Bethe ansatz for two-magnon bound states in anisotropic magnetic chains of arbitrary spin

N. Papanicolaou*
Department of Physics, University of Crete and Research Center of Crete, P.O. Box 1527, Heraklion, Crete GR-711 10, Greece

G. C. Psaltakis
Research Center of Crete, Institute of Electronic Structure and Laser, P.O. Box 1527, Heraklion, Crete GR-711 10, Greece
(Received 14 April 1986; revised manuscript received 11 August 1986)

The two-magnon spectra in anisotropic magnetic chains of arbitrary spin are derived by an elementary method which is an extension of Bethe's original ansatz for spin-$\frac{1}{2}$ systems. Applications are presented for quantum spin chains with uniaxial or Ising Anisotropy as well as chains with quartic exchange interactions. The nature of certain collective modes emerging in a $1/n$ expansion is also clarified.

I. INTRODUCTION

The study of bound states of magnons has been a subject of considerable interest since the early work of Bethe.[1] The Bethe ansatz for multimagnon states provided essentially complete information concerning the bound-state spectrum of spin-$\frac{1}{2}$ magnetic chains. Moreover a variety of one-dimensional problems have been solved exactly by suitable generalizations of the original ansatz.

The applicability of the Bethe ansatz is, however, limited to dynamical systems that are completely integrable. This limitation becomes evident already in the context of anisotropic magnetic chains of general spin $S>\frac{1}{2}$, for which integrability is doubtful except in very special cases.[2] Therefore more conventional methods had to be employed. For the two-magnon spectra, a Green's-function approach initiated by Wortis[3] has practically dominated all studies. This approach works in any dimension, provided the ground state is ferromagnetic, and also yields expressions for measurable quantities, namely the dynamic structure factors. Extensive calculations of the latter in one dimension have been carried out by Schneider and co-workers.[4]

Nevertheless we note that although lack of complete integrability would be crucial for three-magnon and multimagnon states, it puts little restriction on the dynamics of two-magnon states. Indeed, a Bethe-ansatz type of technique for evaluating the two-magnon bound-state frequencies of the completely *isotropic* ferromagnetic chain of arbitrary spin has already been used.[5] In our present work we show that in fact the original Bethe ansatz may be extended to the calculation of the two-magnon states also in *anisotropic* magnetic chains of arbitrary spin. Hence we are able to provide an alternative to Wortis's method for the special case of one-dimensional spin systems.

The present calculation furnishes a simple expression for the two-magnon wave function together with the energy spectrum. Details are given in Sec. II for a chain with an easy axis of magnetization due to a uniaxial anisotropy. The appearance of a single-ion bound state,[6] in addition to the usual exchange bound state, is confirmed and clarified. Section III extends the calculation to a variety of spin chains. Thus we study the effect of Ising anisotropy, planar chains in a spin-flop phase caused by a magnetic field and Heisenberg models incorporating quartic exchange interactions.

A by-product of this analysis is the illumination of the nature of certain collective modes emerging in a $1/n$ expansion, which are identified with the single-ion bound states. This and related issues are discussed in Sec. IV. Our conclusions are summarized in Sec. V.

II. THE TWO-MAGNON STATE

The method will be illustrated in detail for a magnetic chain described by the Hamiltonian

$$H=-\sum_{n=1}^{N}[J(\mathbf{S}_n\cdot\mathbf{S}_{n+1})+D(S_n^z)^2]\ ,\qquad \mathbf{S}_n^2=S(S+1),\ \ J,D\geq 0\ , \tag{2.1}$$

assuming periodic boundary conditions. Since both J and D are positive, the ground state Φ_0 is fully ordered in the z direction and its energy is given by

$$H\Phi_0=E_0\Phi_0,\ \ E_0=-N(J+D)S^2\ . \tag{2.2}$$

Let now Φ_n denote the state obtained from Φ_0 by decreasing the azimuthal spin by one unit at the site n. The one-margon eigenstate is constructed as

$$\Psi_1=\sum_{n=1}^{N}e^{ikn}\Phi_n,\ \ H\Psi_1=E_1\Psi_1\qquad E_1=E_0+\omega,\ \ \omega=2SJ(1-\cos k)+(2S-1)D\ . \tag{2.3}$$

Here ω is the one-magnon excitation energy developing a mass gap for $S>\frac{1}{2}$ due to the anisotropy.

In order to gain some insight about the nature of two-magnon states we consider first the extreme limit of large D, or $J\simeq 0$. The moments in (2.1) uncouple in this limit. Two-magnon states can be constructed either by reducing the azimuthal spin by two units at a single site or by reducing its value by one unit at two different sites. In the former case the excitation energy is

$$\Omega_{\rm I}=D[S^2-(S-2)^2]=4(S-1)D\ , \tag{2.4}$$

whereas in the latter case,

$$\Omega_{\rm II}=2D[S^2-(S-1)^2]=2(2S-1)D\ . \tag{2.5}$$

Clearly then, two distinct two-magnon bound states will emerge when the exchange interaction is taken into consideration. States of type I may be called single-ion bound states[6] while those of type II will denote the usual exchange bound states. No such distinction is possible in the limit of vanishing anisotropy.

The actual construction of these states for arbitrary values of J and D follows steps familiar from the original Bethe ansatz.[7] Keeping with the notation introduced in the preceding paragraphs, $\Phi_{n,m}$ is the state with two spins reduced by one unit at the sites n and m. By convention, the special case $\Phi_{n,n}$ is the state with the spin reduced by two units at the site n. Taking also into consideration the obvious symmetry $\Phi_{n,m}=\Phi_{m,n}$, a general two-magnon state may be written in the form

$$\Psi_2=\sum_{n=1}^{N}\sum_{m=n}^{N}C_{n,m}\Phi_{n,m}\ . \tag{2.6}$$

Our task is to determine the expansion coefficients $C_{n,m}$ so that Ψ_2 becomes an eigenstate of the Hamiltonian,

$$H\Psi_2=E_2\Psi_2=(E_0+\Omega)\Psi_2\ , \tag{2.7}$$

where E_0 is the ground-state energy (2.2) and Ω is the two-magnon excitation energy.

