltonian to that of Heisenberg exchange. (By Heisenberg exchange we mean that the spin-spin interaction is described in terms of linear exchange operators $(\tilde{S}_i \cdot \tilde{S}_j)^1$ only. Generally, Heisenberg exchange requires setting

$G_m^{(i)} = G_1^{(i)}$ for i = 1,2 and m = 1,2,...,2S'.) Consequently if $S' = \frac{1}{2}$ then we need only specify two other parameters, namely b and ΔS.

4.1 Bound States

Case (a) $S' = \frac{1}{2}$ $\Delta S = 0$ $b = 1$

This is the case of a uniform Heisenberg chain with spin magnitude $S = \frac{1}{2}$. The corresponding Hamiltonian has already been discussed somewhat in Chapter 1 (refer to equation (1.9)). Recall that this is a completely integrable system which can be solved using the Bethe ansatz approach [BE]. The two-magnon spectrum (see Figure (1.2) in Chapter 1) contains a single energy continuum along with a single bound state branch lying completely below the continuum for all K. We know from quantum mechanical theory that there must be at least one bound state for all values of K as this is a one-dimensional problem [LL]. The binding energy between continuum and bound state is largest at the Brillouin zone boundary ($K = \pi$) and smallest at $K = 0$.

To help in understanding of nonuniform cases it is informative to consider the spectrum of this uniform chain when plotted in the reduced Brillouin zone $|K| \leq \frac{\pi}{2}$ (i.e., the Brillouin zone for any alternating chain). The bound state branch is folded back at $K = \pi/2$ so that it now consists of both an upper part which lies entirely inside the continuum

and a lower part which lies entirely outside the continuum for all K. Note that these two parts are degenerate at the reduced Brillouin zone boundary. Although the upper portion of the branch overlaps the continuum it remains a true bound state for all K as its "character" has not been altered.

Case (b) $S' = \frac{1}{2}$ $\Delta S = 0$ $b \neq 1$

We now consider the alternating bond Heisenberg chain with uniform spin magnitude $S = \frac{1}{2}$. Because of the alternation in bond strength the single energy continuum of the previous (uniform) case now splits into three distinct continua. In order of increasing energy, these are acoustic-acoustic (A-A), mixed-mode, and optic-optic (O-O). Each of these continua has at least one associated bound state beneath it (the A-A continuum has two). The two-magnon spectrum, depicting bound state branches and continuum boundaries, is shown in Figure (4.1) for $b = \frac{1}{2}$.

The bound state structure below the A-A continuum is similar in form to that of the uniform case (when plotted in the reduced Brillouin zone) except now there is a non-zero gap at $K = \pi/2$ between the upper and lower branches. It has been shown that this gap vanishes linearly with the difference 1-b [BLS]. Also, the character of the state associated with the upper branch has been altered in that it is now a resonant state while inside the continuum. The lower branch does

however remain a true bound state for all K. Its binding energy is smallest at K = 0 and largest at K = $\pi/2$.

The bound state branch below the mixed continuum remains a true bound state for all K with binding energy smallest at K = $\pi/2$ and largest at K = 0. The bound state branch below the O-O continuum corresponds to a resonant state for small values of K until it emerges from the continuum to become a true bound state at large K values. Both of these "new" bound states undergo a change in character in crossing from spectral region III to spectral region V, here referring to the regions as labelled in Figure (2.3). This change in character is a direct consequence of the two allowed values of relative wavevector q being degenerate at the boundary between these regions (see Appendix B for details). In region III, the imaginary parts of the two allowed q values are different while in region V they are equal (with real parts different). In all subsequently examined cases, bound states lying inside the continuum gaps exhibited similar behaviour.

Case (c) $\Delta S = 0 \quad S > \frac{1}{2} \quad b \neq 1 \quad r^{(1)} = r^{(2)} = 1$

We now consider the alternating bond Heisenberg chain with uniform spin of magnitude $S > \frac{1}{2}$. (Note that if $S > 1$ then this may or may not be a true Heisenberg chain as $G_m^{(i)}$ $m = 3,4,\ldots,2S$ have not been specified.) The bound state

spectrum for this case is shown in Figure (4.2) where we have chosen $b = \frac{1}{2}$ and $S = 1$. This spectrum is qualitatively similar to that of the prior case ($S = \frac{1}{2}$ alternating bond chain) except for an additional bound state branch located between the mixed-mode and O-O continua. This branch is isolated from both continua for all K. We presume that this bound state is absent in the spin $S = \frac{1}{2}$ case because it is associated with two spin deviations on the same spin site and hence is unphysical for $S = \frac{1}{2}$ only. Since the magnitude of both spins in the unit cell has been incremented from $S = \frac{1}{2}$ to $S = 1$, one might expect a total of two "new" states. That is, a total of two states that are both unphysical in the $S = \frac{1}{2}$ alternating bond case. This suggests the likelihood of a state inside one of the continua and hence resonant for all values of K.

Increasing the magnitude of spin above $S = 1$ or varying b (provided $b \neq 0$ or 1) does not change the qualitative form of the spectra shown for $S = 1$ and $b = \frac{1}{2}$. However, if we scale energy values by S, then the relative binding energy of each of the five bound states decreases as S increases. This is expected since $S \to \infty$ corresponds to the classical limit at which point the bound states must be absorbed into their respective continua. The bound state midway between the mixed and O-O continua approaches the latter in the large S limit.

If we set b = 1 then we obtain the case of a uniform Heisenberg chain with $S > \frac{1}{2}$. The spectrum corresponding to this case is qualitatively similar to the spectrum for case (a) (uniform Heisenberg chain with $S = \frac{1}{2}$). However when $S > \frac{1}{2}$ there is known to be a resonant state inside the continuum, corresponding to an unphysical state when $S = \frac{1}{2}$. This resonant state can be forced out of the continua by including a single-ion anisotrophy term in the Hamiltonian [PP].

Case (d) $\Delta S = 0$ $S > \frac{1}{2}$ $r^{(1)} = r^{(2)} = 0$

This corresponds to a chain with uniform spin, generally alternating bond strength, and $G_2^{(1)} = G_2^{(2)} = 0$. The significance of this last condition can be seen by considering the set of interacting equations (2.19) which are now as follows:

$$[\xi_2 - S(1+b)]a_{2n,2n} = -S[a_{2n+1,2n+1} + ba_{2n-1,2n-1}] \quad (4.2a)$$

$$[\xi_2 - 2S]a_{2n-1,2n} = -S[a_{2n-1,2n+1} + a_{2n-2,2n}] \quad (4.2b)$$

$$[\xi_2 - 2Sb]a_{2n,2n+1} = -Sb[a_{2n,2n+2} + a_{2n-1,2n+1}] \quad (4.2c)$$

$$[\xi_2 - S(1+b)]a_{2n+1,2n+1} = -S[a_{2n,2n} + ba_{2n+2,2n+2}]. \quad (4.2d)$$

Clearly all the amplitudes with two spin deviations on the

same site have decoupled from all other amplitudes. The same was true in cases (a) and (b); however in those cases the decoupled amplitudes were unphysical since $S = S' = \frac{1}{2}$. For larger values of S we expect the decoupled amplitudes with two spin deviations on the same site to describe physical bound states.

We can obtain explicit analytic expressions for these same site bound states as follows. Substitute for the amplitudes in (4.2a) and (4.2d) with the general forms given by (2.30). We then obtain the following:

$$C_0\{[\xi_2 - S(1+b)]\alpha + [Se^{+iK/2} + Sbe^{-iK/2}]\delta\}$$

$$+ D_0\{[\xi_2 - S(1+b)]\bar{\alpha} + [Se^{+iK/2} + Sbe^{-iK/2}]\bar{\delta}\} = 0 \qquad (4.3a)$$

$$C_0\{[Se^{-iK/2} + Sbe^{+iK/2}]\alpha + [\xi_2 - S(1+b)]\delta\}$$

$$+ D_0\{[Se^{-iK/2} + Sbe^{+iK/2}]\bar{\alpha} + [\xi_2 - S(1+b)]\bar{\delta}\} = 0 . \qquad (4.3b)$$

The secular determinant of this linear homogeneous system is as follows:

$$\xi_2^2 - 2S(1+b)\xi_2 + S^2[(1+b)^2 - 1 - b^2 - 2b\cos(2K)] = 0 . \qquad (4.4)$$

Solving for the two-magnon excitation energy gives the following pair of bound state dispersion curves:

$$E_B^{\pm} = G_1^{(1)} S[1 + b \pm \sqrt{1+b^2+2b\cos(2K)}] \qquad (4.5)$$

both of which describe states with two spin deviations on a single site.

The set of equations involving amplitudes with spin deviations on different sites ((4.2b), (4.2c), and the non-interacting equations (2.17)) is formally identical to the set of equations obtained for case (b). Hence if we scale energy by a factor 2S then the bound states and energy continua are identical to those of the spin $S = \frac{1}{2}$ alternating bond case except for the two additional bound state branches as described by (4.5). The complete spectrum, three continua and all six bound state branches, is shown in Figure (4.3) for $b = \frac{1}{2}$ and $S = 1$. Notice that the bound states for spin deviations on the same site (i.e., E_B^- and E_B^+) lie entirely inside the A-A continuum and mixed-mode continuum respectively. Yet, these are true bound states for all values of K because of the complete decoupling that occurred. However, if we allowed spin to alternate or let $G_2^{(i)}$ take on non-zero (albeit small) values then this decoupling would be broken and the two additional bound states would become resonant states inside the continua.

If we set $b = 1$ then we have a uniform chain with $S > \frac{1}{2}$ and $r^{(1)} = r^{(2)} = 0$. In this case we obtain a scaled spectrum identical to that of case (a) (uniform chain with $S = \frac{1}{2}$) except for an additional bound state lying entirely inside the single continuum. Because of the complete decoupling,

this is a true bound state for all K and the dispersion relation is given by

$$E_B = 4G_1^{(1)} S\sin^2(\tfrac{K}{2}) \tag{4.6}$$

where we have assumed the full Brillouin zone representation ($|K| \leq \pi$). In spite of similarities to case (a), this is generally not a completely integrable system. This is because the remaining values of $G_m^{(i)}$ ($m = 3,4,\ldots,2S$) are yet unspecified. The exception occurs when $S = 1$ because in this case, all exchange coefficients have been specified. In fact, the uniform chain with $S = 1$ and $G_2^{(i)} = 0$ is a special case of a family of completely integrable systems [SU1] which are known as Schrödinger exchange operators [SCH]. Using our notation these correspond to

$$G_m^{(i)} = \frac{1 - (-1)^m}{2} \qquad i = 1,2;\ m = 0,1,\ldots,2S\ . \tag{4.7}$$

Case (e) $\quad S' > \frac{1}{2} \qquad r^{(i)} \to \infty \qquad i = 1,2$

This case describes a chain with generally alternating spins, generally alternating bonds, and $G_1^{(1)} = G_1^{(2)} = 0$. For $S = S' = 1$ this corresponds to a biquadratic exchange Hamiltonian. (By this we mean the spin-spin interaction is described in terms of quadratic exchange operators $(\tilde{S}_i \cdot \tilde{S}_j)^2$ only.) Regardless of S and S', if $G_1^{(1)} = G_1^{(2)} = 0$ then both branches of the one-magnon dispersion relation (2.12)

must vanish for all K. For the two-magnon problem it immediately follows that all three energy continua must also collapse to zero energy for all values of K. These "collapsed continua" make this a very special case.

From (2.27) we see that cos(2q) is infinite and consequently the relative wavevector q must have an infinite imaginary part. Eliminating those values of q corresponding to unphysical (exponentially growing) solutions means that all acceptable values of q have a negative and infinite imaginary part. From (2.29) and (2.30) it is evident that all amplitudes, except those with spin deviations on same or adjacent sites, must vanish due to an exponentially decaying factor. Using this simplification along with Bloch theorem we can express the four interacting equations (2.19) in terms of only four unknown amplitudes. These are equivalent to the relative coordinate amplitudes $U_0^{(1)}$, $U_1^{(2)}$, $U_1^{(3)}$, $U_0^{(4)}$ as defined by (3.15). The secular determinant for this sytem is as follows:

$$E_2^4 - E_2^3(G_2^{(1)} + G_2^{(2)})(2S + 2S' - 1)$$

$$+ E_2^2 G_2^{(1)} G_2^{(2)} \frac{(2S-1)(2S'-1)}{(S+S'-1)^2} [(2S+2S'-1)^2 - 4SS'\cos^2(K)] = 0 . \tag{4.8}$$

Solving this quartic equation we find a two-fold degenerate bound state at $E_2 = 0$ for all K (i.e., inside the collapsed

continua for all K) and two additional bound state branches with dispersion relations given by

$$E_B^{\pm} = \left(\frac{2S+2S'-1}{2}\right)\left(G_2^{(1)} + G_2^{(2)}\right) \pm \left[\left(\frac{2S+2S'-1}{2}\right)^2 \left(G_2^{(1)} + G_2^{(2)}\right)^2 - \frac{(2S-1)(2S'-1)}{(S+S'-1)} G_2^{(1)} G_2^{(2)} \left[(2S+2S'-1)^2 - 4SS'\cos^2(K)\right]\right]^{\frac{1}{2}}. \tag{4.9}$$

The simplicity of the two-magnon spectra for this model is physically justifiable in that the two-magnon states are in some sense equivalent to the "normal" spin waves of other models. In this model, the spin excitation pairs are strictly localized to same or adjacent sites and hence behave as a single entity propogating along the chain.

Now consider the even more special case of a uniform chain with $G_1^{(1)} = G_1^{(2)} = 0$. In this case there are only two bound state branches. One is degenerate with the collapsed continuum and one is given by

$$E_B = G_2^{(1)}\left[(2S-1) + 4S\sin^2\left(\frac{K}{2}\right)\right]. \tag{4.10}$$

Although E_B is only a single branch in the full Brillouin zone ($|K| \leq \pi$), this bound state folds back at $K = \pi/2$ in the reduced zone scheme ($|K| \leq \pi/2$). The dispersion relations for these two reduced zone branches are as follows:

$$E_B^{\pm} = G_2^{(1)}\left[(4S-1) \pm 2S\cos(K)\right]. \tag{4.11}$$

So for a uniform chain, we find that E_B^+ and E_B^- are degenerate at the reduced Brillouin zone boundary. This degeneracy along with the overall simplicity of the model suggests the possibility of a completely integrable system. The uniform chain with S = 1 and $G_1^{(1)} = G_1^{(2)} = 0$ is in fact a special case of a family of completely integrable systems [BB] originally studied by Parkinson [PAR]. In our terminology these are given by

$$\left.\begin{aligned} &G_1^{(i)} = G_2^{(i)} = \ldots = G_{2S-1}^{(i)} = 0 \\ &G_{2S}^{(i)} \neq 0 \end{aligned}\right\} \; i = 1,2 \qquad (4.12)$$

Case (f) $\quad \Delta S = 0 \quad S > \frac{1}{2} \quad b \neq 1 \quad r^{(1)} = r^{(2)}$

Suppose we consider chains with uniform spin only. Then the two previous cases can be interpreted as being extreme or limiting cases of alternating bond system in which we are free to vary the ratio $r \equiv r^{(1)} = r^{(2)}$ from zero to infinity. If r = 0 we obtain case (d) whereas if r diverges we obtain case (e). We anticipate that any intermediate value of r corresponds to a system which is appropriately intermediate between these two extreme cases. In general, the intermediate systems should have more complicated spectra since complete decoupling between sets of amplitudes occurs only in the limiting cases. One such intermediate case was already disucssed in case (c) where r = 1 (i.e., the Heisenberg case).

For case (d) we identify a total of six distinct bound state branches. We can also consider case (e) as having six bound states such that four of these are degenerate with the collapsed continua. We know there are four such states associated with the collapsed continua from examining the spectra with $r >> 1$ but finite. So it follows that any intermediate case ($0 < r < \infty$) should also have six associated states. These could be true bound states but are generally resonant states for some (or all) values of K. Furthermore, we expect this number of six bound or resonant two-magnon states to apply to any chain with some degree of alternation associated with it. However if $S' = \frac{1}{2}$ or $S = S' = \frac{1}{2}$, then one or two of these states would be unphysical.

The six bound/resonant states of any intermediate case in this model can be considered to have "evolved" from the bound states of either of the two limiting cases. We can illustrate this evolution with a few choice examples. For each of these examples we will set $S = 1$ and $b = \frac{1}{2}$. However varying these two parameter does not alter the qualitative form of the spectra provided $S > \frac{1}{2}$ and $b \neq 0,1$.

Figure (4.4) shows the bound state spectrum for the case $r = \frac{1}{5}$. Notice the similarity with case (d) ($r = 0$) except now the states inside the A-A and mixed-mode continuum must be resonant states due to broken decoupling. The state inside the A-A continuum apparently emerges from the top of the

continuum at large values of K where it is a true bound state again. The state inside the mixed continuum will similarily emerge but not until $r \simeq 0.7$. This state first emerges at small values of K.

Recall Figure (4.2) which shows the two-magnon spectrum for the Heisenberg case, $r = 1$. By following the spectral evolution from $r = 0$ to $r = 1$ we can make the following observations regarding the Heisenberg case. The "extra" bound state between the mixed and O-O continua (refer to case (c)) is now identified as having evolved from the bound state inside the mixed continuum at $r = 0$. The bound state inside the A-A continuum at $r = 0$ evolves into the bound state below the mixed continuum at $r = 1$. Meanwhile the bound state originally beneath the mixed continuum (when $r = 0$) gradually rises up into the mixed continuum as r is increased. At $r = 1$, this state is presumably a resonant state for all K. Recall from case (c) that such a resonant state had been predicted using a different line of reasoning.

Finally consider Figure (4.5) which depicts the bound state spectrum for the intermediate case $r = 2$. This case is interesting in that all six bound/resonant states are observed as being true bound states for at least some values of K. As $r \to \infty$ the two bound states above the O-O continuum evolve into the non-trivial states $E_B^{\pm}$ while the other four states are dragged along with the collapsing continua. Note

that the upper of the two branches beneath the A-A continuum has emerged outside the top of this continuum at small values of K.

Case (g) $\Delta S = 0$ $S > \frac{1}{2}$ $r^{(1)} = 0$ $r^{(2)} = \infty$

This case corresponds to a system with uniform spin, alternating bond, $G_1^{(2)} = 0$, and $G_2^{(1)} = 0$. This is another system which can be regarded as being intermediate between the two systems described in cases (d) and (e). Here the alternating chain is composed of two sublattices, each of which corresponds to one of the previously described cases. (For S = 1 this would correspond to pure biquadratic exchange alternating with Schrödinger exchange along the chain.) Since $G_1^{(2)} = 0$ the one-magnon dispersion relations reduce to $E_1 = 0$ and $E_1 = 2SG_1^{(1)}$ for all K. Consequently, the two-magnon energy continua all have zero width and coincide with $E_2 = 0$, $E_2 = 2SG_1^{(1)}$, and $E_2 = 4SG_1^{(1)}$.

From (2.27) we see that cos(2q) has a zero in the denominator. However cos(2q) does not necessarily diverge as the numerator of this expression may also vanish. In fact, the roots of the numerator coincide exactly with the three collapsed energy continua. Therefore, how we choose to take the limit $G_1^{(2)} \to 0$ becomes a crucial factor in properly evaluating the allowed values of relative wavevector q. (Note that we did not have a similar crisis in case (e) where both $G_1^{(1)}$ and $G_1^{(2)}$ vanish. In this case the denominator of

(2.27) will always go to zero more rapidly than the numerator and hence cos(2q) diverges for all E_2.)

To avoid the use of "nasty" limit taking procedures we turn to the scaling formalism (Chapter 3) which does not require explicit calculation of relative wavevector. The scaling formalism is particularily convenient for this case because both $V_p' = V_p M^{-1} V_p$ and $V_m' = V_m M^{-1} V_m$ are exactly zero (M, V_p, V_m as defined in (3.18-3.20)). Hence the scaling transformation described by (3.26) converges after only one iteration. This rapid convergence can be justified as follows. From (2.27) we know that |Imag(q)| even if not infinite, must still be very large. Hence any bound state solution must decay very rapidly to zero as relative coordinate between spin deviations increases. V_p' and V_m' describe the effective range of interaction in relative coordinate space so it follows that both of these matrices should vanish after a minimal number of iterations.

Since $V_p' = 0$ we know from (3.23) that there is no effective interaction between unit cell U_0 and unit cell U_4. However $V_p \neq 0$, so we know from (3.23) that there is a direct interaction taking place between unit cells U_0 and U_2 as well as between U_2 and U_4. The only possible explanation of these two results is the following. Amplitudes describing spin deviations separated by zero, one, or two sites have completely decoupled from all other two-magnon amplitudes. It therefore follows from the formalism of Chapter 3 that bound states

corresponding to spin deviations separated by two sites or less can be obtained from the secular equation

$$\det[M_0'] = 0 \tag{4.13}$$

where: $M_0' = M_0 - V_p M^{-1} V_m$

and where M, M_0, V_p, V_m are defined by (3.18-3.20) and (3.22). Substitution and simplification leads to the following result:

$$\Omega[\Omega+2SG_1^{(1)}]^2\{\Omega^3 + \Omega^2 G_2^{(2)}(1-4S) + \Omega 4S^2 G_1^{(1)}(G_2^{(2)}\cos^2(K) - G_1^{(1)})$$

$$+ 2S^2(G_1^{(1)})^2 G_2^{(2)}(2S-1+4\sin^2(K))\} = 0 . \tag{4.14}$$

Recall from (2.18) that $\Omega = E_2 - 2SG_1^{(1)}$. So the bound state solutions are given by

(1) $E_2 = 0$ twice

(2) $E_2 = 2SG_1^{(1)}$

(3) roots of the cubic { } in (4.14) .

At least three of the bound states are degenerate with the collapsed continua but because of the complete decoupling these remain true bound states for all values of K. Notice the total of six bound states. This coincides with the number predicted for any alternating chain (see case (f)).

Now consider the amplitudes describing spin deviations separated by greater than two sites. For energies not coinciding with the collapsed continua we know that

$|\text{Imag}(q)| \to \infty$. So from (2.29) these amplitudes must vanish outside of the continua due to an exponentially decaying factor. Consequently, such amplitudes have non-trivial solutions only at the collapsed continua energies of $E_2 = 0$, $2SG_1^{(1)}$, $4SG_1^{(1)}$.

The complete two-magnon spectrum (three collapsed continua and three non-degenerate bound states) is shown in Figure (4.6) for $S = 1$ and $G_2^{(2)} = G_1^{(2)}$.

