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Heisenberg Hamiltonian with a Dzyaloshinski–Moriya interaction

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Abstract. The spin-$\frac{1}{2}$ ferromagnetic Heisenberg Hamiltonian with a Dzyaloshinski–Moriya interaction and in the presence of a strong magnetic field is studied in one dimension. Using the exact Bethe *ansatz* analysis, the excitation spectrum of one- and two-magnon states is derived. It is further shown that in certain parameter regimes the two-magnon bound state exists in the full range of allowed values of the centre-of-mass momentum wavevector k.

1. Introduction

The Heisenberg Hamiltonian in one dimension has been widely studied over the years. The ground-state energy and low-lying excitation spectrum are known exactly for both the ferromagnetic (FM) and the antiferromagnetic (AFM) Hamiltonians. The exact results are obtained using the well known Bethe *ansatz* (BA) [1]. Bethe first proposed the *ansatz* in 1931 and used it to find the energy dispersion relations of magnon bound states in the case of the spin-$\frac{1}{2}$ FM Hamiltonian in one dimension. Later the technique has been recognized to be very general and applicable not only to models in magnetism but also to a variety of other models [2]. The Heisenberg Hamiltonian has further been studied by including different anisotropy terms in the Hamiltonian. One such term corresponds to the well known Dzyaloshinski–Moriya (DM) interaction [3, 4]. The effect of this term on the ground state and the excitation spectrum of the Heisenberg Hamiltonian has been studied in the past [5, 6] for both the FM and the AFM Hamiltonians. The BA has been applied in some of the cases studied. In this paper, we consider the $S = \frac{1}{2}$ one-dimensional FM Heisenberg Hamiltonian with an added DM interaction and in the presence of a strong magnetic field. In the absence of the magnetic field, the ground state is never FM [1]. For a sufficiently strong magnetic field and for $J_2 < J_1$, the FM state can become the ground state. We study the effect of the DM interaction on the FM spin-wave spectrum and show using the BA that two magnon bound states exist in suitable parameter regimes.

2. Excitation spectrum

The Hamiltonian that we consider is given by

$$H = -J_1 \sum_{i=1}^{N} S_i \cdot S_{i+1} + J_2 \sum_{i=1}^{N} (S_i \times S_{i+1}) \cdot \hat{z} - h \sum_{i=1}^{N} S_i^z \qquad (1)$$

with J_1, $J_2 > 0$. J_2 is the strength of the DM interaction which is taken to be directed along the z axis, $\hat{z}$ is the unit vector in the z direction and h is the strength of the magnetic field directed along the z axis. We consider J_2 to be less than J_1. The spins have magnitude $\frac{1}{2}$ and a periodic boundary condition (PBC) is assumed, i.e. $N+1 \equiv 1$ where N is the number of spins in the chain. For a sufficiently strong magnetic field and for $J_2 < J_1$, the ground state of H is FM with all spins aligned parallel to each other. This can be verified by exact diagonalization of H when N is small. In terms of the spin-raising and spin-lowering operators, the Hamiltonian H in equation (1) becomes

$$H = -J_1 \sum_{i=1}^{N} [S_i^z S_{i+1}^z + \tfrac{1}{2}(S_i^+ S_{i+1}^- + S_i^- S_{i+1}^+)] - \frac{\mathrm{i}J_2}{2} \sum_{i=1}^{N} (S_i^- S_{i+1}^+ - S_i^+ S_{i+1}^-) - h \sum_{i=1}^{N} S_i^z. \tag{2}$$

The ground state ϕ_0 has all spins pointing upwards, i.e.

$$\phi_0 = \alpha(1)\alpha(2)\ldots\alpha(N)$$

where α denotes an up spin. The ground-state energy $E_g = -J_1 N/4 - hN/2$. One can easily verify that S^z, the z component of the total spin, is a constant of motion, i.e. $[H, S^z] = 0$. We now consider the case in which r spins deviate from the ground-state spin arrangement, i.e. there are r down spins at the sites $m_1, m_2, \ldots, m_r$. These spin functions are written as $\Psi(m_1, m_2, \ldots, m_r)$. The eigenfunction Ψ of H is a linear combination of the ${}^N C_r$ functions $\Psi(m_1, m_2, \ldots, m_r)$:

$$\Psi = \sum_{\{m\}} a(m_1, m_2, \ldots, m_r)\Psi(m_1, m_2, \ldots, m_r). \tag{3}$$

