Scaling approach to two-magnon excitations in quantum spin chains

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(Received 19 September 1988)

A scaling approach to two-magnon excitations in general S quantum spin chains is presented. The local densities of two-magnon excitations can be obtained directly without solving the one-magnon problem beforehand. Special features of the excitation spectrum are related to the complete integrability of the model.

I. INTRODUCTION

The study of excitations in generalized Heisenberg spin chains with general spin S has received considerable attention recently.[1-7] The complete excitation spectrum consists of both bound states and resonant states within the continuum of scattering states. In the case of a ferromagnetic ground state, the one-magnon and two-magnon problems can be solved exactly.[8] For special models, the m-magnon problem can also be solved for arbitrary values of m using the Bethe ansatz[9] or the quantum inverse scattering method.[10,11] These special models are referred to as completely integrable, whereas the general spin S model is not integrable. The work of Chubukov and Khveshenko[1] was concerned with finding the conditions under which the two-magnon excitations of the general model have the same structure as in the integrable models. They suggest that this may be a method for identifying integrable cases. Haldane[12,13] had conjectured earlier that the bound and resonant type of m-magnon states form $p=\min(m,2S)$ branches in the general model but that all branches are real and continuous across p Brillouin zones in an extended zone scheme for the integrable models. In the nonintegrable models, the branches enter the continuum and gaps occur at the Brillouin-zone boundaries.

In the present work we describe a method to calculate two-magnon excitations in ferromagnets using real-space rescaling methods. The pure one-magnon problem as well as the one-magnon problem with impurities has been described previously.[14,15] Our approach to the two-magnon problem maps it onto an effective tight-binding Hamiltonian. General properties are easily extracted for the most general isotropic spin Hamiltonian for spin S. The special cases which correspond to completely integrable models are identified with special properties of the two-magnon excitations, in agreement with the results of Chubukov and Khveschenko. In addition, our results suggest that certain values of the couplings of the general model correspond to systems with limited integrability.

In the next section we describe the general S model and consider the two-magnon excitation spectrum for the ferromagnetic system. The scaling method is described in Sec. III along with our results. Finally, we summarize our findings in Sec. IV.

II. THE MODEL

We consider the following Hamiltonian for a chain of spin S quantum spins

$$H=-\sum_{i=1}^{N}\sum_{n=1}^{2S} J^{(n)}(\mathbf{S}_i\cdot\mathbf{S}_{i+1})^n . \tag{1}$$

The interactions are restricted to nearest neighbors, but further neighbors can also be included as well as various types of anisotropies without difficulty. The Hamiltonian in (1) is the most general form for spin S with SU(2) symmetry. The model with only the $n=1$ term is the usual Heisenberg model. Schrödinger[16] has determined the values of the $J^{(n)}$ which yield the spin-exchange operator for general S which has SU$(2S+1)$ symmetry. This special model is completely integrable.[17] Another special case which is completely integrable corresponds to the values of the $J^{(n)}$ of Takhtajan[10] and Babujian.[11]

These special cases are most easily described by considering an isolated pair of nearest-neighbor spins. The total angular momentum j of the pair can take the values $j=0,1,\ldots,2S$, and the energy eigenvalue of the pair in state j is

$$\lambda_j=-\sum_{n=1}^{2S} J^{(n)}[j(j+1)/2-S(S+1)]^n . \tag{2}$$

It is convenient to define the eigenvalues with respect to the state of maximum j and ratios of these quantities as follows:

$$\alpha_m(S)=\lambda_{2S-m}-\lambda_{2S} ,$$
$$g_m(S)=\frac{\alpha_m(S)}{\alpha_1(S)} , \tag{3}$$

where $m=0,1,\ldots,2S$. Note that $g_0(S)=0$ and $g_1(S)=1$ for all values of the $J^{(n)}$ in (1). The values of the $J^{(n)}$ which give the Schrödinger exchange operator for a pair of spins correspond to

$$g_m(S)=\frac{1-(-1)^m}{2}\ , \tag{4a}$$

for $m=0,1,\ldots,2S$. The values of the $J^{(n)}$ of Takhtajan and Babujian correspond to

$$g_m(S)=2S[\psi(2S+1)-\psi(2S+1-m)]\ , \tag{4b}$$

where ψ is the derivative of the logarithm of the gamma function.