Case (h) $\quad \Delta S > 0 \quad b = 1 \quad r^{(1)} = r^{(2)} = 1$

This case describes an alternating spin Heisenberg chain with uniform bonds. Note that if $S' > 1$ then this may not be a true Heisenberg chain since $G_m^{(i)}$, $m = 3,4,\ldots,2S'$, are yet unspecified. Also note that if $S' = \frac{1}{2}$ then all physical amplitudes are independent of $G_2^{(1)}$ and $G_2^{(2)}$ and so $r^{(1)}$ and $r^{(2)}$ need not be specified.

First consider the specific case with $S' = \frac{1}{2}$ and $S = 1$. The corresponding bound state spectrum is shown in Figure (4.7). This spectrum is very similar to that of case (b), namely the alternating bond Heisenberg chain with uniform spin $S = \frac{1}{2}$. This similarity suggests that the means by which alternation is introduced into the otherwise uniform Heisenberg system is relatively umimportant. In both cases there are four bound state branches such that two are below the A-A continuum and one is below each of the others. The

only qualitative difference between the two spectra is the form of the bound state branch lying immediately below the mixed continuum. In the alternating spin Heisenberg case (with $S' = \frac{1}{2}$ and $S = 1$) this branch is "connected" to the A-A continuum at $K = 0$ whereas for the alternating bond Heisenberg case no such connection occurs.

Next consider the alternating spin, uniform bond Heisenberg chain with $S' = 1$ and $S = \frac{3}{2}$. The corresponding bound state spectrum for this case is shown in Figure (4.8). This spectrum is qualitatively very similar to that obtained for $S' = \frac{1}{2}$, $S = 1$. Notice that the connection between bound state branch and A-A continuum upper edge has remained intact. Now consider the bound state spectrum for the spin combination $S' = \frac{1}{2}$ and $S = \frac{3}{2}$. This is shown in Figure (4.9). Again the spectrum is very similar to that obtained for $S' = \frac{1}{2}$, $S = 1$, except now the connection between bound state and A-A continuum has been broken.

We find that all combinations of S and S' ($S' < S$) in the alternating spin, uniform bond Heisenberg chain result in similar spectra to those shown in Figures (4.7-9). For all combinations of non-equal spin magnitudes there are four observable bound state branches such that two are below the A-A continuum and one is below each of the other continua. (The relative binding energy of each of these branches does decrease as spin magnitudes increase but this is expected

since $S \to \infty$ is the classical limit.) Whether or not there is a $K = 0$ connection between bound state and A-A continuum upper edge depends strictly on the difference in spin magnitudes. The $K = 0$ reduced energy of the bound state below the mixed continuum is empirically given by

$$\xi_B(K = 0) = 2[S + S' - \tfrac{1}{2}] \tag{4.15}$$

while the reduced energy of the A-A continuum upper edge is analytically given by (see Appendix B)

$$\xi_C(K < K_c) = 2(S+S') - [8SS'(1-\cos(K)) + 4(S-S')^2]^{\frac{1}{2}} \tag{4.16}$$

and so at $K = 0$,

$$\xi_C(K = 0) = 4S' . \tag{4.17}$$

Hence this connection occurs in the uniform bond Heisenberg chain if and only if $\Delta S = \frac{1}{2}$. We also find that any degree of bond alternation ($b \neq 1$) or any deviation from the Heisenberg case ($r^{(i)} \neq 1$) results in the breaking of this connection regardless of ΔS. Furthermore, such deviations from the uniform bond Heisenberg case generally result in more complicated spectra.

The connection between "mixed-mode" bound state and A-A continuum upper edge may be an important spectral feature. When it occurs the bound state branch forms a "bridge" between two otherwise isolated continua. However the physical signi-

ficance (if any) of such a spectral feature is so far unclear. We do know that the occurrence of this feature requires that $\Delta S = \frac{1}{2}$, $b = 1$, and $r^{(1)} = r^{(2)} = 1$ all must be satisfied. The only obvious simplification in the two-magnon problem when $\Delta S = \frac{1}{2}$ is (from (2.20)) $\tau^{(1)} = \tau^{(2)} = \theta_{S'}$. Consequently, three of the diagonal entries in the matrix M_0 (3.22) are degenerate. If $r^{(1)} = r^{(2)} = 1$ then the only obvious simplification is (from (2.20)) $\Delta^{(1)} = \Delta^{(2)} = 0$. As a result, there is a partial decoupling in the interacting equations (2.19) between amplitudes with two spin deviations on the same even site and amplitudes with two spin deviations on the same odd site. The two-magnon problem obviously simplifies when bond strength is uniform ($b = 1$). What remains unclear is how these various simplifications are related when they occur simultaneously.

There is another point of interest regarding the alternating spin, uniform bond Heisenberg chain. First consider the interacting equations (2.19) for any case in which $S' = \frac{1}{2}$. Because of the decoupling of the unphysical amplitudes (i.e., those amplitudes with two spin deviations on the same even site) there is an unphysical solution given by

$$E_2 = 2S[G_2^{(1)} + G_2^{(2)}]. \tag{4.18}$$

So it follows that increasing S' from $\frac{1}{2}$ to a larger value

should result in an additional bound (or resonant) state which is physically valid. We have previously observed this to happen for the alternating bond, uniform spin Heisenberg chain, as discussed in cases (b) and (c) for $S' = \frac{1}{2}$ and $S' > \frac{1}{2}$ respectively. However for the alternating spin, uniform bond Heisenberg chain we always observe exactly four bound states, independent of the size of S'. Therefore an "extra" resonant state is anticipated in those cases for which $S' > \frac{1}{2}$. The presence of such a state will be considered in the following section.

4.2 Local Densities of States

In Chapter 3 we formalized a technique for evaluating the local density of states at any two-magnon spectral point (K,E_2) of an alternating ferrimagnetic chain. Each local densities of states calculation is obtained from a response function describing two spin excitations arranged in a particular configuration along the chain. A given configuration is specified by

(1) the number of sites separating the excitations or in other words the relative coordinate r

(2) if r is even; the type of spin sites that are excited (each spin site is labelled by either S or S'); if r is odd; the type of bonds connecting the excited sites (each bond is described by either $G_m^{(1)}$ or $G_m^{(2)}$, m = 1,2) .

We found it most convenient to express these results by plotting local density of states versus excitation energy for a fixed value of total wavevector. The value of K is varied in intervals across the Brillouin zone, thereby giving a series of plots extending over the entire spectral plane (or whatever region we are interested in).

Using the methods described in Chapter 3, it is possible to calculate local densities of states with respect to spin excitations separated by any distance along the chain. However we usually restricted our calculations to spin excitations on same or neighbouring sites only. Calculations corresponding to greater separation of spin excitations are generally redundant. Also, bound and resonant states become harder to identify in the local densities of states as this separation increases. This is because such states are dominated by exponentially decaying factors of the form exp[-|Imag(q)|r] where r is the relative coordinate. Furthermore, the plane wave component of the scattering (continuum) states oscillates more rapidly as separation increases due to a factor exp[±iReal(q)r]. So the larger the separation the more nodes in the corresponding densities of states. These nodes complicate the plots making the "true" resonant states harder to identify. For an example of this latter effect consider Figure (4.10) which shows the local densities of states for (a) two excitations on the same site and (b) two excitations

separated by ten sites (we are considering a uniform spin chain with S = 1 so we do not have to specify whether the excitations take place on even or odd spin sites).

Using Figure (4.10a) as an example of a "typical" densities of states plot we can illustrate the various spectral information which is easily extracted by way of this method. First, consider the scattering state continua. Generally, these are identifiable as extended regions of non-vanishing density of states. Here, the A-A continuum ranges from 0.2 to 1.6 reduced energy units (reu), the mixed continuum ranges from 2.3 to 3.7 reu, and the O-O continuum ranges from 4.5 to 5.8 reu. Next, consider the bound state solutions. These appear in the plots as very sharp peaks outside the continua regions. In Figure (4.10a) three bound states are observed at 0.2, 2.3, and 4.0 reu. Finally, consider the resonant state solutions. These appear in the plots as peaks inside of the continua regions. The relative sharpness of such peaks depends on the particular state and value of K. Although resonant peaks are the most interesting features of these plots, identifying an inner-continuum structure as being resonant or not is often a subjective classification. Hence, such identifications must be made with caution. Candidates for resonant peaks in Figure (4.10a) are located near 1.4 reu and near 3.3 reu. We observe in Figure (4.10b) that one of the bound states (4.0 reu) has vanished and both resonant

states have dissipated. Hence, our choice of plots to study is justified.

Because of the subjectivity in classifying resonances such evaluations are best made by "tracing" said peak across the Brillouin zone to see if it persists, sharpens, shifts, fades, etc. When studying a particular case we usually examine local densities of states for at least five different values of K. However in our subsequent discussions we only display the results for K = 0, $\pi/4$, and $\pi/2$ for the sake of economizing space. We do however calculate (and present) the local densities of states with respect to both same site and nearest-neighbour spin excitations. Both are included because often a particular configuration will not be sensitive to all of the bound and resonant states occuring at a given value of K. There are four possible configurations corresponding to excitations separated by one or zero sites so there are generally four distinct plots for each value of K. These are referred to as "even site" (two spin excitations on same S' site), "odd site" (two spin excitations on same S site), "strong bond" (excitations separated by a bond described by $G^{(1)}_{1,2}$), and "weak bond" (excitations separated by a bond described by $G^{(2)}_{1,2}$). In cases of uniform spin the first two plots are degenerate while for uniform bond chains the latter two are degenerate. If $S' = \frac{1}{2}$ then the even site plot is unphysical.

Case (a) $\Delta S = 0$ $S > \frac{1}{2}$ $b \neq 1$ $r^{(1)} = r^{(2)} = 1$

This is the case of an alternating bond, uniform spin Heisenberg chain with spin magnitude $S > \frac{1}{2}$. Here we choose to study $S = 1$ and $b = \frac{1}{2}$ although any $S > \frac{1}{2}$ and $b \neq 0,1$ will give results that are qualitatively similar. This special case was initially discussed in case (c) of Section 4.1 and the bound state spectrum is depicted in Figure (4.2). The local densities of states are shown in Figure (4.11) for $K = 0$, Figure (4.12) for $K = \pi/4$, and Figure (4.13) for $K = \pi/2$. For each K value the results are plotted for (a) same site spin excitations, (b) spin excitations separated by a strong bond, and (c) spin excitations separated by a weak bond.

Recall there are a total of five bound state branches for this case, only three of which are true bound states for all values of K. These three (the lower of the two below the A-A continuum, the state below the mixed continuum, and the lower of the two below the O-O continuum) are identifiable as sharp peaks at all values of K. The upper bound state below the O-O continuum is only identifiable in plots with $K > K_c$, where K_c is the value of wavevector at which the internal singularity originates in O-O and A-A continua. (See Appendix B for detailed discussion.) Here $K_c \simeq \pi/3$. Strangely enough, we observe no resonant behaviour in the O-O continuum when $K < K_c$.

The upper bound state beneath the A-A continuum is only identifiable as a bound state peak in plots with K near or at $\pi/2$. For all smaller values of K there is a resonant peak in the A-A continuum which appears to correspond to this bound state. At K = 0 this resonant state is observed as a relatively broad peak near the top of the continuum. As K increases the peak gradually sharpens while moving downwards through the continuum. Near $K = \pi/2$ the peak eventually "pops" out of the continuum becoming a true bound state. What is most interesting is the behaviour of this peak relative to the van Hove internal singularity inside the A-A continuum. (Recall from Chapter 2 that this singularity does not exist for small values of K but first occurs at $K = K_c$ where it coincides with the upper edge of the A-A continuum. As K further increases the singularity moves downwards until it coincides with the lower edge at $K = \pi/2$.) The resonant state remains beneath this singularity for all $K > K_c$. That is, the resonant state is unable to "cross-over" the singularity from spectral region II to spectral region IV (refer to Figure (2.3)). Consequently, the state is pushed downwards and eventually out of the continuum as the singularity progresses towards the lower edge.

Recall from Section 4.1 (case (f)) that a total of six distinct bound/resonant type states are anticipated for an alternating chain with no unphysical amplitudes. Up till

now we have only identified five such states for this case. So we now look for states that are resonant for all values of K. The only possibility is the peak in the mixed-mode continuum. This is a very broad structure at $K = \pi/2$ which gradually narrows as K decreases. However the entire continuum narrows as K goes to zero so this is not a well-defined resonant structure. Yet in case (f) of Section 4.1 we did predict a resonant state occurring inside the mixed continuum.

There is a rather sharp peak at the top of the A-A continuum in the $K = \pi/2$ plots that has not yet been accounted for. This peak actually occurs for all $K > K_c$ but it does not correspond to a resonant state. Rather it corresponds to a divergence in the density of states at the continuum edge while inside spectral region IV. This is a common feature of most cases we examined and is probably attributed to the system under study being one-dimensional [AM]. The lower end of the O-O continuum also tends to sharpen while inside spectral region IV, however here the effect is usually not as predominant.

Case (b) $\quad \Delta S = 0 \qquad S > \frac{1}{2} \qquad b \neq 1 \qquad r^{(1)} = r^{(2)} = \frac{1}{5}$

This is a special case of the uniform spin, alternating bond chain such that $G_2^{(i)} = \frac{1}{5} G_1^{(i)}$, $i = 1,2$. As usual we consider the results for $b = \frac{1}{2}$ and $S = 1$. The bound state

spectrum for this system was originally discussed in case (f) of Section 4.1 and is displayed in Figure (4.4). The local densities of states are shown in Figures (4.14), (4.15), and (4.16) for K = 0, $\pi/4$, and $\pi/2$ respectively. For each K value the results are plotted for (a) same site excitations, (b) spin excitations separated by a strong bond, and (c) spin excitations separated by a weak bond.

In this case there are five bound state branches, only two of which are bound states for all values of K. These two (the lower of the two states below the A-A continuum and the state directly below the mixed continuum) are identifiable as sharp peaks for all values of K. The bound state below the O-O continuum is not identifiable at small values of K, either as a bound state or resonant state.

The upper bound state below the A-A continuum shows similar behaviour to its counterpart in case (a). At K = 0 it is a broad peak in the middle of the continuum (near 0.6 reu). As K increases the peak gradually sharpens and when K increases past K_c (again $K_c \simeq \pi/3$) the peak is pushed downwards, seemingly unable to cross-over the internal singularity. The state is finally forced out of the continuum near $K = \pi/2$. The bound state directly above the A-A continuum (at large values of K) also originates as a resonant peak inside the A-A continuum. At K = 0 this state corresponds to the resonant

peak at the upper end of the continuum (near 1.5 reu). This peak sharpens as K increases and at $K = K_c$ it leaves the continuum, becoming a true bound state. Notice that this state's emergence from the continuum coincides exactly with the appearance of the internal singularity. So this resonant state (like the previously discussed one) is effectively forced out of the A-A continuum by its inability to cross-over the internal singularity.

Unlike case (a), there is a very well defined resonant structure inside the mixed-mode continuum for all values of K. At $K = \pi/2$ there is a relatively sharp peak near 2.2 reu and the peak continues to sharpen as K decreases. The corresponding resonant state is probably related to the decoupled bound state inside the mixed continuum when $r^{(1)} = r^{(2)} = 0$. Because of this resonant state we are able to identify a total of six distinct bound and resonant states which is the number expected for any alternating chain with $S' > \frac{1}{2}$.

Case (c) $\quad S' = \frac{1}{2} \qquad \Delta S \neq 0 \qquad b = 1$

We now consider the alternating spin, uniform bond Heisenberg chain with $S' = \frac{1}{2}$. This model was originally discussed in case (h) of Section 4.1 with the bound state spectra shown in Figures (4.7) and (4.9) for $\Delta S = \frac{1}{2}$ and $\Delta S = 1$ respectively. Here we will examine the local densities of states for $\Delta S = \frac{1}{2}$

(i.e., S = 1). Increasing ΔS breaks the special connection between A-A continuum and bound state at K = 0 but otherwise gives qualitatively similar results. The local densities of states are shown in Figures (4.17), (4.18), and (4.19) for K = 0, $\pi/4$, and $\pi/2$ respectively. For each K value the results are included for (a) two spin excitations on the same odd site, and (b) two spin excitations on neighbouring sites. (Remember, two spin excitations on the same even site is unphysical if $S' = \frac{1}{2}$.)

In this case there are four bound state branches only two of which are bound states for all values of K. These two (the lower of the two states below the A-A continuum and the state below the mixed continuum) are identifiable as sharp peaks for all values of K. As in the previous two cases the bound state below the O-O continuum is not identifiable at small values of K either as a resonant state or bound state. Also as in the previous two cases, the upper bound state below the A-A continuum starts off at small values of K as a resonant state inside this continuum. As before, the corresponding resonant peak gradually sharpens and moves downwards as K increases, eventually emerging near $K = \pi/2$.

Because of the unphysical state corresponding to two spin deviations on a $S' = \frac{1}{2}$ site we only expect five distinct bound or resonant states for this case. However, besides

the four states already mentioned the only other resonant structure is a very broad peak in the mixed-mode continuum. Similarily to case (a) this is not a well defined resonance even though it sharpens as K decreases (due to continuum collapsing at K = 0.) The overall similarity of these results to that of case (a), the alternating bond Heisenberg chain, suggests the mechanism for alternation (bond or spin) is relatively unimportant.

Case (d) $S' > \frac{1}{2}$ $\Delta S > 0$ $b = 1$ $r^{(1)} = r^{(2)} = 1$

Finally we consider the alternating spin, uniform bond Heisenberg chain with $S' > \frac{1}{2}$. This system was originally discussed in case (h) of Section 4. 1 and the bound state spectra is shown in Figure (4.8) for $S' = 1$, $S = \frac{3}{2}$. The local densities of states are shown for these same spin magnitudes in Figures (4.20), (4.21), and (4.22) for $K = 0$, $\pi/4$, and $\pi/2$ respectively. For each K value the results are considered for (a) two spin excitations on the same even site, (b) two spin excitations on the same odd site, and (c) spin excitations on adjacent sites. As for case (c), increasing ΔS breaks the connection between mixed-mode bound state and A-A continuum upper edge but otherwise gives qualitatively similar results.

The bound state below the O-O continuum is now identifiable for all values of K but otherwise there are no signi-

ficant differences between these results and those obtained for case (c). This is surprising because when $S' = \frac{1}{2}$ there is a decoupled unphysical state (4.18). Hence, we expect a corresponding physical state (either bound or resonant) to arise when S' is increased to a larger value. However no additional bound or resonant states are evident in any of the local densities of states for this case. Since fewer bound states implies a simpler system, this result now suggests that alternation of bond strength is a more severe "disturbance" than alternation of spin magnitude. So an alternating spin system is (possibly) a more likely candidate for complete integrability.

4.3 Two-Magnon Spectra

In this section we present Figures (4.1) to (4.22) inclusive. These are the two-magnon bound state spectra and two-magnon local densities of states referred to in the previous sections. In all proceeding figures, energy is in units of $G_1^{(1)}$.

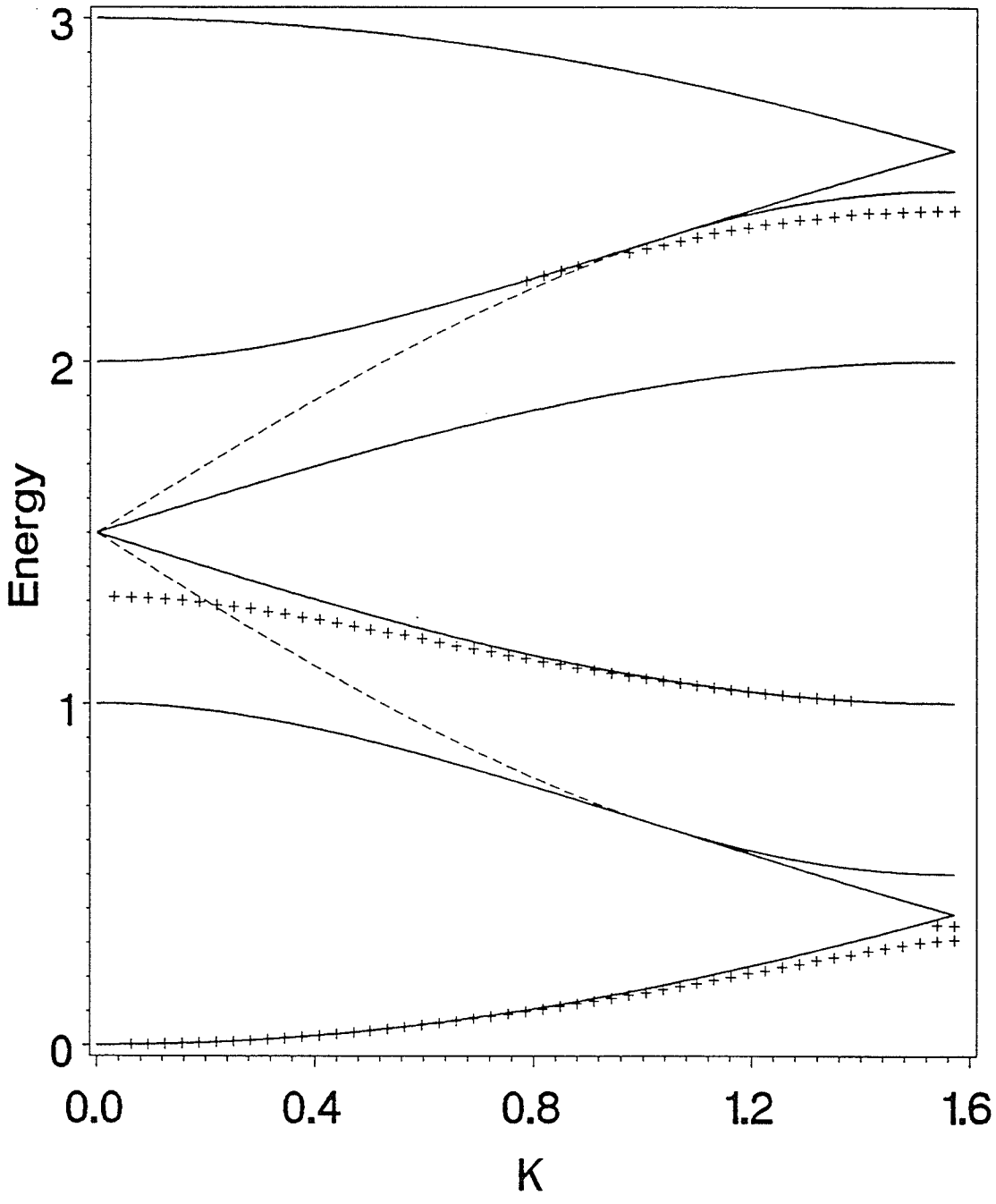

FIGURE 4.1 : Two-magnon spectrum for an alternating bond Heisenberg chain (S=S'=1/2 b=1/2). Regions bounded by solid curves are continua. Dashed lines separate spectral regions III and V. Crosses indicate bound state branches.