Each of the numbers $m_1, \ldots, m_r$ runs over the possible values 1 to N subject to the condition

$$m_1 < m_2 < \cdots < m_r \tag{4}$$

to avoid double counting. We write the eigenvalue equation as

$$E\Psi = H\Psi = E \sum_{\{m\}} a(\{m\})\Psi(m_1, m_2, \ldots, m_r). \tag{5}$$

Multiplying by a particular $\Psi^*(m_1, m_2, \ldots, m_r)$ and using orthogonality properties, one obtains

$$\varepsilon a(m_1, m_2, \ldots, m_r) = -\frac{J_1 + \mathrm{i}J_2}{2} \sum_{\{m'\}} a(m_1', m_2', \ldots, m_r') - \frac{J_1 - \mathrm{i}J_2}{2} \times \sum_{\{m''\}} a(m_1'', m_2'', \ldots, m_r'') + \tfrac{1}{2} J_1 N' a(m_1, m_2, \ldots, m_r) + hra(m_1, m_2, \ldots, m_r) \tag{6}$$

where $\varepsilon = E + J_1 N/4 + hN/2$ is the excitation energy with respect to the ground-state energy E_g and N' is the number of antiparallel spin pairs. The first sum on the right-hand side is over the distributions $m_1', \ldots, m_r'$ which arise from a nearest-neighbour exchange of antiparallel spins of the type $\uparrow\downarrow$ in $(m_1, \ldots, m_r)$ and the second sum is over the distributions

$m_1'', \ldots, m_r''$ which arise from interchange of spins in antiparallel pairs of the type $\downarrow\uparrow$ in $(m_1, \ldots, m_r)$.

Consider the case of one spin deviation, i.e. $r = 1$. In this case, $N' = 2$ and equation (6) becomes

$$\varepsilon a(m) = -[(J_1 + \mathrm{i}J_2)/2]a(m+1) - [(J_1 - \mathrm{i}J_2)/2]a(m-1) + J_1 a(m) + ha(m). \tag{7}$$

The solution for $a(m)$ is given by

$$a(m) = \exp(\mathrm{i}km)$$

so that

$$\varepsilon = J_1(1 - \cos k) + J_2 \sin k + h. \tag{8}$$

From the PBC, $k = (2\pi/N)\lambda$, $\lambda = 0, 1, \ldots, N-1$.

Now consider the case $r = 2$, i.e. there are two spin deviations. We distinguish between two cases.

(i) The two down spins are not neighbours, i.e.

$$\varepsilon a(m_1, m_2) = -[(J_1 + \mathrm{i}J_2)/2][a(m_1+1, m_2) + a(m_1, m_2+1)] - [(J_1 - \mathrm{i}J_2)/2] \times [a(m_1-1, m_2) + a(m_1, m_2-1)] + 2J_1 a(m_1, m_2) + 2ha(m_1, m_2). \tag{9}$$

(ii) The two down spins are neighbours, i.e.

$$\varepsilon a(m_1, m_1+1) = -[(J_1 + \mathrm{i}J_2)/2]a(m_1, m_1+2) - [(J_1 - \mathrm{i}J_2)/2] \times a(m_1-1, m_1+1) + J_1 a(m_1, m_1+1) + 2ha(m_1, m_1+1). \tag{10}$$

Equation (9) is satisfied by the BA

$$a(m_1, m_2) = C_1 \exp[\mathrm{i}(k_1 m_1 + k_2 m_2)] + C_2 \exp[\mathrm{i}(k_2 m_1 + k_1 m_2)] \tag{11}$$

with the eigenvalue

$$\varepsilon = J_1[(1 - \cos k_1) + (1 - \cos k_2)] + J_2(\sin k_1 + \sin k_2) + 2h \tag{12}$$

where C_1, C_2, k_1 and k_2 are to be determined. Equation (10) can also be satisfied if C_1 and C_2 are chosen in such a manner that

$$(J_1/2)[a(m_1, m_1) + a(m_1+1, m_1+1) - 2a(m_1, m_1+1)] - (\mathrm{i}J_2/2) \times [a(m_1, m_1) - a(m_1+1, m_1+1)] = 0. \tag{13}$$

The amplitudes $a(m, m)$ have no physical meaning, since we are dealing with spin-$\frac{1}{2}$ particles, and are actually defined by equation (13). Putting equation (11) into equation (13) and choosing $C_1 = \exp(\mathrm{i}\phi/2)$ and $C_2 = \exp(-\mathrm{i}\phi/2)$, one derives the condition

$$\cot\left(\frac{\phi}{2}\right) = \frac{-J_1 \sin[(k_1 - k_2)/2]}{J_1 \cos[(k_1 - k_2)/2] - J_1 \cos[(k_1 + k_2)/2] + J_2 \sin[(k_1 + k_2)/2]}. \tag{14}$$

From the PBC, one obtains $a(m_1, m_2) = a(m_2, m_1 + N)$, leading to the relations

$$Nk_1 - \phi = 2\pi\lambda_1 \qquad Nk_2 + \phi = 2\pi\lambda_2 \qquad \lambda_1, \lambda_2 = 0, 1, 2, \ldots, N-1. \tag{15}$$

The sum of k_1 and k_2 is a constant of motion by translational symmetry:

$$k = k_1 + k_2 = (2\pi/N)(\lambda_1 + \lambda_2). \tag{16}$$

For real k_1, k_2 and $\phi(-\pi \leqslant \phi \leqslant \pi)$, the eigenvalue spectrum is given by equation (12) and corresponds to a continuum of scattering states.

