Quantum spin ladder with dynamic phonons. Bound states of magnons and phonons.

O.P. Sushkov
School of Physics, University of New South Wales, Sydney 2052, Australia

We consider the two-chain Heisenberg ladder with antiferromagnetic interactions. Our approach is based on the description of spin excitations as triplets above a strong-coupling singlet ground state. It is shown that interaction with dynamic phonons drastically changes the dispersion of the elementary triplet excitation (magnon) and the spin structure factor. It is also shown that a new triplet excitation appears in the spectrum: the bound state of a magnon and a phonon.

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Quantum spin ladders have recently become a subject of considerable interest, mainly because of their relevance to a variety of quasi one-dimensional materials. It is well established that the two-leg \( S = 1/2 \) spin ladder has a gapped excitation spectrum. Quite recently a state with the energy above the one-particle excitation level but below the two-particle continuum was observed in \((\text{VO})_2\text{P}_2\text{O}_7\) which can be described as a dimerized chain. This result triggered theoretical work on two-particle bound states in this model. The above results raise the important issue of possible low-lying two-particle excitations in quasi one-dimensional models with a gapped spectrum. It has been shown that in a two-leg ladder bound states with total spin \( S=0 \) and total spin \( S=1 \) always exist below the continuum. Similar bound states exist also in many two-dimensional quantum spin systems. To complete the overview of pure spin systems (no dynamic phonons) we should mention that for spin chains with small explicit dimerization the spectrum can be even more complex consisting of multiple triplet and singlet states.

The importance of dynamic phonons was realized a long time ago in relation to the spin-Peiers transition. In the paper a simple model Hamiltonian for description of the combined spin-phonon dynamics in a spin chain has been suggested. Numerical study of this Hamiltonian has shown that many physical properties differ substantially from those derived in the static limit. This important observation raises the question of the role of phonons in the dynamics of the spin ladder. In the present work, using the analytical approach developed in, we demonstrate that dynamic phonons qualitatively change the spectrum of triplet excitations in the two-leg spin ladder: 1) an additional triplet appears as a magnon-phonon bound state, 2) the magnon dispersion attains discontinuity. 3)q-dependence of the spin structure factor is substantially different from that without phonons. Following the idea of work we consider the Hamiltonian of two coupled \( S = 1/2 \) chains (spin ladder) with local phonons coupled to the rung spin-spin interaction:

\[
H = \sum_i \{ J S_i^z S_{i+1}^z + J S_i^\alpha S_{i+1}^\alpha + J_{\perp} S_i^x S_{i+1}^x \} + \sum_i \left\{ g(b_i^\dagger + b_i)S_i^x S_i^z + \omega_0 b_i^\dagger b_i \right\}.
\]

Here \( b_i^\dagger \) and \( b_i \) are the phonon creation and annihilation operators. We assume the optical phonon to be dispersionless. The intra-chain (\( J \)) and the inter-chain (\( J_{\perp} \)) interactions are assumed antiferromagnetic \( J, J_{\perp} > 0 \).

Following works we consider the set of the rung singlets as the unperturbed ground state, introduce a triplet creation operator on the rung \( t_{\alpha i}^\dagger, \alpha = x, y, z \), and hence map the Hamiltonian to

\[
H = \sum_{i,\alpha,\beta} \left\{ J_{\perp} t_{\alpha i}^\dagger t_{\alpha i} + \frac{J}{2} \left( t_{\alpha i}^\alpha t_{\alpha i+1}^\alpha + t_{\alpha i+1}^\alpha t_{\alpha i}^\alpha + h.c. \right) \right\} + \frac{J}{2} \left( t_{\alpha i}^\alpha t_{\beta i+1}^\alpha t_{\beta i+1}^\alpha + t_{\beta i}^\alpha t_{\beta i+1}^\alpha + t_{\beta i+1}^\alpha t_{\beta i+1}^\alpha \right) + \sum_{i,\alpha} \left\{ g(b_i^\dagger + b_i) t_{\alpha i}^\dagger t_{\alpha i} + \omega_0 b_i^\dagger b_i \right\} + U \sum_{i,\alpha,\beta} t_{\alpha i}^\dagger t_{\alpha i}^\dagger t_{\beta i} t_{\alpha i} + \sum_{i,\alpha} \left\{ g(b_i^\dagger + b_i) t_{\alpha i}^\dagger t_{\alpha i} + \omega_0 b_i^\dagger b_i \right\},
\]

where \( U \to \infty \) is a fictitious interaction which enforces no double occupancy constraint \( t_{\alpha i}^\dagger t_{\alpha i}^\dagger t_{\beta i} t_{\alpha i} = 0 \). For shortness we call the excitation corresponding to \( t_{\alpha i}^\dagger \) ("elementary" triplet) a magnon.