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 ground-state energy per site is

$$E_0=\lambda_{2S}=-\sum_{n=1}^{2S} J^{(n)}S^{2n}\ . \tag{5}$$

The one-magnon eigenstates are plane waves with excitation energy

$$E_1=\alpha_1(S)(1-\cos Ka)\ , \tag{6a}$$

where using (2) and (3) we have

$$\alpha_1(S)=\sum_{n=1}^{2S} J^{(n)}S^n[S^n-(S-2)^n]\ . \tag{6b}$$

For stability of the ground state with respect to one-magnon excitations we require $\alpha_1(S)$ to be positive or zero. Parkinson[6] has recently studied an $S=1$ model with pure biquadratic exchange which has $\alpha_1=0$.

The two-magnon excitations are solutions of the Schrödinger equation which can be written in the basis of two-spin deviation states $|l,m\rangle=S_l^+S_m^+|0\rangle$, $(l\geq m)$. Using center of mass and relative coordinates for the sites l and m, the normalized amplitudes $C_{l,m}$ in this basis can be expressed as[18,19]

$$C_{l,m}=e^{iKa(l+m)/2}c_{|l-m|}\ . \tag{7}$$

In this mixed orthonormal basis $|K,r\rangle$, K represents the total momentum of the pair and $r=|l-m|$ is their relative separation in units of the lattice spacing a. The equations for the relative amplitudes c_r take the following form:

$$\begin{aligned}&(E-\varepsilon_0)c_0=V_0c_1\ ,\\&(E-\varepsilon_1)c_1=V_0c_0+Vc_2\ ,\\&(E-\varepsilon)c_r=V(c_{r-1}+c_{r+1})\ (r>1)\ ,\end{aligned} \tag{8}$$

where E is measured relative to the ground-state energy E_0 and

$$\begin{aligned}&\varepsilon_0=\alpha_1(S)(1-\cos Ka)+\frac{2S\alpha_2(S)}{4S-1}(1+\cos Ka)\ ,\\&\varepsilon_1=\alpha_1(S)+\frac{(2S-1)\alpha_2(S)}{4S-1}\ ,\\&\varepsilon=2\alpha_1(S)\ ,\\&V_0=\frac{-2\sqrt{S(2S-1)}\alpha_2(S)}{4S-1}\cos(Ka/2)\ ,\\&V=-\alpha_1(S)\cos(Ka/2)\ .\end{aligned} \tag{9}$$

The two-magnon spectrum depends only on α_1 and α_2, which from (2) and (3) is given by

$$\alpha_2(S)=\sum_{n=1}^{2S} J^{(n)}[S^{2n}-(S^2-4S+1)^n]\ . \tag{10}$$

The above equations are equivalent to those that are encountered in tight binding systems with defects. In the present case, the relative coordinate describes the separation of one-magnon excitations which interact on the same site or when on nearest-neighbor sites. The problem can be solved using real-space rescaling methods.

However even before solving (8) it is apparent from (9) that special cases arise. For example, if $V_0=0$, then the amplitude c_0 is completely decoupled from the others. This is true for $S=\frac{1}{2}$ where c_0 is an unphysical amplitude corresponding to two deviations on the same site. This is also the case for all $S\geq 1$ when $\alpha_2=0$. Now c_0 is a physical amplitude, and the solution $E=\varepsilon_0$ has the same form as the one-magnon excitations in (6a) and represents a propagating quadrupolar wave.[20] The equations for the remaining amplitudes reduce to the $S=\frac{1}{2}$ case with α_1 replacing the usual exchange constant $J^{(1)}$. Hence in this case, the two-magnon bound states have the same structure as in the $S=\frac{1}{2}$ integrable model. Note that $\alpha_2=0$ corresponds to the value of g_2 in (4a). This special property of the two-magnon excitations does not specify the remaining values of the g_m $(m>2)$ and hence occurs on a hypersurface of the couplings $J^{(n)}$ when $S\geq\frac{3}{2}$.

A second special case occurs when α_2/α_1 takes the value of g_2 in (4b). At $Ka=\pi$, we have both V and V_0 equal to zero and $\varepsilon_0=\varepsilon_1=\varepsilon$. That is, all two-magnon excitations are degenerate at the first Brillouin-zone boundary and there are no gaps. As above, this property occurs on a hypersurface of the couplings $J^{(n)}$ for $S\geq\frac{3}{2}$. For $S=1$ the hypersurface collapses to a point.[2] For general values of g_2 there is a gap at $Ka=\pi$ given by $|\varepsilon_0-\varepsilon_1|$.

A third special situation arises when $\alpha_1=0$ as in the model studied by Parkinson.[6] In this case only the amplitudes c_0 and c_1 are coupled and a propagating two-magnon solution $E=\varepsilon_0+\varepsilon_1$ is stable for $\alpha_2>0$.

