

Magnon mode truncation in a rung-dimerized asymmetric spin ladder

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(Received 17 June 2007; revised manuscript received 23 August 2007; published 19 November 2007)

An effective model is suggested for an asymmetric spin ladder with dimerized rungs. Magnon mode truncation that originated from magnon decay (recently observed in the one compound IPA-CuCl₃) is naturally described within this model. Using Bethe *Ansätze*, we studied a one-magnon sector and obtained relations between interaction constants of the model and experimentally observable quantities such as the gap and truncation energies, spin velocity, and truncation wave vector. It is also shown that the structure factor turns to zero at the truncation point.

DOI: [10.1103/PhysRevB.76.174431](https://doi.org/10.1103/PhysRevB.76.174431)

PACS number(s): 75.10.Jm, 75.50.Ee

I. INTRODUCTION

A spin ladder with strong antiferromagnetic rung coupling gives an ideal example of a gapped spin-dimerized system.¹ Actually, the majority of spins in its ground state are coupled in rung singlets (rung dimers) so that the relative coupling energy estimates a value of the gap. For this reason, all low-temperature effects depend on dynamical properties of states with a few number of excited rungs. A theoretical study of excitations in spin ladders with strong antiferromagnetic rung coupling was developed in a number of papers.²⁻⁵ It was pointed out that the lowest excitations form a coherent magnon branch. When the gap energy is smaller than the energy width of the magnon zone, the latter may intersect the two-magnon scattering continuum. For a *symmetric* spin ladder (with equal couplings along both legs as well as along both diagonals), these two sectors do not hybridize so a one-magnon state is always stable. The situation is quite different for an *asymmetric* spin ladder with nonequal couplings along legs or along diagonals. As it was pointed out in Ref. 6-9, the coupling asymmetry entails hybridization between the “bare” (related to a symmetric case) one- and two-magnon sectors. If the system has a wide magnon band intersecting with the two-magnon scattering continuum, this hybridization results in magnon instability and truncation of the magnon mode at some value k_{trunc} of wave vector. Experimentally a magnon mode truncation was observed in neutron scattering from the one dimensional (1D) compound IPA-CuCl₃ [(CH₃)₂CHNH₃CuCl₃].⁶ The latter is considered as an asymmetric spin ladder with strong ferromagnetic rungs and is effectively equivalent to a 1D Haldane antiferromagnet.

In this paper, starting from an asymmetric rung-dimerized spin ladder, we present an effective model which produces an explicit realization of magnon mode truncation related to magnon decay. Within our model, we study the one-magnon excitations and obtain explicit relations between the coupling constants and experimentally observable quantities.

II. HAMILTONIAN FOR AN ASYMMETRIC SPIN LADDER

In the present paper, we shall study an asymmetric spin ladder with the following Hamiltonian:^{4,9}

$$\hat{H} = \sum_n H_{n,n+1}, \quad (1)$$

where $H_{n,n+1} = H_{n,n+1}^{rung} + H_{n,n+1}^{leg} + H_{n,n+1}^{diag} + H_{n,n+1}^{cyc} + H_{n,n+1}^{norm}$ and

$$H_{n,n+1}^{rung} = \frac{J_{\perp}}{2} (\mathbf{S}_{1,n} \cdot \mathbf{S}_{2,n} + \mathbf{S}_{1,n+1} \cdot \mathbf{S}_{2,n+1}),$$

$$H_{n,n+1}^{leg} = J_{\parallel} (\mathbf{S}_{1,n} \cdot \mathbf{S}_{1,n+1} + \mathbf{S}_{2,n} \cdot \mathbf{S}_{2,n+1}),$$

$$H_{n,n+1}^{diag} = J_d \mathbf{S}_{1,n} \cdot \mathbf{S}_{2,n+1},$$

$$H_{n,n+1}^{cyc} = J_c [(\mathbf{S}_{1,n} \cdot \mathbf{S}_{1,n+1})(\mathbf{S}_{2,n} \cdot \mathbf{S}_{2,n+1}) + (\mathbf{S}_{1,n} \cdot \mathbf{S}_{2,n}) \times (\mathbf{S}_{1,n+1} \cdot \mathbf{S}_{2,n+1}) - (\mathbf{S}_{1,n} \cdot \mathbf{S}_{2,n+1})(\mathbf{S}_{2,n} \cdot \mathbf{S}_{1,n+1})]. \quad (2)$$