We thus insert (2.6) in (2.7) and derive a set of linear equations for the $C_{n,m}$. The calculation is straightforward but requires some care concerning the following point. Three cases have to be distinguished, namely,

$$\begin{aligned}
H\Phi_{n,n}&=[E_0+4SJ+4(S-1)D]\Phi_{n,n}-J[S(2S-1)]^{1/2}(\Phi_{n,n+1}+\Phi_{n-1,n})\ ,\\
H\Phi_{n,n+1}&=[E_0+(4S-1)J+2(2S-1)D]\Phi_{n,n+1}-J[S(2S-1)]^{1/2}(\Phi_{n,n}+\Phi_{n+1,n+1})-SJ(\Phi_{n,n+2}+\Phi_{n-1,n+1})\ ,\\
H\Phi_{n,m}&=[E_0+4SJ+2(2S-1)D]\Phi_{n,m}-SJ(\Phi_{n+1,m}+\Phi_{n-1,m}+\Phi_{n,m+1}+\Phi_{n,m-1})\ ,\quad m\geq n+2\ .
\end{aligned} \tag{2.8}$$

The corresponding linear equations for the $C_{n,m}$ read

$$\begin{aligned}
&[\Omega-4SJ-4(S-1)D]C_{n,n}+J[S(2S-1)]^{1/2}(C_{n,n+1}+C_{n-1,n})=0\ ,\\
&[\Omega-(4S-1)J-2(2S-1)D]C_{n,n+1}+J[S(2S-1)]^{1/2}(C_{n,n}+C_{n+1,n+1})+SJ(C_{n-1,n+1}+C_{n,n+2})=0\ ,\\
&[\Omega-4SJ-2(2S-1)D]C_{n,m}+SJ(C_{n-1,m}+C_{n,m-1}+C_{n+1,m}+C_{n,m+1})=0\ .
\end{aligned} \tag{2.9}$$

Before presenting the complete solution of Eqs. (2.9) we wish to consider some special cases which anticipate important features of the general result. Hence

$$\begin{aligned}
&C_{n,n}=(-1)^n,\ \ C_{n,n+1}=0=C_{n,m}\ ,\\
&\Omega=4SJ+4(S-1)D\equiv\Omega_{\rm I}\ ,
\end{aligned} \tag{2.10}$$

and

$$\begin{aligned}
&C_{n,n}=0,\ \ C_{n,n+1}=(-1)^n,\ \ C_{n,m}=0\ ,\\
&\Omega=(4S-1)J+2(2S-1)D\equiv\Omega_{\rm II}\ ,
\end{aligned} \tag{2.11}$$

are obvious solutions of (2.9). The significance of these solutions becomes evident by comparing them with (2.4) and (2.5) in the limit $J\to 0$. As expected, the distinction between single-ion and exchange bound states persists in the full problem. However, the simplicity of the exact results (2.10) and (2.11) was, perhaps, more difficult to anticipate. As we shall see later these solutions correspond to momenta at the zone boundary.

We now turn to the main point of this paper. The linear system (2.9) is solved through a Bethe ansatz. More specifically, the third equation in (2.9) is solved by

$$\begin{aligned}
C_{n,m}&=\exp[i(k_1n+k_2m+\phi/2)]\\
&\quad+\exp[i(k_1m+k_2n-\phi/2)]\ ,\\
\Omega&=2(2S-1)D+4SJ[1-\tfrac{1}{2}(\cos k_1+\cos k_2)]\ ,
\end{aligned} \tag{2.12}$$

where the wave vectors k_1,k_2 and the phase shift ϕ are at this point arbitrary constants which may be complex. Restrictions on these constants arise from extending (2.12) to the first two equations in (2.9). This is accomplished in two steps.

We solve the first equation in (2.9) for $C_{n,n}$,

$$C_{n,n}=-\frac{J[S(2S-1)]^{1/2}}{\Omega-4SJ-4(S-1)D}(C_{n,n+1}+C_{n-1,n})\ , \tag{2.13}$$

which is then inserted into the second equation to yield

$$\begin{aligned}
&[\Omega-(4S-1)J-2(2S-1)D]C_{n,n+1}+SJ(C_{n-1,n+1}+C_{n,,n+2})\\
&\qquad=\frac{S(2S-1)J^2}{\Omega-4SJ-4(S-1)D}(2C_{n,n+1}+C_{n-1,n}+C_{n+1,n+2})\ .
\end{aligned} \tag{2.14}$$

This equation may be viewed as an algebraic constraint on the constants k_1, k_2 and ϕ by virtue of (2.12). Lengthy but straightforward algebra leads to the constraint

$$\cot\left[\frac{\phi}{2}\right]=\frac{[1+(2S-1)R]\sin[(k_1-k_2)/2]}{2S\cos[(k_1+k_2)/2]-[1+(2S-1)R]\cos[(k_1-k_2)/2]}\ ,$$
$$R=\frac{1+\cos(k_1+k_2)}{\cos k_1+\cos k_2-d},\quad d=D/SJ\ . \tag{2.15}$$

It is worth noting that in the absence of anisotropy ($d=0$), Eq. (2.15) becomes

$$\cot\left[\frac{\phi}{2}\right]=\frac{1}{2}\left[\cot\frac{k_1}{2}-\cot\frac{k_2}{2}\right]\left[1+(2S-1)\frac{\cos[(k_1+k_2)/2]}{\cos[(k_1-k_2)/2]}\right]\ . \tag{2.16}$$

and reduces to Bethe's expression at $S=\frac{1}{2}$.

To complete the solution of (2.9) we note that Eq. (2.13) may be written as

$$C_{n,n}=\left[\frac{2S-1}{S}\right]^{1/2}\frac{\cos(k_1-\phi/2)+\cos(k_2+\phi/2)}{\cos k_1+\cos k_2-d}\exp[i(k_1+k_2)n]\ . \tag{2.17}$$

The wave function constructed through Eqs. (2.12), (2.15), and (2.17) is the general two-magnon state depending on the wave vectors k_1 and k_2, the latter being restricted only by the periodic boundary conditions. This wave function describes scattering as well as bound states of magnons. We concentrate on bound states which are characterized by parameters k_1, k_2, and ϕ of the form

$$k_1=u+iv,\quad k_2=u-iv,\quad \phi=iNv\ , \tag{2.18}$$

where u and v are real. The expression for ϕ given in (2.18) follows from the boundary conditions.[7] It can also be shown that v may be assumed positive, negative v leading to identical results.