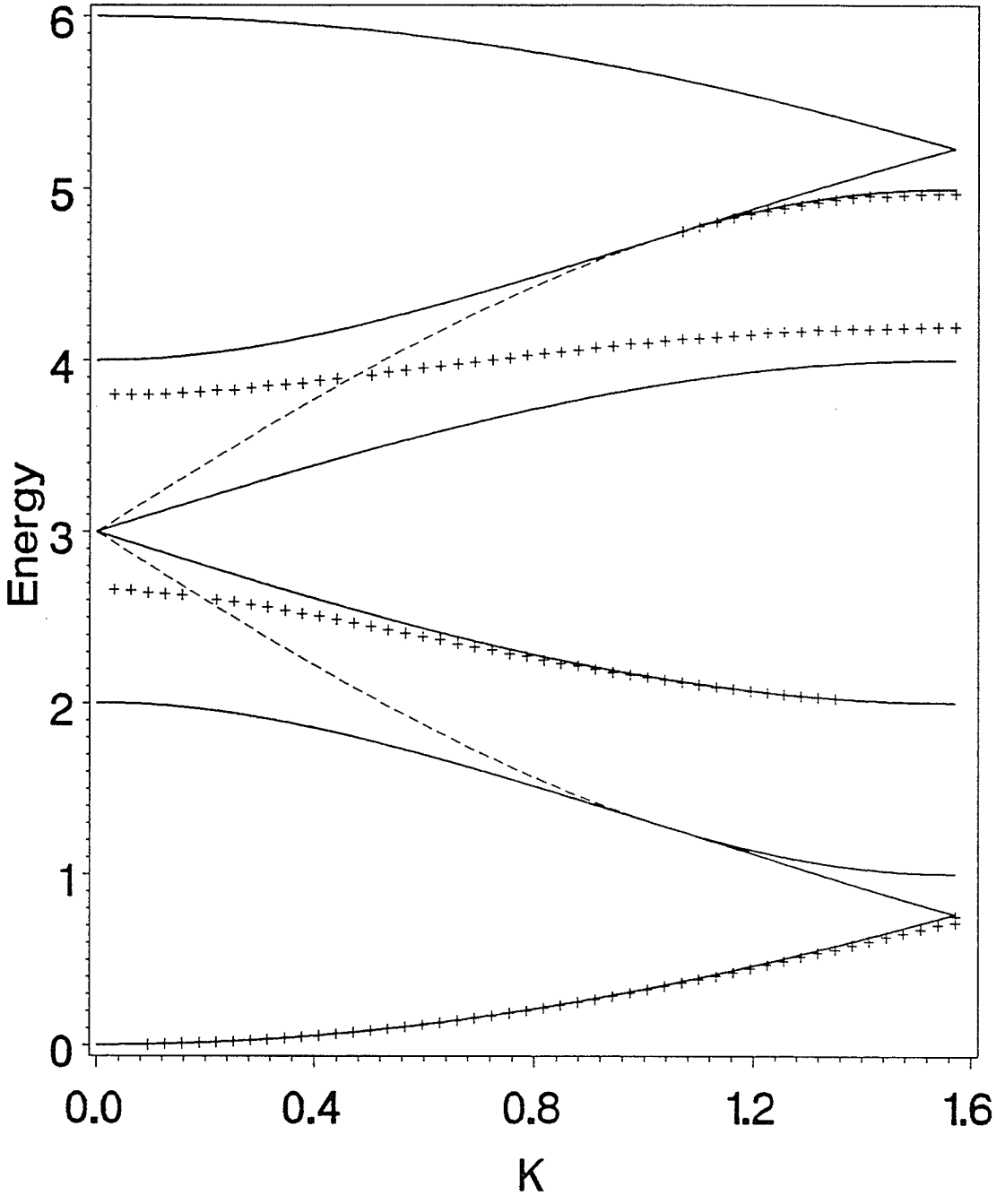

FIGURE 4.2 : Two-magnon spectrum for an alternating bond Heisenberg chain (S=S'=1 b=1/2). Regions bounded by solid curves are continua. Dashed lines separate spectral regions III and V. Crosses indicate bound state branches.

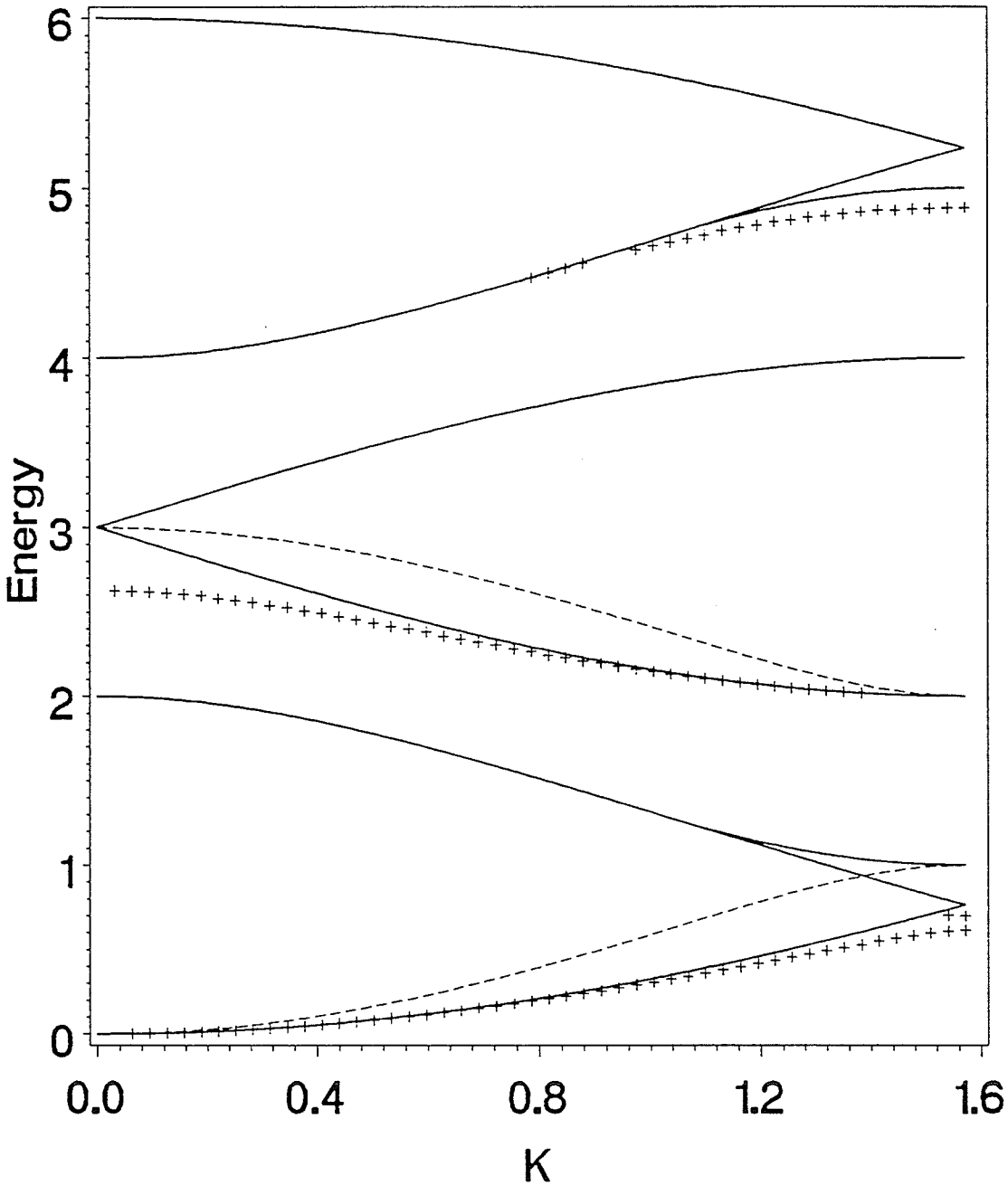

FIGURE 4.3 : Two-magnon spectrum for an alternating bond chain with r(1)=r(2)=0 (S=S'=1 b=1/2). Regions bounded by solid curves are continua. Dashed lines indicate bound states for spin deviations on the same site while crosses indicate bound states for spin deviations on different sites.

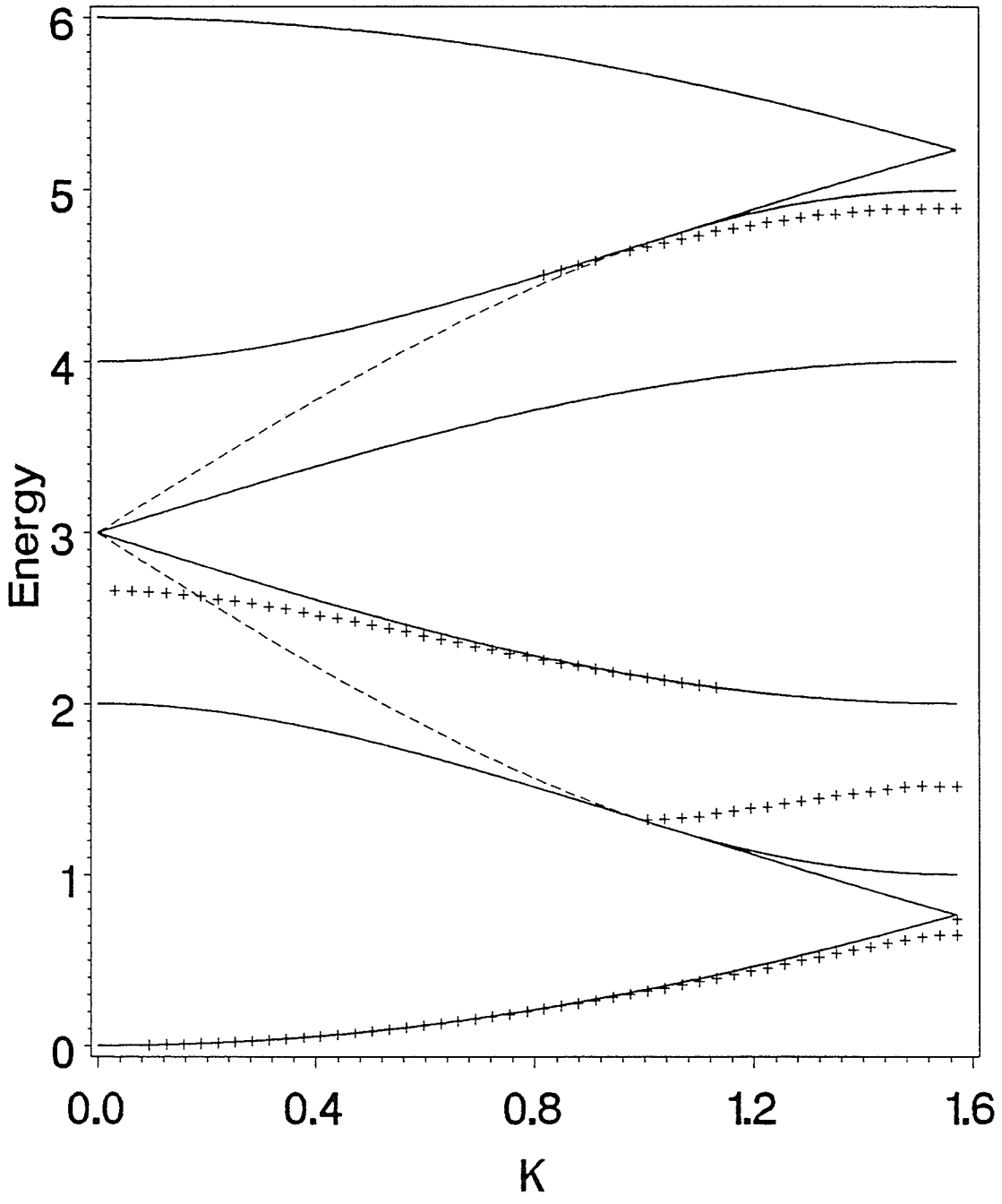

FIGURE 4.4 : Two-magnon spectrum for an alternating bond chain with r(1)=r(2)=1/5 (S=S'=1 b=1/2). Regions bounded by solid curves are continua. Dashed lines separate spectral regions III and V. Crosses indicate bound state branches.

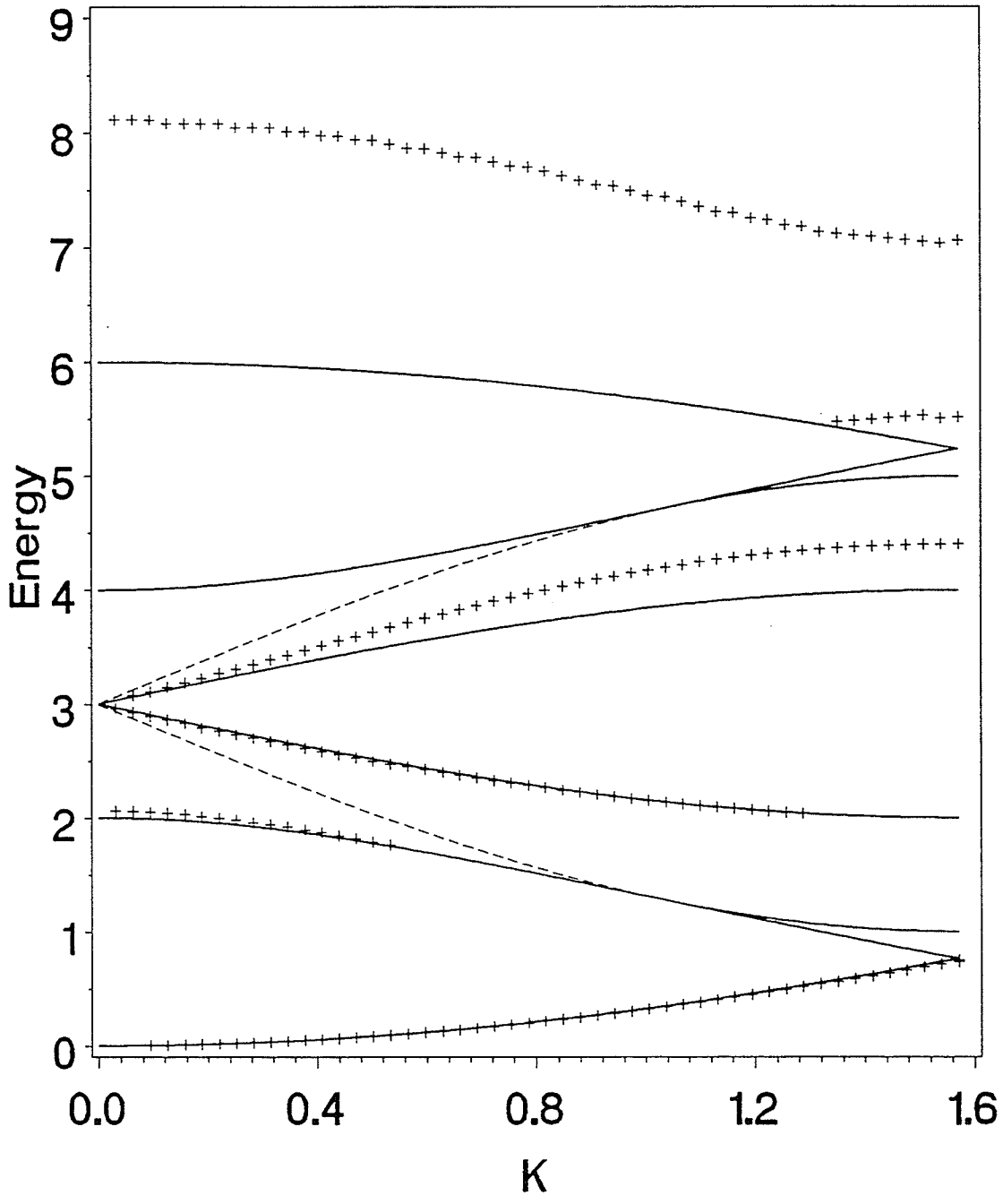

FIGURE 4.5 : Two-magnon spectrum for an alternating bond chain with r(1)=r(2)=2 (S=S'=1 b=1/2). Regions bounded by solid curves are continua. Dashed lines separate spectral regions III and V. Crosses indicate bound state branches.

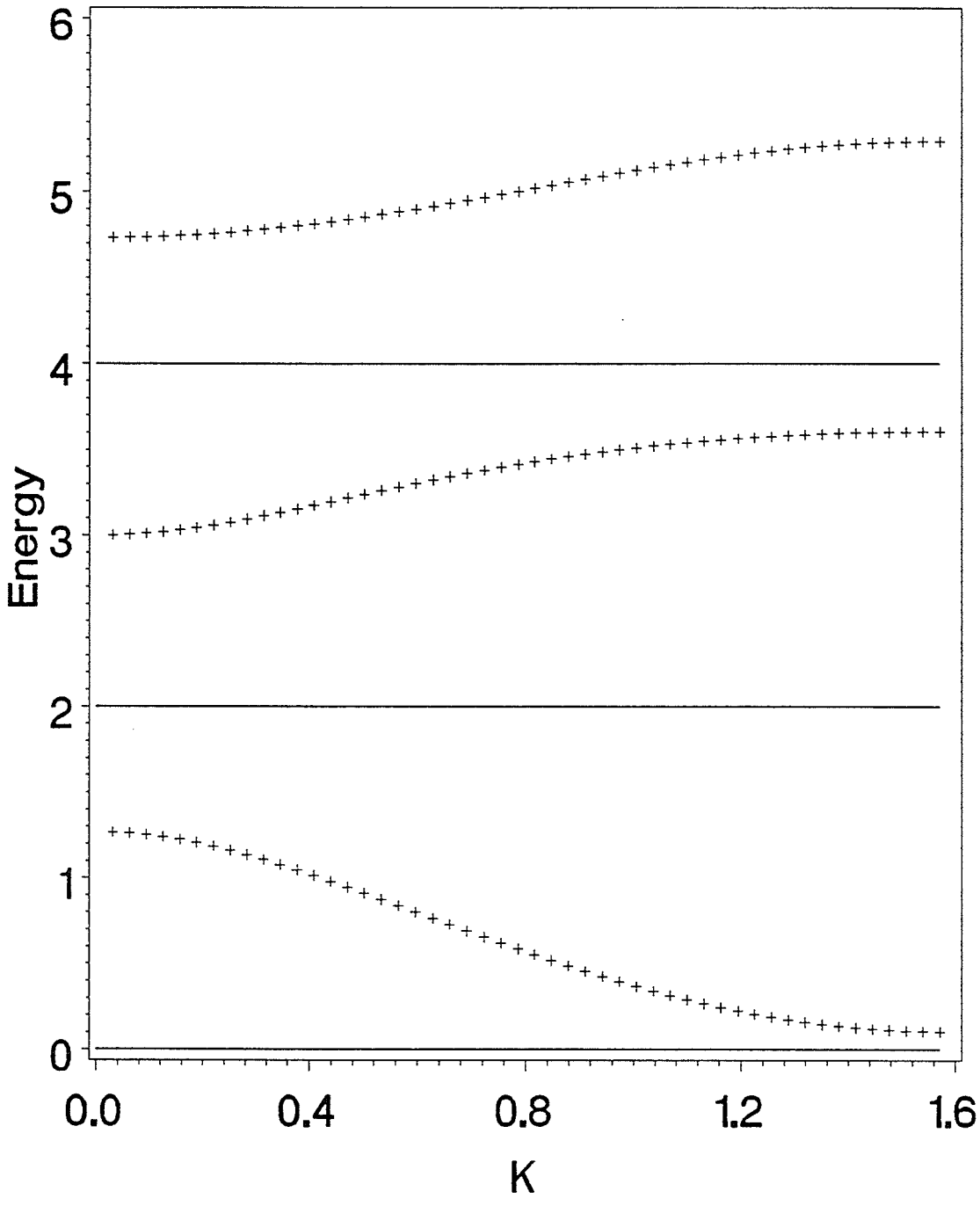

FIGURE 4.6 : Two-magnon spectrum for an alternating bond chain with $r(1)=\infty$ and $r(2)=0$ ($S=S'=1$). Solid lines are collapsed continua and crosses indicate bound state branches.