Here, $\mathbf{S}_{j,n}$ ($j=1,2$) are the $S=1/2$ spin operators related to the n th rung. The auxiliary term $H_{n,n+1}^{norm} = J_{norm} I$ (I is an identity matrix) is added for the zero normalization of the ground state energy.

The condition

$$J_d + J_c = 2J_{\parallel}, \quad (3)$$

suggested in Ref. 4, guarantees that the vector $|0\rangle_n \otimes |0\rangle_{n+1}$ (where $|0\rangle_n$ is the n th rung singlet or, equivalently, rung dimer) is an eigenstate for $H_{n,n+1}$, so the vector

$$|0\rangle = \prod_n |0\rangle_n \quad (4)$$

is an eigenstate for \hat{H} . An additional system of inequalities,

$$J_{\perp} > 2J_{\parallel}, \quad J_{\perp} > \frac{5}{2}J_c, \quad J_{\perp} + J_{\parallel} > \frac{3}{4}J_c,$$

$$3J_{\perp} - 2J_{\parallel} - J_c > \sqrt{J_{\perp}^2 - 4J_{\perp}J_{\parallel} + 20J_{\parallel}^2 - 16J_{\parallel}J_c + 4J_c^2}, \quad (5)$$

together with a condition $J_{norm} = 3/4J_{\perp} - 9/16J_c$, guarantees that the vector [Eq. (4)] is the (zero energy) ground state for \hat{H} . The full system of the “ground state tuning” conditions

[Eqs. (3) and (5)] belongs to the mathematical basis of our model.

For $J_d=0$, the Hamiltonian \hat{H} commutes with the operator, $\hat{Q}=\frac{1}{2}\sum_n(\mathbf{S}_{1,n}+\mathbf{S}_{2,n})^2$, considered as a number of bare magnons.^{5,9} Therefore, the Hilbert space splits into an infinite sum: $\mathcal{H}=\sum_{m=0}^{\infty}\mathcal{H}^m$, where $\hat{Q}|_{\mathcal{H}^m}=m$. The subspace \mathcal{H}^0 is one dimensional and is generated by the ground state [Eq. (4)].

III. SPECTRAL PROBLEM FOR THE REDUCED HAMILTONIAN RELATED TO THE EFFECTIVE MODEL

Despite the fact that the ground state [Eq. (4)] for the Hamiltonian [Eqs. (1)–(3) and (5)] is known, it is not clear how to obtain its excitations. In the symmetric case,^{4,5} the one-magnon state corresponds to \mathcal{H}^1 , but even for a small asymmetry it already lies in $\sum_{n=0}^{\infty}\mathcal{H}^{2n+1}$.⁹ For this reason, the related spectral problem seems to be unsolvable. However, for a strong rung coupling, the states with a rather big number of bare magnons have a large energy and may therefore be effectively reduced. In the first order, with respect to the dimerization energy, the reduced Hilbert space $\mathcal{H}^{red}=\mathcal{H}^0\oplus\mathcal{H}^1\oplus\mathcal{H}^2$ contains, in addition to the ground state [Eq. (4)], only the bare one- and two-magnon sectors. The corresponding effective Hamiltonian \hat{H}^{eff} is defined as the restriction of \hat{H} on \mathcal{H}^{red} , or

$$\hat{H}^{eff}=P^{(0,1,2)}\hat{H}P^{(0,1,2)}, \quad (6)$$

where $P^{(0,1,2)}$ is the projector on \mathcal{H}^{red} .