Hence we introduce (2.18) in (2.15) and take the thermodynamic limit $N\to\infty$ to obtain the algebraic equation

$$\left[1+(2S-1)\frac{\cos^2 u}{\cos u\cosh v-d/2}\right]\exp(-v)=2S\cos u\ , \tag{2.19}$$

which may be viewed as an equation for v, for a given momentum $u=(k_1+k_2)/2=K/2$. It proves convenient to work with the variable $x=\exp(-v)$ which satisfies the cubic equation

$$x^3+\left[2(S-1)\cos u-\frac{d}{\cos u}\right]x^2+(1+2dS)x-2S\cos u=0\ . \tag{2.20}$$

Since v may be assumed positive, the only relevant roots of (2.20) are real roots in the interval [0,1].

Once a root of the cubic equation is found in the interval [0,1], for a given total wave vector K, the energy is calculated from Eq. (2.12) which may be written as

$$\Omega=2(2S-1)D+4SJ\left[1-\frac{1}{2}\left[x+\frac{1}{x}\right]\cos u\right]\ . \tag{2.21}$$

In practice, Eqs. (2.20) and (2.21) summarize all the information needed for calculating the spectrum of two-magnon bound states. Some attention should be paid to the fact that the total wave vector $K=k_1+k_2$ takes values over a double Brillouin zone. A consistent calculation requires folding of the zone, as usual, when the cubic equation yields a root in the interval [0,1] for values of K outside the fundamental zone. As it turns out, the preceding remarks are irrelevant for the model considered in this section because the cubic equation possesses roots in the interval [0,1] only for $|K|\leq\pi$. However, folding of the zone is essential for some models studied in Sec. III.

We are now in a position to analyze in detail the two-magnon excitation spectrum. We first note that Wortis's original result for $d=0$ follows easily from Eqs. (2.20) and (2.21). The presence of the anisotropy leads to some interesting new aspects pointed out by Silberglitt and Torrance.[6] The bound-state spectrum emerging from Eqs. (2.20) and (2.21) is shown in Fig. 1 for various values of the anisotropy and $S=1$. The conspicuous feature of that figure is that two separate branches develop for $d\neq 0$.

In order to better understand this spectrum we consider (2.20) at the zone boundary ($\cos u\simeq 0$). Two real roots are found in the interval [0,1] for $d\neq 0$,

$$x_1\simeq(\cos u)/d,\quad x_2\simeq 2S\cos u\ . \tag{2.22}$$

The corresponding energies calculated from (2.21) read

$$\Omega_{\mathrm{I}}=4SJ+4(S-1)D\ ,$$
$$\Omega_{\mathrm{II}}=(4S-1)J+2(2S-1)D\ . \tag{2.23}$$

These are precisely the values found earlier in the text for the special solutions given in (2.10) and (2.11). It can also be shown that the wave functions calculated from the general results (2.12) and (2.17), restricted to the zone boundary, lead to the simple wave functions given in (2.10) and (2.11). We should warn the reader that the last calculation involves a somewhat difficult limiting procedure.

Simple inspection of the wave functions (2.10) and (2.11) suggests that the terminology introduced in Ref. 6 is quite appropriate; that is, states of type I and II should be called single-ion and exchange bound states, respectively. Of course, such a distinction is not entirely meaningful inside the zone because the wave function of either type acquires both single-ion and exchange components. However, we find this classification instructive and will adopt it in the following.

The dominant feature of the spectrum for small values of D is the exchange bound state (type II). This can be seen from Eqs. (2.23) by forming the difference

$$\Omega_{\rm I}-\Omega_{\rm II}=J-2D\ , \tag{2.24}$$

which is positive for $D<J/2$. In this range of couplings the exchange bound state extends throughout the zone whereas the single-ion state occupies only a small portion of the zone near the boundary. For $D>J/2$, the role of the two modes is interchanged and the single-ion bound state occupies the entire zone. It becomes dispersionless for very large anisotropy, with energy $\Omega \simeq 4(S-1)D$, in agreement with Eq. (2.4).

To conclude this section we establish that for $D<J/2$ the exchange bound state at the zone center is separated from the two-magnon continuum by a finite gap, in spite first appearances in Fig. 1. A perturbative solution of (2.20) in powers of d at $\cos u=1$ yields

$$x=1-\frac{2S-1}{4S}d+\frac{2S-1}{(4S)^3}[1+4S(S-2)]d^2+\cdots\ ,$$
$$\Omega=2(2S-1)D\left[1-\frac{2S-1}{16S^3}\frac{D}{J}+\cdots\right]. \tag{2.25}$$

This energy is always lower than the threshold of the two-magnon continuum at the zone center.

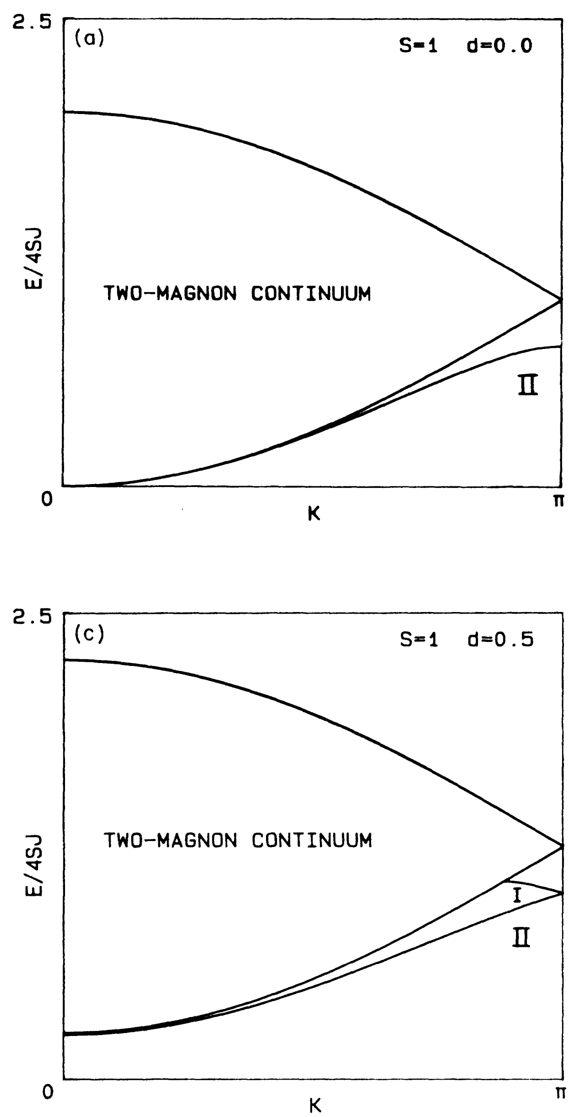

FIG. 1. Two-magnon spectra for an easy-axis magnetic chain with uniaxial anisotropy. I and II stand for the single-ion and exchange bound state, respectively.

