Two-magnon states of the alternating-bond ferrimagnetic chain

A. J. M. Medved and B. W. Southern
Department of Physics, University of Manitoba, Winnipeg, Manitoba, Canada R3T 2N2

D. A. Lavis
Department of Mathematics, King's College, The Strand, London WC2R 2LS, United Kingdom

(Received 12 June 1990)

In this paper we examine the nature of two-magnon excitations in the alternating-bond ferrimagnetic spin chain for general values S and S' of the two species of spin. Both a direct analytic approach as well as a method based on a scaling transformation are used to study the bound-state branches and their relationship to the two-magnon continuum.

I. INTRODUCTION

In the past few years exotic arrays of metal ions exhibiting unusual magnetic behavior have been discovered.[1–3] Some of these systems can be described in terms of isotropic exchange interactions which alternate in strength along a chain. The chains are composed of two sublattices which have unequal spin magnitudes S and S'. These ferrimagnetic chains usually have antiferromagnetic interactions which favor antiparallel arrangements of spins on nearest-neighbor sites. Although many exact results for the excitations in uniform-spin chains have been obtained, the nature of excitations in ferrimagnetic chains has not been widely studied. The spectrum of the uniform-spin $S=\frac{1}{2}$ chain is known from the Bethe ansatz.[4,5] However, for larger values of S, the isotropic Heisenberg chain is not solvable by this method. Takhtajan[6] and Babujian[7] have independently constructed a generalization of the integrable $S=\frac{1}{2}$ Heisenberg model for general values of S which is solvable by the Bethe ansatz. The general model is a polynomial in the scalar product of neighboring spins which includes all powers up to $2S$.

In a previous paper[8] we have studied the excitations of an alternating-bond system in which all spins have the same magnitude $S=\frac{1}{2}$. Here we will extend this study to $S>\frac{1}{2}$ as well as the case where both the interactions and the spin magnitudes alternate along the chain. We consider only the case where the ground state is *ferromagnetic* corresponding to the state of maximum total spin and we obtain exact results for the two-magnon excitations. The motivation for our study is to try to identify systems which may be completely integrable. Such systems are of interest because exact results for the corresponding antiferromagnetic systems can then be obtained. Haldane[9] and Chubukov and Khveshenko[10] have observed that completely integrable systems have certain special features in their m-magnon spectra. Haldane[9] observed that, in the uniform-spin S integrable models, the bound-state branches are all real and continuous across $p=\min(m,2S)$ Brillouin zones in an extended zone scheme. Hence special features of the two-magnon spectrum might be a way of identifying integrable models involving alternating spins.

We carry out our calculations using two complementary methods. The two-magnon problem can be described as an interaction between one-magnon states and the solution can be expressed in terms of the one-magnon energies and eigenvalues. This is convenient for studying the bound states in the spectrum. We also use a scaling approach to calculate local densities of states directly. This latter approach is more convenient for the study of scattering states.

In Sec. II we describe the model and write down the equations for the two-magnon states. In Sec. III we solve for the bound states and study the dependence on both bond and spin alternation. Section IV describes our results for the continuum states obtained using a scaling approach. Section V summarizes our findings.

II. THE MODEL

We begin by introducing a very general Hamiltonian which describes an infinite alternating quantum spin chain with rotationally invariant interactions restricted to nearest neighbors. This can be expressed in terms of the alternating-spin operators $\mathbf{S}'_{2n}$ and $\mathbf{S}_{2n+1}$ as follows:

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

where the total number of sites N is even and we have assumed, without loss of generality, that $S'\leq S$. The couplings $J_1^{(p)},J_2^{(p)}$ represent the interactions which alternate in strength along the chain. For uniform spins and bonds, the above Hamiltonian includes the spin S integrable models[6,7] as special cases.

The Hamiltonian (1) can be described in terms of the set of couplings $J_i^{(p)}$ or, equivalently, in terms of parameters related to the eigenvalues of the operator $(\mathbf{S}\cdot\mathbf{S}')$. If λ_m $(m=0,1,2,\ldots,2S')$ denotes the eigenvalues in descending order with $\hbar=1$, then we have

$$\lambda_m=SS'-m(S+S')+\tfrac{1}{2}m(m-1) , \quad (2)$$

and we define

$$G_m^{(i)}=\frac{g_0^{(i)}-g_m^{(i)}}{\lambda_0-\lambda_m}\quad (m=1,2,\ldots,2S')\ ,$$
$$g_m^{(i)}=\sum_p J_i^{(p)}\lambda_m^p\quad (i=1,2)\ . \tag{3}$$

We shall use the $G_m^{(i)}$ to describe the Hamiltonian. The advantage of using the $G_m^{(i)}$ rather than the $J_i^{(p)}$ is that the m-magnon problem only involves the first m of the former combinations. In the following we assume that the ground state of (1) corresponds to the ferromagnetic state $|0\rangle$ with all spins aligned along the negative z direction. The constraints on the $J_i^{(p)}$ for this to be the case correspond to having the $G_m^{(i)}$ non-negative.