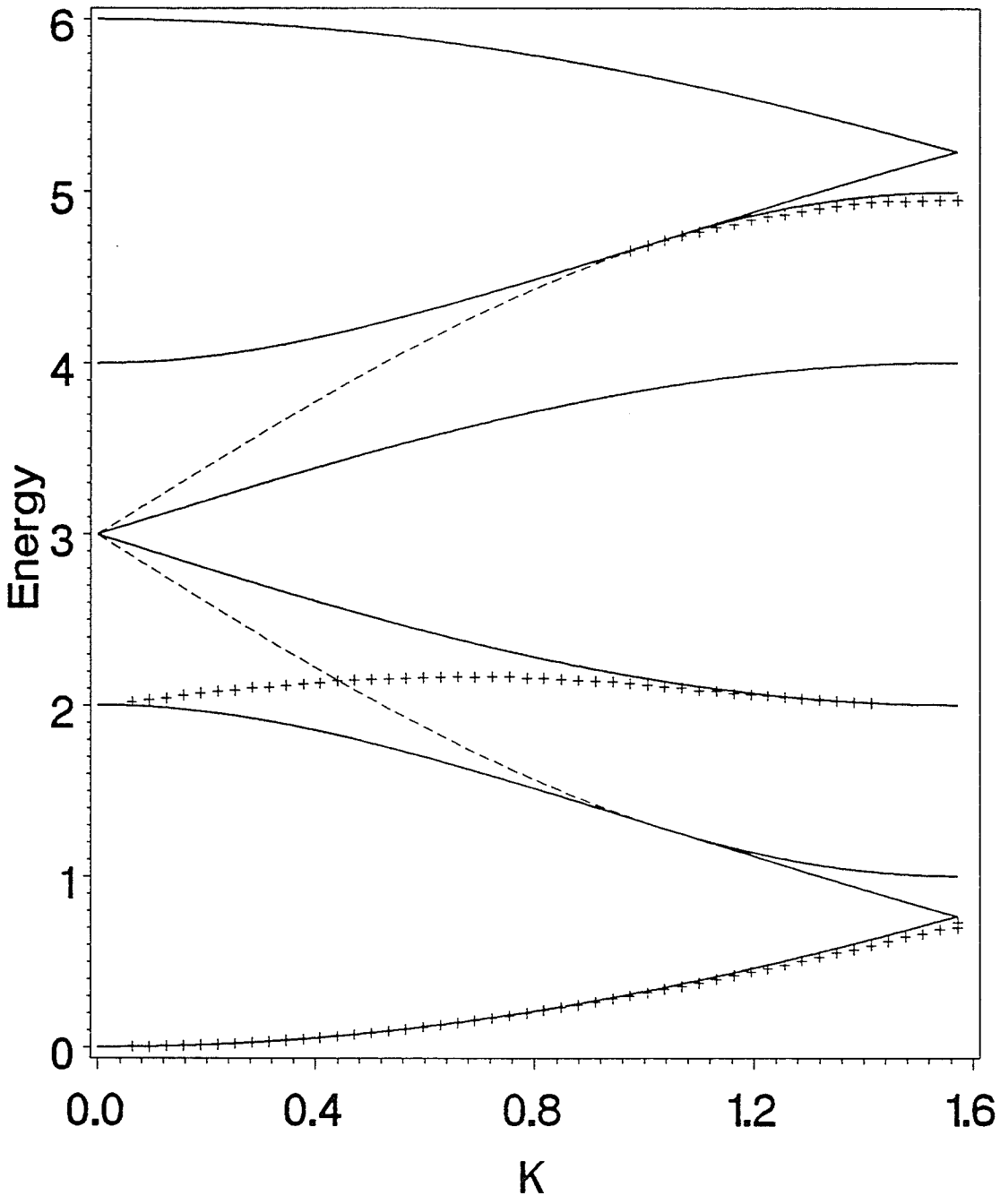

FIGURE 4.7 : Two-magnon spectrum for an alternating spin Heisenberg chain (S'=1/2 S=1 b=1). Regions bounded by solid curves are continua. Dashed lines separate spectral regions III and V. Crosses indicate bound state branches.

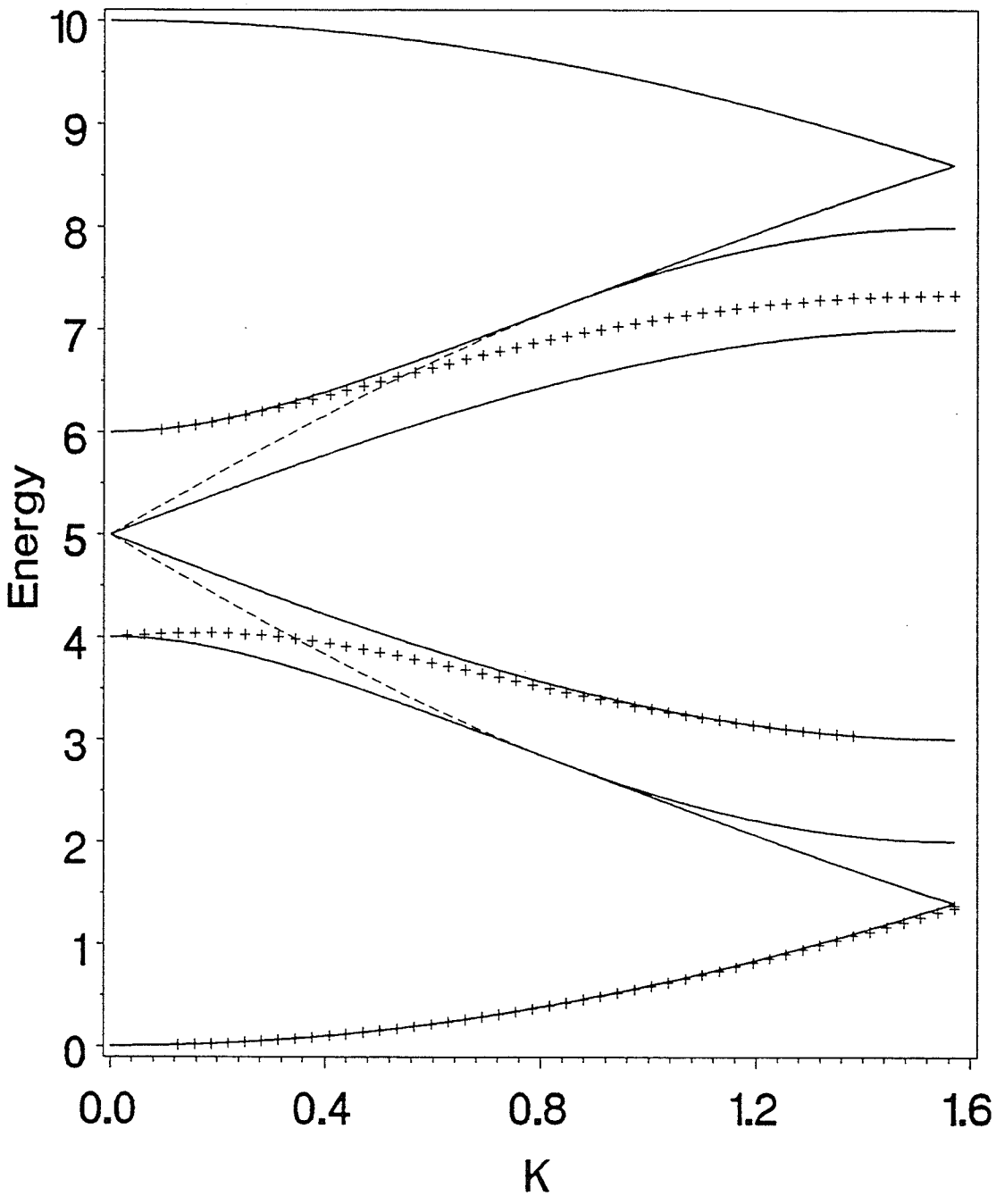

FIGURE 4.8 : Two-magnon spectrum for an alternating spin Heisenberg chain (S'=1 S=3/2 b=1). Regions bounded by solid curves are continua. Dashed lines separate spectral regions III and V. Crosses indicate bound state branches.

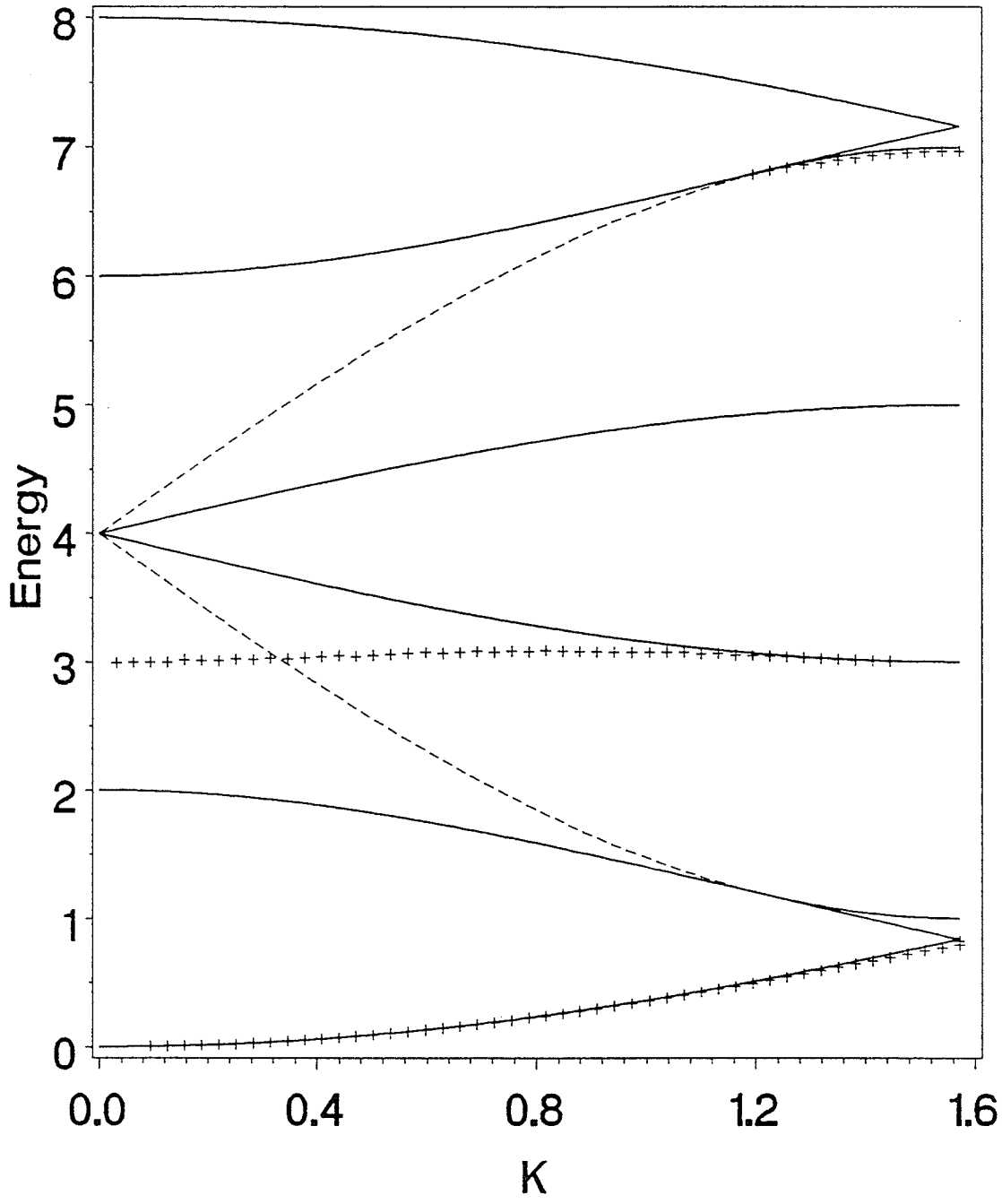

FIGURE 4.9 : Two-magnon spectrum for an alternating spin Heisenberg chain ($S'=1/2$ $S=3/2$ $b=1$). Regions bounded by solid curves are continua. Dashed lines separate spectral regions III and V. Crosses indicate bound state branches.

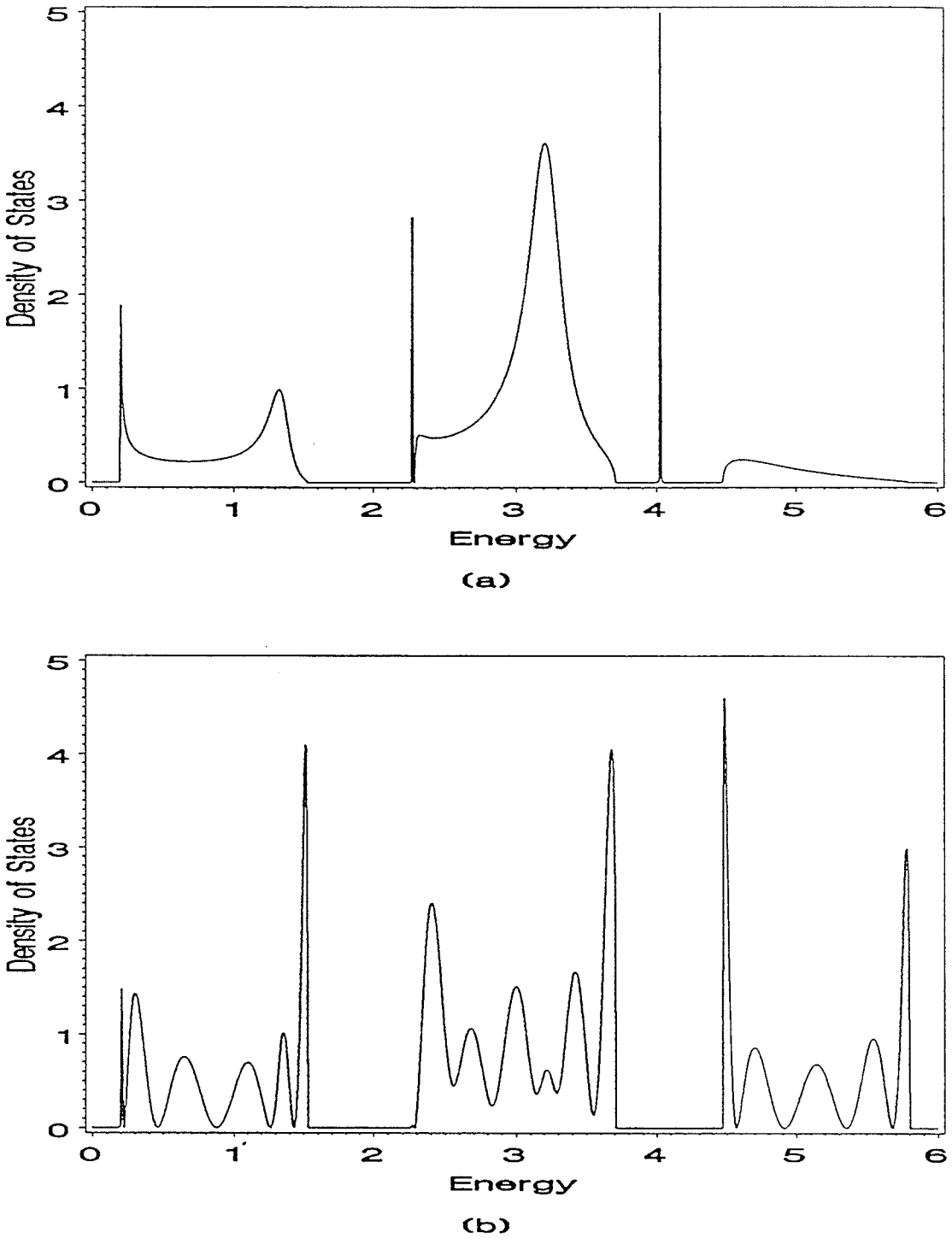

FIGURE 4.10: Local densities of states for (a) two spin deviations on the same site and (b) two spin deviations separated by ten sites for an alternating bond Heisenberg chain (S=S'=1 b=1/2) at K=PI/4.

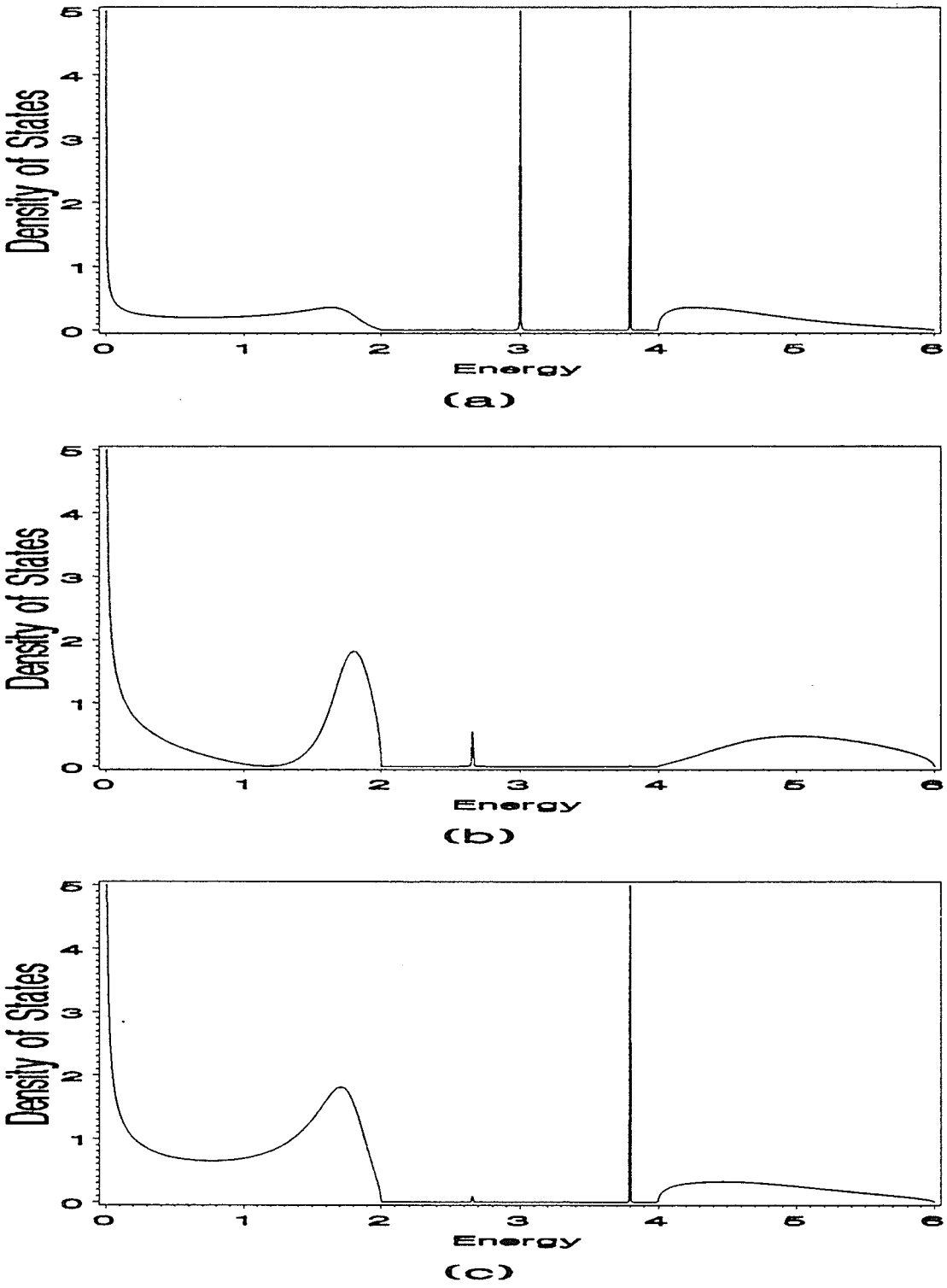

FIGURE 4.11: Local densities of states for two spin deviations (a) on the same site (b) separated by a strong bond and (c) separated by a weak bond for an alternating bond Heisenberg chain (S=S'=1 b=1/2) at K=0.

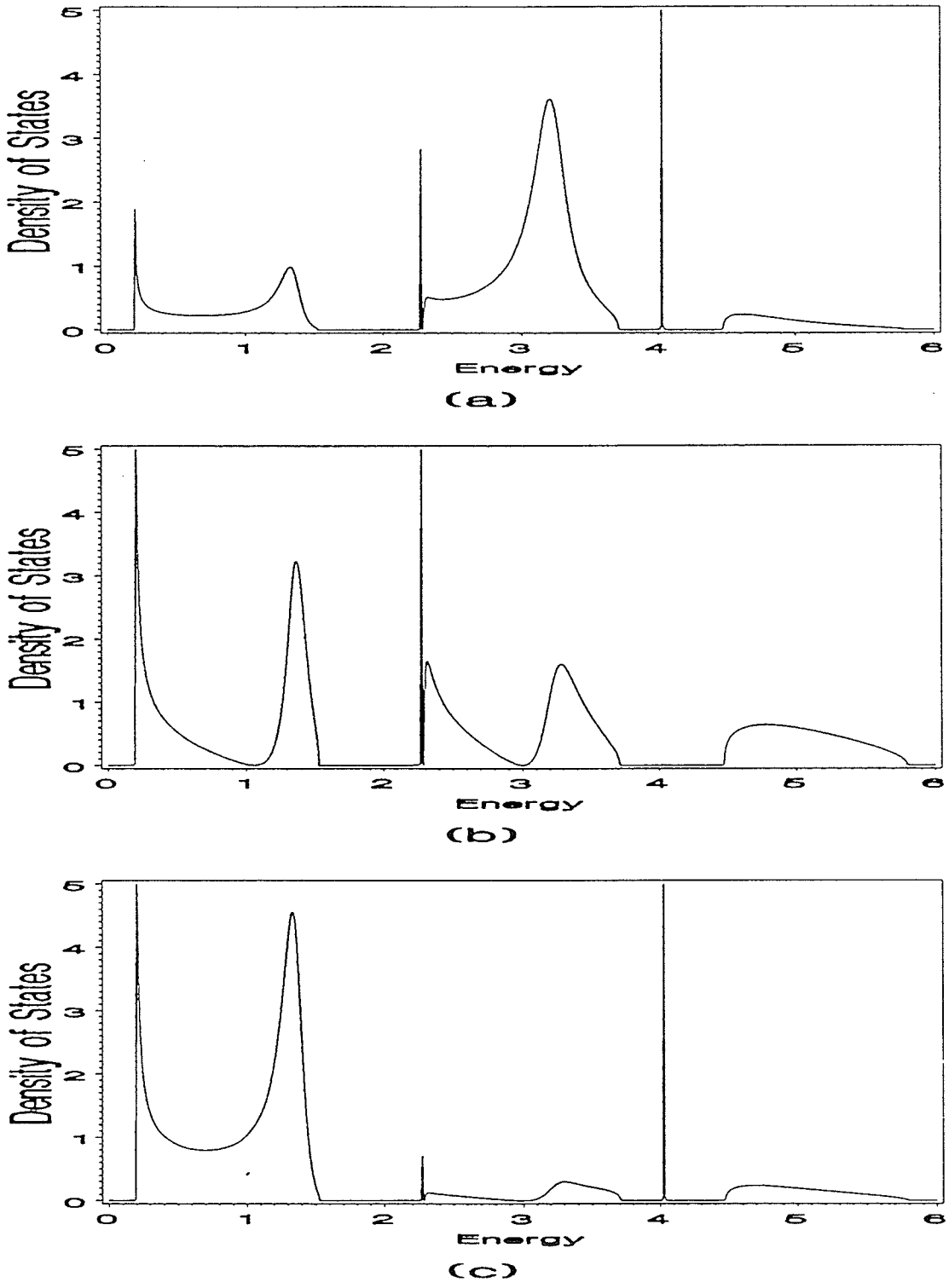

FIGURE 4.12: Local densities of states for two spin deviations (a) on the same site (b) separated by a strong bond and (c) separated by a weak bond for an alternating bond Heisenberg chain (S=S'=1 b=1/2) at K=PI/4.