III. MISCELLANEOUS GENERALIZATIONS

A natural variation of (2.1) is the easy-plane ferromagnetic chain described by the Hamiltonian

$$H=\sum_n[-J(\mathbf{S}_n\cdot\mathbf{S}_{n+1})+A(S_n^z)^2-BS_n^z] \,, \tag{3.1}$$

where the anisotropy constant A $(=-D)$ is assumed positive. Therefore, for weak magnetic fields B, the system develops a nontrivial ground state with planar behavior. Any attempt to derive the excitation spectrum by the method developed in the preceding section fails in this case.

However, the ground state of (3.1) is ordered in the z direction if the magnetic field B exceeds a critical value B_c, namely,

$$B\geq B_c=(2S-1)A \,. \tag{3.2}$$

This value is feasible for some planar spin chains of current interest; e.g., $B_c=56$ kG for the spin-1 chain observed in $CsNiF_3$. We will assume in the following that (3.2) is satisfied so that the calculation of the preceding section may be carried over with minor modifications. We briefly describe the results.

The one-magnon excitation energy reads

$$\omega=[B-(2S-1)A]+2SJ(1-\cos k) \,. \tag{3.3}$$

The two-magnon bound-state spectrum is calculated from

$$\Omega=2[B-(2S-1)A]+4SJ\left[1-\frac{1}{2}\left[x+\frac{1}{x}\right]\cos u\right] \,, \tag{3.4}$$

where x is a real root in the interval [0,1] of the algebraic equation

$$x^3+\left[2(S-1)\cos u+\frac{a}{\cos u}\right]x^2+(1-2aS)x-2S\cos u=0 \,, \quad a=A/SJ \,. \tag{3.5}$$

This equation follows from (2.20) by the simple replacement $d\rightarrow -a$. Note that the magnetic field does not enter Eq. (3.5), its role being solely to ensure positive excitation energies in (3.4) provided that (3.2) is satisfied.

Examples of two-magnon bound states are shown in Fig. 2. The single-ion bound state appears above the two-magnon continuum and extends throughout the zone for sufficiently strong anisotropy ($a\gtrsim 1.4$). An important calculational detail is that the single-ion bound state occurs for wave vectors $K=2u$ outside the fundamental zone. Figure 2 was thus obtained through an appropriate folding of the zone.

As a further example we consider a generalization of the Hamiltonian (2.1) to include Ising anisotropy,

$$H=-\sum_n\{J[S_n^xS_{n+1}^x+S_n^yS_{n+1}^y+(1+\sigma)S_n^zS_{n+1}^z] +D(S_n^z)^2\} \,. \tag{3.6}$$

The spectrum of the two-magnon bound states is now determined by

$$\Omega=2(2S-1)D+4SJ\left[1+\sigma-\frac{1}{2}\left[x+\frac{1}{x}\right]\cos u\right] \,,$$
$$(1+\sigma)x^3+\left[2(S-1)\cos u-\frac{(1+\sigma)d}{\cos u}\right]x^2 +(1+\sigma+2dS)x-2S\cos u=0 \,. \tag{3.7}$$

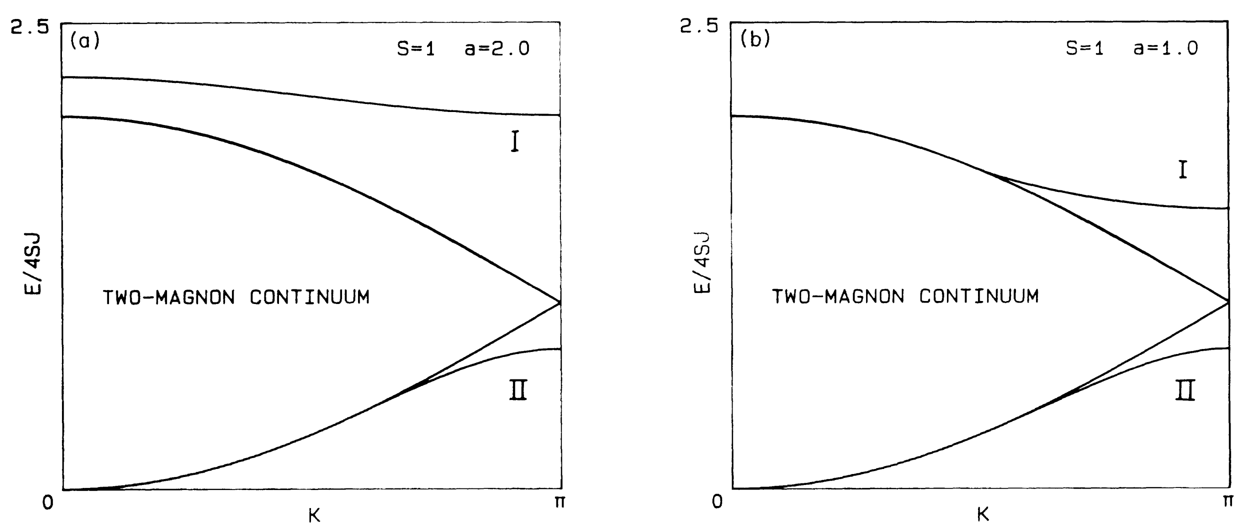

FIG. 2. Two-magnon spectra for an easy-plane magnetic chain in a spin-flop phase caused by an external magnetic field. The field was taken equal to its critical value $B=(2S-1)A$.

