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LETTER TO THE EDITOR

Two-magnon bound states in an alternating Heisenberg chain

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Abstract
The behaviour of a singlet two-magnon bound state in an $S = 1/2$ alternating Heisenberg antiferromagnetic chain is investigated by a quantum self-consistent theory with the help of the bosonization technique in the continuum limit approach. The singlet two-magnon bound state exists for any dimerization $\delta > 0$ at total momentum $q = 0$. Its dispersion relation is given analytically in the vicinity of zero momentum. In the case of weak dimerization, the binding energy of the singlet two-magnon bound state monotonically increases with increasing dimerization parameter. Our results are consistent with recent experimental data of $CuGeO_3$.

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The alternating Heisenberg chain (AHC) is a simple quantum spin system. It is a straightforward generalization of the uniform Heisenberg antiferromagnetic chain. The AHC has a rather complicated spectrum of states at higher energies, including multimagnon continua and bound states, and has been used to model the magnetic behaviour of a wide range of materials.

On the other hand, the AHC may also arise as a result of the spin–Peierls (SP) effect. A spontaneous spatial dimerization in the one-dimensional (1D) antiferromagnet results in an AHC. $CuGeO_3$ [1] is a typical SP chain, although interactions beyond nearest neighbour are also thought to be important. Pure $CuGeO_3$ has a SP transition at $T_{SP} = 14.3$ K. Below T_{SP}, the system is in a dimerized spin singlet state, and the gap of spin triplet excitations is $\Delta \approx 24.5$ K. Kuroe *et al* [2] observed additional peaks in the Raman intensity on cooling below T_{SP} for $CuGeO_3$. The lowest Raman excitation in the dimerized phase was observed at 30 cm^{-1}, i.e. slightly below 2Δ. Previously, it was indicated that a singlet excitation might result from a bound state of two triplet excitations [2]. In particular, the observation of a two-magnon continuum in $CuGeO_3$ with an onset close to 2Δ [3] has motivated recent theoretical studies of the continuum and two-magnon bound states in the AHC [4–7]. The existence of well defined magnon modes, i.e. two-magnon bound states which split from the continuum, has been recently addressed by Uhrig and Schulz [4] within an RPA. They found evidence in the whole range of dimerization ($\delta > 0$) for a singlet ($S = 0$) bound state below the continuum for all total momenta q and predicted a triplet ($S = 1$) bound state around $q = \pi/2$ (the zone boundary) for not too small δ. By numerical diagonalization, Bouzerar *et al* [5] similarly concluded that the $S = 1$ two-magnon bound state only exists for a range of q around the zone boundary, but, inconsistent with the above, there is no well defined singlet excitation at $q = 0$. Recently, by using perturbation theory and numerical methods based on multiple precision programming, Barnes *et al* [6] obtained the singlet bound state for all q and the triplet bound state only for a range of q around π/b (equivalent to the $q = \pi/2$ point, the zone boundary), where b represents the length of the unit cell. In addition, Fledderjohann and Gros [7] searched for evidence of the bound states in a numerical study of the dynamical structure factor for any finite value of δ on chains of up to $L = 24$, and concluded that a two-magnon bound state does indeed lie below the two-magnon continuum for any $\delta > 0$. Very recent Monte Carlo studies [8] also showed the existence of massive singlet excitation in the AHC. As a result, it is highly desirable to give an analytical approach to studying the possible two-magnon bound states.

It is well known that the SP system in the case of weak dimerization can be mapped onto a 1D sine–Gordon (SG) model via the Jordan–Wigner transformation and bosonization [9]. On the other hand, in recent years an analytical quantum self-consistent theory [10] was developed to study the low-energy excitation of the SG model. Moreover, it was successfully used to study a two-dimensional classical Coulomb gas [11]. The main advantage of the theory is that the infrared divergence of the SG model can be effectively treated and the low-energy excitation, such as the single-particle excitation spectrum and bound states, can be obtained in a self-consistent way. In this Letter we investigate the singlet two-magnon bound state in the AHC with the help of this method.