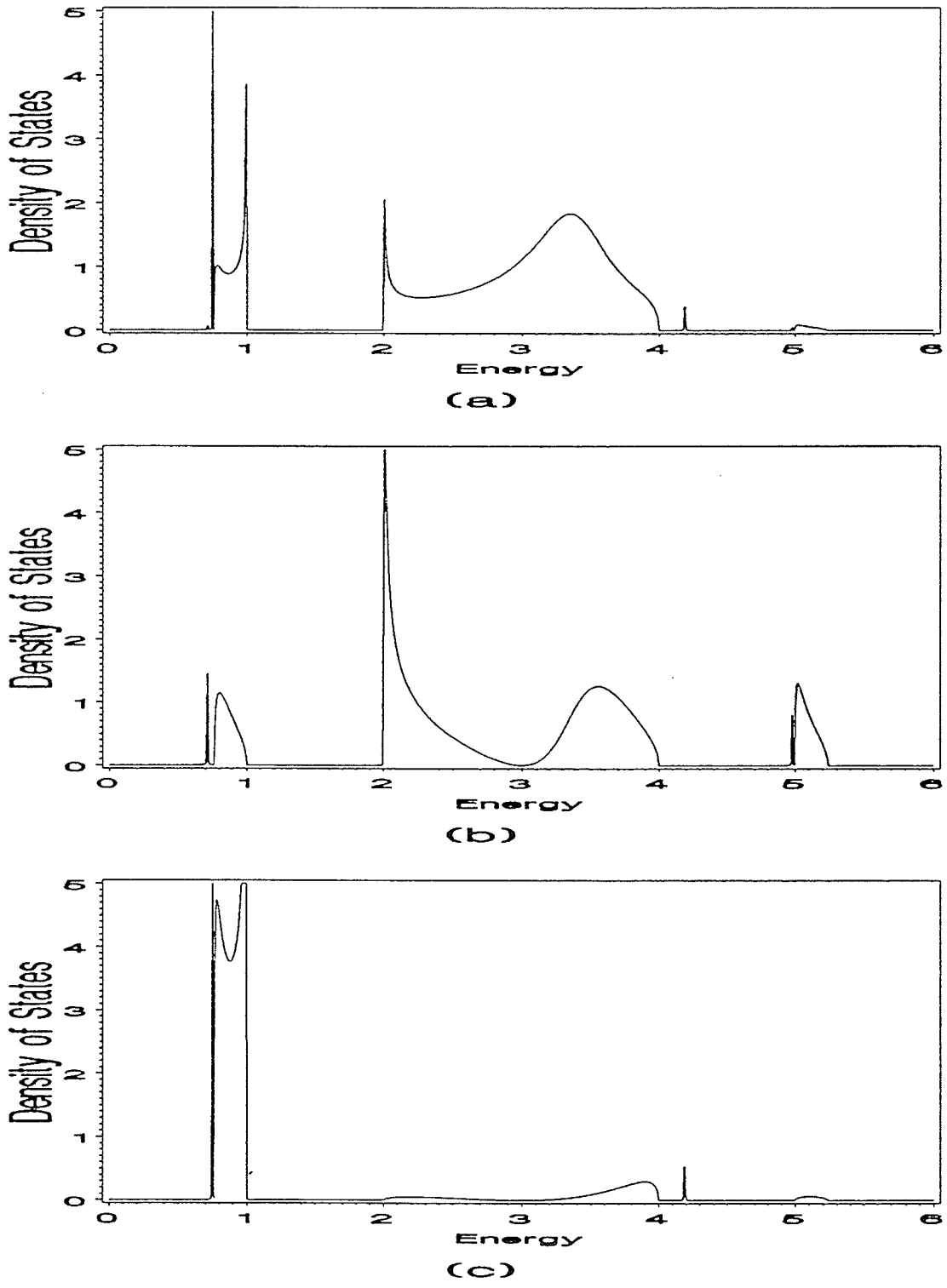

FIGURE 4.13: Local densities of states for two spin deviations (a) on the same site (b) separated by a strong bond and (c) separated by a weak bond for an alternating bond Heisenberg chain (S=S'=1 b=1/2) at K=PI/2.

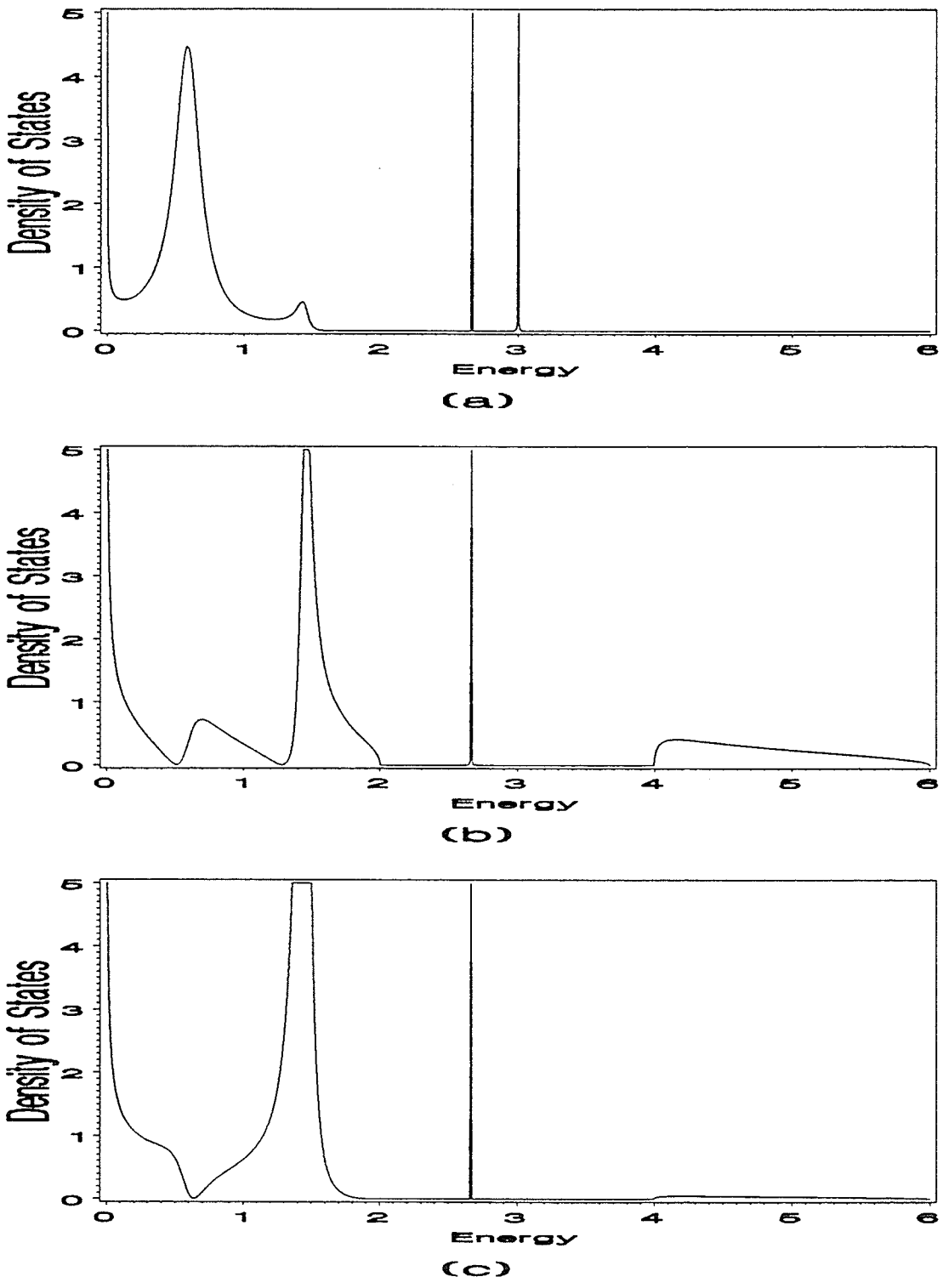

FIGURE 4.14: Local densities of states for two spin deviations (a) on the same site (b) separated by a strong bond and (c) separated by a weak bond for an alternating bond chain with r(1)=r(2)=1/5 (S=S'=1 b=1/2) at K=0.

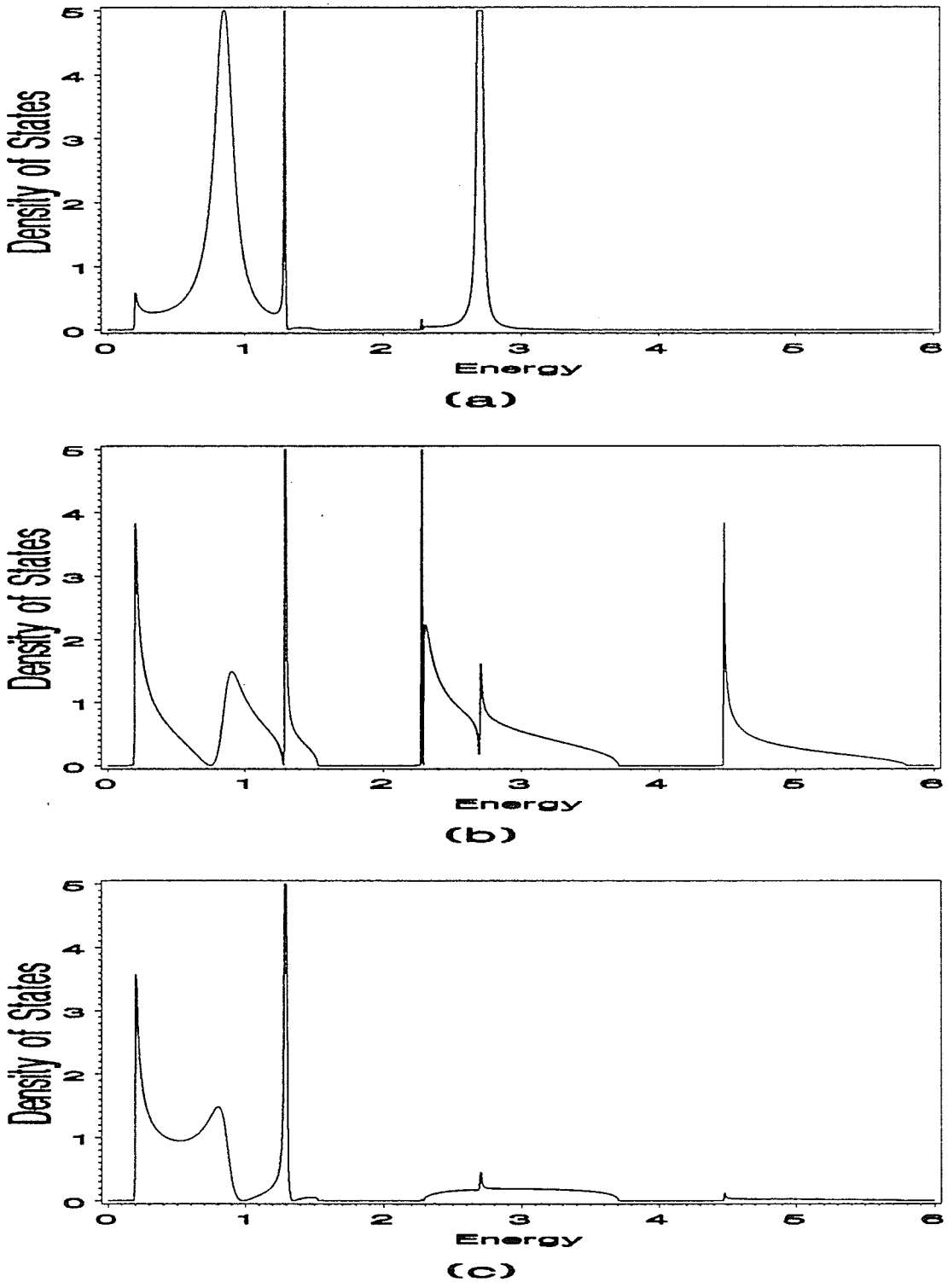

FIGURE 4.15: Local densities of states for two spin deviations (a) on the same site (b) separated by a strong bond and (c) separated by a weak bond for an alternating bond chain with r(1)=r(2)=1/5 (S=S'=1 b=1/2) at K=PI/4.

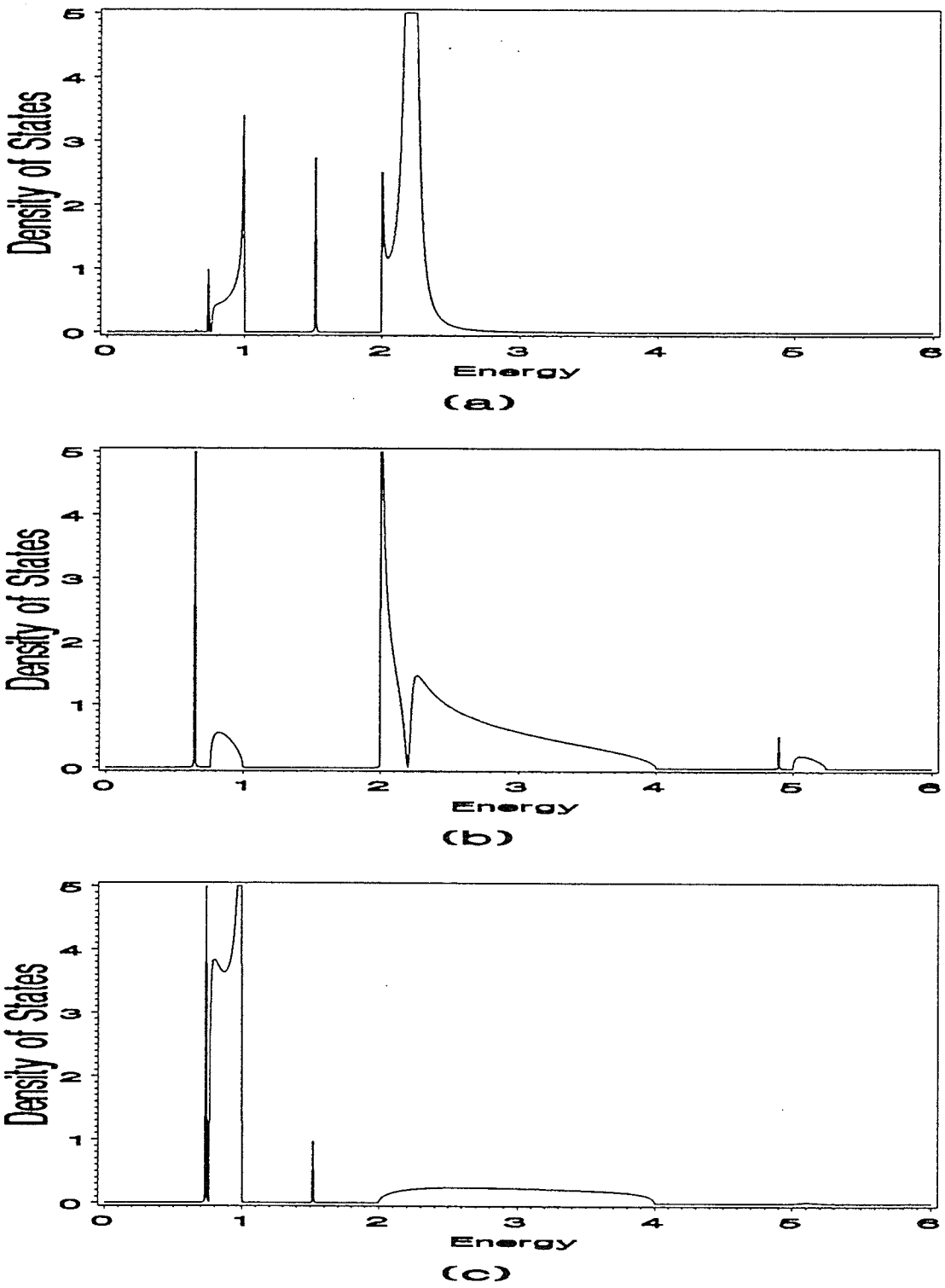

FIGURE 4.16: Local densities of states for two spin deviations (a) on the same site (b) separated by a strong bond and (c) separated by a weak bond for an alternating bond chain with r(1)=r(2)=1/5 (S=S'=1 b=1/2) at K=PI/2.

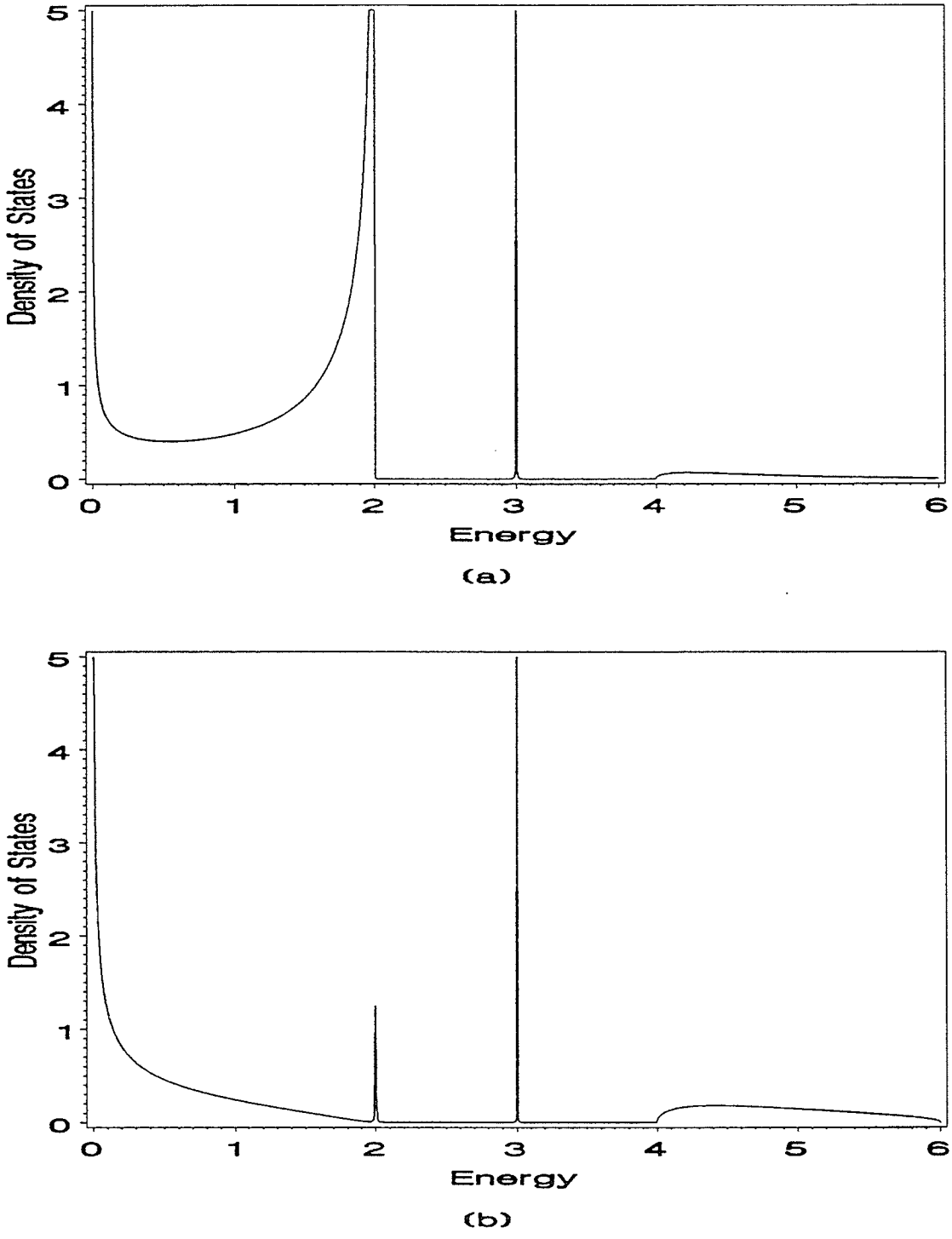

FIGURE 4.17: Local densities of states for (a) two spin deviations on the same odd site and (b) two spin deviations on adjacent sites for an alternating spin Heisenberg chain (S'=1/2 S=1 b=1) at K=0.

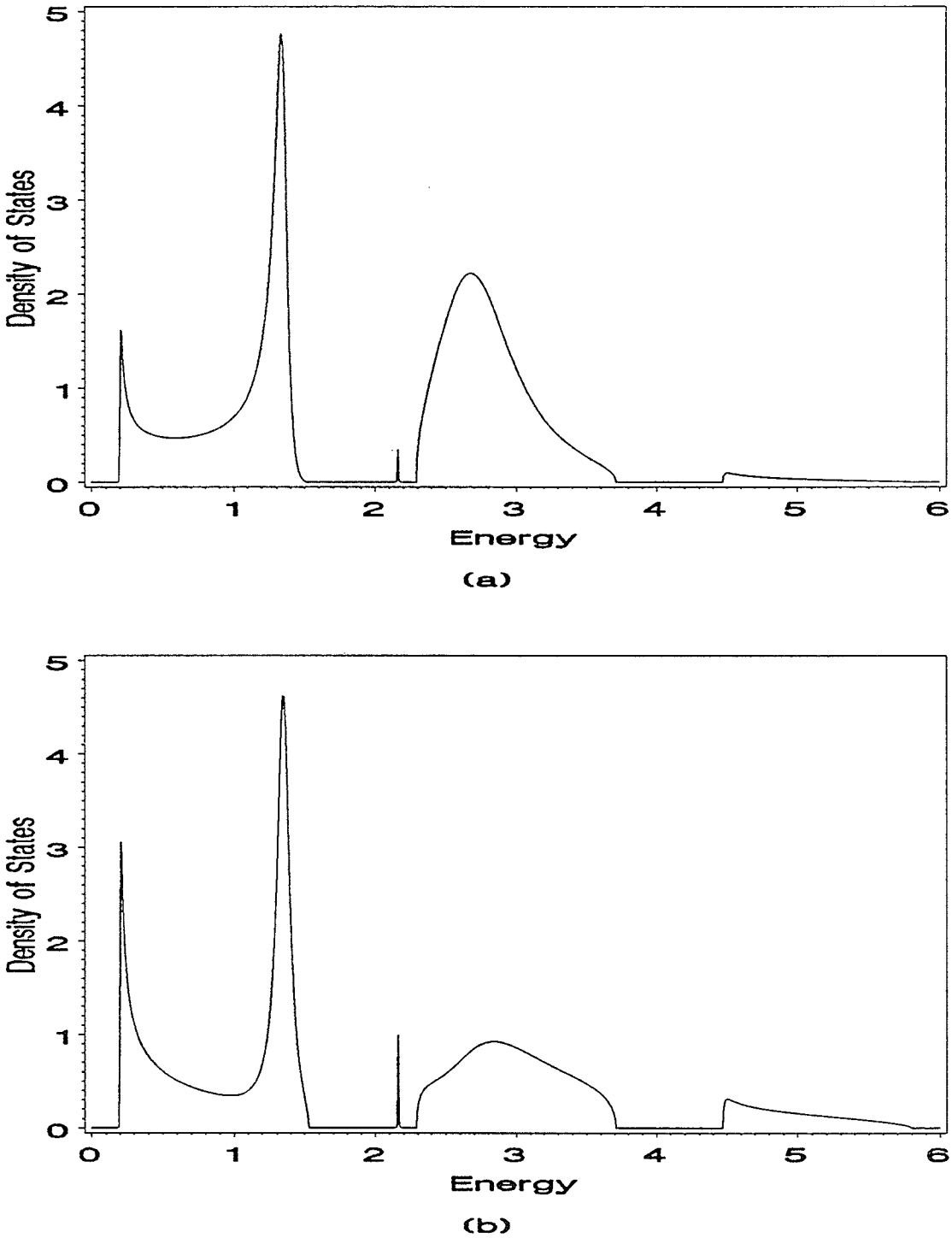

FIGURE 4.18: Local densities of states for (a) two spin deviations on the same odd site and (b) two spin deviations on adjacent sites for an alternating spin Heisenberg chain (S'=1/2 S=1 b=1) at K=PI/4.