III. SCALING METHOD

In a previous series of papers[14,15] we have described a rescaling method for excitations in tight-binding systems. The basic idea is to construct a transformation on the system of equations which leaves their form invariant but renormalizes the various parameters appearing in them. The spectral properties of the system can then be determined by iterating the transformation. In the present problem, we can obtain a transformation for a general scaling factor b as follows. The index 0 is used as a reference point and the amplitudes $(r=1,\ldots,b-1,$ $b+1,\ldots,)$ are eliminated from the equations. The transformation is

$$
\begin{aligned}
V_0' &= \frac{V_0 V}{(E-\varepsilon_1)U_{b-2}-VU_{b-3}} , \\
\varepsilon_1' &= \varepsilon + V\left[\frac{(E-\varepsilon_1)U_{b-3}-VU_{b-4}}{(E-\varepsilon_1)U_{b-2}-VU_{b-3}} + \frac{U_{b-2}}{U_{b-1}}\right] , \\
\varepsilon_0' &= \varepsilon_0 + \frac{V_0^2 U_{b-2}}{(E-\varepsilon_1)U_{b-2}-VU_{b-3}} , \\
\varepsilon' &= \varepsilon + \frac{2VU_{b-2}}{U_{b-1}} , \\
V' &= \frac{V}{U_{b-1}} ,
\end{aligned}
\tag{11}
$$

where $U_b = \sin(b+1)\theta/\sin\theta$ and $\cos\theta = (E-\varepsilon)/2V$.

It is easily verified that for $b=1$ all parameters remain unchanged. The transformation for $b=2$ corresponds to the usual decimation procedure where every other amplitude is eliminated and has been used previously to calculate the local Green's functions for defects in an infinite chain. Analytic results for the two-magnon response functions can be obtained by taking the limit $b \to \infty$. Assuming the two-magnon excitation energy E to have a small positive imaginary part, we find that in the limit $b \to \infty$ the parameters in (11) approach the following values:

$$
\begin{aligned}
&\varepsilon_0' \to \varepsilon_0^{(\infty)} = \varepsilon_0 + \frac{V_0^2}{E-\varepsilon_1 - VQ} , \\
&\varepsilon_1' \to \varepsilon_1^{(\infty)} = \varepsilon + 2VQ , \\
&\varepsilon' \to \varepsilon^{(\infty)} = \varepsilon + 2VQ , \\
&V_0' \to V_0^{(\infty)} = 0 , \\
&V' \to V^{(\infty)} = 0 ,
\end{aligned}
\tag{12}
$$

where

$$
\begin{aligned}
Q &= \Delta + (\Delta^2 - 1)^{1/2}, \quad \Delta > +1 ; \\
&= \Delta - (\Delta^2 - 1)^{1/2}, \quad \Delta < -1 ; \\
&= \Delta + i(1-\Delta^2)^{1/2}, \quad |\Delta| < 1 ;
\end{aligned}
\tag{13}
$$

and $\Delta = (E-\varepsilon)/2V$. Hence, solutions of (8) which have $c_0 \neq 0$ are given by $E = \varepsilon_0^{(\infty)}$. In general, this relation leads to a cubic equation for E. However, in the special cases mentioned in the preceding section, the cubic reduces to either a quadratic or linear equation.

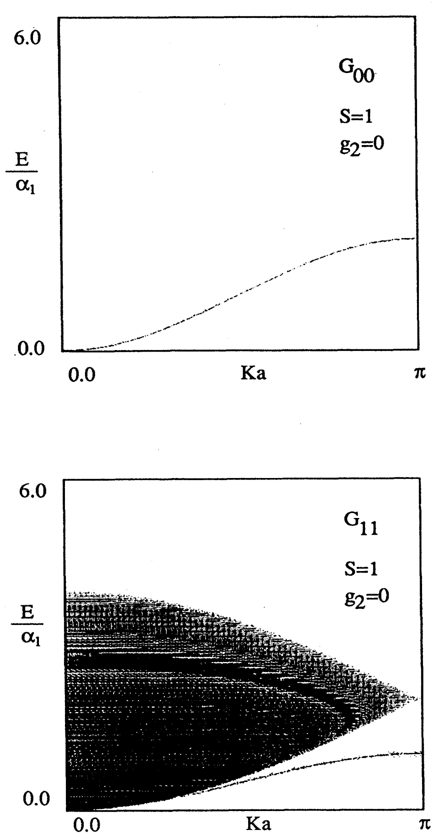

FIG. 1. The imaginary parts of the two-magnon response functions G_{00} and G_{11} are represented by gray scales in the E/α_1-Ka plane. The spin value is $S=1$ and $g_2=0$.