The AHC Hamiltonian is

$$H = \sum_{i=1}^{N_{\mathrm{d}}=L/2} (\mathcal{J} \boldsymbol{S}_{2i-1} \boldsymbol{S}_{2i} + \alpha \mathcal{J} \boldsymbol{S}_{2i} \boldsymbol{S}_{2i+1}) \tag{1}$$

where N_{d} is the number of independent dimers or unit cells, which are coupled by the interaction $\alpha\mathcal{J}$, with $\mathcal{J}$ the coupling within each dimer. We impose periodic boundary conditions, with identified spins at both sites 1 and $L+1$, and assume that $\mathcal{J} > 0$ and $0 < \alpha < 1$. An equivalent form often used in the discussion of SP transitions is written as

$$H = \sum_{j=1}^{N} J[1 + (-1)^j \delta] \boldsymbol{S}_j \boldsymbol{S}_{j+1} \tag{2}$$

which is related to equation (1) by $J = (1+\alpha)\mathcal{J}/2$ and $\delta = (1-\alpha)/(1+\alpha)$.

Following the standard steps of the Jordan–Wigner transformation and bosonization, we obtain the quantum SG Hamiltonian, which describes large-distance behaviour of a weakly dimerized system [9, 12],

$$H = \frac{1}{2} \int \left[(vK) P^2 + \left(\frac{v}{K} \right) (\partial_x \phi)^2 \right] \mathrm{d}x - C \int \cos g\phi \, \mathrm{d}x \tag{3}$$

where v is the spin wave velocity and $g = \sqrt{2\pi}$. P is the momentum density field conjugate to ϕ, with the commutation relation $[\phi(x), P(x')] = \mathrm{i}\delta(x - x')$. The coefficients v, K and C are related to J and δ by $v = 2\sqrt{AB}$, $K = \sqrt{B/A}/2\pi$ and $C = \delta J/a$ with $A = Ja(1+3/\pi)/8\pi$, and $B = 2\pi Ja(1 - 1/\pi)$, where a is a short-distance cutoff or lattice spacing. For the convenience of the following discussion, by rescaling the field operator and its conjugate momentum, equation (3) can be further transformed into the standard SG model,

$$H = v \int \left[\frac{1}{2}(\partial_x \phi)^2 + \frac{1}{2} P^2 - \frac{m_0}{a^2\beta^2} \cos\beta\phi \right] \mathrm{d}x \tag{4}$$

where $m_0 = Ca^2/2A = 4\pi^2\delta/(\pi + 3)$ and $\beta^2 = (B/A)^{\frac{1}{2}} = 4\pi\sqrt{(\pi - 1)/(\pi + 3)}$. The canonical commutation relation remains unchanged.

The excitation spectrum of the SG model at $\beta = \sqrt{2\pi}$ is exactly known [13, 14], which provides valuable information about the spectrum consisting of single-soliton and single-antisoliton excitations with masses $M_{\mathrm{s}} = M_{\bar{\mathrm{s}}} = M$ and two bound states (breathers) with masses $M_1 = M$ and $M_2 = \sqrt{3}M$. We note that in a bosonized picture of the fermonic theory [15, 16] a particle, a hole and an exciton correspond to a soliton, an antisoliton and a breather mode, respectively. The single-particle excitation (one magnon) and the single-hole excitation carry $S^z = 1$ and -1, respectively, while the two exciton-like particle–hole (two-magnon) bound states have opposite parity ($S^z = 0$) in spin language. The two-magnon bound-state mode with lower energy is degenerate with the two one-magnon excited states, and these three excitations correspond to a triplet excitation branch. An applied magnetic field would split this triplet into its three components. Another two-magnon bound state with higher energy has its counterpart in a spin singlet excitation [12]. We will focus our attention on the latter below.