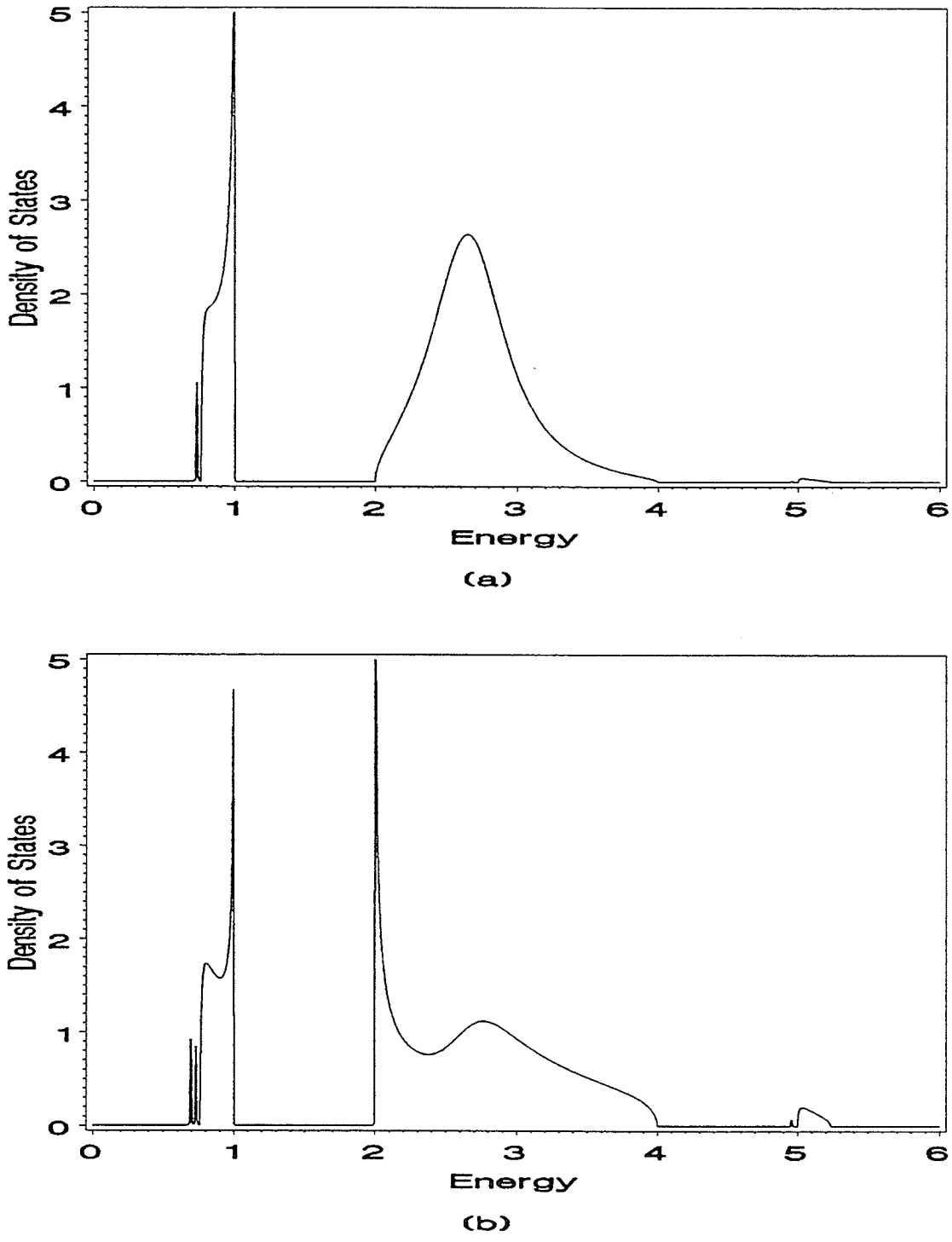

FIGURE 4.19: Local densities of states for (a) two spin deviations on the same odd site and (b) two spin deviations on adjacent sites for an alternating spin Heisenberg chain (S'=1/2 S=1 b=1) at K=PI/2.

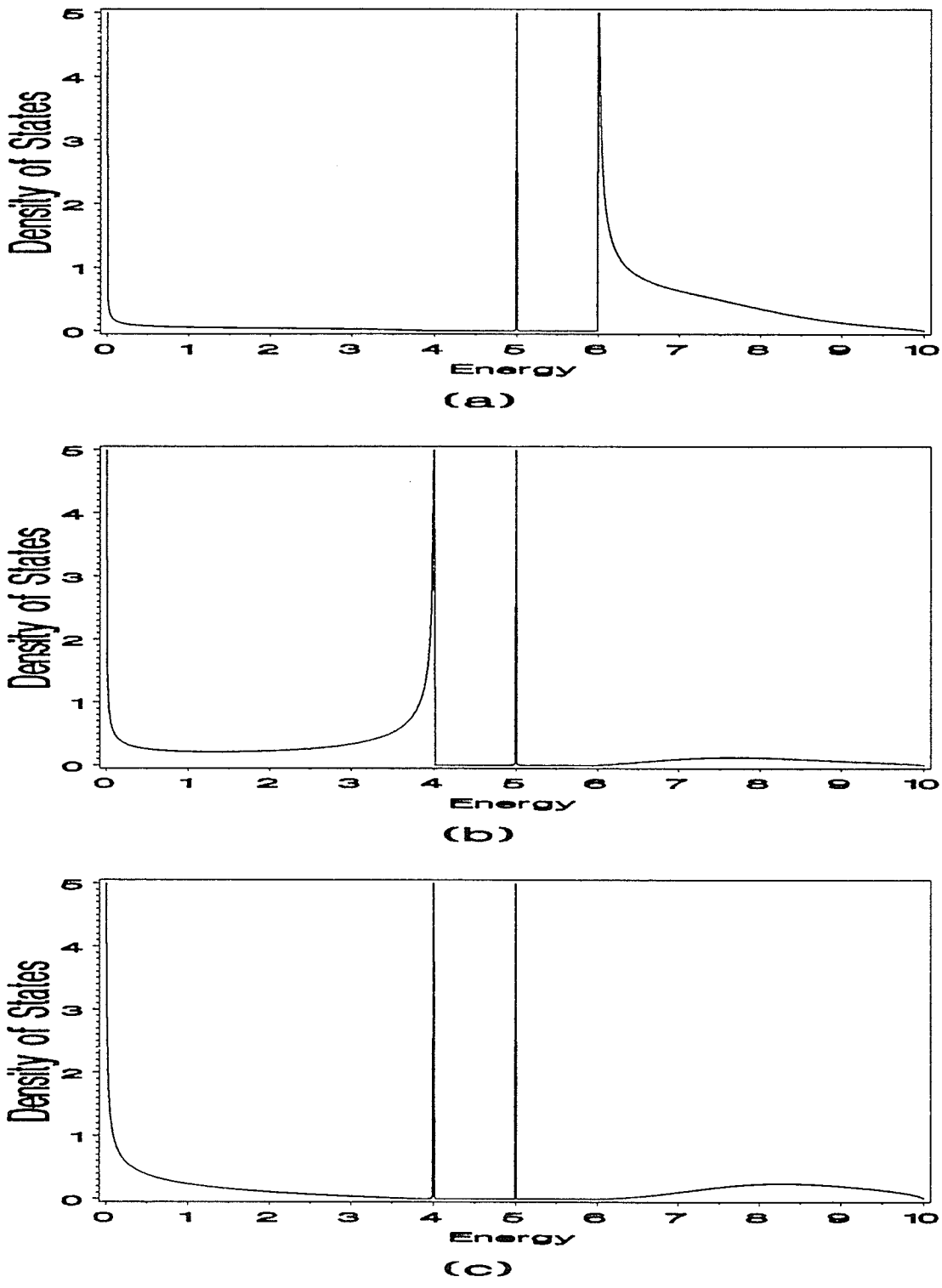

FIGURE 4.20: Local densities of states for two spin deviations (a) on the same even site (b) on the same odd site and (c) on adjacent sites for an alternating spin Heisenberg chain (S'=1 S=3/2 b=1) at K=0.

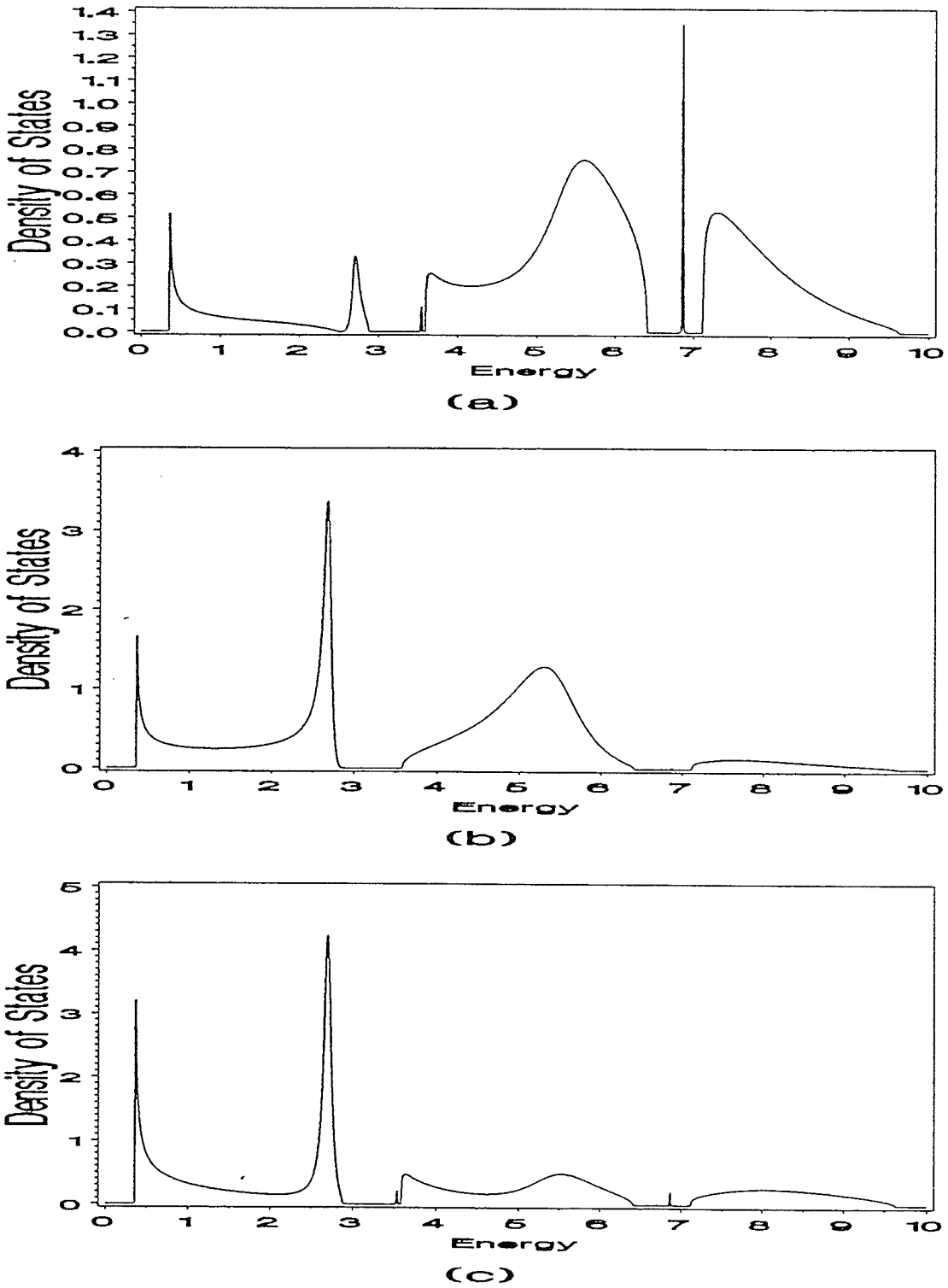

FIGURE 4.21: Local densities of states for two spin deviations (a) on the same even site (b) on the same odd site and (c) on adjacent sites for an alternating spin Heisenberg chain (S'=1 S=3/2 b=1) at K=PI/4.

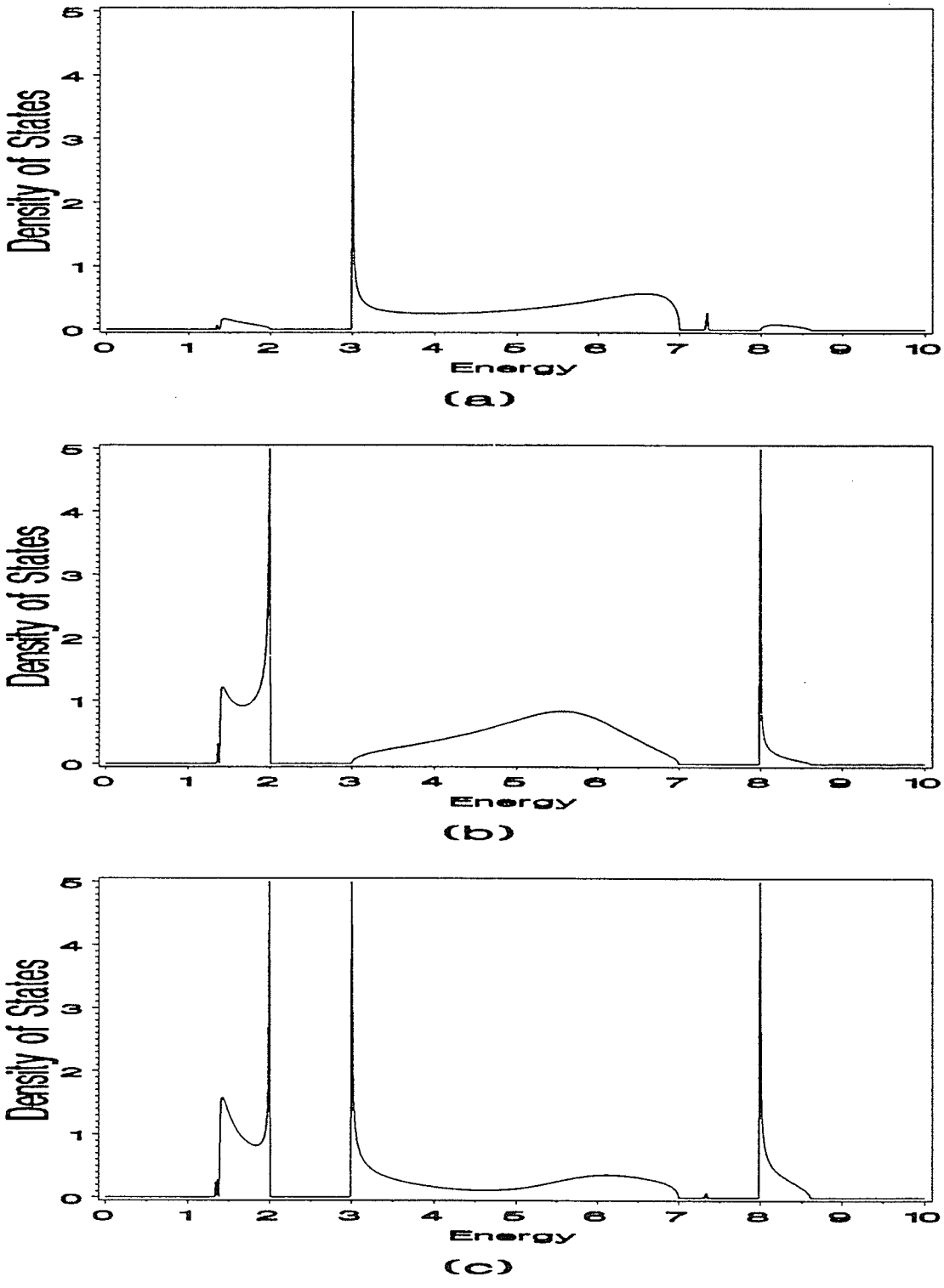

FIGURE 4.22: Local densities of states for two spin deviations (a) on the same even site (b) on the same odd site and (c) on adjacent sites for an alternating spin Heisenberg chain (S'=1 S=3/2 b=1) at K=PI/2.

Chapter 5

SUMMARY

In this thesis we studied the two-magnon excitations of an alternating ferrimagnetic chain. We only considered systems in which the ground state is ferromagnetic and in which the spin-spin interactions are restricted to being isotropic, rotationally invariant, and between nearest neighbours. However we did allow for systems in which spin magnitude and/or spin exchange interactions could alternate along the chain. Both the strength and the form of these interactions could be allowed to alternate.

Two distinct methods were used for obtaining solutions of the two-magnon problem. The first of these methods involved a direct analytic approach. This approach allowed us to solve for the complete set of bound state branches and continua boundaries for any system conforming to our model. The second method used a real-space rescaling approach to solve for the two-magnon Green's functions. Using these response functions the local densities of states could be calculated throughout the two-magnon spectrum. Together, these two techniques provided an efficient means of assessing both bound and scattering state contributions to the two-magnon wavefunction.

Using the above methods, we studied the two-magnon spectral properties of a number of special cases of the alternating ferrimagnetic chain. These cases included various uniform, alternating bond, and alternating spin systems. For some of these cases we were able to use the analytic approach to derive explicit expressions for the bound state dispersion relations. However in general, these bound state dispersion branches were generated using an exact numerical procedure. The scaling approach provided additional information regarding the relative contribution of states inside the scattering continua. This included the spectral locality of resonant state solutions.

Besides enhancing our understanding of two-magnon spectra and how these spectra relate for different cases, there was an additional motivation in my research. This was the possible identification of completely integrable systems. Such systems are of particular interest because the arbitrary m-magnon problem can be solved using the Bethe ansatz approach [BE]. As a result, it is possible to calculate the complete energy spectrum of integrable systems, independent of the choice of ground state.

The two-magnon spectra were checked for "special features" which might indicate complete integrability. In particular we checked for cases which satisfy Haldane's criteria [HAL].

(Haldane conjectured that the m-magnon bound state branches of completely integrable models are both real and continuous across minimum (m,2S) Brillouin zones of an extended zone scheme.) However the only cases we identified were uniform chains already known to correspond to families of completely integrable systems [IS], [BB], [SU1].

We did manage to observe a special feature in the two-magnon spectra for alternating spin, uniform bond Heisenberg chains when spins on adjacent sites differed in magnitude by exactly $\frac{1}{2}$. In these spectra, we identified a bound state branch which forms a connection between two otherwise isolated continua. Furthermore, the scaling approach revealed alternating spin Heisenberg chains as having relatively simple spectra when compared to their alternating bond counterparts. We conclude that the uniform bond Heisenberg chain with spin magnitudes differing by $\frac{1}{2}$ is a possible candidate for solution by a Bethe ansatz approach.

Although we restricted our study to relatively simple (one-dimensional and isotropic) lattices such systems are not too far removed from the "real world". Layered materials exhibiting quasi-one-dimensional character can often be described in terms of spin exchange interactions [RRR]. In fact, there is recent interest in metal ion arrays which can be described by isotropic exchange interactions along an alternating chain [DCG], [JVL], [SCD]. Such real systems

generally have an antiferromagnetic nature, stressing the importance of searching for completely integrable models.

Both the scaling and analytic formalism of this thesis can be easily extended to the study of chains with anisotropic interactions or to the study of chains with longer range interactions or both. The analytic approach can also be extended to the study of higher-dimensional lattices. Unfortunately, the scaling method is essentially limited to use in one-dimensional problems. When applied to higher dimensional systems the effective range of interaction between lattice sites increases as the scaling transformation is iterated. Hence, using the scaling approach to study two- or three-dimensional lattices would require construction of a transformation valid for any range of interaction. Such a transformation generally cannot be formulated.

A further extension of the scaling formalism could be to study the three-magnon problem of alternating ferrimagnetic chains. We know that for most cases the three-magnon problem is insoluble and the scaling approach particularily fails because of the previously described problem in studying higher-dimensional systems. (Whereas the two-magnon problem of a ferrimagnetic chain maps to a semi-infinite chain in relative coordinate space, the corresponding three-magnon problem maps to a semi-infinite wedge. That is, the three-magnon problem maps to a two-dimensional tight-binding model.) However we anticipate for special cases (such as completely

integrable models) that there is sufficient decoupling in the three-magnon interacting equations so that the scaling approach can be directly applied. Along with known integrable models the alternating spin, uniform bond Heisenberg chain would be a possible candidate for such studies.

APPENDIX A

In Chapter 2 of this thesis we presented, without proof, the sets of equations determining the various one- and two-magnon amplitudes. (That is, the amplitudes needed in describing the one- and two-magnon wavefunctions.) In this appendix we will consider the explicit derivation of these results.

We will begin by discussing some general properties of the spin exchange operators which make up the Hamiltonian of interest (2.1). We follow this with the derivation of the pair of equations (2.10) which determine the one-magnon amplitudes a_j. Finally, we will derive the sets of equations (2.17), (2.19) which determine the two-magnon amplitudes a_{ij}, $i \leq j$. In the process of these derivations we will also show that single spin deviation states $|i\rangle$ and two spin deviation states $|i,j\rangle$ are not eigenstates of the Hamiltonian.