3. Bound states

To obtain bound states of two spin deviations, consider k_1, k_2 to be complex, i.e.

$$k_1 = u + \mathrm{i}v \qquad k_2 = u - \mathrm{i}v. \tag{17}$$

From equation (15),

$$N(k_1 - k_2) = 2N\mathrm{i}v = 2\pi(\lambda_1 - \lambda_2) + 2\phi. \tag{18}$$

Put $\phi = \psi + \mathrm{i}\chi$ so that

$$\psi = \pi(\lambda_2 - \lambda_1) \qquad \chi = Nv. \tag{19}$$

For non-zero v, χ is large. So

$$\cos\left(\frac{\phi}{2}\right) = \frac{\sin\psi - \mathrm{i}\sinh\chi}{\cosh\chi - \cos\psi} \simeq -\mathrm{i}. \tag{20}$$

From equations (14), (17) and (20), one obtains the condition

$$J_1 \exp(-v) = J_1 \cos u - J_2 \sin u. \tag{21}$$

Thus, from equation (12), the excitation energy for two spin deviations with complex k_1, k_2 is given by

$$\varepsilon = J_1 - J_1[(J_1 \cos u - J_2 \sin u)/J_1]^2 + 2h. \tag{22}$$

The possible values of u are given by equation (21) ($1 \geqslant \exp(-v) \geqslant 0$). The centre-of-mass momentum wavevector k (defined modulo 2π) $= 2u + 2n\pi$ where n is an integer and is limited to the range $0 \leqslant k \leqslant 4\tan^{-1}(J_1/J_2)$.

4. Results

From equation (12), the continuum of scattering states have bounds ε_1 and ε_2 given by

$$\begin{aligned} \varepsilon_1 &= J_1[2 - 2\cos(k/2)] + 2J_2 \sin(k/2) + 2h \\ \varepsilon_2 &= J_1[2 + 2\cos(k/2)] - 2J_2 \sin(k/2) + 2h. \end{aligned} \tag{23}$$

Figure 1 shows the plots of ε_b (the two-magnon bound-state energy given by equation (22)), ε_1 and ε_2 versus k ($0 \leqslant k \leqslant 4\tan^{-1}(J_1/J_2)$) for $J_1 = 1.0$, $J_2 = 0.5$ and $h = 1.0$. One finds that a two-magnon bound state exists in the full range of allowed k-values. There are two points of degeneracy at which $\varepsilon_b = \varepsilon_1$ or ε_2. From equations (22) and (23), the condition for the energies to be the same is

$$J_1 \cos u - J_2 \sin u = J_1 \tag{24}$$

which leads to the relation

$$\sin(u/2)[J_1 \sin(u/2) + J_2 \cos(u/2)] = 0. \tag{25}$$

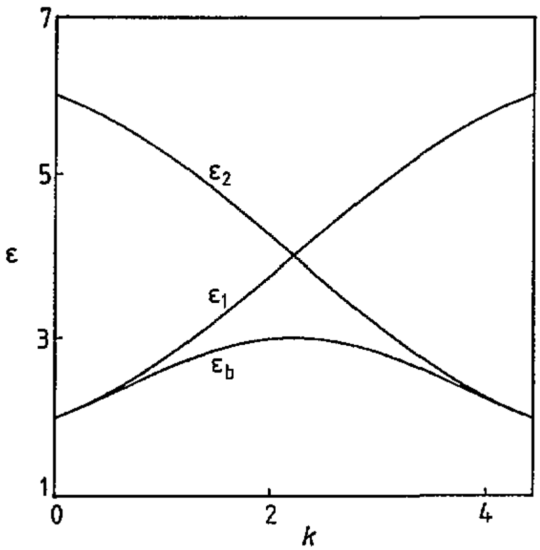

Figure 1. Two-magnon bound-state energy ε_b and energies of two free magnons, with bounds given by ε_1 and ε_2, versus k, the centre-of-mass momentum wavevector, for $J_1 = 1.0$, $J_2 = 0.5$ and $h = 1.0$. The values of k are in the range $0 \leqslant k \leqslant 4\tan^{-1}(J_1/J_2)$.