A general $S=1$ excited state for \hat{H}^{eff} related to a wave vector k and the energy $E(k)$ is the superposition of bare one- and two-magnon components,

$$|k\rangle^\alpha = \frac{1}{Z(k)\sqrt{N}} \sum_m \left[a(k)e^{ikm} \cdots |1\rangle_m^\alpha \cdots + \varepsilon_{\alpha\beta\gamma} \sum_{n>m} e^{ik(m+n)/2} b(k, n-m) \cdots |1\rangle_m^\beta \cdots |1\rangle_n^\gamma \cdots \right], \quad (7)$$

where $|1\rangle_n^\alpha=(\mathbf{S}_{1,n}^\alpha-\mathbf{S}_{2,n}^\alpha)|0\rangle_n$ and “ \cdots ” means an infinite product of dimers related to the remaining rungs. The normalization factor $Z(k)$ is defined as

$$Z^2(k)=|a(k)|^2+2\sum_{n=1}^{\infty}|b(k,n)|^2. \quad (8)$$

The system of Schrödinger equations on the amplitudes $a(k)$ and $b(k, n)$ directly follows from the local action of the operator $H_{n, n+1}$,

$$H_{n, n+1}|0\rangle_n|1\rangle_{n+1}^\alpha = \left(\frac{1}{2}J_\perp - \frac{3}{4}J_c\right)|0\rangle_n|1\rangle_{n+1}^\alpha + \frac{J_c}{2}|1\rangle_n^\alpha|0\rangle_{n+1} - \frac{iJ_d}{2}\varepsilon_{\alpha\beta\gamma}|1\rangle_n^\beta|1\rangle_{n+1}^\gamma,$$

$$H_{n, n+1}|1\rangle_n^\alpha|0\rangle_{n+1} = \left(\frac{1}{2}J_\perp - \frac{3}{4}J_c\right)|1\rangle_n^\alpha|0\rangle_{n+1} + \frac{J_c}{2}|0\rangle_n|1\rangle_{n+1}^\alpha,$$

$$H_{n, n+1}\varepsilon_{\alpha\beta\gamma}|1\rangle_n^\beta|1\rangle_{n+1}^\gamma = (J_\perp - J_\parallel - J_c/4)\varepsilon_{\alpha\beta\gamma}|1\rangle_n^\beta|1\rangle_{n+1}^\gamma + iJ_d|0\rangle_n|1\rangle_{n+1}^\alpha. \quad (9)$$

From Eqs. (7) and (9), one can obtain an infinite set of recurrent equations,

$$(2J_\perp - 3J_c)b(k, n) + J_c \cos \frac{k}{2}[b(k, n-1) + b(k, n+1)] = E(k)b(k, n), \quad n > 1, \quad (10)$$

related to non-neighbor excited rungs and two additional equations related to neighbor rungs,

$$\left(J_\perp - \frac{3}{2}J_c + J_c \cos k\right)a(k) + iJ_d \cos \frac{k}{2}b(k, 1) = E(k)a(k),$$

$$\left(2J_\perp - \frac{9}{4}J_c - \frac{J_d}{2}\right)b(k, 1) + J_c \cos \frac{k}{2}b(k, 2) - \frac{iJ_d}{2} \cos \frac{k}{2}a(k) = E(k)b(k, 1). \quad (11)$$

For a coherent excitation originated from the hybridization of the one-magnon and bound two-magnon states there must be

$$\lim_{n \rightarrow \infty} b(k, n) = 0. \quad (12)$$

With regard to this condition, Eq. (10) has the following general solution:

$$b(k, n) = B(k)z^n(k), \quad (13)$$

where

$$|z(k)| < 1 \quad (14)$$

and

$$E(k) = 2J_\perp - 3J_c + J_c \left(z(k) + \frac{1}{z(k)} \right) \cos \frac{k}{2}. \quad (15)$$