The one-magnon or spin-waves states $|\psi_1\rangle$ can be expanded in the basis of the single spin deviation states as follows:

$$|\psi_1\rangle=\sum_n (a_{2n}|2n\rangle+a_{2n+1}|2n+1\rangle)\ . \tag{4}$$

The Schrödinger equation $H|\psi_1\rangle=E_1|\psi_1\rangle$ results in equations relating the amplitudes a_r which can be conveniently expressed using the $G_1^{(i)}$. The equations for the spin-wave amplitudes are given by

$$[E_1-S(G_1^{(1)}+G_1^{(2)})]a_{2n}=-\sqrt{SS'}(G_1^{(1)}a_{2n+1}+G_1^{(2)}a_{2n-1})\ ,$$
$$[E_1-S'(G_1^{(1)}+G_1^{(2)})]a_{2n+1}=-\sqrt{SS'}(G_1^{(1)}a_{2n}+G_1^{(2)}a_{2n+1})\ , \tag{5}$$

where the one-magnon energy E_1 is measured relative to the ground-state energy $E_0=-(N/2)(g_0^{(1)}+g_0^{(2)})$. The solution of these equations are plane waves with different amplitudes on the even and odd sites. The dispersion relation can be written as

$$E_k^\mu=B+\frac{\mu}{2}(\xi^2+4A^+A^-)^{1/2}\ , \tag{6}$$

where

$$B=\tfrac{1}{2}(S+S')(G_1^{(1)}+G_1^{(2)})\ , \tag{7}$$

$$\xi=(S-S')(G_1^{(1)}+G_1^{(2)})\ , \tag{8}$$

and

$$A^\pm=\sqrt{SS'}G_1^{(1)}e^{\pm ik}+\sqrt{SS'}G_1^{(2)}e^{\mp ik}\ . \tag{9}$$

The index $\mu=\pm1$ labels the two branches which by convention are referred to as "optic" for the upper branch and "acoustic" for the lower branch and the dimensionless wave vector k lies in the range 0 to $\pi/2$. In general there is a nonzero gap between the two branches at the Brillouin-zone boundary ($k=\pi/2$). It can be easily shown that this gap vanishes only in the uniform case where $S=S'$ and $G_1^{(1)}=G_1^{(2)}$.

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

$$|\psi_2\rangle=\sum_{n\le m}(a_{2n,2m}|2n,2m\rangle+a_{2n,2m+1}|2n,2m+1\rangle+a_{2n-1,2m}|2n-1,2m\rangle+a_{2n+1,2m+1}|2n+1,2m+1\rangle)\ , \tag{10}$$

where the ket $|r,s\rangle$ with $r<s$ represents the state with single deviations on the rth and sth spins relative to the ground state while the ket $|r,r\rangle$ represents the state with two spin deviations on the same (rth) site. The equations which determine the various amplitudes are obtained by substituting into the Schrödinger equation $H|\psi_2\rangle=E_2|\psi_2\rangle$. For the case $m>n$ this procedure yields

$$(\Omega-\xi)a_{2n,2m}=-\sqrt{SS'}[G_1^{(1)}(a_{2n,2m+1}+a_{2n+1,2m})+G_1^{(2)}(a_{2n,2m-1}+a_{2n-1,2m})]\ ,$$
$$\Omega a_{2n-1,2m}=-\sqrt{SS'}[G_1^{(1)}(a_{2n-2,2m}+a_{2n-1,2m+1})+G_1^{(2)}(a_{2n,2m}+a_{2n-1,2m-1})]\ ,$$
$$\Omega a_{2n,2m+1}=-\sqrt{SS'}[G_1^{(1)}(a_{2n,2m}+a_{2n+1,2m+1})+G_1^{(2)}(a_{2n-1,2m+1}+a_{2n,2m+2})]\ , \tag{11}$$
$$(\Omega+\xi)a_{2n+1,2m+1}=-\sqrt{SS'}[G_1^{(1)}(a_{2n,2m+1}+a_{2n+1,2m})+G_1^{(2)}(a_{2n+2,2m+1}+a_{2n+1,2m+1})]\ ,$$

where

$$\Omega=E_2-2B \tag{12}$$

and E_2 is measured with respect to E_0. We shall refer to the equations above as the "noninteracting" equations since they only involve amplitudes with spin deviations separated by at least two spin sites. The equations involving excitations on the same or neighboring sites will be referred to as the "interacting" equations. These have the following form:

$$(E_2-\Theta_S)a_{2n,2n}=-\Phi_{S'}^{(1)}a_{2n,2n+1}-\Phi_{S'}^{(2)}a_{2n-1,2n}-\Delta^{(1)}a_{2n+1,2n+1}-\Delta^{(2)}a_{2n-1,2n-1}\ ,$$
$$(E_2-\tau^{(1)})a_{2n-1,2n}=-\Phi_S^{(2)}a_{2n-1,2n-1}-\Phi_{S'}^{(2)}a_{2n,2n}-\sqrt{SS'}G_1^{(1)}(a_{2n-1,2n+1}+a_{2n-2,2n})\ ,$$
$$(E_2-\tau^{(2)})a_{2n,2n+1}=-\Phi_S^{(1)}a_{2n+1,2n+1}-\Phi_{S'}^{(1)}a_{2n,2n}-\sqrt{SS'}G_1^{(2)}(a_{2n,2n+2}+a_{2n-1,2n+1})\ , \tag{13}$$
$$(E_2-\Theta_{S'})a_{2n+1,2n+1}=-\Phi_S^{(1)}a_{2n,2n+1}-\Phi_S^{(2)}a_{2n+1,2n+2}-\Delta^{(2)}a_{2n+2,2n+2}-\Delta^{(1)}a_{2n,2n}\ ,$$

with

$$\Theta_S=\frac{S}{S+S'-1}[(2S'-1)(G_1^{(1)}+G_1^{(2)})+(2S-1)(G_2^{(1)}+G_2^{(2)})] ,$$
$$\tau^{(1)}=(S+S')G_1^{(1)}+\frac{1}{S+S'-1}[(S-S')^2G_1^{(2)}+(2S-1)(2S'-1)G_2^{(2)}] ,$$
$$\Phi_S^{(i)}=\frac{\sqrt{(2S-1)S'}}{S+S'-1}[(S-S')G_1^{(i)}+(2S'-1)G_2^{(i)}] ,\tag{14}$$
$$\Delta^{(i)}=\frac{\sqrt{SS'(2S-1)(2S'-1)}}{S+S'-1}(G_1^{(i)}-G_2^{(i)})\quad (i=1,2) ,$$

and where $\Theta_{S'}$ and $\Phi_{S'}^{(i)}$ have S and S' interchanged while $\tau^{(2)}$ has the superscripts 1 and 2 interchanged. Note that the unphysical amplitudes with two excitations on the same site are decoupled from the rest when the spin on that site is $\frac{1}{2}$.