Thus the two points of degeneracy are

$$\begin{aligned} &u = 2n\pi \qquad n = 0 \qquad \text{or integer} \\ &\tan(u/2) = -J_2/J_1. \end{aligned} \tag{26}$$

In figure 1, the points correspond to $k = 0$ and $4\tan^{-1}(J_1/J_2)$, respectively, which are the end points of the range of k-values.

For $J_2 = 0$ and $h = 0$, equations (21)–(23) reduce to those for the isotropic FM Hamiltonian and the values of k are in the range $0 \leqslant k \leqslant 2\pi$. As J_2 increases from zero, the range of k-values decreases. The magnetic field enters only into the energy expressions and has no effect on the range of k-values. The same linear term $2h$ is contributed by the magnetic field to the energies of the continuum and the bound states. The magnetic field is needed to ensure that the FM state is the ground state. In the FM state, the magnetic field has the largest contribution to the energy equal to $-hN/2$. Since S^z, the z component of the total spin, is a conserved quantity, the other states are obtained by deviating spins from the parallel spin arrangement of the FM state. The FM state has the highest possible value of $S^z = N/2$. The other states have lower values of S^z. For states with low values of S^z, the contribution of the magnetic field to the energy term is much smaller than in the FM state. Thus for strong magnetic fields the FM state definitely has a lower energy. For one and two spin deviations ($S^z = N/2 - 1$ and $N/2 - 2$, respectively), we have calculated the excitation energies measured with respect to that of the FM state. If these excitation energies are greater than zero for a certain choice of the parameters J_1, J_2 and h, the assumption that the FM state is the ground state is correct.

We next consider the general case of r spin deviations. Again, two cases are to be considered.

(i) No two spin deviations are neighbours.
(ii) Two spin deviations are neighbours.

In case (i), the general eigenvalue equation (equation (6)) is satisfied by the full BA [1]:

$$a(m_1, \ldots, m_r) = \sum_{P=1}^{r!} \exp\left[\mathrm{i} \left(\sum_{j=1}^{r} k_{Pj} m_j + \tfrac{1}{2} \sum_{j<l} \phi_{Pj,Pl} \right) \right]. \tag{27}$$

P is any permutation of r numbers $1, 2, \ldots, r$. Pj is the number obtained by operating P on j. The ϕ-values are the phase shifts in analogy with scattering theory. Equation (11) with $C_1 = \exp(\mathrm{i}\phi/2)$ and $C_2 = \exp(-\mathrm{i}\phi/2)$ is a special case of equation (27) for $r = 2$. The eigenvalue ε is given by

$$\varepsilon = J_1 \sum_{l=1}^{r} (1 - \cos k_l) + J_2 \sum_{l=1}^{r} \sin k_l + rh. \tag{28}$$

Equations (8) and (12) are special cases of equation (28) for $r = 1$ and 2, respectively. The wavevectors k_i are determined as before by applying the PBC which leads to the r equations

$$Nk_i = 2\pi\lambda_i + \sum_j \phi_{ij}. \tag{29}$$

The phase shifts ϕ_{ij} are determined, as in the case of $r = 2$, by demanding that the BA (equation (27)) is also a solution for case (ii) (two spin deviations are neighbours). This leads to $r(r-1)/2$ equations identical with equation (14) since there are as many distinct $\phi(\phi_{ij} = -\phi_{ji})$. These equations together with the r equations, equation (29), constitute a total number of $r(r+1)/2$ equations for as many unknowns and so are expected to have solutions. The excitation spectrum is given by equation (28). The full analysis of the BA equations for both real and complex k_i is beyond the scope of this paper.

To summarize, we have considered the $S = \frac{1}{2}$ quantum Heisenberg chain with a DM interaction and in the presence of a strong magnetic field. We have considered the case when the ground state has a FM alignment of spins. Such a ground state is possible because of the presence of the magnetic field. In [6], the magnetic field term is not considered. The ground state in the classical limit has a spiral structure with neighbouring spins making a fixed angle with one another. The spiral structure persists even for weak DM interactions and the FM state can never be the ground state. We have derived the ground-state energy and the excitation spectrum. We have also specifically shown that bound states of two spin deviations can occur. In [6], some ground-state properties and the excitation spectrum have been derived by relating the quantum Hamiltonian to the anisotropic Heisenberg Hamiltonian with a certain type of boundary condition and using the BA. The possibility of bound-state formation has not been considered. Our analysis is similar to Bethe's [1] original work which explicitly showed the existence of magnon bound states for the FM Heisenberg Hamiltonian.

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