The ground state of equation (4) has been well studied in [10]. Choose a trial ground state: $|G\rangle = \exp\left[\sum_k(\gamma_k/2)(b_k b_{-k} - b_k^+ b_{-k}^+)\right]|\mathrm{vac}\rangle$, where b_k is the Fourier component of the Bose field in momentum space and $|\mathrm{vac}\rangle$ denotes the vacuum state; γ_k is a variational parameter, which can be determined by the stable point of the ground-state energy. As a result, the ground-state energy per site can be obtained as

$$E_0 = v \left(\sum_k \frac{|k|}{2} \cosh(2\gamma_k) - \frac{m_0}{a^2\beta^2}\xi \right) \tag{5}$$

with $\xi = \exp\left(-\beta^2/4 \sum_k \mathrm{e}^{-2\gamma_k}/|k|\right)$. The variational parameter, γ_k, is determined by $\partial E_0/\partial\gamma_k = 0$: $\gamma_k = \frac{1}{4}\ln[1 + m_0\xi/(a^2k^2)]$. Substituting γ_k into ξ, then ξ is given self-consistently by

$$\xi = \exp\left[\frac{\beta^2}{\beta^2 - 8\pi} \ln\left(\sqrt{\xi + \frac{1}{m_0}} + \sqrt{\frac{1}{m_0}} \right)^2 \right]. \tag{6}$$

The one-magnon excited state takes the form $|\psi_1(k)\rangle = b_k^+|G\rangle$. After straightforward calculation the expectation value of the Hamiltonian in the one-magnon excited state yields $E_1(k) = E_0 + \omega_1(k)$, where the one-magnon excitation spectrum is

$$\omega_1(k) = \sqrt{v^2k^2 + \Delta_1^2} \tag{7}$$

with $\Delta_1 = v\mu$ representing the energy gap of one-magnon excitation and $\mu = \sqrt{m_0\xi}/a$.

Similarly, the two-magnon state can be constructed by the action of two creation operators on the ground state. We may write the general two-magnon state as [17]

$$|\psi_2(p)\rangle = \int \mathrm{d}k\ \Sigma(k) b_{p+k}^+ b_{p-k}^+ |G\rangle \tag{8}$$

where $q = 2p$ is the total wavenumber which is still a good quantum number. The amplitude $\Sigma(k)$ will be determined by the variation method. The expectation of the Hamiltonian in the state equation (8) becomes

$$E_2(p) = \frac{\langle\psi_2(p)|H|\psi_2(p)\rangle}{\langle\psi_2(p)|\psi_2(p)\rangle} = E_0 + \omega_2(p). \tag{9}$$

The energy of the two-magnon state relative to the ground state is given as

$$\omega_2(p) = \frac{v}{\int[\Sigma(k)]^2\,\mathrm{d}k}\int\left[\sqrt{(p+k)^2+\mu^2}+\sqrt{(p-k)^2+\mu^2}\right][\Sigma(k)]^2\,\mathrm{d}k - \frac{v\beta^2\mu^2}{16\pi\int[\Sigma(k)]^2\,\mathrm{d}k}\left\{\int\frac{\Sigma(k)\,\mathrm{d}k}{[(p+k)^2+\mu^2]^{\frac{1}{4}}[(p-k)^2+\mu^2]^{\frac{1}{4}}}\right\}^2. \tag{10}$$

The amplitude $\Sigma(k)$ can be determined by the variation method: the result is an integral equation which is just the secular equation in the two-particle subspace [17]. Finally, we obtain a equation for $\omega_2(p)$ as

$$1 = \frac{\beta^2\mu^2}{16\pi}\int\frac{\left[\sqrt{(p+k)^2+\mu^2}\sqrt{(p-k)^2+\mu^2}\right]^{-1}}{\sqrt{(p+k)^2+\mu^2}+\sqrt{(p-k)^2+\mu^2}-\omega_2(p)/v}\,\mathrm{d}k. \tag{11}$$