It follows from Eqs. (14) and (15) that

$$\text{Im } z(k) = 0. \quad (16)$$

Substituting Eqs. (13) and (15) into Eq. (11), we obtain a pair of equations on $a(k)$ and $B(k)$ represented in the following matrix form:

$$M(k) \begin{pmatrix} a(k) \\ B(k) \end{pmatrix} = 0, \quad (17)$$

where

$$M(k) = \begin{pmatrix} \frac{3}{2}J_c + J_c \cos k - J_c \left(z(k) + \frac{1}{z(k)} \right) \cos \frac{k}{2} - J_\perp & iz(k)J_d \cos \frac{k}{2} \\ -\frac{iJ_d}{2} \cos \frac{k}{2} & \left(\frac{3}{4}J_c - \frac{J_d}{2} \right) z(k) - J_c \cos \frac{k}{2} \end{pmatrix}. \quad (18)$$

Equation (17) is solvable only for $\det M(k)=0$, or

$$\begin{aligned} & \left[z^2(k)J_c \cos \frac{k}{2} + \left(J_\perp - \frac{3}{2}J_c - J_c \cos k \right) z(k) + J_c \cos \frac{k}{2} \right] \\ & \times \left[\left(\frac{3}{2}J_c - J_d \right) z(k) - 2J_c \cos \frac{k}{2} \right] + z^2(k)J_d^2 \cos^2 \frac{k}{2} = 0. \end{aligned} \quad (19)$$

Equation (19) added by conditions (14) and (16) completely defines the coherent spectrum for \hat{H}^{eff} . The truncation originates from a failure of any of conditions (14) and (16). For the first possibility, the truncation wave vector k_{trunc} coincides with the critical wave vector k_c defined as

$$|z(k_c)| = 1. \quad (20)$$

For the second one, it coincides with the branching wave vector k_b related to the passing of solutions of Eq. (19) into the complex plane.

In order to clear the nature of the truncation point for an arbitrary set of coupling parameters [however limited by Eqs. (3) and (5)], let us first examine the case when condition (20) is satisfied just at the branching point. In other words, we are interested in $k_c=k_b=k_{bc}$ when Eq. (19) has a twice-degenerate solution $z(k_{bc})$ so that the same one has the equation obtained from Eq. (19) by differentiating its left side with respect to $z(k)$. Using an auxiliary variable $f = z(k_{bc}) \cos \frac{k_{bc}}{2}$ and keeping in mind that according to Eqs. (16) and (20) $z^2(k_{bc})=1$, we represent (at $k=k_{bc}$) Eq. (19) and its “derivative” equation in the following system:

$$\begin{aligned} & 4J_c^2 f^3 + (J_d^2 + 2J_d J_c - 7J_c^2) f^2 + J_c(4J_c - 2J_d - 2J_\perp) f + \left(\frac{3}{2}J_c \right. \\ & \left. - J_d \right) \left(J_\perp - \frac{J_c}{2} \right) = 0, \\ & 2J_c^2 f^3 + (J_d^2 + 2J_d J_c - 5J_c^2) f^2 + J_c \left(\frac{7}{2}J_c - 2J_d - J_\perp \right) f + \left(\frac{3}{2}J_c \right. \\ & \left. - J_d \right) \left(J_\perp - \frac{J_c}{2} \right) = 0, \end{aligned} \quad (21)$$

which is solvable only for

$$J_c J_d (2J_\perp - J_c) (3J_c - 2J_d) = 0. \quad (22)$$

[The left side of Eq. (22) was obtained from the result of the two polynomials in the left side of Eq. (21)]. The solution $J_c=0$ of Eq. (22) is not interesting because in this case Eq. (19) is singular and solvable only for $k=\pi$. The solution $J_c=2J_\perp$ is inconsistent with Eq. (5). The solution $3J_c=2J_d$ is