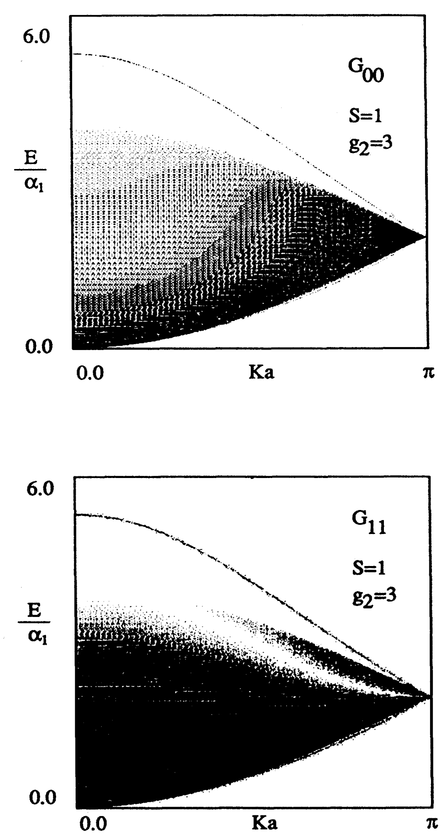

FIG. 2. The imaginary parts of the two-magnon response functions G_{00} and G_{11} are represented by gray scales in the E/α_1-Ka plane. The spin value is $S=1$ and $g_2 = g_* = 3$.

We define the two-magnon Green's functions as follows:

$$G_{rs}(E,K)=\left\langle K,r\left|\frac{1}{E-H}\right|K,s\right\rangle . \tag{14}$$

The imaginary part of $G_{00}=1/E-\varepsilon_0^{(\infty)}$ gives the density of states for two magnons on the same site. A similar transformation to that in (11) can be used to obtain an analytic expression for G_{11} by using the amplitude c_1 in (8) as a reference point.

For $\alpha_1>0$, the ferromagnetic ground state is stable provided $\alpha_2\geq 0$. The behavior is special for $g_2=0$ and $g_2=g_*=(4S-1)/(2S-1)$ corresponding to the integrable cases. For $g_2=0$, the poles of G_{00} correspond to a propagating quadrupolar wave which has the same energy as the one-magnon excitation. G_{11} has a contribution from the continuum and a bound state below with

$$E=\frac{\alpha_1}{2}(1-\cos Ka) ,$$

which is the solution for $S=\frac{1}{2}$ with α_1 replacing $J^{(1)}$. The imaginary parts of G_{00} and G_{11} are represented in Fig. 1 for $S=1$ and $g_2=0$ using a gray scale plot. At the other integrable point, $g_2=g_*$, both G_{00} and G_{11} have contributions from the continuum and two bound states which lie entirely outside the continuum and meet at $Ka=\pi$ with no gap, as shown in Fig. 2. The energies of these branches are

$$\frac{E}{2\alpha_1}=1+\frac{u\delta^2\pm\delta[1-u(1-\delta^2)]^{1/2}}{1-u} , \tag{15}$$

where $\delta=\cos(Ka/2)$ and $u=1/4S^2$. This expression agrees with that obtained by Chubukov and Khveshenko.[1]

In the range $0<g_2<2$, there is only one bound state below the continuum with the one above first appearing at $K=0$ when $g_2=2$. Figure 3 shows a typical spectrum for $S=1$ and $g_2=1$. For all values of $0<g_2<g_*$, the imaginary part of G_{11} has a node within the continuum extending across the entire zone and is located at $E=\varepsilon_0$. For $2<g_2<g_*$ there is one bound state below, which extends across the entire zone, and another one above entering the continuum when

$$\delta=\delta^*=\frac{g_*-g_2}{\frac{2S}{2S-1}g_2-g_*} . \tag{16}$$

A typical spectrum for $S=1$ and $g_2=2.5$ is shown in Fig. 4. When $g_2>g_*$ the situation is reversed with the lower bound state entering the continuum when $\delta=-\delta^*$. For $S=1$, our results are in complete agreement with Chiu-Tsao *et al.*[20]