Nonvanishing values of σ yield significant quantitative changes in the spectrum but the qualitative picture remains more or less the same.

As a last example we consider the effect of quartic exchange interactions:[8]

$$H=-\sum_n[J(\mathbf{S}_n\cdot\mathbf{S}_{n+1})+2G(T_n^{ab}T_{n+1}^{ab})]\ ,$$
$$T_n^{ab}=\tfrac{1}{2}(S_n^aS_n^b+S_n^bS_n^a)\ , \tag{3.8}$$

where summation over the repeated indices $a,b=x,y,z$ is assumed. The exchanged constants J and G are taken to be positive. Hamiltonian (3.8) reduces to the usual Heisenberg model only for $S=\frac{1}{2}$. We shall study the case $S=1$ for which (3.8) is the most general isotopic Hamiltonian involving two-site exchange interactions.

An equivalent form of (3.8) reads

$$H=-\sum_n[(J+G)(\mathbf{S}_n\cdot\mathbf{S}_{n+1})+2G(\mathbf{S}_n\cdot\mathbf{S}_{n+1})^2]\ . \tag{3.9}$$

It is more or less evident that the state with all spins ordered in, say, the z direction, is an eigenstate of (3.9) with energy $E_0=-N(J+3G)$, for all values of the exchange constants. It is known, however, that the ordered state ceases to be the ground state for couplings such that $G>J$. A demonstration of this fact obtains by deriving the two-magnon spectrum in the region $G\leq J$ and showing[9] that the excitation energy becomes negative for $G>J$.

We will derive the two-magnon spectrum for $S=1$ using the method of Sec. II. For this special spin value, (3.9) may also be written as

$$H=-\sum_n[(J-G)(\mathbf{S}_n\cdot\mathbf{S}_{n+1})+2GP_{n,n+1}+2G]\ ,$$
$$P_{n,n+1}=(\mathbf{S}_n\cdot\mathbf{S}_{n+1})^2+(\mathbf{S}_n\cdot\mathbf{S}_{n+1})-1\ , \tag{3.10}$$

where $P_{n,n+1}$ is the exchange operator for $S=1$ given sometime ago by Schrödinger.[10] This form of the Hamiltonian simplifies considerably the intermediate steps of the calculation.

Hence the one-magnon excitation energy is found to be

$$\omega_k=2(J+G)(1-\cos k)\ . \tag{3.11}$$

The general two-magnon state may again be written in the form (2.6) with coefficients $C_{n,m}$ satisfying the system of algebraic equations:

$$(\Omega-4J)C_{n,n}+2G(C_{n+1,n+1}+C_{n-1,n-1})+(J-G)(C_{n,n+1}+C_{n-1,n})=0\ ,$$
$$(\Omega-3J-G)C_{n,n+1}+(J-G)(C_{n,n}+C_{n+1,n+1})+(J+G)(C_{n-1,n+1}+C_{n,n+2})=0\ , \tag{3.12}$$
$$[\Omega-4(J+G)]C_{n,m}+(J+G)(C_{n-1,m}+C_{n+1,m}+C_{n,m-1}+C_{n,m+1})=0\ ,$$

where Ω is the corresponding two-magnon excitation energy. This linear system can be solved by the Bethe ansatz. Indeed, for $n\neq m$, the $C_{n,m}$ are given by Eq. (2.12) with Ω now determined as

$$\Omega=4(J+G)[1-\tfrac{1}{2}(\cos k_1+\cos k_2)]\ . \tag{3.13}$$

At coinciding arguments we have

$$C_{n,n}=\frac{(J-G)[\cos(k_1-\phi/2)+\cos(k_2+\phi/2)]}{(J+G)(\cos k_1+\cos k_2)-2G[1+\cos(k_1+k_2)]}\exp[i(k_1+k_2)n]\ . \tag{3.14}$$

The phase shift ϕ is related to the wave vectors k_1 and k_2 by

$$\cot\left[\frac{\phi}{2}\right]=\frac{(J+3G+R)\sin[(k_1-k_2)/2]}{2(J+G)\cos[(k_1+k_2)/2]-(J+3G+R)\cos[(k_1-k_2)/2]}\ ,$$
$$R=\frac{(J-G)^2[1+\cos(k_1+k_2)]}{(J+G)(\cos k_1+\cos k_2)-2G[1+\cos(k_1+k_2)]}\ . \tag{3.15}$$

In the special limit $G=J$ the above expressions reduce to

$$\cot\left[\frac{\phi}{2}\right]=\frac{1}{2}\left[\cot\frac{k_1}{2}-\cot\frac{k_2}{2}\right]\ , \tag{3.16}$$

which coincides with Bethe's result for the $S=\frac{1}{2}$ ideal ferromagnet. Such a coincidence could have been anticipated observing that the Hamiltonian (3.10) is expressed entirely in terms of the exchange operator when $G=J$.

The remaining steps are identical to those described in Sec. II. The two-magnon bound-state energies are calculated from

$$\Omega=4(J+G)\left[1-\frac{1}{2}\left[x+\frac{1}{x}\right]\cos u\right]\ , \tag{3.17}$$

where x is a real root of the algebraic equation

$$(J+3G)x^3-12G\cos u\,x^2+(J+3G+8G\cos^2u)x-2(J+G)\cos u=0\ , \tag{3.18}$$

in the interval [0,1].

As is shown in Fig. 3, only one branch arises in the two-magnon spectrum, in contrast with the situation analyzed in Sec. II. To understand this result in more detail we first examine (3.17) and (3.18) at the zone center ($\cos u = 1$):

$$\Omega = 4(J+G)\left[1-\frac{1}{2}\left[x+\frac{1}{x}\right]\right], \tag{3.19}$$

$$(J+3G)x^3 - 12Gx^2 + (J+11G)x - 2(J+G) = 0 .$$

The roots of this equation are

$$x_1 = 1$$

$$x_2 = \frac{1}{2(J+3G)}\{9G - J + [(G-J)(57G+7J)]^{1/2}\} \tag{3.20}$$

$$x_3 = \frac{1}{2(J+3G)}\{9G - J - [(G-J)(57G+7J)]^{1/2}\} .$$

We should distinguish three cases:

(i) $G < J$: Clearly the only real root is $x = x_1 = 1$ which yields a vanishing mass gap. There is only one bound state in this coupling region, which is the usual exchange bound state extending throughout the zone.