artificial because in this case $\cos \frac{k}{2}$ factorizes from the left side of Eq. (19), and therefore at $k=\pi$ Eq. (19) is identically satisfied for all $z(\pi)$. The solution $J_d=0$ relates to zero asymmetry when the corresponding truncation wave vector k_0 ,

$$\cos \frac{k_0}{2} = \frac{1}{2} \left(\sqrt{\frac{2J_\perp}{J_c} - 1} \right), \quad (23)$$

may be easily obtained from Eq. (19), which also gives

$$z(k_0) = -1. \quad (24)$$

Formula (23) has a clear physical interpretation. Actually, as it follows from the results of Refs. 4 and 5 (related to symmetric spin ladders) at $k=k_0$, the bare one-magnon branch with dispersion $E_{bare}^{magn}(k) = J_\perp - \frac{3}{2}J_c + J_c \cos k$ intersects the lower bound of the scattering two-magnon continuum,⁵

$$E_{bare}^{2magn,low}(k) = 2J_\perp - 3J_c - 2J_c \cos \frac{k}{2}. \quad (25)$$

The above result confirms the general statement suggested in Refs. 6–8 that even an extremely small asymmetry may drastically change a magnon mode. As it follows from Eq. (23), at $J_d \rightarrow 0$, the truncation occurs only for $9J_c > 2J_\perp$. Since $J_\perp > 0$, the parameter J_c must also be positive.

In order to find a nature of the truncation at $J_d \neq 0$, let us study an evolution of $z(k_b)$ for small J_d . If condition (14) is satisfied for $k=k_b$, then the truncation originates from branching and $k_{trunc}=k_b$. However, in the opposite side for $|z(k_b)| > 1$, it will be $k_{trunc}=k_c$.

Taking for $J_d/J_c \ll 1$ and $k \approx k_0$ the following infinitesimal representation $z(k) = -1 + \epsilon(k)$, using the notations $t(k) = \cos k/2$ and $t_0 = \cos k_0/2$ and the formula

$$\frac{J_\perp}{J_c} - \frac{3}{2} - \cos k = 2[t_0^2 + t_0 - t^2(k)], \quad (26)$$

which follows from Eq. (23), we obtain the following equation from Eq. (19) by omitting the term $\epsilon^3(k)$:

$$\alpha(k)\epsilon^2(k) + \beta(k)\epsilon(k) + \gamma(k) = 0. \quad (27)$$

Here,

$$\begin{aligned} \alpha(k) &= 1 + \frac{t(k)}{\Delta_1} + 2 \frac{[t(k) - t_0][t(k) + t_0 + 1]}{t(k)} - \frac{J_d^2 t(k)}{2J_c^2 \Delta_1}, \\ \beta(k) &= 2 \frac{[t_0 - t(k)][t(k) + t_0 + 1]}{t(k)} \left(2 + \frac{t(k)}{\Delta_1} \right) + \frac{J_d^2 t(k)}{J_c^2 \Delta_1}, \end{aligned}$$

$$\gamma(k) = 2 \frac{[t(k) - t_0][t(k) + t_0 + 1]}{t(k)} \left(1 + \frac{t(k)}{\Delta_1} \right) - \frac{J_d^2 t(k)}{2J_c^2 \Delta_1}, \quad (28)$$

and $\Delta_1 = 3/4 - J_d/(2J_c)$.

The branching wave vector is characterized by the following condition:

$$D(k_b) = \beta^2(k_b) - 4\alpha(k_b)\gamma(k_b) = 0. \quad (29)$$

After its linearization with respect to small parameters $t(k) - t_0$ and J_d^2/J_c^2 , this equation reduces, at first, to $\gamma(k_b) = 0$ and then to

$$\cos \frac{k_b}{2} \approx t_0 + \frac{J_d^2 t_0^2}{4J_c^2(2t_0 + 1)(t_0 + \Delta_1)}. \quad (30)$$