First we consider the noninteracting equations. These are easily solved in terms of products of one-magnon solutions having wave vectors k_1 and k_2, respectively, as follows:

$$\begin{aligned} a_{2n,2m}&=\alpha e^{2ink_1}e^{2imk_2} ,\\ a_{2n-1,2m}&=\beta e^{i(2n-1)k_1}e^{2imk_2} ,\\ a_{2n,2m+1}&=\gamma e^{2ink_1}e^{i(2m+1)k_2} ,\\ a_{2n+1,2m+1}&=\delta e^{i(2n+1)k_1}e^{i(2m+1)k_2} . \end{aligned}\tag{15}$$

Substitution into the noninteracting equations leads to a 4×4 matrix eigenvalue equation. The dispersion relation for the energy is simply the sum of the energy of two noninteracting magnons. That is,

$$E_{K,q}^{\mu_1,\mu_2}=E_{k_1}^{\mu_1}+E_{k_2}^{\mu_2} ,\tag{16}$$

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

$$\begin{aligned} \frac{\alpha}{\delta}&=\frac{\Omega^2+\Omega\xi-A_1^+A_1^- -A_2^+A_2^-}{2A_1^-A_2^-} ,\\ \frac{\beta}{\delta}&=\frac{A_1^+A_1^- -A_2^+A_2^- -\Omega^2-\Omega\xi}{2\Omega A_2^-} ,\\ \frac{\gamma}{\delta}&=\frac{A_2^+A_2^- -A_1^+A_1^- -\Omega^2-\Omega\xi}{2\Omega A_1^-} , \end{aligned}\tag{17}$$

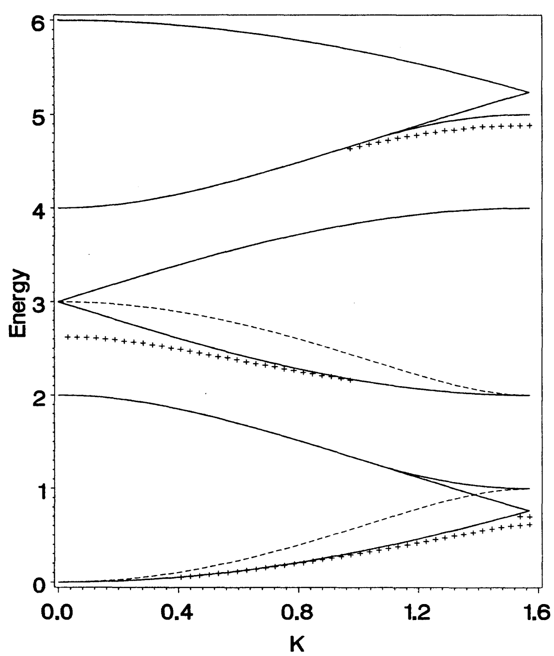

FIG. 1. Two-magnon continua (regions bounded by solid curves) and bound-state branches for $S=1$ and $a=0.5$ for case 1. The energy is the dimensionless quantity $E/G_1^{(1)}$. The branches indicated by crosses correspond to amplitudes with spin deviations on different sites. The dashed lines indicate bound states for spin deviations on the same site. These latter states lie entirely within the two-magnon continua and are identical to the one-magnon dispersion curves.

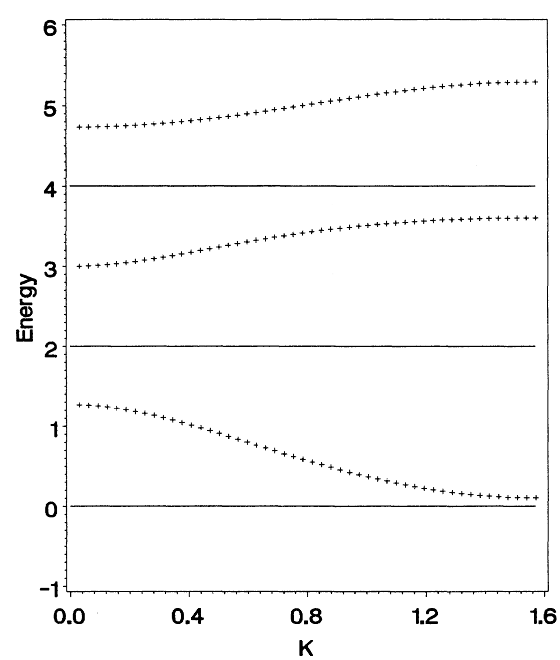

FIG. 2. Two-magnon bound-state branches (crosses) and collapsed continua (solid lines) corresponding to case 3. The energy is the dimensionless quantity $E/G_1^{(1)}$. The results are shown for $S=1$ and $G_1^{(1)}=G_2^{(2)}=1$. As the value of $G_2^{(2)}$ decreases, each of the bound-state branches approaches the continuum below it.

with Ω related to the energy eigenvalue $E_{K,q}^{\mu_1,\mu_2}$ as in (12) and $A_1^{\pm}$ and $A_2^{\pm}$ given by (9) with k_1 and k_2, respectively, replacing k. For given values of k_1 and k_2 (or equivalently K and q), there are four energies which form three distinct energy continua for real wave vectors. These continua arise because of the gap in the one-magnon dispersion curve and a given continuum can be identified as being either "acoustic-acoustic," "optic-optic," or "mixed-mode," depending on which pair of spin-wave branches are involved. Alternatively[8,11] we can use the two-magnon dispersion relation (16) to solve for q with fixed values of K and energy E_2. Both K and E_2 (or equivalently Ω) are real but q can be complex. The expression for q as a function of K and Ω is

$$\cos(2q)=\frac{-\Omega^2\cos K}{4SS'G_1^{(1)}G_1^{(2)}\sin^2K}\pm\frac{\{[\Omega^2-4SS'(G_1^{(1)}\sin K)^2][\Omega^2-4SS'(G_1^{(2)}\sin K)^2]-(\Omega\xi\sin K)^2\}^{1/2}}{4SS'G_1^{(1)}G_1^{(2)}\sin^2K}\ . \tag{18}$$

There are in general four distinct complex values of q for a given spectral point (K,E_2). For each value of q there is a corresponding eigenvector and hence any linear combination of these four eigenvectors is a solution of the noninteracting two-magnon problem. However, only certain combinations will also satisfy the interacting equations as well.