We will treat the interaction with phonons by perturbation theory and therefore at the first step we have to diagonalize the Hamiltonian at \( g = 0 \). The technique to perform this diagonalization was suggested in Ref. with further improvement (rainbow diagrams and attraction in the singlet channel) developed in relation to the analysis of the two-dimensional \( J_1 - J_2 \) model. Applying these techniques we find that the normal Green’s function of the magnon is of the form

\[
G(k, \epsilon) = \frac{u_k^2}{\epsilon - \Omega_k + i\delta} + \frac{v_k^2}{\epsilon + \Omega_k + i\delta} + G_{\text{inc}}.
\]

Coupled Dyson’s equations for the effective Bogoliubov’s parameters \( u_k \) and \( v_k \) and for the magnon dispersion \( \Omega_k \) are derived in Refs. In the limit \( J_\perp \gg J \) the solution is very simple: \( u_k \approx 1, v_k \approx -(J/2J_\perp) \cos k \), and

\[
\Omega_k \approx J_\perp + J \cos k.
\]

The magnon dispersion at \( J_\perp = J \) found as a result of numerical solution of Dyson’s equations is presented in...
Fig. 1 (long-dashed line). For comparison we show by dots the results obtained from dimer series expansions [3].

Probing with neutrons is the experimental method commonly used to measure excitation spectra of magnetic materials. The inelastic neutron scattering cross-section is directly proportional to the dynamic structure factor: $S_u(k,\epsilon) = \int e^{i\epsilon t} \langle \hat{S}_{\alpha}(k, t) \hat{S}_{\alpha}(-k, 0) \rangle dt$, where we assume that the transverse (along the rungs) momentum $k_\perp = \pi_\perp$, i.e. $S_{\alpha,\perp}^\perp = S_{\alpha,\perp}^\perp - S_{\alpha,\perp}^\perp$. Magnon contribution to the dynamic structure factor is $S_u(k,\epsilon) = S_u(k,\epsilon)\delta(\epsilon - \Omega_k)$, where $S_u(k) = (u_k + v_k)^2$. At $J_{\perp} \gg J$ the structure factor is $S_u(k) \approx 1$. The plot of $S_u(k)$ at $J_{\perp} = J$ is shown in Fig. 2 (long-dashed line).

To find the interaction between the magnon and the phonon we have to substitute transformed magnon operator $t_{ak} = u_k t_{ak} + v_k t_{a-k}$ into the interaction term (g-term) of the Hamiltonian [2]. This gives

$$H_{int} = \sum_{k,q,a} \left\{ \Gamma_{k,q} \tilde{t}_{a,k}^\dagger \tilde{t}_{a,k} + \frac{1}{2} \frac{\gamma_{k,q}}{\epsilon - \omega_0 - \Omega_k} \right\} b_q + h.c. \quad (5)$$

$$\Gamma_{k,q} = g(u_k + v_k + u_{k+q}v_q), \quad \gamma_{k,q} = g(u_k + v_k + v_{k+q}v_q),$$

where $b_q$ is the Fourier transform of $b_i$.

We consider weak coupling with phonons, $g^2 \ll J^2$. Therefore the magnon self energy, given by the diagram in Fig. 3a, is of the form

$$\Sigma(k,\epsilon) = \sum_q \frac{\Gamma_{k,q}^2}{\epsilon - \omega_0 - \Omega_k}. \quad (6)$$

Let us consider the limit $J_{\perp} \gg J$. In this case $\Omega_k$ is given by (7) and therefore the integration in (8) can be performed analytically. This gives the correction to the triplet dispersion

$$\delta \Omega_k = \Sigma(k,\epsilon = \Omega_k) = -\frac{g^2}{\sqrt{\omega_0 - J \cos k}^2 - J^2}. \quad (7)$$

This answer is satisfactory if $\omega_0 > 2J$. However for lower phonon energy ($\omega_0 < 2J$) equation (7) gives an infinite correction at $k = k_c$, where $\cos k_c = (\omega_0 - J)/J$. The reason for this is clear: the integrand in (8) has a pole and therefore in spite of the weak coupling the perturbation theory is not valid in the vicinity of $k_c$. To improve the situation we have to use the exact Green’s function

$$\hat{G}(k,\epsilon) = \frac{1}{\epsilon - \Omega_k - \Sigma'(k,\epsilon)}, \quad (8)$$

where $\hat{G}$ is defined as $\hat{G}(k, t) = -i \langle \hat{T} [\tilde{t}_{k,\alpha}(t), \tilde{t}_{k,\alpha}^\dagger(0)] \rangle$ [17]. The dispersion $\epsilon_k$ is given by the pole of this Green’s function.

$$[\hat{G}(k,\epsilon)]^{-1} = 0 \quad (9)$$

Note that the self energy $\Sigma'$ in (8) is different from $\Sigma$ given by (7). The difference is very simple: to get $\Sigma'$ one has to use the same eq. (7), but with $\Omega_k$ replaced by $\epsilon_k$. This replacement is equivalent to summation of rainbow diagrams, Fig. 3b. Simple analysis shows that the vertex corrections (Fig. 3c) are negligible at small $g$.