(ii) $G = J$: This is a special coupling, as is already evident from Eq. (3.10). All three roots in Eq. (3.20) become equal to unity. One would think that more than one branch will arise in the two-magnon spectrum for nonvanishing momenta. However, solving the full equation (3.18) for arbitrary momenta, one finds again only one stable bound state.

(iii) $G < J$: The picture changes drastically in this region. All three roots in Eq. (3.20) are real and distinct. The root x_2 lies outside the interval [0,1] and need not be considered further. Similarly, the generalization of the root $x_1 = 1$ to nonvanishing momenta does not lead to a stable bound state except at the zone center. On the other hand, the root x_3 lies in the interval [0,1] for all momenta but leads to negative excitation energies near the zone center (see Fig. 3). One should thus conclude that ferromagnetic order is impossible for $G > J$.

Since the derived two-magnon spectrum contains only one bound state, one may think that the single-ion mode does not play any role in the present model. However, a closer look reveals a different picture. At the critical coupling $G = J$ the Hamiltonian (3.10) becomes

$$H = -2G\sum_n (1 + P_{n,n+1}) . \tag{3.21}$$

Since this Hamiltonian depends on the spin operators only through the exchange operator, it admits a two-magnon exchange bound state in complete analogy with the spin-$\frac{1}{2}$ ideal ferromagnet. This fact was noted earlier in the text following Eq. (3.16). Moreover a single-ion eigenstate of (3.21) is easily constructed as

$$\Psi_2 = \sum_n e^{ikn}\Phi_{n,n} , \tag{3.22}$$

where we use the notation developed in Sec. II. The corresponding eigenvalue reads

$$\Omega = 4G(1 - \cos k) . \tag{3.23}$$

At first sight, the preceding result appears puzzling. Had we plotted the energy (3.23) in Fig. 3, we would have found that the single-ion bound state lies within the boundaries of the two-magnon continuum. On the other hand, the excitation energy (3.23) is real and degenerate with the one-magnon energy (3.11) restricted to the critical coupling $G = J$. One may conclude that (3.22) is the limiting form of a single-ion bound state which is a resonance for all couplings in the region $G < J$. For $G > J$, ferromagnetic order is not possible and a nematic phase is realized which is characterized by a twofold magnon spectrum.[11]

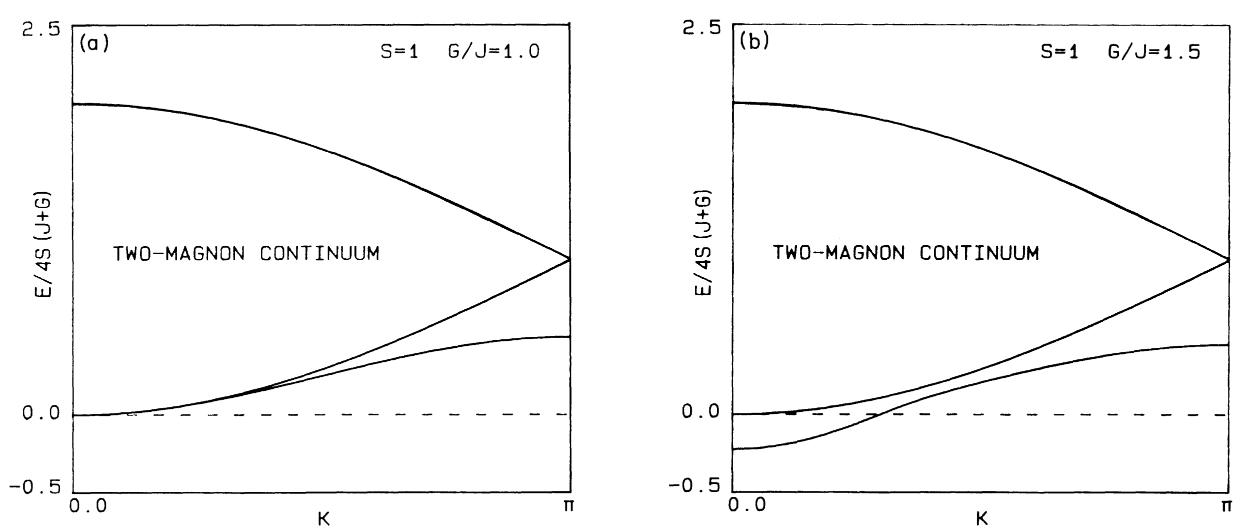

FIG. 3. Two-magnon spectra for a spin-1 model involving quartic exchange interactions. Note that there is only one stable bound state for $G \leq J$ which acquires a negative mass gap for $G > J$.

It is tempting at this point to assume that the single-ion bound state and the one-magnon state join up at the critical coupling $G=J$ to form a doublet which remains degenerate for all couplings in the region $G>J$. Such an interpretation can be made more precise in the context of the $1/n$ expansion discussed in the following section.

IV. THE $1/n$ EXPANSION

The original calculation of Wortis[3] as well as the method presented in Sec. II are limited to magnetic systems that develop ferromagnetic order in their ground state. Alternative methods are therefore necessary to study spin systems with more complicated ground states. A spin-wave theory based on a $1/S$ expansion is, perhaps, the most commonly used approach for approximate calculations.

A more sophisticated spin-wave approach based on a $1/n$ expansion was developed recently in order to account for the special characteristics of magnetic systems with planar behavior[12] and systems involving quartic exchange interactions.[13] Since the $1/n$ expansion predicts certain collective modes in addition to magnons, we thought it appropriate to examine this issue in the light of exact bound-state calculations. For the sake of simplicity we will restrict our attention to $S=1$. A generalization to arbitrary spin is also available.

Consider the set of operators

$$T^a=S^a,\quad T^{ab}=\tfrac{1}{2}(S^aS^b+S^bS^a)\;, \tag{4.1}$$

at a given site whose label will often be suppressed for notational convenience. For $S=1$, these operators are viewed as 3×3 matrices in some definite spin basis. Convenient choices of the basis are dictated by the special dynamical characteristics of the system of interest. There are nine independent matrices in (4.1), because of the symmetry $T^{ab}=T^{ba}$, which close the unitary algera U(3).