According to Eqs. (27) and (29), $\epsilon(k_b) = -\beta(k_b)/[2\alpha(k_b)]$, or using Eqs. (30) and (28),

$$\epsilon(k_b) \approx - \left(\frac{J_d t_0}{2J_c(t_0 + \Delta_1)} \right)^2. \quad (31)$$

Since $\epsilon(k_b) < 0$, condition (14) fails for $z(k_b)$. Therefore, for $J_d^2 \ll J_c^2$, there must be

$$k_{trunc} = k_c. \quad (32)$$

Since for $J_d \neq 0$ the wave vector k_c evolves continuously from k_0 , Eqs. (24), (20), and (16) give

$$z(k_c) = -1. \quad (33)$$

Although Eqs. (32) and (33) were proven for $J_d^2 \ll J_c^2$, they are also right for all J_d . Actually, if for some region of J_d it will be $k_{trunc} = k_b$, then there must be a point where $k_c = k_b$. However, as it was shown above, k_0 is the only one point of such type.

Equations (15) and (33) give the following representation for the magnon energy at the truncation point:

$$E_{trunc} = 2J_\perp - 3J_c - 2J_c \cos \frac{k_c}{2}. \quad (34)$$

The magnon branch approaches the bottom of the two-magnon continuum tangentially,

$$\left. \frac{\partial E_{bare}^{2magn,low}(k)}{\partial k} \right|_{k=k_c} = \left. \frac{\partial E(k)}{\partial k} \right|_{k=k_c} = J_c \sin \frac{k_c}{2}. \quad (35)$$

Equation (35) may be easily derived from Eqs. (25) and (15) using an auxiliary relation,

$$\left. \frac{\partial}{\partial k} \left(z(k) + \frac{1}{z(k)} \right) \right|_{k=k_c} = 0, \quad (36)$$

which follows from Eq. (33). The same result was obtained in Ref. 7 by a different approach.

Let us notice that the singularity at $t_0 + \Delta_1 = 0$ in formulas (30) and (31) originates from a resonance between the one-magnon and bound two-magnon states. Actually, for $t_0 = -\Delta_1$, Eq. (19) has the thrice-degenerate solution related to both these states. This special case is not considered in the present paper.

IV. MAGNON DISPERSION NEAR THE GAP

Let us turn to the opposite side of the spectrum related to $k = \pi$. As it follows from Eq. (19), $z(k)$ is an odd function and $z(\pi) = 0$. Therefore, for $k \approx \pi$, we may put

$$z(k) \approx z_1(\pi - k) + z_3(\pi - k)^3. \quad (37)$$

Then, from Eqs. (15) and (37) it follows that for $z_1^3 - z_1/12 - z_3 > 0$ the dispersion at $k \approx \pi$ takes the form

$$E(k) \approx E_{gap} \left(1 + \frac{v_{spin}^2}{2E_{gap}^2} (\pi - k)^2 \right), \quad (38)$$

where the gap energy E_{gap} and the spin velocity v_{spin} are given by

$$E_{gap} = 2J_\perp - 3J_c + \frac{J_c}{2z_1}, \quad \frac{v_{spin}}{E_{gap}} = \sqrt{\frac{J_c \left(z_1 - \frac{1}{12z_1} - \frac{z_3}{z_1^2} \right)}{2J_\perp - 3J_c + \frac{J_c}{2z_1}}}. \quad (39)$$

Since both E_{gap} and v_{spin} may be obtained by an experiment⁶ we shall express them explicitly from the coupling constants.