A.1 General

First consider the operators which comprise the Hamiltonian of interest (2.1). These are

$$\tilde{S}'_{2n} \cdot \tilde{S}_{2n+1} = S'^{x}_{2n} S^{x}_{2n+1} + S'^{y}_{2n} S^{y}_{2n+1} + S'^{z}_{2n} S^{z}_{2n+1}$$

$$= \frac{1}{2} S'^{+}_{2n} S^{-}_{2n} + \frac{1}{2} S'^{-}_{2n} S^{+}_{2n+1} + S'^{z}_{2n} S^{z}_{2n+1} \qquad \text{(A.1a)}$$

$$\tilde{S}_{2n+1}\cdot\tilde{S}'_{2n+2} = \frac{1}{2} S^{+}_{2n+1}S^{'-}_{2n+2} + \frac{1}{2} S^{-}_{2n+1}S^{'+}_{2n+2} + S^{z}_{2n+1}S^{'z}_{2n+2} \tag{A.1b}$$

where: $n = 1,2,\ldots,\frac{N}{2}$ (N is the number of sites on the chain).

Here we are using the usual definition of quantum raising and lowering operators: $S^{\pm} = S^{x} \pm iS^{y}$. The subsequent derivations require knowing the effect of these operators (A.1) on the various one and two spin deviation states. (Deviations are always assumed to be with respect to the ferromagnetic ground state which has all spins alligned with maximum projection along the negative z-direction.)

Any m deviation state can be expanded as a product of N kets such that each ket is an eigenket of spin localized at a specific site along the chain. In other words, an m deviation can be expressed by

$$|\alpha_1\rangle_1|\alpha_2\rangle_2 \cdots |\alpha_\ell\rangle_\ell \cdots |\alpha_N\rangle_N \tag{A.2}$$

where if ℓ is odd

$$S^{z}_{\ell}|\alpha_\ell\rangle_\ell = \alpha_\ell|\alpha_\ell\rangle \tag{A.3a}$$

$$S^{\pm}_{\ell}|\alpha_\ell\rangle_\ell = \sqrt{S(S+1)-\alpha_\ell(\alpha_\ell\pm 1)}\ |\alpha_\ell\pm 1\rangle_\ell \tag{A.3b}$$

$$\alpha_\ell = \{-S,-S+1,\ldots,+S\} \tag{A.3c}$$

and where if ℓ is even

$$S'^{z}_{\ell}|\alpha_{\ell}>_{\ell} = \alpha_{\ell}|\alpha_{\ell}> \tag{A.4a}$$

$$S'^{\pm}_{\ell}|\alpha_{\ell}>_{\ell} = \sqrt{S'(S'+1)-\alpha_{\ell}(\alpha_{\ell}\pm 1)}\ |\alpha_{\ell}\pm 1>_{\ell} \tag{A.4b}$$

$$\alpha_{\ell} = \{-S',-S'+1,\ldots,+S'\}\ . \tag{A.4c}$$

(A.3) and (A.4) follow directly from the usual quantum spin (i.e., angular momenta) commutation relations [SAK]. Furthermore, we assume that spin operators corresponding to different sites commute. As a result, a given ket $|\alpha_{\ell}>_{\ell}$ is independent of all spin operators not corresponding to the ℓ^{th} site.

Using this notation we can write the ferromagnetic ground state as follows:

$$|0> = |-S>_1|-S'>_2 \ \ldots\ |-S>_{N-1}|-S'>_N\ . \tag{A.5}$$

A single spin deviation state such that the deviation occurs on an arbitrary even site can be written

$$|2n> = |-S>_1|-S'>_2 \ \ldots\ |-S>_{2n-1}|-S'+1>_{2n}|-S>_{2n+1} \ \ldots\ |-S'>_N\ . \tag{A.6}$$

A two spin deviation state such that the deviations occur on different sites labelled by 2n and 2m+1 (m > n) can be written

$$|2n,2m+1> = |-S>_1|-S'>_2 \ \ldots\ |-S>_{2n-1}|-S'+1>_{2n}|-S>_{2n+1}\ \ldots$$

$$\ldots\ |-S'>_{2m}|-S+1>_{2m+1}|-S'>_{2m+2} \ \ldots\ |-S'>_N\ . \tag{A.7}$$

A two spin deviation state such that both deviations occur on the same arbitrary odd site can be written

$$|2n+1,2n+1\rangle = |-S\rangle_1|-S'\rangle_2 \ldots$$

$$\ldots |-S'\rangle_{2n}|-S+2\rangle_{2n+1}|-S'\rangle_{2n+2} \ldots |-S'\rangle_N \tag{A.8}$$

And so on.

To illustrate the effect of the operators in (A.1) on the various one and two spin deviation states we consider the following "sample calculation":

$$\tilde{S}'_{2n}\cdot\tilde{S}_{2n+1}|2n,2m+1\rangle = [\tfrac{1}{2} S'^{+}_{2n}S^{-}_{2n+1} + \tfrac{1}{2} S'^{-}_{2n}S^{+}_{2n+1}$$

$$+ S'^{z}_{2n}S^{z}_{2n+1}]|2n,2m+1\rangle, \quad m > n . \tag{A.9}$$

Since each spin operator acts only on the ket corresponding to its specific site, to evaluate (A.9) it is sufficient to know how the operators on the right-hand side effect the kets $|-S'+1\rangle_{2n}$ and $|-S\rangle_{2n+1}$. From (A.3) and (A.4) we can write

$$S'^{+}_{2n}|-S'+1\rangle_{2n} = \sqrt{S'(S'+1)-(-S'+1)(-S'+2)}\ |-S'+1+1\rangle_{2n}$$

$$= \sqrt{2(2S'-1)}\ |-S+2\rangle_{2n} \tag{A.10a}$$

$$S'^{-}_{2n}|-S'+1>_{2n} = \sqrt{S'(S'+1)-(-S'+1)(-S')}\ |-S'+1-1>_{2n}$$

$$= \sqrt{2S'}\ |-S'>_{2n} \qquad \text{(A.10b)}$$

$$S'^{z}_{2n}|-S'+1>_{2n} = (-S'+1)|-S'+1>_{2n} \qquad \text{(A.10c)}$$

$$S^{+}_{2n+1}|-S>_{2n+1} = \sqrt{S(S+1)-(-S)(-S+1)}\ |-S+1>_{2n+1}$$

$$= \sqrt{2S}\ |-S+1>_{2n+1} \qquad \text{(A.10d)}$$

$$S^{-}_{2n+1}|-S>_{2n+1} = 0 \qquad \text{(A.10e)}$$

$$S^{z}_{2n+1}|-S>_{2n+1} = -S|-S>_{2n+1}\ . \qquad \text{(A.10f)}$$

The following expressions are equivalent to those in (A.10):

$$S'^{+}_{2n}|2n\ldots> = \sqrt{2(2S'-1)}\ |2n,2n\ldots> \qquad \text{(A.11a)}$$

$$S'^{-}_{2n}|2n\ldots> = \sqrt{2S'}\ |\ldots> \qquad \text{(A.11b)}$$

$$S'^{z}_{2n}|2n\ldots> = (-S'+1)|2n\ldots> \qquad \text{(A.11c)}$$

$$S^{+}_{2n+1}|\ldots> = \sqrt{2S}\ |2n+1\ldots> \qquad \text{(A.11d)}$$

$$S^{-}_{2n+1}|\ldots> = 0 \qquad \text{(A.11e)}$$

$$S^{z}_{2n+1}|\ldots> = -S|\ldots> \qquad \text{(A.11f)}$$

where "..." allows for the possibility of additional spin deviations provided they do not occur at the site acted on by the indicated operator. Using (A.11) we can now evaluate (A.9) as follows:

$$\tilde{S}'_{2n}\cdot\tilde{S}_{2n+1}|2n,2m+1\rangle = \frac{1}{2}\,S'^{+}_{2n}[S^{-}_{2n+1}|2n,2m+1\rangle]$$

$$+ \frac{1}{2}\,S'^{-}_{2n}[S^{+}_{2n+1}|2n,2m+1\rangle] + S'^{z}_{2n}[S^{z}_{2n+1}|2n,2m+1\rangle]$$

$$= \frac{1}{2}\,S'^{+}_{2n}[0] + \frac{1}{2}\,\sqrt{2S}\,S'^{-}_{2n}|2n,2n+1,2m+1\rangle$$

$$+ (-S)S'^{z}_{2n}|2n,2m+1\rangle$$

$$= \sqrt{SS'}\,|2n+1,2m+1\rangle + S(S'-1)\,|2n,2m+1\rangle\,. \tag{A.12}$$

Similar calculations as (A.12) lead to the following catalog of results (where $i,j \neq 2n,2n+1$):

$$\tilde{S}'_{2n}\cdot\tilde{S}_{2n+1}|i\rangle = SS'|i\rangle \tag{A.13a}$$

$$\tilde{S}'_{2n}\cdot\tilde{S}_{2n+1}|2n\rangle = S(S'-1)\,|2n\rangle + \sqrt{SS'}\,|2n+1\rangle \tag{A.13b}$$

$$\tilde{S}'_{2n}\cdot\tilde{S}_{2n+1}|2n+1\rangle = S'(S-1)\,|2n+1\rangle + \sqrt{SS'}\,|2n\rangle \tag{A.13c}$$

$$\tilde{S}'_{2n}\cdot\tilde{S}_{2n+1}|i,j\rangle = SS'|i,j\rangle \tag{A.13d}$$

$$\tilde{S}'_{2n}\cdot\tilde{S}_{2n+1}|2n,j\rangle = S(S'-1)|2n,j\rangle + \sqrt{SS'}\ |2n+1,j\rangle \qquad \text{(A.13e)}$$

$$\tilde{S}'_{2n}\cdot\tilde{S}_{2n+1}|2n+1,j\rangle = S'(S-1)|2n+1,j\rangle + \sqrt{SS'}\ |2n,j\rangle \qquad \text{(A.13f)}$$

$$\tilde{S}'_{2n}\cdot\tilde{S}_{2n+1}|i,2n\rangle = S(S'-1)|i,2n\rangle + \sqrt{SS'}\ |i,2n+1\rangle \qquad \text{(A.13g)}$$

$$\tilde{S}'_{2n}\cdot\tilde{S}_{2n+1}|i,2n+1\rangle = S'(S-1)|i,2n+1\rangle + \sqrt{SS'}\ |i,2n\rangle \qquad \text{(A.13h)}$$

$$\tilde{S}'_{2n}\cdot\tilde{S}_{2n+1}|2n,2n\rangle = S(S'-2)|2n,2n\rangle + \sqrt{S(2S'-1)}\ |2n,2n+1\rangle \qquad \text{(A.13i)}$$

$$\tilde{S}'_{2n}\cdot\tilde{S}_{2n+1}|2n,2n+1\rangle = (S-1)(S'-1)|2n,2n+1\rangle + \sqrt{S(2S'-1)}\ |2n,2n\rangle + \sqrt{S'(2S-1)}\ |2n+1,2n+1\rangle \qquad \text{(A.13j)}$$

$$\tilde{S}'_{2n}\cdot\tilde{S}_{2n+1}|2n+1,2n+1\rangle = S'(S-2)|2n+1,2n+1\rangle + \sqrt{S'(2S-1)}\ |2n,2n+1\rangle \qquad \text{(A.13k)}$$

An analgous set of relations is similarily obtained for the operator $\tilde{S}_{2n+1}\cdot\tilde{S}'_{2n+2}$.

A.2 One-Magnon Amplitudes

From (A.13) we now know the effect of the operator $\tilde{S}'_{2n}\cdot\tilde{S}_{2n+1}$ on all single spin deviation states. We can express these results in matrix form as follows:

$$(\tilde{S}'_{2n}\cdot\tilde{S}_{2n+1})\begin{bmatrix}|1>\\|2>\\\vdots\\|N>\end{bmatrix} = A\begin{bmatrix}|1>\\|2>\\\vdots\\|N>\end{bmatrix} \tag{A.14}$$

where A is an N×N matrix such that

$$A_{2n,2n} = S(S'-1) \tag{A.15a}$$

$$A_{2n,2n+1} = A_{2n+1,2n} = \sqrt{SS'} \tag{A.15b}$$

$$A_{2n+1,2n+1} = S'(S-1) \tag{A.15c}$$

otherwise:

$$A_{ij} = \delta_{ij} SS' \tag{A.15d}$$

where: δ_{ij} is the Kronecker delta function .

It follows that:

$$(\tilde{S}'_{2n}\cdot\tilde{S}_{2n+1})^p\begin{bmatrix}|1>\\|2>\\\vdots\\|N>\end{bmatrix} = A^p\begin{bmatrix}|1>\\|2>\\\vdots\\|N>\end{bmatrix}. \tag{A.16}$$

Since A is a symmetric matrix we can easily evaluate A^p for any p = 2,3,... by applying standard linear algebraic technique [KRE]. For arbitrary p we find

$$A^{p}_{2n,2n} = \frac{S'\lambda_0^p + S\lambda_1^p}{S + S'} \tag{A.17a}$$

$$A^{p}_{2n,2n+1} = A^{p}_{2n+1,2n} = \frac{\sqrt{SS'}\ (\lambda_0^p - \lambda_1^p)}{S + S'} \tag{A.17b}$$

$$A^{p}_{2n+1,2n+1} = \frac{S\lambda_0^p + S'\lambda_1^p}{S + S'} \tag{A.17c}$$

otherwise:

$$A^{p}_{ij} = \delta_{ij}\lambda_0^p \tag{A.17d}$$

where from (2.5) λ_m (m = 0,1,...,2S') denotes the eigenvalues of $\tilde{S}\cdot\tilde{S}'$ in descending order.

From (A.16) and (A.17) we can obtain the following result:

$$\sum_{p=1}^{2S'} J_1^{(p)} (\tilde{S}'_{2n}\cdot\tilde{S}_{2n+1})^p \begin{bmatrix} |1> \\ |2> \\ \vdots \\ |N> \end{bmatrix} = A' \begin{bmatrix} |1> \\ |2> \\ \vdots \\ |N> \end{bmatrix} \tag{A.18}$$

where:

$$A'_{2n,2n} = \frac{S'g_0^{(1)} + Sg_1^{(1)}}{S + S'} \tag{A.19a}$$

$$A'_{2n,2n+1} = A'_{2n+1,2n} = \sqrt{SS'}\ G_1^{(1)} \tag{A.19b}$$

$$A'_{2n+1,2n+1} = \frac{Sg_0^{(1)} + S'g_1^{(1)}}{S + S'} \tag{A.19c}$$

otherwise:

$$A'_{ij} = \delta_{ij} g_0^{(1)} \tag{A.19d}$$

where the parameters $g_m^{(i)}$ and $G_m^{(i)}$ are as defined in (2.6).

From this result we can obtain the following:

$$\sum_{n=1}^{N/2} \sum_{p=1}^{2S'} J_1^{(p)} (\tilde{S}'_{2n} \cdot \tilde{S}_{2n+1})^p \begin{bmatrix} |2m> \\ |2m+1> \end{bmatrix}$$

$$= \begin{bmatrix} \frac{N}{2} g_0^{(1)} - S G_1^{(1)} & \sqrt{SS'}\, G_1^{(1)} \\ \sqrt{SS'}\, G_1^{(1)} & \frac{N}{2} g_0^{(1)} - S' G_1^{(1)} \end{bmatrix} \begin{bmatrix} |2m> \\ |2m+1> \end{bmatrix}$$

$$m = 1, 2, \ldots, \frac{N}{2}. \tag{A.20}$$

And similarily we find

$$\sum_{n=1}^{N/2} \sum_{p=1}^{2S'} J_2^{(p)} (\tilde{S}_{2n+1} \cdot \tilde{S}'_{2n+2})^p \begin{bmatrix} |2m+1> \\ |2m+2> \end{bmatrix}$$

$$= \begin{bmatrix} \frac{N}{2} g_0^{(2)} - S' G_1^{(2)} & \sqrt{SS'}\, G_1^{(2)} \\ \sqrt{SS'}\, G_1^{(2)} & \frac{N}{2} g_0^{(2)} - S G_1^{(2)} \end{bmatrix} \begin{bmatrix} |2m+1> \\ |2m+2> \end{bmatrix} \tag{A.21}$$

Recall from (2.1) the Hamiltonian of interest:

$$H = - \sum_{n=1}^{N/2} \sum_{p=1}^{2S'} [J_1^{(p)} (\tilde{S}'_{2n} \cdot \tilde{S}_{2n+1})^p + J_2^{(p)} (\tilde{S}_{2n+1} \cdot \tilde{S}'_{2n+2})^p] . \tag{A.22}$$

Clearly (A.20) and (A.21) are all that is required to explicitly write down the representation of the Hamiltonian in the basis of single spin deviation states. If we let $H' = H - E_0$ where E_0 is the ground state energy (2.7) then we obtain the following:

$$H'|2m\rangle = S(G_1^{(1)}+G_1^{(2)})|2m\rangle - \sqrt{SS'}\,[G_1^{(1)}|2m+1\rangle + G_1^{(2)}|2m-1\rangle] \qquad \text{(A.23a)}$$

$$H'|2m+1\rangle = S'(G_1^{(1)}+G_1^{(2)})|2m+1\rangle - \sqrt{SS'}\,[G_1^{(1)}|2m\rangle + G_1^{(2)}|2m+2\rangle]\,. \qquad \text{(A.23b)}$$

Note that we have now explicitly shown that single spin deviation states are not eigenstates of the Hamiltonian.

Now consider the one-magnon Schrödinger equation (2.9). This can be written

$$H'|\psi_1\rangle = E_1|\psi_1\rangle\,. \qquad \text{(A.24)}$$

Substituting for the general form of the one-magnon wavefunction (2.8) gives

$$\sum_{n=1}^{N/2} (E_1-H')[a_{2n}|2n\rangle + a_{2n+1}|2n+1\rangle] = 0\,. \qquad \text{(A.25)}$$

Using the results of (A.23) we can eliminate H' from (A.25) and obtain the following:

$$\sum_{n=1}^{N/2} \Big\{ \sqrt{SS'}\, G_1^{(2)} a_{2n} |2n-1\rangle + [(E_1 - S(G_1^{(1)} + G_1^{(2)}))a_{2n} + G_1^{(1)} \sqrt{SS'}\, a_{2n+1}] |2n\rangle + [(E_1 - S'(G_1^{(1)} + G_1^{(2)}))a_{2n+1} + G_1^{(1)} \sqrt{SS'}\, a_{2n}] |2n+1\rangle + \sqrt{SS'}\, G_1^{(2)} a_{2n+1} |2n+2\rangle \Big\} = 0 . \tag{A.26}$$

The single spin deviation states $\{|1\rangle, |2\rangle, \ldots, |N\rangle\}$ form an orthogonal set (this can be seen by explicitly calculating $\langle i|j\rangle$, $i \neq j$, with both states expressed as the product of N kets as in (A.2)). Consequently, the coefficient of each state in (A.26) must vanish independently. To determine the coefficients of the states $|2m\rangle$ and $|2m+1\rangle$ we need only consider the terms in which the summation index n takes on values m, m±1. Equating both of these coefficients to zero gives is the following expressions:

$$[E_1 - S(G_1^{(1)} + G_1^{(2)})]a_{2m} + \sqrt{SS'}\, [G_1^{(1)} a_{2m+1} + G_1^{(2)} a_{2m-1}] = 0 \tag{A.27a}$$

$$[E_1 - S'(G_1^{(1)} + G_1^{(2)})]a_{2m+1} + \sqrt{SS'}\, [G_1^{(1)} a_{2m} + G_1^{(2)} a_{2m+2}] = 0 \tag{A.27b}$$

And these are the one-magnon amplitude equations as reported in (2.10) of Chapter 2.