The complete solution to the two-magnon equations can be obtained by writing each amplitude as a linear combination of the components of the four degenerate eigenvectors (one for each value of q) and then determining what particular combination (if any) satisfies the complete set of interacting equations. For points (K,E_2) inside the energy continua there will always be a nontrivial solution for the wave function. These solutions inside the continua are referred to as "scattering states" and will be discussed later in the paper. However, for points (K,E_2) outside of the energy continua there will always be four complex values of q occurring in pairs with equal and opposite imaginary parts. For an infinite chain, only decaying solutions are acceptable and hence each amplitude can be written as a combination of at most two eigenvectors. A nonvanishing solution for the wave function only exists for certain values of E_2 and K. Such solutions are referred to as "bound states."

The procedure to locate the bound-state solutions is as follows. If q and $\bar{q}$ denote the two surviving values of q for any point (K,E_2) outside the continua, then general expressions for the amplitudes can be written as

$$\begin{aligned}
a_{2n,2n}&=e^{2inK}(C_0\alpha+D_0\bar{\alpha})\ ,\\
a_{2n,2m}&=e^{iK(n+m)}(C\alpha e^{-iq(2m-2n)}+D\bar{\alpha}e^{-i\bar{q}(2m-2n)})\ ,\\
a_{2n-1,2m}&=e^{iK(n+m-1/2)}(C\beta e^{-iq(2m-2n+1)}\\
&\qquad+D\bar{\beta}e^{-i\bar{q}(2m-2n+1)})\ ,\\
a_{2n,2m+1}&=e^{iK(n+m+1/2)}(C\gamma e^{-iq(2m-2n+1)}\\
&\qquad+D\bar{\gamma}e^{-i\bar{q}(2m-2n+1)})\ ,\\
a_{2n+1,2n+1}&=e^{iK(2n+1)}(C_0\delta+D_0\bar{\delta})\ ,\\
a_{2n+1,2m+1}&=e^{iK(n+m+1)}(C\delta e^{-iq(2m-2n)}\\
&\qquad+D\bar{\delta}e^{-i\bar{q}(2m-2n)})\ ,
\end{aligned} \tag{19}$$

where $m>n$ and where $\alpha,\beta,\gamma,\delta$ and $\bar{\alpha},\bar{\beta},\bar{\gamma},\bar{\delta}$ are the components of the "noninteracting" eigenvectors corresponding to q and $\bar{q}$, respectively. Substituting these expressions into the interacting equations results in a 4×4 matrix eigenvalue and hence a nonvanishing solution occurs at the point (K,E_2) only if the secular determinant for this equation vanishes. In our work we searched for bound-state solutions by fixing the value of K and varying the energy throughout the regions outside of the continua. These results are described in the next section.

III. BOUND STATES

Using the procedure described at the end of Sec. II it is possible to obtain the complete set of bound-state solutions for a system with alternating bonds or alternating spins or both. As we are able to vary the parameters $S,S',G_1^{(1)},G_1^{(2)},G_2^{(1)},G_2^{(2)}$ there are many different systems that we can examine. We will use the following ratios:

$$\begin{aligned}
\eta&=S/S'\ ,\\
r^{(i)}&=G_2^{(i)}/G_1^{(i)}\ ,\\
a&=G_1^{(2)}/G_1^{(1)}\ ,
\end{aligned} \tag{20}$$

to describe our results. The ratio η indicates the degree of spin alternation, $r^{(i)}$ indicates the form of interaction between neighbors, and a indicates the degree of bond alternation. The uniform-spin S chain has both η and a equal to unity and $r^{(1)}=r^{(2)}$. For special values of these ratios, the equations for the bound states reduce to simple forms for which analytic expressions for the energies can be obtained. We examine these special cases first and then examine the more general situations.

Case 1. $\eta=1$, $r^{(i)}=0$. This case corresponds to a system with uniform spins, alternating bonds, and $G_2^{(1)}=G_2^{(2)}=0$. This special case with both $r^{(1)}$ and $r^{(2)}$ equal zero is a member of a family of systems which includes a spin-S Hamiltonian which has the form of an alternating-bond Schrödinger exchange operator.[12,13] It can be easily seen from the interacting equations (13) that in this case the amplitudes with two spin deviations on the same site decouple from all other amplitudes. For $S=\frac{1}{2}$ these amplitudes are unphysical and can be ignored. For larger values of S they describe physical bound states. The set of equations involving spin deviations on different sites are formally identical to the equations for the $S=\frac{1}{2}$ alternating-bond Heisenberg chain with all energies scaled by a factor of $2S$. The two-magnon spectrum of this latter system has been studied previously by Bell, Loly, and Southern.[8] The spectrum consists of three separate continua referred to as acoustic-acoustic, optic-optic, and mixed-mode as well as four bound-state branches. Two of these are associated with the acoustic-acoustic continuum, whereas the others are each associated with the mixed and optic-optic continua, respectively. The branches below the acoustic-acoustic continuum have a gap between them at the Brillouin-zone boundary and the upper branch enters the continuum to become a resonance at smaller K. The equations involving two spin deviations on the same site are easily solved for two additional bound-state branches and they have the following form:

$$E_b^{\pm}=S\{G_1^{(1)}+G_1^{(2)}\pm[(G_1^{(1)})^2+(G_1^{(2)})^2+2G_2^{(1)}G_1^{(2)}\cos 2K]^{1/2}\} . \tag{21}$$

Both E_b^- and E_b^+ lie completely inside of an energy continuum (acoustic-acoustic and mixed-mode, respectively) but because of the decoupling these are true bound states and not resonant states. The above dispersion relation is precisely that of the one-magnon excitations in an alternating-bond spin S chain. Hence the complete spectrum consists of the three continua and six bound-state branches as shown in Fig. 1 for $S=1$ and $a=0.5$. If the spin alternates as well, the different parts of the spectrum are coupled and the two additional bound states become resonances inside the continua.