Using the notation of (4.1) Hamiltonian (2.1) reads

$$H=-\left[\tfrac{1}{2}\sum_{i,j}J_{ij}(T_i^aT_j^a)+D\sum_i T_i^{zz}\right] \tag{4.2}$$

and Hamiltonian (3.8) is written as

$$H=-\tfrac{1}{2}\sum_{i,j}[J_{ij}(T_i^aT_j^a)+2G_{ij}(T_i^{ab}T_j^{ab})]\;, \tag{4.3}$$

where we assume summation over the repeated indices $a,b=x,y,z$. The notation for the exchange constants used in Eqs. (4.2) and (4.3) indicates that the current calculation may be carried out in an arbitrary space dimension. Hamiltonian (4.2) was studied in Refs. 12 for negative values of D for which the ground state exhibits nontrivial planar behavior. Similar Hamiltonian (4.3) was examined in Ref. 13 for couplings such that $G>J$ where a nematic phase develops. Here we would like to address the simpler cases with $D\geq0$ and $G\leq J$ for which the ground state is ferromagnetic and both one- and two-magnon spectra are known exactly.

The $1/n$ expansion is derived through a generalized Holstein-Primakoff (HP) representation of the operators T^a and T^{ab}. Since the ground state is ferromagnetic in the current examples, a convenient basis for the spin operators is the canonical spin-1 basis. The appropriate HP representation may then be extracted from the work of Sec. II in Ref. 12. We quote the final result

$$\begin{aligned}
&T^z=n-a^*a-2b^*b\;,\\
&T^+=T^x+iT^y=\sqrt{2}(Ra+a^*b)\;,\\
&T^{zz}=n-a^*a\;,\\
&A^+=T^{xx}+iT^{xy}=\tfrac{1}{2}(n+a^*a)+Rb\;,\\
&B^+=T^{yy}+iT^{xy}=\tfrac{1}{2}(n+a^*a)-b^*R\;,\\
&C^+=\sqrt{2}(T^{xz}+iT^{yz})=Ra-a^*b\;,
\end{aligned} \tag{4.4}$$

where a and b are ordinary Bose operators and

$$R=(n-a^*a-b^*b)^{1/2}\;. \tag{4.5}$$

The ensuing method of calculation consists of inserting the Bose representation (4.4) in (4.2) and (4.3) and systematically expanding in inverse powers of n, setting $n=1$ at the end of the calculation.

Hamiltonian (4.2) is expanded holding $\bar{J}_{ij}=nJ_{ij}$ fixed. We thus obtain

$$H=nE_0+H_0+\frac{1}{\sqrt{n}}H_1+\frac{1}{n}H_2+\cdots\;, \tag{4.6}$$

with

$$\begin{aligned}
E_0&=-\left[ND+\tfrac{1}{2}\sum_{i,j}\bar{J}_{ij}\right]\\
H_0&=\tfrac{1}{2}\sum_{i,j}\bar{J}_{ij}[a_i^*a_i+a_j^*a_j-a_i^*a_j-a_j^*a_i)\\
&\qquad+2(b_i^*b_i+b_j^*b_j)]+D\sum_i a_i^*a_i\\
H_1&=-\sum_{i,j}\bar{J}_{ij}(a_i^*a_j^*b_i+a_ia_jb_j^*)\\
H_2&=-\tfrac{1}{2}\sum_{i,j}\bar{J}_{ij}[2a_i^*b_ib_j^*a_j+(N_i+b_i^*b_i)(N_j+b_j^*b_j)\\
&\qquad-a_ia_j^*N_j-N_ia_ia_j^*]\\
N_i&\equiv a_i^*a_i+b_i^*b_i\;.
\end{aligned} \tag{4.7}$$

E_0 is the usual ferromagnetic ground-state energy and H_0 contains information about the normal modes of the system. Higher-order terms in (4.7) account for a variety of physical processes which can be calculated perturbatively.

The excitation energies obtained from the diagonalization of H_0 read (at $n=1$)

$$\omega_k=D+[J(0)-J(k)],\quad \Omega_k=2J(0)\;, \tag{4.8}$$

where $J(k)$ is the Fourier transform of J_{ij} defined from

$$J_{ij}=\frac{1}{N}\sum_k e^{-ik(R_i-R_j)}J(k)\;. \tag{4.9}$$

In (4.8), ω_k denotes the excitation energy of the one-magnon state created by the operator a and Ω_k the excitation energy of a two-magnon state created by b.

In the one-dimensional case, we may set $J(k)=2J\cos k$, so that $\omega_k=D+2J(1-\cos k)$ is identified with the one-magnon dispersion (2.3). Furthermore, $\Omega_k = 2J(0) = 4J$ is found to be equal to the single-ion bound state energy $\Omega_{\rm I}$ given by (2.23) with $S=1$. Recall that $\Omega_{\rm I}$ is the exact value of the single-ion dispersion at the zone boundary, and its limiting value throughout the zone for large anisotropy. Clearly then the dispersionless frequency Ω_k found in (4.8) must be identified with the large-n approximation of the single-ion bound state energy.

Systematic $1/n$ corrections are calculated with ordinary perturbation theory applied to the effective Hamiltonian (4.6). Since H_1 is an odd function of the Bose operators, the first $1/n$ correction is obtained by performing second-order perturbation theory in H_1 and first-order perturbation theory in H_2. As expected, the corrections to the ground state and the one-magnon state vanish. It can also be shown that H_2 does not contribute to Ω_k to leading order. Hence we write $\Omega_k \simeq 4J + \delta\Omega_k$ where $\delta\Omega_k$ is calculated through second-order perturbation theory in H_1. In the one-dimensional case and $n=1$ we find that

$$\Omega_k = 4J\left[1+\frac{1}{8\pi}\int_{-\pi}^{\pi}dp\,\frac{[\cos p+\cos(p-k)]^2}{\cos p+\cos(p-k)-d}\right], \quad d=D/J\,. \tag{4.10}$$

The integral in (4.10) is well defined as it stands only for $d \geq 2$, i.e., $D \geq 2J$. In this region we perform the integral explicitly to find

$$\Omega_k = 4J\left[1+\frac{d}{4}\left[1-\frac{d}{[d^2-4\cos^2(k/2)]^{1/2}}\right]\right]. \tag{4.11}$$

This approximate result is compared with the exact single-ion dispersion in Fig. 4. It is evident that (4.11) is accurate near the zone boundary, and adequate at the zone center, for strong anisotropy $d>2$.