Substituting Eq. (37) into Eq. (19), we obtain the following system of equations on the coefficients z_1 and z_3 :

$$\left[\left(J_\perp - \frac{J_c}{2} \right) z_1 + \frac{J_c}{2} \right] \left[\left(\frac{3}{2} J_c - J_d \right) z_1 - J_c \right] = 0, \quad (40)$$

$$\left[\left(J_\perp - \frac{J_c}{2} \right) z_1 + \frac{J_c}{2} \right] \left[\left(\frac{3}{2} J_c - J_d \right) z_3 + \frac{J_c}{12} \right] + \left[\frac{J_c}{2} (z_1^2 - z_1 - \frac{1}{12}) + z_3 \left(J_\perp - \frac{J_c}{2} \right) \right] \left[\left(\frac{3}{2} J_c - J_d \right) z_1 - J_c \right] + \frac{J_d^2 z_1^2}{4} = 0. \quad (41)$$

Equation (40) has two solutions,

$$z_1^{magn} = -\frac{J_c}{2J_\perp - J_c}, \quad z_1^{bound} = \frac{2J_c}{3J_c - 2J_d}, \quad (42)$$

related to magnon and bound two-magnon branches.^{4,5} According to the first equation in Eq. (42), $z_3^{magn}(J_\perp - J_c/2) = -J_c z_3^{magn}/(2z_1^{magn})$, so from Eq. (41) it follows that

$$z_1^{magn} - \frac{1}{12z_1^{magn}} - \frac{z_3^{magn}}{(z_1^{magn})^2} = 1 - \frac{J_d^2}{J_c(4J_\perp + J_c - 2J_d)}, \quad (43)$$

and according to Eq. (39) one can obtain,

$$E_{gap} = J_\perp - \frac{5}{2} J_c, \quad (44)$$

$$\frac{v_{spin}}{E_{gap}} = \sqrt{\frac{2J_c}{2J_\perp - 5J_c} \left(1 - \frac{J_d^2}{J_c(4J_\perp + J_c - 2J_d)} \right)}.$$

As it follows from Eq. (44), the point $k = \pi$ corresponds to an energy minimum (the gap) only for $J_c(4J_\perp + J_c - 2J_d) > J_d^2$.

[According to the comment after Eq. (24), we suppose that $J_c > 0$.]

Using Eqs. (33) and (34), we may represent Eq. (19) in the point $k=k_c$ as follows:

$$\left(\frac{(E_{trunc} - 2E_{gap})\cos^2 \frac{k_c}{2}}{1 - \cos \frac{k_c}{2}} + E_{gap} - E_{trunc} \right) \times \left[\frac{(E_{trunc} - 2E_{gap})\left(3 + 4 \cos \frac{k_c}{2}\right)}{4\left(1 - \cos \frac{k_c}{2}\right)} - J_d \right] = J_d^2 \cos^2 \frac{k_c}{2}, \quad (45)$$

where the parameters J_\perp and J_c are excluded by Eqs. (34) and (44). Equation (45) may be used for obtaining the parameter J_d directly from an experimental data.

V. ONE-MAGNON DYNAMICAL STRUCTURE FACTOR NEAR THE THRESHOLD

We use the following representation for the dynamical structure factor (DSF):

$$S_{\alpha\beta}(\mathbf{q}, \omega) = \lim_{N \rightarrow \infty} \frac{1}{N} \sum_{\mu} \langle 0 | \mathbf{S}^\alpha(\mathbf{q}) | \mu \rangle \langle \mu | \mathbf{S}^\beta(-\mathbf{q}) | 0 \rangle \delta(\omega - E_\mu). \quad (46)$$

Here, $\mathbf{S}(\mathbf{q})$ is the spin Fourier transformation associated with the two-dimensional vector $\mathbf{q}=(q, q_{rung})$ with leg and rung components. Since the latter has only two possible values, 0 and π , we may study them separately,

$$\mathbf{S}(q, 0) = \sum_n e^{-iqn} (\mathbf{S}_{1,n} + \mathbf{S}_{2,n}), \quad (47)$$

$$\mathbf{S}(q, \pi) = \sum_n e^{-iqn} (\mathbf{S}_{1,n} - \mathbf{S}_{2,n}).$$

According to the following pair of relations, $\mathbf{S}(q, 0)|0\rangle = 0$, $\mathbf{S}(-q, \pi)|0\rangle = \sum_n e^{iqn} \dots |1\rangle_n \dots$, we may reduce the matrix elements in Eq. (46),

$$\langle \mu | \mathbf{S}(q, 0) | 0 \rangle = 0, \quad \langle \mu | \mathbf{S}^\beta(-q, \pi) | 0 \rangle = \delta_{\alpha\beta} \delta_{kq} \frac{\sqrt{N} a(q)}{Z(q)}. \quad (48)$$