Case 2. $r^{(1)}=r^{(2)}=\infty$. This case describes a system with alternating spins, alternating bonds, but with $G_1^{(1)}=G_1^{(2)}=0$. As an example, this case describes a $S=1$ system with alternating purely biquadratic exchange interactions. All three continua collapse to zero energy since the one-magnon energies are all zero. We can see from Eq. (18) that the relative wave vector q is imaginary with infinite amplitude. As a result all amplitudes, except those with spin deviations on the same or adjacent sites, must vanish due to an exponentially decaying factor. This simplification leads to equations which can be easily solved for the bound-state energies. We find there to be a twofold degenerate bound state at $E=0$ for all K (i.e., inside the collapsed continua) while there are two additional bound states with energies given by

$$E_b^{\pm}=\left[\frac{2S+2S'-1}{2}\right](G_2^{(1)}+G_2^{(2)})\pm\left[(G_2^{(1)}+G_2^{(2)})^2-4\frac{(2S-1)(2S'-1)}{(S+S'-1)^2}\left[1-\frac{SS'\cos^2K}{(2S+2S'-1)^2}\right]G_2^{(1)}G_2^{(2)}\right]^{1/2} . \tag{22}$$

If either spin is $\frac{1}{2}$, then one of these bound states has zero energy and the other is unphysical. For uniform-spin S chains, the bound states in (22) have no gap at the Brillouin-zone boundary and form one continuous branch in an extended zone scheme. The pure biquadratic exchange model for $S=1$ is one member of this family and corresponds to a integrable system.[14,15] The results for $S=1$ are shown in Fig. 2. In this case the form of H for $S=1$ would be purely biquadratic exchange alternating with Schrödinger exchange along the chain.

Case 3. $\eta=1$, $r^{(1)}=0$, $r^{(2)}=\infty$. If we consider chains with uniform spin only ($\eta=1$) then the two previous cases can be interpreted as limiting cases of an alternating-bond system in which we are free to vary the ratios $r^{(i)}=G_2^{(i)}/G_1^{(i)}$ from 0 (former case) to infinity (latter case). Hence we would anticipate any intermediate values of the $r^{(i)}$ to correspond to a system intermediate between the two extremes. If either $G_1^{(1)}$ or $G_1^{(2)}$ is zero, then the one-magnon energies are 0 or $2B$ independent of the wave vector. Hence the width of the two-magnon continua collapse to zero and have energies equal to 0, $2B$, or $4B$. For the choice $G_1^{(2)}=G_2^{(1)}=0$, there is a decoupling of the amplitudes describing two-spin deviations separated by zero, one, and two sites from the rest. The amplitudes for separations greater than two sites only have nontrivial solutions at energies corresponding to the collapsed continua. The amplitudes for separations less than three sites have six bound-state contributions. Two of these have the same energy as the acoustic-acoustic ($E=0$) continuum and one has the same energy as the mixed ($E=2B$) continuum but they remain decoupled from them. Each of the other three bound states can be associated with having originated from each of three continua. Analytic expressions for the bound-state dispersion curves can be obtained as solutions of a cubic equation but will not be presented here.

Case 4. $\eta=1$, $r^{(1)}=r^{(2)}=1$. Each of the cases above represent special limits in which analytic expressions for the two-magnon energies can be found. For $S=1$ uniform chains, the first two cases correspond to Hamiltonians which are members of a family of completely integrable systems.[5] When the ratios in (20) are different from these values, the spectrum of bound-state branches is more complicated.[13] In general, the bound states either become resonances for all K or they can enter or emerge from the continua at intermediate values of K. As an example, consider the general S alternating-bond Heisenberg chain ($r^{(i)}=1$). For $S=\frac{1}{2}$ the Hamiltonian is an alternating-bond exchange operator and corresponds to case 1. The amplitudes for two deviations on the same site are unphysical and are decoupled from the rest. For larger values of S, these amplitudes are physical. As the $r^{(i)}$ are increased from zero, the two additional bound-state branches described in case 1 interact with the continua. In the limit when $r^{(i)}=1$, one lies entirely in the gap between the mixed and optic continua while the other becomes a resonant state inside the acoustic continuum. Figure 3 shows the bound-state branches for $S=1$ and $a=0.5$. The resonant states will be discussed further in the Sec. IV.

Case 5. $\eta\neq 1$, $a=1$. A final case that we consider is a system with uniform bonds but alternating spin such that $S'=\frac{1}{2}$ and $S>S'$. Amplitudes with two spin deviations on an even spin site are unphysical and they decouple completely from the rest. The remaining equations are