In the limit $J_{\perp} \gg J$ eq. (8) has an analytical solution. Away from $k_c$ this solution reproduces the perturbation theory result (7), however at $k = k_c$ it gives a discontinuity in dispersion. At $k = k_c + 0$ the dispersion is pushed down as $\epsilon_k \approx \Omega_k - (g^2/\sqrt{2J})^{2/3}$. Immediately on the left from $k_c$ ($k = k_c - 0$) the dispersion disappears because of the huge decay width. However away from this point ($k = k_c - \Delta k$) the width drops down and at $\Delta k \gtrsim g^2/(2J^2 \sin k_c)\sin \omega_0/k_c$ the halfwidth becomes smaller than the energy. It means that the magnon reappears as a relatively narrow state. At $J_{\perp} \sim J$ the equation (7) can be solved only numerically. As an example we present in Fig. 1 (solid line) the plot of the magnon dispersion at $J_{\perp} = J$, $\omega_0 = 0.5J$, $g^2/J^2 = 0.2$. In spite of the relatively weak coupling to phonons the dispersion is substantially different from that without phonons (dashed line).

The magnon contribution to the the dynamic structure factor is $S_u^{(m)}(k)\delta(\epsilon - \epsilon_k)$, where $S_u^{(m)}(k) = Z_k(u_k + v_k)^2$, and $Z_k = (1 - \frac{\omega_0}{\omega_0 - \Omega_k})^{-1}$ is the quasiparticle residue.

The plot of $S_u^{(m)}(k)$ is presented in Fig. 2 by solid line. It is also very much different from that without phonons (long-dashed line). Concluding the discussion of magnons we would like to note that the discontinuity in the spectrum is similar to the roton spectrum endpoint in liquid $^4$He, see e.g. Ref. [3].

Consider now a phonon-magnon bound state. The binding arises due to the diagrams shown in Figs. 4a, b. To solve the problem in general case one has to use the Bethe-Salpeter equation with account of retardation.

However for small phonon-magnon coupling ($g^2 \ll J^2$) which we consider in the present work, the binding is relatively weak and we can use simple second order Schrödinger perturbation theory. In this approximation the diagrams Fig. 4a, b give the following effective interaction

$$M(Q, k, p) = M_a(Q, k, p) + M_b(Q, k, p) \quad (10)$$

$$\frac{\Gamma_{k,q-p} \Gamma_{p-Q-k}}{E_Q - 2\omega_0 - \epsilon_{k+p-Q} + \epsilon_k - \epsilon_p - \epsilon_{k+p-Q}} + \frac{\gamma_{k,q-p} \gamma_{p,q-k}}{E_Q - \epsilon_k - \epsilon_p - \epsilon_{k+p-Q}},$$

where $E_Q$ and $Q$ is the energy and the momentum of the bound state. As soon as the interaction is known the bound state is defined by usual equation

$$[E_Q - \omega_0 - \epsilon_k] \psi(k) = \int \frac{dp}{2\pi} M(Q, k, p) \psi(p). \quad (11)$$

In the limit $J_{\perp} \gg J$ the kernel is very simple $M_a \approx M_a \approx -g^2/(\omega_0 + 2J \cos^2 Q/2)$, and solution of equation (11)
gives \( E_Q = J_\perp - J + \omega_0 - \epsilon_b \), with the wave function and binding energy equal to

\[
\psi(p) = \frac{(8J^2g^2)^{1/4}}{\epsilon_b + 2J\cos^2 p/2} \quad (12)
\]

\[
\epsilon_b(Q) = \frac{g^4}{2J(\omega_0 + 2J\cos^2 Q/2)^2}.
\]

At \( J_\perp \sim J \) equation (11) can be solved only numerically. We present it Fig.1 (dashed line) the plot of the bound state dispersion at \( J_\perp = J, \omega_0 = 0.5J \), \( g^2/J^2 = 0.2 \). Shadowed areas show phonon-magnon continuum. It is clear that binding is maximum at \( Q = \pi \).