For the bound state in this Letter, we first consider the case of the static centre of mass, i.e. $p = 0$. The energy gap of two-magnon excitation is that of $\Delta_2 = \omega_2(0)$. For $\Delta_2 < 2\Delta_1$, equation (11) becomes

$$\frac{8\pi}{\beta^2} = \frac{1}{2\tau}\left[\frac{1}{\sqrt{1-\tau^2}}\left(\arcsin\tau + \frac{\pi}{2}\right) - \frac{\pi}{2}\right] \tag{12}$$

with $\tau = \Delta_2/2\Delta_1$. The binding energy E_b of the two-magnon bound state is defined by

$$E_\mathrm{b} = 2\Delta_1 - \Delta_2. \tag{13}$$

For the general case of $p \neq 0$, it is difficult to obtain an exactly analytical formula for the dispersion of the two-magnon bound state. Instead, we can expand $\omega_2(p)$ around $\omega_2(0)$ up to second order, which is presumably the minimum of the energy of the two-magnon bound state. By a straightforward procedure starting from equation (11), the final form of $\omega_2(p)$ is

$$\omega_2(p) = \omega_2(0) + \Omega(\tau)\frac{v}{\mu}p^2 + \mathcal{O}(p^4) \tag{14}$$

where

$$\Omega(\tau) = \left\{\frac{\pi}{2}\left[-\frac{1}{2\tau}+\frac{1}{\tau^3}+\frac{2\tau^2-3}{\tau^3(1-\tau^2)^{3/2}}\right]+\frac{1}{\tau^2(1-\tau^2)}+\frac{2\tau^2-3}{\tau^3(1-\tau^2)^{3/2}}\arcsin\tau\right\} \times\left[\frac{\pi}{2\tau^2}+\frac{1}{\tau(1-\tau^2)}-\frac{1}{\tau^2(1-\tau^2)^{3/2}}(\arcsin\tau+\pi/2)\right]^{-1}. \tag{15}$$

Equations (13) and (14) are the main results in this Letter. It is well known that the AHC undergoes a transition at $\delta = 0$, and a gap opens in the spectrum of elementary excitation. The power law which characterizes the opening of the one-magnon gap has been estimated by many authors [9,18,19]. For the case of $\delta \ll 1$, the same results are obtained analytically [20]. We wish to connect the calculated results with recent experimental data of $CuGeO_3$. In order to fix the parameters J and δ, we follow the analysis of Riera and Dobry [21], which is based on susceptibility data and calculations of Lanczos diagonalization techniques by Bouzerar *et al* [22], to take $J = 160$ K and $\delta = 0.012$, respectively. It then follows that the singlet–triplet gap is equal to $\Delta_1 = 0.140J$, close to $\Delta_1^{\mathrm{exp}} \approx 2.15$ meV $= 0.156J$ as measured by INS [23], and the singlet–singlet gap is equal to $\Delta_2 = 0.262J$, which is consistent with the

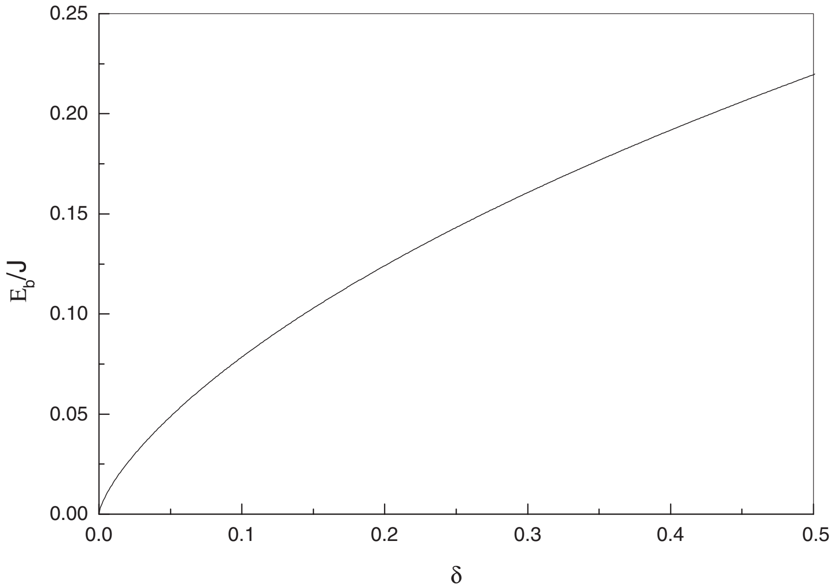

Figure 1. Binding energy of the singlet two-magnon bound state versus δ at $q = 0$ in units of J.