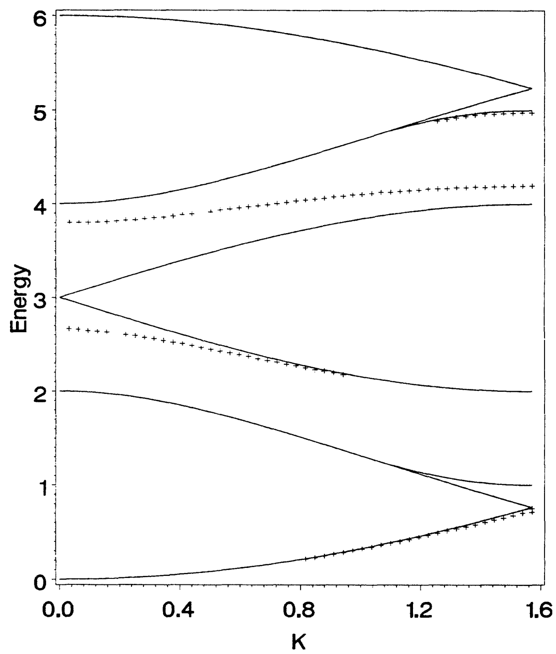

FIG. 3. Two-magnon spectrum of the alternating-bond $S=1$ Heisenberg chain. Compared to the $S=\frac{1}{2}$ chain, an additional bound-state branch lies in the gap between the optic-optic and mixed continua. The energy is the dimensionless quantity $E/G_1^{(1)}$.

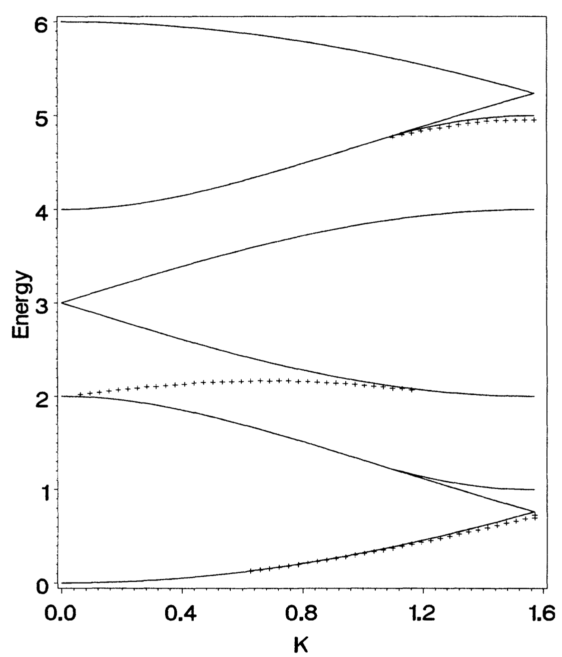

FIG. 4. Two-magnon branches of the alternating spin Heisbenberg chain are indicated by crosses. The results correspond to the values $S=1$, $S'=\frac{1}{2}$, and $a=1$. The energy is the dimensionless quantity $E/G_1^{(1)}$.

independent of the parameters $G_2^{(1)}$ and $G_2^{(2)}$ which is expected since setting $S'=\frac{1}{2}$ restricts the form of the Hamiltonian to Heisenberg exchange. The bound states for this system are again similar to those obtained for the $S=\frac{1}{2}$ alternating-bond Heisenberg chain, however, there are some interesting differences. Figure 4 shows the bound-state spectrum for the case $S=1$ and $S'=\frac{1}{2}$. The binding energy of the two bound states below the acoustic-acoustic continuum decreases at $K=\pi/2$ as S increases and hence the energy gap at the Brillouin-zone boundary also decreases with S. Similarly the binding energy of the state below the optic-optic continuum decreases at $K=\pi/2$ as S increases. These differences are what we would expect as the large-S limit is approached. However, the behavior of the state below the mixed-mode continuum is unusual. For $S=1$ this bound-state branch touches the acoustic-acoustic continuum at $K=0$ and also touches the mixed constraints at $K=\pi/2$. The energy of this state is $E/G_1^{(1)}=2S$ at $K=0$ for all $S>\frac{1}{2}$, whereas the energy of the continuum at $K=0$ is $4S'$. Consequently, it is only for $S=1$ that this state is connected to the upper edge of the acoustic-acoustic continuum at $K=0$. For any $S>1$ this connection is broken. More generally, this connection between bound state and continuum edge was found to be present for larger values of S'. When $S'>\frac{1}{2}$, the Hamiltonian is not restricted to the Heisenberg form. However, if we choose the Heisenberg form and have $S=S'+\frac{1}{2}$, then the connection between the two continua is preserved for all S'.

IV. REAL-SPACE SCALING APPROACH

The equations [(11) and (13)] for the two-magnon excitations were solved in Sec. III by first expanding the various amplitudes in terms of the eigenvectors of the noninteracting one-magnon states. Another approach to solving these equations is based upon the ideas of the real-space rescaling methods used to study critical phenomena. As described in the paper by Bell, Loly, and Southern,[8] if we group the four amplitudes for two spin deviations within a unit cell in the form of a column vector U_{2r}, then the two-magnon equations can be expressed concisely as follows:

$$\begin{aligned} MU_{2r} &= V_p U_{2r+2} + V_m U_{2r-2}, \quad r>0 \\ M_0 U_0 &= V_p U_2, \quad r=0 \end{aligned} \tag{23}$$

where $r=0,1,2,\ldots$ labels the unit cells. The 4×4 matrices M, M_0, V_p, V_m are functions of the $G_m^{(i)}$, the total wave vector K, and the two-magnon energy E_2. The rescaling approach to solving these equations involves constructing a transformation for these matrices which uses a cell of interest as a reference point and which eliminates every other unit cell. The equations for the remaining cells have the same general form as the original set but the matrices are renormalized. For example, using the cell $r=0$ as a reference, we have

$$
\begin{aligned}
M' &= M - V_m M^{-1} V_p - V_p M^{-1} V_m \, , \\
M'_0 &= M_0 - V_p M^{-1} V_m \, , \\
V'_p &= V_p M^{-1} V_p \, , \\
V'_m &= V_m M^{-1} V_m \, .
\end{aligned} \tag{24}
$$

The spectral properties of the system can be easily obtained by iterating this transformation until the matrices V_p and V_m approach zero. A small imaginary part must be added to the two-magnon excitation energy E_2 for convergence.