A.3 Two-Magnon Amplitudes

From (A.13) we know the effect of the operator $\tilde{S}'_{2n} \cdot \tilde{S}_{2n+1}$

on all two spin deviation states. We can summarize these results using matrix notation as follows:

$$\tilde{S}'_{2n}\cdot\tilde{S}_{2n+1}|i,j\rangle = L|i,j\rangle \qquad i,j \neq 2n,2n+1 \tag{A.28a}$$

$$\tilde{S}'_{2n}\cdot\tilde{S}_{2n+1}\begin{bmatrix}|2n,j\rangle\\ |2n+1,j\rangle\end{bmatrix} = M\begin{bmatrix}|2n,j\rangle\\ |2n+1,j\rangle\end{bmatrix}, \; j \neq 2n,2n+1 \tag{A.28b}$$

$$\tilde{S}'_{2n}\cdot\tilde{S}_{2n+1}\begin{bmatrix}|2n,2n\rangle\\ |2n,2n+1\rangle\\ |2n+1,2n+1\rangle\end{bmatrix} = N\begin{bmatrix}|2n,2n\rangle\\ |2n,2n+1\rangle\\ |2n+1,2n+1\rangle\end{bmatrix} \tag{A.28c}$$

where

$$L = SS' \tag{A.29a}$$

$$M = \begin{bmatrix}S(S'-1) & \sqrt{SS'}\\ \sqrt{SS'} & S'(S-1)\end{bmatrix} \tag{A.29b}$$

$$N = \begin{bmatrix}S(S'-2) & \sqrt{S(2S'-1)} & 0\\ \sqrt{S(2S'-1)} & (S-1)(S'-1) & \sqrt{S'(2S-1)}\\ 0 & \sqrt{S'(2S-1)} & S'(S-2)\end{bmatrix} \tag{A.29c}$$

Clearly the effect of the operator $(\tilde{S}'_{2n}\cdot\tilde{S}_{2n+1})^p$ on two spin deviation states is described by the matrices L^p, M^p, and N^p. Since the matrices L, M, and N are all symmetric we can easily evaluate L^p, M^p, and N^p for any p = 2,3,4,... by applying standard linear algebra techniques [KRE] . For arbitrary p the results are as follows:

$$L^p = \lambda_0^p \tag{A.30a}$$

$$M^p = \frac{1}{(S+S')}\begin{bmatrix} S'\lambda_0^p + S\lambda_1^p & \sqrt{SS'}\,(\lambda_0^p - \lambda_1^p) \\ \sqrt{SS'}\,(\lambda_0^p - \lambda_1^p) & S\lambda_0^p + S'\lambda_1^p \end{bmatrix} \tag{A.30b}$$

$$(N^p)_{11} = (2S'-1)S'\sigma_0^p + (2S'-1)S\sigma_1^p + (2S-1)S\sigma_2^p \tag{A.30c}$$

$$(N^p)_{22} = 4SS'\sigma_0^p + (S-S')^2\sigma_1^p + (2S-1)(2S'-1)\sigma_2^p \tag{A.30d}$$

$$(N^p)_{33} = (2S-1)S\sigma_0^p + (2S-1)S'\sigma_1^p + (2S'-1)S'\sigma_2^p \tag{A.30e}$$

$$(N^p)_{12} = (N^p)_{21} = \sqrt{S(2S'-1)}\,[2S'\sigma_0^p + (S-S')\sigma_1^p - (2S-1)\sigma_2^p] \tag{A.30f}$$

$$(N^p)_{23} = (N^p)_{32} = \sqrt{S'(2S-1)}\,[2S\sigma_0^p - (S-S')\sigma_1^p - (2S'-1)\sigma_2^p] \tag{A.30g}$$

$$(N^p)_{31} = (N^p)_{13} = \sqrt{SS'(2S-1)(2S'-1)}\,[\sigma_0^p - \sigma_1^p + \sigma_2^p] \tag{A.30h}$$

where

$$\sigma_m^p = \lambda_m^p \prod_{\substack{\ell=0 \\ \ell\neq m}}^{2} (\lambda_m - \lambda_\ell)^{-1} \qquad m = 0,1,2 \tag{A.31}$$

and from our previous definition of λ_m (2.5) note that

$$\lambda_0 = SS' \tag{A.32a}$$

$$\lambda_1 = SS' - (S+S') \tag{A.32b}$$

$$\lambda_2 = SS' - 2(S+S') + 1 . \tag{A.32c}$$

Next consider the operator $\sum_{p=1}^{2S'} J_1^{(p)} (\tilde{S}'_{2n} \cdot \tilde{S}_{2n+1})^p$. The effect of this operator on two spin deviation states is described by the following matrices:

$$L' = \sum_{p=1}^{2S'} J_1^{(p)} L^p \tag{A.33a}$$

$$M' = \sum_{p=1}^{2S'} J_1^{(p)} M^p \tag{A.33b}$$

$$N' = \sum_{p=1}^{2S'} J_1^{(p)} N^p . \tag{A.33c}$$

In terms of the parameters $G_m^{(i)}$ and $g_m^{(i)}$ (2.6) these matrices are as follows:

$$L' = g_0^{(1)} \tag{A.34a}$$

$$M' = \begin{bmatrix} \frac{S'g_0^{(1)} + Sg_1^{(1)}}{S+S'} & \sqrt{SS'}\, G_1^{(1)} \\ \sqrt{SS'}\, G_1^{(1)} & \frac{Sg_0^{(1)} + S'g_1^{(1)}}{S+S'} \end{bmatrix} \tag{A.34b}$$

$$N'_{11} = g_0^{(1)} - \left(\frac{S}{S+S'-1}\right)\left[(2S'-1)G_1^{(1)} + (2S-1)G_2^{(1)}\right] \qquad \text{(A.34c)}$$

$$N'_{22} = g_0^{(1)} - \left(\frac{1}{S+S'-1}\right)\left[(S-S')^2 G_1^{(1)} + (2S-1)(2S'-1)G_2^{(1)}\right] \qquad \text{(A.34d)}$$

$$N'_{33} = g_0^{(1)} - \left(\frac{S'}{S+S'-1}\right)\left[(2S-1)G_1^{(1)} + (2S'-1)G_2^{(1)}\right] \qquad \text{(A.34e)}$$

$$N'_{12} = N'_{21} = \sqrt{S(2S'-1)}\ \left(\frac{1}{S+S'-1}\right)\left[-(S-S')G_1^{(1)} + (2S-1)G_2^{(1)}\right] \qquad \text{(A.34f)}$$

$$N'_{23} = N'_{32} = \sqrt{S'(2S-1)}\ \left(\frac{1}{S+S'-1}\right)\left[(S-S')G_1^{(1)} + (2S'-1)G_2^{(1)}\right] \qquad \text{(A.34g)}$$

$$N'_{31} = N'_{13} = \sqrt{SS'(2S-1)(2S'-1)}\ \left(\frac{1}{S+S'-1}\right)\left[G_1^{(1)} - G_2^{(1)}\right]. \qquad \text{(A.34h)}$$

Next consider the operator $Q \equiv \sum_{n=1}^{N/2} \sum_{p=1}^{2S'} (\tilde{S}'_{2n} \cdot \tilde{S}_{2n+1})^p$. Using the previous set of results (A.34) we can determine the effect of the operator on the various two spin deviation states. Doing so gives the following relations (where $m > \ell$):

$$Q|2\ell,2m\rangle = \left[\frac{N}{2} g_0^{(1)} - 2SG_1^{(1)}\right]|2\ell,2m\rangle + \sqrt{SS'}\, G_1^{(1)}\left(|2\ell+1,2m\rangle + |2\ell,2m+1\rangle\right) \qquad \text{(A.35a)}$$

$$Q|2\ell-1,2m\rangle = \left[\frac{N}{2} g_0^{(1)} - (S+S')G_1^{(1)}\right]|2\ell-1,2m\rangle + \sqrt{SS'}\, G_1^{(1)}\left(|2\ell-2,2m\rangle + |2\ell-1,2m+1\rangle\right) \qquad \text{(A.35b)}$$

$$Q|2\ell,2m+1\rangle = [\frac{N}{2} g_0^{(1)} - (S+S')G_1^{(1)}]|2\ell,2m+1\rangle$$

$$+ \sqrt{SS'}\, G_1^{(1)} (|2\ell+1,2m+1\rangle + |2\ell,2m\rangle) \qquad (A.35c)$$

$$Q|2\ell+1,2m+1\rangle = [\frac{N}{2} g_0^{(1)} - 2S'G_1^{(1)}]|2\ell+1,2m+1\rangle$$

$$+ \sqrt{SS'}\, G_1^{(1)} (|2\ell,2m+1\rangle + |2\ell+1,2m\rangle) \qquad (A.35d)$$

$$Q|2m-1,2m\rangle = [\frac{N}{2} g_0^{(1)} - (S+S')G_1^{(1)}]|2m-1,2m\rangle$$

$$+ \sqrt{SS'}\, G_1^{(1)} (|2m-2,2m\rangle + |2m-1,2m+1\rangle) \qquad (A.35e)$$

$$Q|2m,2m+1\rangle = [(\frac{N-2}{2}) g_0^{(1)} + N'_{22}]|2m,2m+1\rangle$$

$$+ N'_{12}|2m,2m\rangle + N'_{23}|2m+1,2m+1\rangle \qquad (A.35f)$$

$$Q|2m,2m\rangle = [(\frac{N-2}{2}) g_0^{(1)} + N'_{11}]|2m,2m\rangle$$

$$+ N'_{12}|2m,2m+1\rangle + N'_{31}|2m+1,2m+1\rangle \qquad (A.35g)$$

$$Q|2m+1,2m+1\rangle = [(\frac{N-2}{2}) g_0^{(1)} + N'_{33}]|2m+1,2m+1\rangle$$

$$+ N'_{23}|2m,2m+1\rangle + N'_{31}|2m,2m\rangle . \qquad (A.35h)$$

Using the preceding results (A.35) as well as the analagous set of results with respect to the operator $\tilde{S}_{2n+1} \cdot \tilde{S}'_{2n+2}$ we can now write down the representation of the Hamiltonian (A.22) in the basis of two spin deviation states.

If we again let $H' = H - E_0$ then we obtain the following where $(m > \ell)$:

$$H'|2\ell,2m> = 2S(G_1^{(1)} + G_1^{(2)})|2\ell,2m> - \sqrt{SS'}\,G_1^{(1)}(|2\ell+1,2m> + |2\ell,2m+1>) - \sqrt{SS'}\,G_1^{(2)}(|2\ell,2m-1> + |2\ell-1,2m>) \quad (A.36a)$$

$$H'|2\ell-1,2m> = (S+S')(G_1^{(1)} + G_1^{(2)})|2\ell-1,2m> - \sqrt{SS'}\,G_1^{(1)}(|2\ell-2,2m> + |2\ell-1,2m+1>) - \sqrt{SS'}\,G_1^{(2)}(|2\ell,2m> + |2\ell-1,2m-1>) \quad (A.36b)$$

$$H'|2\ell,2m+1> = (S+S')(G_1^{(1)} + G_1^{(2)})|2\ell,2m+1> - \sqrt{SS'}\,G_1^{(1)}(|2\ell+1,2m+1> + |2\ell,2m>) - \sqrt{SS'}\,G_1^{(2)}(|2\ell-1,2m+1> + |2\ell,2m+2>) \quad (A.36c)$$

$$H'|2\ell+1,2m+1> = 2S'(G_1^{(1)} + G_1^{(2)})|2\ell+1,2m+1> - \sqrt{SS'}\,G_1^{(1)}(|2\ell,2m+1> + |2\ell+1,2m>) - \sqrt{SS'}\,G_1^{(2)}(|2\ell+2,2m+1> + |2\ell+1,2m+2>) \quad (A.36d)$$

$$H'|2m-1,2m> = \tau^{(1)}|2m-1,2m> - \Phi_{S'}^{(2)}|2m,2m> - \Phi_S^{(2)}|2m-1,2m-1> - \sqrt{SS'}\,G_1^{(1)}(|2m-2,2m> + |2m-1,2m+1>) \quad (A.36e)$$

$$H'|2m,2m+1\rangle = \tau^{(2)}|2m,2m+1\rangle - \Phi_{S'}^{(1)}|2m,2m\rangle - \Phi_{S}^{(1)}|2m+1,2m+1\rangle$$
$$- \sqrt{SS'}\, G_1^{(2)}(|2m-1,2m+1\rangle + |2m,2m+2\rangle) \quad (A.36f)$$

$$H'|2m,2m\rangle = \theta_S|2m,2m\rangle - \Phi_{S'}^{(1)}|2m,2m+1\rangle - \Phi_{S'}^{(2)}|2m-1,2m\rangle$$
$$-\Delta^{(1)}|2m+1,2m+1\rangle - \Delta^{(2)}|2m-1,2m-1\rangle \quad (A.36g)$$

$$H'|2m+1,2m+1\rangle = \theta_{S'}|2m+1,2m+1\rangle - \Phi_{S}^{(1)}|2m,2m+1\rangle - \Phi_{S}^{(2)}|2m+1,2m+2\rangle$$
$$- \Delta^{(1)}|2m,2m\rangle - \Delta^{(2)}|2m+2,2m+2\rangle \quad (A.36h)$$

where: $\ell,m = 1,2,\ldots,\frac{N}{2}$ $(\ell < m)$

and where the parameters $\tau^{(i)}$, θ_S, $\Phi_S^{(i)}$, $\Delta^{(i)}$ are as defined in (2.20). Notice that we have now explicitly shown that two spin deviation states are not eigenstates of the Hamiltonian.

Now consider the two-magnon Schrödinger equation (2.16). This can be written

$$H'|\psi_2\rangle = E_2|\psi_2\rangle . \quad (A.37)$$

Substituting for the general form of the two-magnon wavefunction (2.15) gives

$$\sum_{\substack{n=1 \\ n\le m}}^{N/2}\sum_{m=1}^{N/2}(E_2-H')[a_{2n,2m}|2n,2m\rangle + a_{2n-1,2m}|2n,2m-1\rangle$$
$$+ a_{2n,2m+1}|2n,2m+1\rangle + a_{2n+1,2m+1}|2n+1,2m+1\rangle] = 0 \quad (A.38)$$

Using the results of (A.36) we can eliminate H' from (A.38). This gives an expression analagous to (A.26) of the one-magnon problem, except much more complicated.

The two spin deviation states $\{|ij\rangle | i \leq j;\ i,j = 1,2,..,N\}$ form an orthogonal set. (As for the single spin deviation states this can be shown explicitly by using the formalism of Section A.1.) Consequently, the coefficient of each state in (A.38) must vanish independently. To determine the coefficients of the states $|2r,2s\rangle$, $|2r-1,2s\rangle$, $|2r,2s+1\rangle$, $|2r+1,2s+1\rangle$ we need only consider the terms in which the summation indices take on the values $n = r,\ r \pm 1$ and $m = s,\ s \pm 1$ such that $n \leq m$. For any $r < s$, equating the coefficients of each of these four states to zero results in the set of four non-interacting equations (2.17). Meanwhile, if $r = s$ then equating the coefficients gives us the four interacting equations (2.19).

APPENDIX B

In Chapter 2 we found that the two-magnon spectrum for an alternating ferrimagnetic chain contains three distinct energy continua. In this appendix we will solve explicitly for the spectral curves which describe the various continua boundaries.

The approach used here will be to consider the conditions required for relative wavevector q to take on real values. This leads to the continua boundaries because q can only be real valued if the corresponding spectral point (K,E_2) lies inside one of the three continua. (As discussed in Chapter 2 $q = (k_1-k_2)/2$ where $\mathrm{Imag}(k_1) = -\mathrm{Imag}(k_2)$. So $q \in \mathbb{R}$ only if $k_1,k_2 \in \mathbb{R}$ and k_1,k_2 are real only inside the continua.) An alternative approach would be to use the secular determinant equation (2.23), to solve for the turning points of excitation energy E_2 as a function of q [KRU].

Recall the expression (2.27) for cos(2q) as a function of energy E_2 and total wavevector K, which we obtained directly from the two-magnon dispersion relation. We now rewrite (2.27) in a more convenient form:

$$\cos(2q) = \frac{-\Omega^2\cos(K) \pm \sqrt{\Omega^4 - \Omega^2 F\sin^2(K) + P^2\sin^4(K)}}{P\sin^2(K)} \qquad \text{(B.1)}$$

where

$$\Omega = E_2 - 2B \tag{B.2a}$$

$$F = 4SS'[(G_1^{(1)})^2 + (G_1^{(2)})^2] + D^2 \tag{B.2b}$$

$$P = 4SS'G_1^{(1)}G_1^{(2)} \tag{B.2c}$$

and where parameters $G_m^{(i)}$, B, and D are defined in equations (2.6), (2.14a), and (2.14c) respectively. There are four (generally different) values of q which satisfy (B.1) once E_2 and K (and all other parameters) have been set. In general all four of these allowed q values are complex. However at least two allowed values must be real provided that both cos(2q) is real and $|\cos(2q)| \leq 1$. If either of these criteria is violated then all four values of q will have non-zero imaginary parts. Note that cos(2q) will be real provided that the square root on the right-hand side of (B.1) has a positive argument.

A continuum boundary separates regions of the spectral plane for which real values of q do and do not exist. So it follows that any point on a continuum boundary satisfies one of the following two conditions:

$$(1) \quad \cos(2q) = \pm 1 \tag{B.3}$$

$$(2) \quad \Omega^4 - \Omega^2 F\sin^2(K) + P^2\sin^4(K) = 0 , \quad \text{and} \tag{B.4a}$$

$$|\cos(2q)| \leq 1 . \tag{B.4b}$$

Consider condition (1). If we set the right-hand side (B.1) equal to λ (where $\lambda = \pm 1$) then we obtain

$$\lambda P\sin^2(K) + \Omega^2\cos(K) = \pm\sqrt{\Omega^4 - \Omega^2 F\sin^2(K) + P^2\sin^4(K)} \; . \qquad (B.5)$$

Square both sides and rearrange (using $\lambda^2 = +1$):

$$-\Omega^4\sin^2(K) + \Omega^2[2\lambda P\cos(K) + F]\sin^2(K) = 0 \qquad (B.6)$$

or

$$\Omega^2\sin^2(K)[\Omega^2 - 2\lambda P\cos(K) - F] = 0 \; . \qquad (B.7)$$

The factor $\Omega^2\sin^2(K)$ is independent of λ and hence has no bearing on the reality of q. So this condition becomes

$$\Omega = \pm[2P\lambda\cos(K) + F]^{\frac{1}{2}} \qquad (B.8)$$

where: $\lambda = \pm 1$.

Each of the four spectral curves described by (B.8) is a potential continuum boundary. In order of increasing energy these spectral curves are as follows:

$$E_2(K) = 2B - [F + 2P\cos(K)]^{\frac{1}{2}} \qquad (B.9a)$$

$$E_2(K) = 2B - [F - 2P\cos(K)]^{\frac{1}{2}} \qquad (B.9b)$$

$$E_2(K) = 2B + [F - 2P\cos(K)]^{\frac{1}{2}} \qquad (B.9c)$$

$$E_2(K) = 2B + [F + 2P\cos(K)]^{\frac{1}{2}} \; . \qquad (B.9d)$$

Subsequent discussion will refer to these curves as $E_2(K) = W_\nu$ where ν = a,b,c,d respectively. It is important to note that all sections of these curves do not necessarily correspond to continuum boundaries. Suppose there is a local extrema (i.e., von Hove singularity) in the expression for cos(2q) which lies inside a continuum region. Such an internal singularity (if it exists) must satisfy condition (1) and hence will coincide with at least one of these curves for some range of K.

Now consider condition (2). The first part of this condition (B.4a) is a quadratic equation in Ω^2. Solving gives

$$\Omega^2 = \frac{\sin^2(K)}{2}\left[F \pm \sqrt{F^2 - 4P^2}\right]. \qquad \text{(B.10)}$$

Each of the four spectral curves described by (B.10) is a potential continuum boundary. In order of increasing energy these curves are as follows:

$$E_2(K) = 2B - \sin(K)\left[\frac{F+\sqrt{F^2-4P^2}}{2}\right]^{\frac{1}{2}} \qquad \text{(B.11a)}$$

$$E_2(K) = 2B - \sin(K)\left[\frac{F-\sqrt{F^2-4P^2}}{2}\right]^{\frac{1}{2}} \qquad \text{(B.11b)}$$

$$E_2(K) = 2b + \sin(K)\left[\frac{F-\sqrt{F^2-4P^2}}{2}\right]^{\frac{1}{2}} \qquad \text{(B.11c)}$$

$$E_2(K) = 2B + \sin(K)\left[\frac{F+\sqrt{F^2-4P^2}}{2}\right]^{\frac{1}{2}} \qquad \text{(B.11d)}$$

Subsequent discussion will refer to these curves as $E_2(K) = Z_\nu$ where ν = a,b,c,d respectively. Note that each of these spectral curves can only describe a continuum boundary when the second part of condition (2) (namely (B.4b)) is also satisfied. That is, the curve $E_2(K) = Z_\nu$ corresponds to a continuum boundary only for values of K in which $|\cos(2q)| \leq 1$ is satisfied along the curve.

We can consider the second part of condition (2) as follows. If we substitute (B.10) back into (B.1) we obtain

$$\cos(2q) = -\frac{\cos(K)}{2P}\left[F \pm \sqrt{F^2 - 4P^2}\right] . \qquad (B.12)$$

Choosing the plus sign in (B.12) (in front of the square root) gives the value of con(2q) for points along the curves Z_a and Z_d while choosing the minus sign gives the value of cos(2q) for points along the curves Z_b and Z_c. Regardless of whether we choose the plus or minus sign, cos(2q) will take on a finite absolute value at K = 0 and will gradually decrease in magnitude as we move across the Brillouin zone until cos(2q) = 0 at $K = \pi/2$. If the minus sign is chosen then it can be shown that $|\cos(2q)| < 1$ at K = 0 and hence $|\cos(2q)| \leq 1$ is satisfied for all K. However if the plus sign is chosen then it can be shown that $|\cos(2q)| > 1$ at K = 0. As a result, $|\cos(2q)| \leq 1$ only for $K > K_c$ where K_c is some special value of total wavevector. We can solve for K_c by choosing the plus sign and then equating the right-hand

side of (B.12) with -1. Solving for $K = K_c$ gives

$$K_c = \text{ARCOS}\left[\frac{2P}{F+\sqrt{F^2-4P^2}}\right] . \qquad (B.13)$$

To summarize, $E_2(K) = Z_b$ and $E_2(K) = Z_c$ are continuum boundaries for all values of K whereas $E_2(K) = Z_a$ and $E_2(K) = Z_d$ are continuum boundaries only for $K > K_c$.

The special value of wavevector denoted by K_c has additional significance. At this point in the Brillouin zone we find that $W_b = Z_a$ and $W_c = Z_d$. Further investigation reveals that for $K > K_c$, then $E_2(K) = W_b$ and $E_2(K) = W_c$ both lie inside energy continua. Hence for $K > K_c$ these two spectral curves correspond to internal van Hove singularities rather than continuum boundaries.

We know from Chapter 2 that there are three distinct continua (optim-optic, mixed-mode, and acoustic-acoustic) so there must be six continua boundaries. Appropriately, we have indentified six distinct expressions for continua boundaries at any given value of K. If we order these boundaries in energy and match them up with the appropriate continua then we have the following correspondence:

1. acoustic-acoustic lower boundary, $E_2(K) = W_a$
2. acoustic-acoustic upper boundary, $E_2(K) = \begin{cases} W_b & K < K_c \\ Z_c & K > K_c \end{cases}$
3. mixed-mode lower boundary $E_2(K) = Z_b$

4. Mixed-mode upper boundary $E_2(K) = Z_b$

5. optic-optic lower boundary $E_2(K) = \begin{cases} W_c & K < K_c \\ Z_d & K > K_c \end{cases}$

6. optic-optic upper boundary $E_2(K) = W_d$.

A plot of these continua boundaries is shown in Figure (2.2) for $S = S' = \frac{1}{2}$, $G_1^{(1)} = \frac{1}{2} G_1^{(2)}$.

If we plot all eight spectral curves given by (B.9) and (B.11) continuously across the Brillouin zone then the resulting E_2 versus K spectral plane is separated into eleven distinct regions. In Figure (2.3) we have plotted all eight curves (for $S = S' = \frac{1}{2}$, $G_1^{(1)} = \frac{1}{2} G_1^{(2)}$) and the resulting regions are labelled in the same manner as by Krupennikov in his study of the alternating Heisenberg chain [KRU]. The significance of these spectral regions is that the "nature" of the allowed values of relative wavevector q depends upon which particular region is under consideration. (By nature, we mean the distribution of the four allowed values of q in the complex plane.) As a result, the nature of solution of the two-magnon problem varies from region to region.

Notice that the regions labelled by odd numerals (I, III, V) are all outside the energy continua while those labelled by even numerals (II, IV, VI) are all inner continuum regions. It is obvious (from Chapter 2) that crossing over a continuum boundary should change the nature of solution. In crossing from region II to region IV we do not leave the

continuum in question (either A-A or O-O). However the nature of solution generally changes as a result of crossing over an internal van Hove singularity. In crossing from region III to region V we do not leave the continua gap in question. However the nature of solution generally changes because of a degeneracy on the curve separating these two regions. For spectral points on this curve the square root in (B.1) vanishes and hence there are only two allowed values of q rather than four.

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