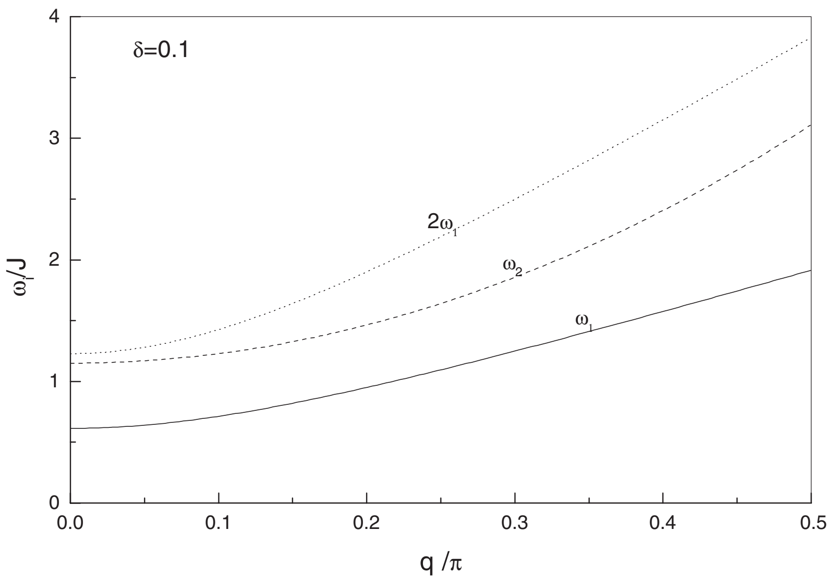

Figure 2. Dispersion $\omega_i(q) = E_i(q) - E_0$ of the two excited modes for $\delta = 0.1$ in units of J. The solid curve is ω_2 and the dashed curve corresponds to ω_1. The dotted curve represents the edge of the two-magnon continuum.

lowest Raman excitation energy $\Delta_2^{\exp} = 30\ \mathrm{cm}^{-1} = 0.268J$ [2, 24]. From equation (12) we also obtain the singlet–triplet gap ratio $R = 2\tau = 1.87$ compared with $R^{\exp} = 1.72$. The dependence of the binding energy of the singlet two-magnon bound state on dimerization is shown in figure 1 at $q = 0$, in reduced units of J. It is found that the binding energy E_b

monotonically increases with increasing dimerization, δ, implying the existence of the singlet bound state at $q = 0$ for any $\delta > 0$.

In figure 2 we show the dispersion of the singlet two-magnon excitations for $0 < q < \pi/2$ considered appropriate within the present method and fixed $\delta = 0.1$. From figure 2 we see that the singlet two-magnon bound state always appears below the edge of the two-magnon continuum. It is concluded that the singlet two-magnon bound state exists for a considerable range of momentum, which is also qualitatively consistent with [4] and [6].

In summary we have presented a theoretical method which combines the bosonization technique and the quantum self-consistent theory to study elementary excitations of the $S = 1/2$ alternating Heisenberg antiferromagnetic chain. It is found that a singlet two-magnon bound state exists below the two-magnon continuum for $\delta > 0$ in the $S = 1/2$ alternating Heisenberg antiferromagnetic chain. The binding energy of the singlet two-magnon bound state increases with increasing dimerization for weakly dimerized chains. Our results of the singlet two-magnon bound state are consistent with recent experimental data of $CuGeO_3$.

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