The local densities of states for two excitations separat-

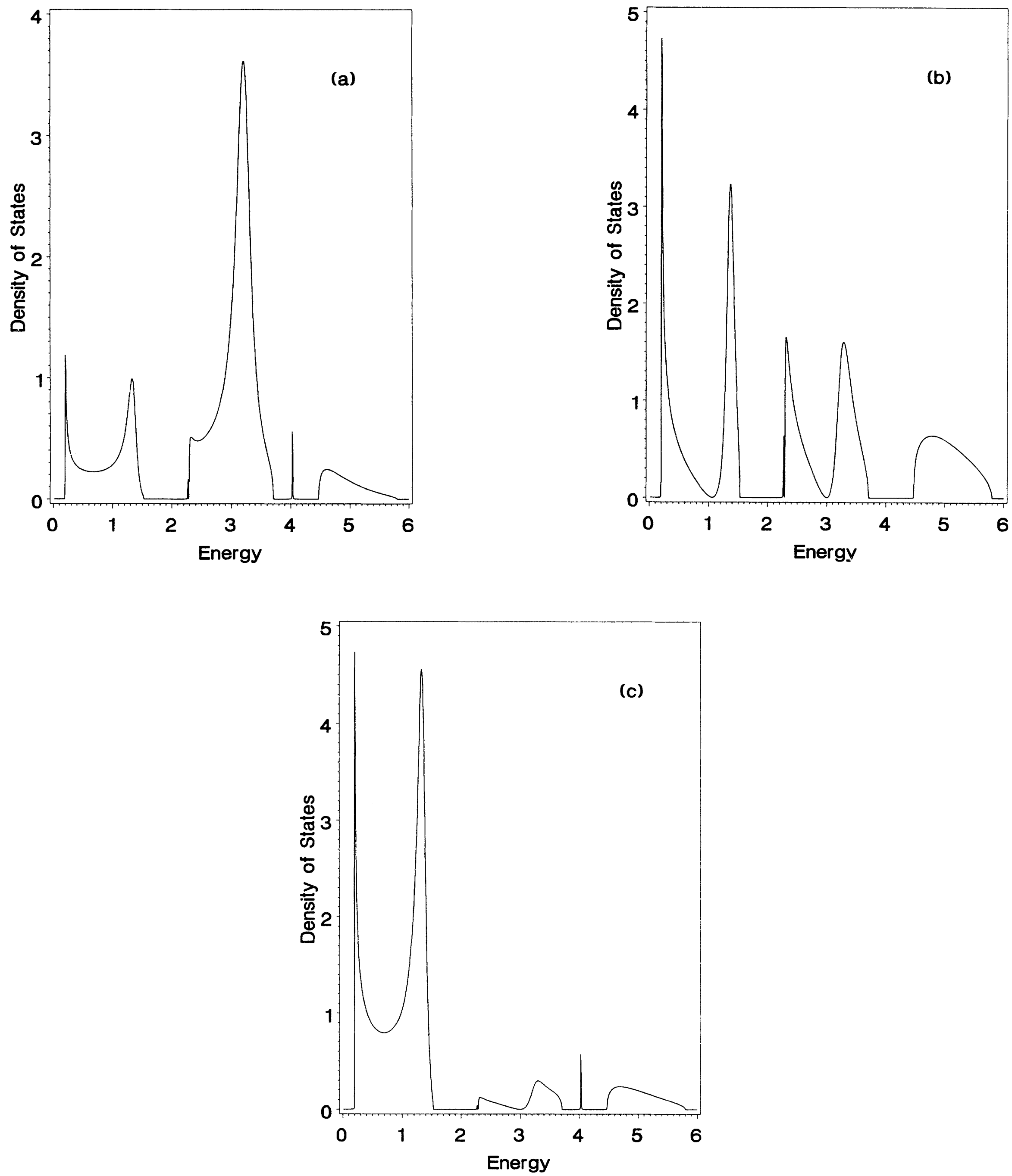

FIG. 5. Densities of states for (a) two deviations on the same site, (b) two deviations separated by a strong bond, and (c) two deviations separated by a weak bond for the $S=1$ alternating-bond Heisenberg chain at $K=\pi/4$. The energy is the dimensionless quantity $E/G_1^{(1)}$.