The bound state has spin \( S = 1 \) and therefore it can be excited in neutron scattering. The mechanism for this excitation is shown in Fig.4c: first a virtual magnon is excited and then it emits a phonon with formation of the bound state. The corresponding contribution to the dynamic structure factor is \( S_u^{(b)}(k)\delta(\epsilon - E_k) \) with \( S_u^{(b)}(k) \) given by

\[
S_u^{(b)}(k) = \frac{(u_k + v_k)}{E_k - \Omega_k - \Sigma'(k, E_k)} \sum_p \Gamma_{k,k-p}\psi(p)^2. \quad (13)
\]

At \( J_\perp \gg J \) integration in this formula with account of eqs. (12) gives

\[
S_u^{(b)}(k) = \frac{g^2}{(2\epsilon_b(k)/J)(\omega_0 - 2J\cos^2 k/2)^2}. \quad (14)
\]

It is assumed that the denominator in this formula is not too small. At small denominator there is strong mixing between the magnon and the bound state and therefore a more accurate consideration is necessary. The structure factor \( S_u^{(b)}(k) \) for \( J_\perp = J, \omega_0 = 0.5J \) and \( g^2 = 0.2J^2 \) obtained by numerical integration in (13) is shown in Fig.2 by the dashed line. At \( k = \pi \) the bound state excitation probability is 10 times smaller than that for the magnon. However at \( k \sim 0.8\pi \) the probabilities are comparable.

Above we have considered the magnon and the bound state of the magnon with a phonon. In addition to these states there are bound states of two magnons considered in Ref. [4]. The dynamic phonon does not qualitatively influence these bound states. However additional phonon diagrams shown in Fig.5 push down the energies of these states. To illustrate this for \( J_\perp = J, \omega_0 = 0.5J \) and \( g^2 = 0.2J^2 \) we show in Fig.1 (dashed-dotted line) the dispersion of the two-magnon bound state with \( S = 1 \). Because of the decay to the phonon and two magnons this state attains finite width \( \Gamma \sim 0.15J \). This is why the state disappears at \( k \sim 0.6\pi \) where splitting from the corresponding continuum is getting smaller than halfwidth. The structure factor for this state is

\[
S_g(k, \epsilon) = S_g(k)\delta_T(\epsilon - E_k), \quad \text{where} \quad \delta_T \text{ is a function with finite width.}
\]

The index \( g \) indicates that the state can be excited at \( k_\perp = 0 \), i.e. by \( S_1 + S'_1 \). The formula for \( S_g(k) \) is presented in [6]. Integration in this formula gives the plot shown in Fig.2 by the dotted-dashed line. At \( k = \pi \) the excitation probability is 4 times smaller than that for the magnon. However at \( k \sim 0.8\pi \) they become equal.

In conclusion, we have studied the two-leg antiferromagnetic Heisenberg ladder with spins coupled to dynamic phonons. In the analysis we use the bond operator representation together with the diagram technique and Brueckner approximation. It has been demonstrated that the phonons qualitatively change spectrum of triplet excitations: 1) An additional triplet appears as a magnon-phonon bound state. Dispersion of this triplet for some particular parameters is shown in Fig.1 (dashed line); 2) the magnon (elementary triplet) dispersion attains a discontinuity, Fig.1, solid line; 3) k-dependence of the spin structure factor (Fig 2, solid line) is substantially different from that without phonons (Fig 2, long-dashed line).

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FIG. 1. Triplet excitations on the isotropic ($J_\perp = J$) ladder. The long-dashed line is the magnon dispersion obtained by the Brueckner method without coupling to phonons. Dots represent the same dispersion obtained in Ref.[5] using series expansion. Solid line gives the magnon dispersion with account of coupling to phonons. The phonon energy is $\omega_0 = 0.5J$ and the coupling constant $g^2/J^2 = 0.2$. The dashed line corresponds to the bound state of the magnon and the phonon. The dashed-dotted line corresponds to the bound state of the two magnons with total spin $S=1$. Shaded areas gives magnon-phonon continuum.

FIG. 2. Spin structure factors (excitation probabilities) for isotropic ladder, $J_\perp = J$. The long-dashed line corresponds to the magnon without coupling to phonons. Solid line describes the same magnon coupled to phonons ($\omega_0 = 0.5J$, $g^2/J^2 = 0.2$). The dashed line describes bound state of the magnon and the phonon. The dashed-dotted line corresponds to the bound state of the two magnons.

FIG. 3. Magnon self energy due to the phonons. Dashed line corresponds to the phonon Green’s function. (a) Single loop, (b) rainbow diagrams, (c) vertex correction.

FIG. 4. Diagrams (a) and (b) represent the phonon - magnon scattering amplitudes responsible for the binding. Solid line describes the magnon and dashed line describes the phonon. The diagram (c) shows mechanism for the bound state contribution to the spin structure factor.

FIG. 5. Phonon corrections for the two magnon bound state.