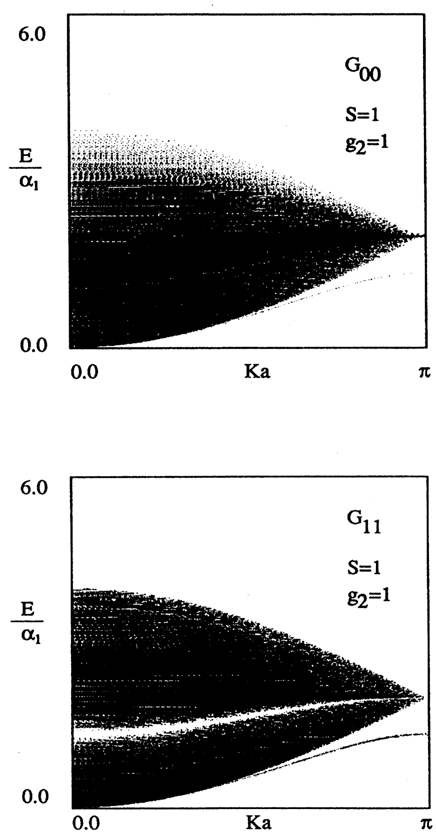

FIG. 3. The imaginary parts of the two-magnon response functions G_{00} and G_{11} are represented by gray scales in the E/α_1-Ka plane. The spin value is $S=1$ and $g_2=g_*/3=1$.

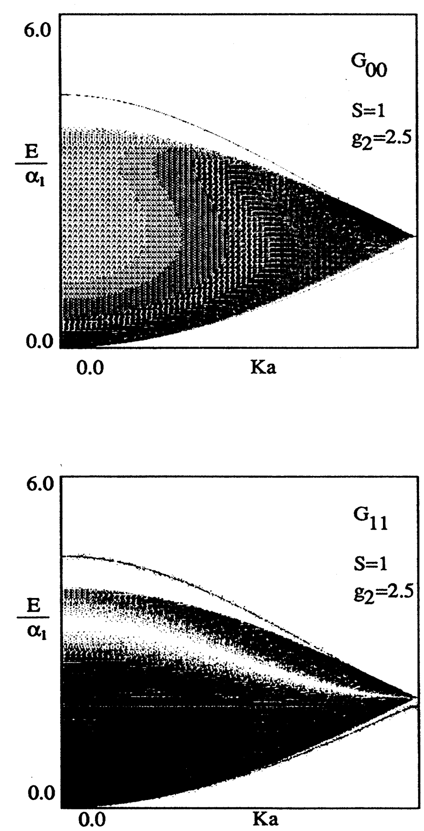

FIG. 4. The imaginary parts of the two-magnon response functions G_{00} and G_{11} are represented by gray scales in the E/α_1-Ka plane. The spin value is $S=1$ and $g_2=5g_*/6=2.5$.

Affleck *et al.*[4] have studied antiferromagnetic models based on projection operators which have limited integrability. The ferromagnetic version of these models which project into the $j=2S$ state of a neighboring pair of spins has $\alpha_1>0$ and $g_m=1$ for $m=1,2,\ldots,2S$. We do not find any special behavior of the two-magnon spectrum when $g_2=1$.

IV. SUMMARY

We have presented a real-space rescaling approach to two-magnon excitations in general S quantum spin chains. The method can be used to calculate the two-magnon response functions directly, without the need to solve the one-magnon problem beforehand. For nearest-neighbor interactions, we have used a general scaling factor b to obtain analytic results for the two-magnon response functions. We have confirmed the earlier results of Chubukov and Khveshenko[1] and Haldane[12,13] that the two-magnon bound-state branches are real and continuous across the Brillouin-zone boundary when the general spin S model is completely integrable. The method is easily extended to the case of further-neighbor interactions or alternating bond systems.

The approach outlined in Sec. III can be used to study m-magnon excitations in the general S model. For three-magnon excitations[21,22] the resulting equations will involve $g_m(S)$, $m=1,2,3$ and special features are expected to be present when the g_m have values corresponding to the integrable cases. These special features occur on a hypersurface of the couplings $J^{(n)}$ in the two-magnon case when $S\geq\frac{3}{2}$. For the three-magnon case, this hypersurface will be reduced to a point if $S=\frac{3}{2}$. For $S\geq 2$, there should be special cases where both the two-magnon and three-magnon excitations have the same structure as in the integrable cases but not the excitations involving four or more magnons. These cases would correspond to situations with limited integrability. We are currently studying these possibilities.

ACKNOWLEDGMENTS

We would like to thank P. D. Loly for many useful discussions. 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.) acknowledge the support of North Atlantic Treaty Organization (NATO) under Research Grant No. 0087/87. T.S.L. is grateful to the Physics Department at the University of Manitoba for its kind hospitality.

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