Ground state fluctuations in rung-dimerized spin ladders

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Treating an exactly rung-dimerized spin ladder as a reference model we study perturbatively zero temperature quantum fluctuations in spin ladders with slightly destroyed rung-dimerization. Analytic expressions are obtained for the gas parameter (density of rung-triplets) and the ground state energy per rung. At a strong diagonal frustration as well as at a rather strong antiferromagnetic rung coupling these results well agree with the previous numerical calculations.

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I. INTRODUCTION

Perturbation theory for rung-dimerized spin ladders first considered in seminal works was then developed in a number of papers. In all of them an array of isolated rungs was treated as the exact zero-order reference model. The main virtue of this approach is a possibility to perform calculations up to a very high order. From the other hand its principal defect is triviality of dispersion in excitation spectrum of the reference (isolated rungs) model. According to this obstacle it seems reliable that obtained results will be well applicable only to narrow band spin ladders with \( \Delta \gtrsim E_{\text{gap}} \) (\( E_{\text{gap}} \) is a gap, \( \Delta E_{\text{magn}} \) is a magnon bandwidth). However this condition may be failed for real compounds. For example a recent neutron scattering experiment in the spin ladder compound \((\text{CsD}_{12}\text{N})_2\text{CuBr}_4\) gives \( \Delta E_{\text{magn}}/E_{\text{gap}} \approx 0.72 \) while for the spin ladder compound \(\text{La}_6\text{Ca}_9\text{Cu}_{24}\text{O}_{44}\) this ratio is about 5.3.

In this paper we suggest a more general perturbative approach to magnetic excitations in spin ladders by treating the exactly rung-dimerized spin ladder as a reference model. As in the isolated-rungs case the corresponding ground state still is an array of rung-dimers (singlets)

\[
|0\rangle_{e-d} = \prod_n |0\rangle_n, \tag{1}
\]

(\( |0\rangle_n \) is a singlet state associated with \( n \)-th rung), however now an excited triplet (denoted by \( |F_n\rangle \)) can move along the ladder from one rung to another. This process entails a nontrivial dispersion for an elementary excitation of the reference model. The latter will be called a rungon because in fact it is an excited single rung coherently propagating inside the rung-dimers bulk. It will be implied that the perturbed model belongs to the rung-dimerized phase, so its ground state is a dilute gas of excited rungon pairs. In this picture an elementary excitation magnon should be considered as a bare rungon interacting with the perturbed ground state.

The main technical difficulty of the suggesting approach is non integrability of the reference model. Indeed as it will be shown in forward an evaluation of the lowest (second) order perturbative correction to the ground state energy utilizes only two-rungon wave functions of the reference model. The next, i.e. one-magnon level requires a knowledge of the three-rungon spectrum. Due to the non integrability this problem is of a principal mathematical difficulty. Nevertheless for 5 integrable cases the three-magnon problem may be solved by the Bethe Ansatz.

In this paper the manifested approach is applied for an evaluation of two main ground state parameters, namely the gas parameter (or equivalently the density of rung triplets)

\[
\rho = \lim_{N \to \infty} \frac{1}{N} \langle 0 | \hat{Q} | 0 \rangle. \tag{2}
\]

and the normalized energy density

\[
\varepsilon = - \lim_{N \to \infty} \frac{\langle 0 | \hat{H} | 0 \rangle}{N E_{\text{rung}}} \tag{3}
\]

Here \( \hat{H} \), \( N \) and \( E_{\text{rung}} \) are correspondingly the Hamiltonian, a number of rungs and the excitation energy of an isolated rung. The operator \( \hat{Q} = \sum_n Q_n \), whose local density satisfies the following relations

\[
Q_n |0\rangle_n = 0, \quad Q_n |1\rangle_n = |1\rangle_n, \tag{4}
\]

is the number operator for rung-triplets. Probably it is better to denote the gas parameter by \( n \) (concentration) instead of \( \rho \) (density). However in this paper the index “\( n \)” is utilized especially for enumerating of ladder rungs.