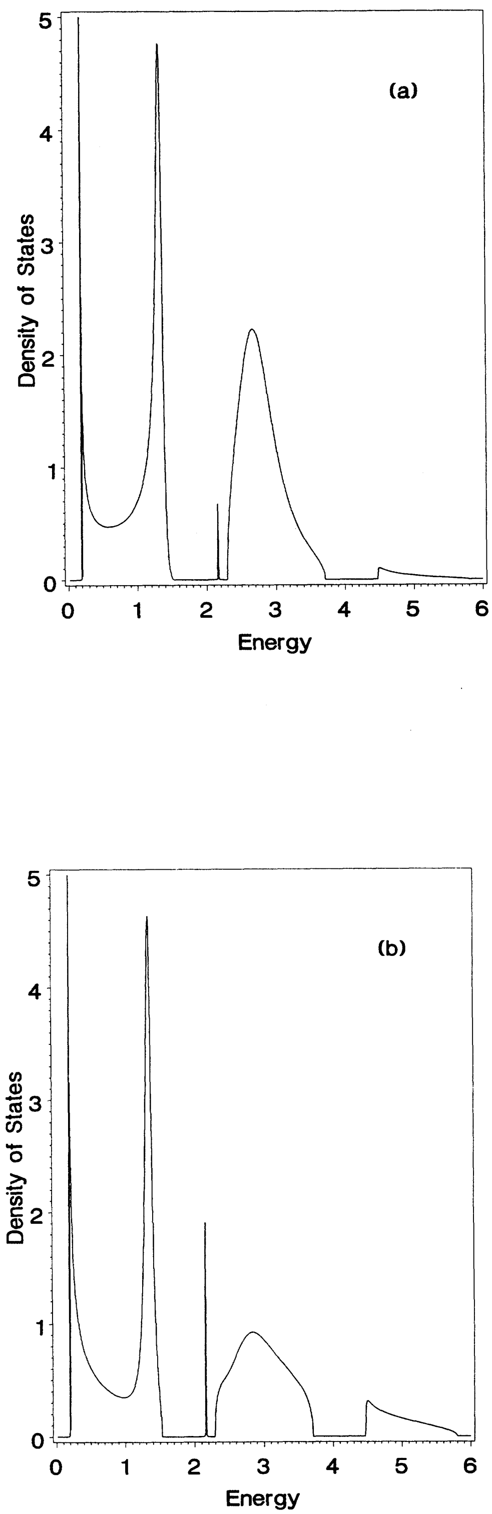

FIG. 6. Densities of states for (a) two deviations on the same $S=1$ site and (b) two deviations on neighboring sites for the $S=1$, $S'=\frac{1}{2}$ alternating-spin Heisenberg chain at $K=\pi/4$. The energy is the dimensionless quantity $E/G_1^{(1)}$.

ed by any distance can be obtained from the inverse of the limiting form of M_0. If we fix the value of K and plot these spectral functions against E_2, then contributions from both bound states and scattering states are easily identified. In the regions of energy outside the two-magnon continua, the procedure requires only five or six iterations for convergence. Inside these regions, the convergence depends upon the magnitude of the imaginary part in the energy. We have used an imaginary part equal to 10^{-5} and convergence requires typically 20 to 25 iterations. In Fig. 5 we show the local densities of states for case 4 in Sec. III which describes a uniform-spin $S=1$ Heisenberg chain with bonds that alternate in strength ($a=0.5$). The results for spin deviations on the same and neighboring sites for $K=\pi/4$ are presented. There are two of the latter kind corresponding to having the deviations at the ends of the two types of bonds. The bound states discussed in Sec. III are clearly visible in all three response functions as δ-function contributions. The resonant states show up as sharp peaks within the continua. Only the acoustic-acoustic continuum can be identified as having a resonant state. As K increases towards the Brillouin-zone boundary, this peak narrows and approaches the lower edge of the continuum finally emerging as a true bound state.

Finally in Fig. 6 we show the response functions for case 5 of Sec. III which corresponds to a system with alternating spins. The spins have magnitudes $S=1$ and $S'=\frac{1}{2}$, respectively, and the total wave vector K has the value $\pi/4$. Again, only the acoustic-acoustic continuum has a resonant mode and its behavior across the zone is similar to the alternating-bond case. Hence, for the Heisenberg Hamiltonian, both the alternating-bond and alternating-spin chains have similar bound state and resonant structure in their two-magnon spectra. However, the alternating-spin chain seems to have some special bound-state features when the spin magnitudes differ by $\frac{1}{2}$.

V. SUMMARY

We have obtained exact results for the two-magnon excitation spectrum for the general case of an alternating-bond and alternating-spin chain. In special cases analytic results for the bound-state branches were found. In more general cases, a numerical procedure based on real-space rescaling methods was used. This procedure provides a very direct way of obtaining information about both the bound-state and resonant-state contributions to the spectral properties.

The motivation for our study was to try to identify systems which may be completely integrable. These systems have been shown[9,10] to have special features in their two-magnon spectra. Although we have not been able to identify any new cases with these features, we did observe that in the case of alternating Heisenberg spin chains that a bound-state branch forms a connection between two of the continua when the spin magnitudes differ by $\frac{1}{2}$. We are currently studying this case using the Bethe ansatz[4,5] to ascertain if it corresponds to an integrable system. The antiferromagnetic version of such a model would be quite interesting and its low-energy excitation spectrum could then be obtained. These results could then be used to calculate the thermodynamic properties of bimetallic chains.[1-3]

ACKNOWLEDGMENTS

This work was supported by the Natural Sciences and Engineering Research Council of Canada. Two of the authors (B.W.S.) and (D.A.L.) also acknowledge the support of NATO under Research Grant No. 0087/87.

[1] Y. Journaux, P. Van Koningsbruggen, F. Lloret, K. Nakatani, Y. Pei, O. Kahn, and J. P. Renard, J. Phys. (Paris) Colloq. **49**, C8-851 (1988).

[2] F. Sapiña, E. Coronado, M. Drillon, R. Georges, and D. Beltrán, J. Phys. (Paris) Colloq. **49**, C8-1423 (1988).

[3] M. Drillon, E. Coronado, R. Georges, J. C. Gianduzzo, and J. Curely, Phys. Rev. B **40**, 10 992 (1989).

[4] H. A. Bethe, Z. Phys. **71**, 205 (1931).

[5] Y. A. Izyumov and Y. N. Skryabin, *Statistical Mechanics of Magnetically Ordered Systems* (Plenum, New York, 1988).

[6] L. A. Takhtajan, Phys. Lett. **87A**, 479 (1982).

[7] H. M. Babujian, Phys. Lett. **90A**, 479 (1982).

[8] S. C. Bell, P. D. Loly, and B. W. Southern, J. Phys. Condens. Matter **1**, 9899 (1989).

[9] F. D. M. Haldane, J. Phys. C **15**, L1309 (1982).

[10] A. V. Chubukov and D. V. Khveshenko, J. Phys. C **20**, L505 (1987).

[11] N. A. Krupennikov, Phys. Met. Metall. **44**, 10 (1979).

[12] E. Schrödinger, Proc. R. Ir. Acad. Sect. A **47**, 39 (1941).

[13] B. W. Southern, T. S. Liu, and D. A. Lavis, Phys. Rev. B **39**, 12 160 (1989).

[14] J. B. Parkinson, J. Phys. C **21**, 3793 (1988).

[15] M. T. Batchelor and M. N. Barber, J. Phys. A **23**, L15 (1990).