Therefore, the DSF has a purely diagonal form, $S_{\alpha\beta}(q, \pi, \omega) = \delta_{\alpha\beta} S(q, \pi, \omega)$, while the one-magnon contribution is purely coherent,

$$S_{magn}(q, \pi, \omega) = A_{magn}(q) \delta[\omega - E^{magn}(q)], \quad (49)$$

where

$$A_{magn}(q) = \left| \frac{a_{magn}(q)}{Z_{magn}(q)} \right|^2. \quad (50)$$

According to Eqs. (8) and (13),

$$Z_{magn}(k) = \sqrt{|a_{magn}(k)|^2 + \frac{2|B_{magn}(k)|^2 z^2(k)}{1 - z^2(k)}}. \quad (51)$$

For $q \rightarrow k_c$, it will be $A_{magn}(q) \propto 1 - z^2(q)$, so as it follows from Eq. (33), $A_{magn}(k_c) = 0$. The same result was obtained in Ref. 7 by a different approach.

Finally, let us notice that a rather similar effect of hybridization between magnon and phonon modes was studied in Ref. 10. However, in the latter case a magnon mode does not truncate (because there is no decay), and therefore the corresponding structure factor does not turn to zero.

VI. SUMMARY AND DISCUSSION

In this paper, for a rung-dimerized asymmetric spin ladder, we suggested an effective model which neglects all states with $n > 2$ bare magnons. Using Bethe *Ansätze*, we studied the effect of magnon mode truncation resulting from magnon decay and clarified its mathematical nature [see Eq. (32)]. We obtained the four equations [see Eqs. (34), (44), and (45)] coupling the interaction constants of our model (namely, J_\perp , J_c , and J_d) with the truncation wave vector, gap and truncation energies, and spin velocity.

Of course, the neglect of the states with $n > 2$ bare magnons is a rather rough approximation. In reality, an intersection between the one- and two-magnon scattering modes is possible only for a wide band system. In this case, the bare $n > 2$ zones also lie not so far from the magnon mode and therefore give a rather essential contribution to it. However, if we are concerned only about the gap and truncation points, then our model produces a good approximation. Near the gap, the magnon energy is minimal and lies far below the bare $n > 2$ magnon modes. For example, as it follows from Eq. (44) for $J_d \ll J_\perp, J_c$, even the $n=2$ correction is small. From the other side, since the $1 \rightarrow 2$ decay threshold lies on a *finite* distance below the $1 \rightarrow 3$ one, the latter is not sufficient at the vicinity of the truncation point where the parameters $[E(k_c) - E(k)]/E_{gap}$ and $[E(k_c) - E(k)]/(E_{trunc} - E_{gap})$ are small. Therefore, the infinitesimal analysis of Sec. III [Eqs. (27)–(32)] gives the right picture of the truncation [Eq. (33)].

There is only one known asymmetric rung-dimerized spin ladder compound, namely, the CuHpCl (see Ref. 11 and references therein). However, the effect of truncation was not observed in this material. This fact is clear because the gap energy in CuHpCl (0.9 meV) is bigger than the magnon bandwidth (0.5 meV), so the magnon mode does not intersect with the scattering two-magnon continuum.

Although no wideband asymmetric rung-dimerized spin ladder compound was found up to now, we suppose that this will likely happen in the not so remote future. Then, the results of our paper will probably be useful for a theoretical study of such compound.

ACKNOWLEDGMENTS

The author is grateful to S. L. Ginzburg, S. V. Maleyev, and A. V. Syromyatnikov for the interest and helpful discussion.

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