Both the quantities \( \rho \) and \( \varepsilon \) are of interest for ascertaining of boundaries of the rung-dimerized phase. Also \( \rho \) may be considered as the governing parameter for the dilute gas approximation. The parameter \( \varepsilon \) was used for evaluation of the spin ladder entropy.

For a future development of the perturbation theory both \( \rho \) and \( \varepsilon \) may be considered as the corresponding governing parameters. Indeed it is crucial to obtain a system of conditions on the coupling constants under which the perturbative approach is valid. In fact it should be a requirement for some relevant dimensionless governing parameters to be small. Usually only \( \rho \) was suggested on this role. Namely the mean field Green function approach to rung-dimerized spin ladders may be developed only at \( \rho \ll 1 \). The quasiclassical approximation is valid...
only at $\rho \lambda(T) \ll 1$, where $\lambda(T)$ is the average de Broglie wavelength of thermally excited magnons expressed in lattice units. Despite the parameter $\varepsilon$ was not yet utilized for establishing of the perturbative approach validity we suppose that this energetic quantity also is very important.

In this light it seems reasonable that besides numerical estimations\textsuperscript{11,12} it is necessary to have for $\rho$ and $\varepsilon$ reliable analytic formulas. The latter are just obtained in the present paper in the second order of perturbation theory near the exact rung-dimerized ground state (1). As it was already mentioned technically these calculations are possible because the first order correction term in the perturbative expansion for $|0\rangle$ contains only (previously obtained by the authors\textsuperscript{10} two-rung excitations around $|0\rangle$\textsubscript{r-d}. At $\rho \ll 1$ and $\varepsilon \ll 1$ the obtained formulas agree with the corresponding numerical data\textsuperscript{11}.

II. STRUCTURE OF THE HAMILTONIAN

It is more convenient to represent the general spin ladder Hamiltonian in the following form\textsuperscript{10}

\[
\hat{H} = \hat{H}_{r-d} + J_0 \hat{V},
\]

where

\[
\hat{H}_{r-d} = \sum_n J_1 (Q_n + Q_{n+1}) + J_2 (\Psi_n \cdot \bar{\Psi}_{n+1} + \bar{\Psi}_n \cdot \Psi_{n+1})
+ J_3 Q_n Q_{n+1} + J_4 S_n \cdot S_{n+1} + J_5 (S_n \cdot S_{n+1})^2,
\]

and

\[
\hat{V} = \sum_n \bar{\Psi}_n \cdot \bar{\Psi}_{n+1} + \Psi_n \cdot \Psi_{n+1}.
\]

Here

\[
\Psi_n = \frac{1}{2} (S_{1,n} - S_{2,n}) - i [S_{1,n} \times S_{2,n}],
\]

\[
\bar{\Psi}_n = \frac{1}{2} (S_{1,n} - S_{2,n}) + i [S_{1,n} \times S_{2,n}],
\]

\[
S_n = S_{1,n} + S_{2,n},
\]

\[
Q_n = \frac{1}{2} S_n^2 = \bar{\Psi}_n \cdot \Psi_n,
\]

(\(S_{i,n}\) (i = 1, 2) are spin-1/2 operators associated with \(n\)-th rung). According to

\[
\Psi_n^a |0\rangle_n = |1\rangle_n^a, \quad \bar{\Psi}_n |0\rangle_n = 0, \quad \Psi_n^a |1\rangle_n = 0, \quad \bar{\Psi}_n^a |1\rangle_n = \delta_{ab} |0\rangle_n,
\]

the operators $\bar{\Psi}$ and $\Psi$ may be considered as (neither Bose, nor Fermi) creation-annihilation operators for rung-triplets. Correspondence between (5)-(7) and the traditional representation

\[
\hat{H} = \sum_{n=-\infty}^{\infty} H_{n,n+1}^r + H_{n,n+1}^d + H_{n,n+1}^{dd}
+ H_{n,n+1}^{rr} + H_{n,n+1}^{ll} + H_{n,n+1}^{dd} + J_{\text{norm}},
\]

where

\[
H_{n,n+1}^r = \frac{J_1}{2} (S_{1,n} \cdot S_{2,n} + S_{1,n+1} \cdot S_{2,n+1}),
\]