In the weak-anisotropy region $d<2$ the integral (4.10) develops an imaginary part for momenta at the zone center signaling instability of the single-ion mode. The real part of the integral must be evaluated with a principal-value prescription. Hence the $1/n$ expansion overestimates the anisotropy below which the single-ion mode ceases to extend throughout the zone. Recall that the exact calculation of Sec. II yields a critical value $d=\frac{1}{2}$ above which the single-ion bound state is stable for all momenta.

Nevertheless the overall qualitative picture emerging from the $1/n$ expansion is in agreement with the exact results of Sec. II. Perhaps we should mention that the exchange bound state does not arise as a fundamental mode in the $1/n$ expansion, just as it does not arise in the $1/S$ expansion.

To conclude the discussion of this model we comment on the fate of the single-ion mode for negative values of D ($D=-A$, with A positive), in the absence of external magnetic fields. As was shown in Refs. 12 the single-ion mode appears as a resonance together with a gapless magnon for anisotropies A below a critical value A_c. At the critical coupling A_c this mode becomes degenerate with the magnon and a twofold spectrum arises in the region $A \geq A_c$ with nonvanishing mass gap.

Our final task is to discuss briefly the $1/n$ expansion for the Hamiltonian (4.3) with couplings such that $G \leq J$. The spectrum in the harmonic approximation was found to be

$$\omega_k = 2(J+G)(1-\cos k), \quad \Omega_k = 4(J-G\cos k)\,. \tag{4.12}$$

The magnon frequency ω_k coincides with (3.11) and Ω_k should again be identified with the single-ion mode. At the critical coupling $G=J$, we find that $\Omega_k = 4G(1-\cos k) = \omega_k$, in agreement with Eq. (3.23).

However, the exact calculation of Sec. III revealed that the single-ion bound state cannot be stable for any momentum. To see how the $1/n$ expansion copes with this situation we have calculated the next correction to Ω_k

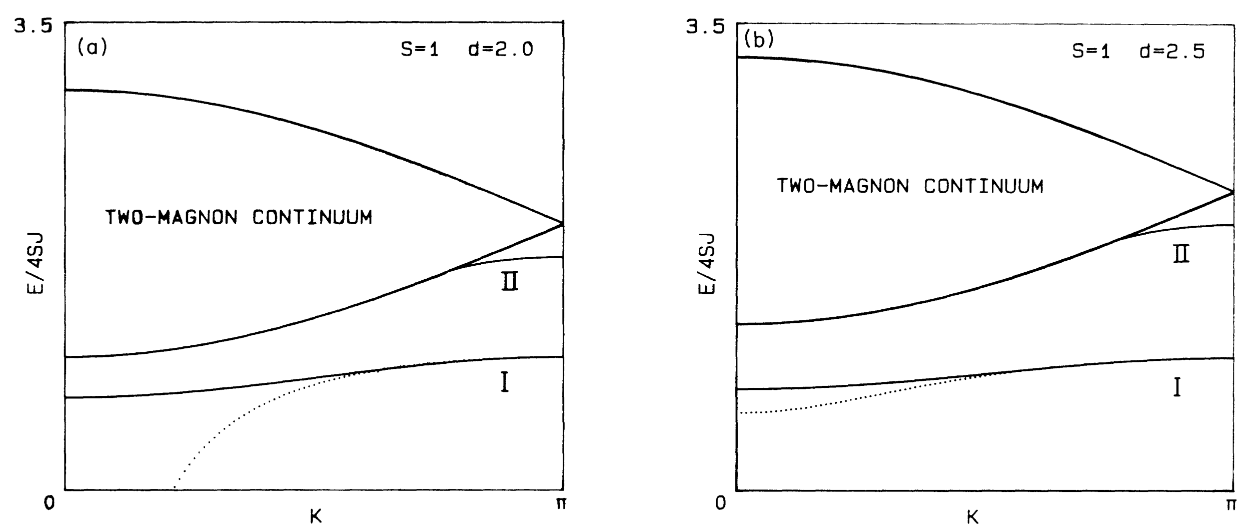

FIG. 4. Comparison of an approximate $1/n$ calculation of the single-ion mode (dotted line) with the exact result for an easy-axis magnetic chain.

by analogy with Eq. (4.10),

$$\Omega_k = 4(J - G\cos k) + 2(J-G)^2 \int_{-\pi}^{\pi} \frac{dp}{2\pi} \frac{[\cos p + \cos(p-k)]^2}{\Omega_p - \omega_k - \omega_{p-k}} . \quad (4.13)$$

It is easily seen that the denominator in the integral of (4.13) develops a zero in p for all values of k and couplings in the region $G < J$. Therefore the single-ion mode is indeed unstable over the entire zone. It becomes degenerate with the magnon at the critical coupling $G = J$ and a twofold spectrum emerges for $G > J$ (see Ref. 13).

V. CONCLUDING REMARKS

One-dimensional spin systems were originally thought of as convenient mathematical models serving as a testing ground for various theoretical ideas. While an abundance of exact results became available, the well-known peculiarities of one-dimensional models appeared to hinder their relevance to realistic three-dimensional systems. However, the situation has changed recently because a number of quasi-one-dimensional magnetic chains have been identified experimentally.[14]

Most of the current work in this area is concerned with the possible appearance of solitons and other exotic modes. Therefore it is important to obtain unambiguous evidence for more conventional magnon bound states. Experimental progress in that direction seems to be slow mainly because it proved difficult to directly observe two-magnon states through standard linear-response methods.[15-17] We hope that the theoretical calculations presented in this paper will aid future work on this subject.

ACKNOWLEDGMENT

This work was supported in part by the U.S. Department of Energy.

*On leave from Washington University, St. Louis, MO 63130.

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