\[
H_{n,n+1}^l = J_1 (S_{1,n} \cdot S_{1,n+1} + S_{2,n} \cdot S_{2,n+1}),
\]

\[
H_{n,n+1}^d = J_d (S_{1,n} \cdot S_{2,n+1} + S_{2,n} \cdot S_{1,n+1}),
\]

\[
H_{n,n+1}^{rr} = J_{rr} (S_{1,n} \cdot S_{2,n}) (S_{1,n+1} \cdot S_{2,n+1}),
\]

\[
H_{n,n+1}^{ll} = J_{ll} (S_{1,n} \cdot S_{1,n+1}) (S_{2,n} \cdot S_{2,n+1}),
\]

\[
H_{n,n+1}^{dd} = J_{dd} (S_{1,n} \cdot S_{2,n+1}) (S_{2,n} \cdot S_{1,n+1}),
\]

\[
J_{\text{norm}} = \frac{3}{4} (J_r + J_l - J_d) - \frac{9}{16} J_{rr} - \frac{3}{8} J_{ll},
\]

is given by the formulas\textsuperscript{10}

\[
J_1 = \frac{1}{4} \left( 2 J_r - 3 J_{rr} - J_{ll} - J_{dd} \right),
\]

\[
J_2 = \frac{1}{8} \left( 4 (J_l - J_d) + J_{ll} - J_{dd} \right),
\]

\[
J_3 = J_{rr},
\]

\[
J_4 = \frac{1}{8} \left( 4 (J_l + J_d) + J_{ll} + J_{dd} \right),
\]

\[
J_5 = \frac{1}{4} \left( J_l + J_{dd} \right),
\]

\[
J_6 = \frac{1}{8} \left( 4 (J_l - J_d) - J_{ll} + J_{dd} \right).
\]

Let us notice that one can inverse the relations (8) and express the spin operators

\[
S_{1,n} = \frac{1}{2} \left( \Psi_n + \bar{\Psi}_n - i [\bar{\Psi}_n \times \Psi_n] \right),
\]

\[
S_{2,n} = \frac{1}{2} \left( - \Psi_n - \bar{\Psi}_n - i [\bar{\Psi}_n \times \Psi_n] \right).
\]

As it was already mentioned\textsuperscript{10} the operators (8) do not coincide with very similar ones introduced in Refs. 3 and 17,18 (as well as in other papers of these authors). Indeed the representation (14) is similar to the ones suggested in Refs. 17 and 3, but in fact is not identical to any of them because the analogs of $\Psi_n$ and $\bar{\Psi}_n$ treated in these Refs. act in extended vector spaces. That is why for example the "inverse" formula (8) fails for these operators. The operators suggested in Ref. 18 in fact act in the same vector space as (8) but have a slightly different form.

According to (6)

\[
E_{\text{rung}} = 2 J_1,
\]

\[
\rho = -\frac{\partial}{\partial J_1} (J_1 \varepsilon).
\]

Without loss of generality one can imply $J_2 > 0$ because a substitution $J_2 \rightarrow -J_2$ is equivalent to permutation of spins in all odd (or even) rungs.

As it readily follows from (4), (6) and (10) $[\hat{Q}, \hat{H}_{r-d}] = 0$. So the Hilbert space related to $\hat{H}_{r-d}$ splits into a direct sum

\[
\mathcal{H} = \sum_{m=0}^{\infty} \mathcal{H}^m, \quad \hat{Q}|\mathcal{H}^m = m,
\]
where each $\mathcal{H}^m$ corresponds to $m$-rungon sector.

For rather big $J_1$ vector (1) is the (zero energy) ground state of $H_{r-d}$. The complete set of inequalities on $J_1$ which guarantees the exact rung-dimerization is not yet obtained except the following one.\footnote{Note: 10.}

$$J_1 - J_2 > 0. \tag{18}$$

According to (7) and (10)

$$\hat{V} : \mathcal{H}^m \to \mathcal{H}^{m-2} \oplus \mathcal{H}^{m-2}. \tag{19}$$

So the operator $\hat{V}$ destroys the exact rung-dimerization. However, it seems reliable that the region $J_1 > J_2, J_3, J_4, J_5 > J_6$ should contain the rung-dimerized phase for which the operator $J_6 \hat{V}$ may be treated perturbatively and

$$\rho \ll 1, \quad \varepsilon \ll 1. \tag{20}$$

The parameter $J_1$ characterizes a chemical potential of an exited rung (or rungon mass) while $J_2$ its kinetic energy. The couplings $J_3 - J_5$ describe a spin-dependent rungon-rungon interaction. Finitely the parameter $J_6$ governs creation-annihilation of singlet rungon pairs.

### III. EVALUATION OF THE GOVERNING PARAMETERS

According to Eqs. (3) and (19) $\langle 0 | \hat{V} | 0 \rangle_{r-d} = 0$, so

$$\varepsilon = \varepsilon_{\text{bound}} + \varepsilon_{\text{scatt}} + o(J_6^2), \tag{21}$$

where

$$\varepsilon_{\text{bound}} = \frac{J_6^2}{2J_1} \lim_{N \to \infty} \frac{\langle \text{bound} | \hat{V} | 0 \rangle_{r-d}^2}{2N \varepsilon_{\text{bound}}},$$

$$\varepsilon_{\text{scatt}} = \frac{J_6^2}{2\pi J_1} \int_0^\pi \frac{|q, \text{scatt} | \hat{V} | 0 \rangle_{r-d}^2}{E_{\text{scatt}}(q)} dq \tag{22}$$

(we have utilized $1/N \sum_q \to 1/(2\pi) \int_0^{2\pi} d(2q)$) are contributions from singlet, translationary invariant bound and scattering two-rungon states.\footnote{Note: 10.}

$$|\text{bound} \rangle = \sqrt{\frac{\Delta^2 - 1}{3N}} \sum_{m<n} \Delta_{m-n}^{m-n-1} |1\rangle_n |1\rangle_m \ldots,$$

$$|q, \text{scatt} \rangle = \sqrt{\frac{2}{3(\Delta^2 - 2\Delta_0 \cos q + 1)N}} \times \sum_{m<n} a(q, n - m) \ldots |1\rangle_n |1\rangle_m \ldots \tag{23}$$

Here $0 < q < \pi$ is a half of relative wave number

$$a(q, n) = \sin nq - \Delta_0 \sin (n-1)q, \tag{24}$$

and $\Delta_0 = (J_3 - 2J_4 + 4J_5)/(2J_2)$.

The corresponding energies are the following

$$E_{\text{bound}} = 4J_1 + 2J_2 \left( \Delta_0 + \frac{1}{\Delta_0} \right) = 2E_{\text{gap}} + \frac{(\Delta_0 + 1)^2}{2\Delta_0} \Delta E_{\text{rung}}, \tag{25}$$

$$E_{\text{scatt}}(q) = 4(J_1 + J_2 \cos q). \tag{26}$$

where $E_{\text{gap}} = 2(J_1 - J_2)$ and $\Delta E_{\text{rung}} = 4J_2$ are the rungon gap and energy width.\footnote{Note: 10.}

As it follows from (23) the translationary invariant bound state exists only for

$$|\Delta_0| > 1. \tag{27}$$

(although as it follows from (25) and (26) in a real compound it should metastable at $\Delta_0 > 1$).

According to (7), (10) and (23)

$$\langle q, \text{scatt} | \hat{V} | 0 \rangle_{r-d} = \frac{\sqrt{6} \sin q}{\sqrt{(\Delta_0^2 - 2\Delta_0 \cos q + 1)}},$$

$$\langle \text{bound} | \hat{V} | 0 \rangle_{r-d} = \sqrt{N} \frac{\sqrt{3(\Delta_0^2 - 1)}}{\Delta_0}. \tag{28}$$

Substituting (28) into (22) and utilizing (25)-(27) one can readily obtain

$$\varepsilon_{\text{scatt}} = \frac{3J_6^2}{8J_1 \Delta_0^2} I,$$

$$\varepsilon_{\text{bound}} = \Theta(\Delta_0^2 - 1) \frac{3J_6^2(\Delta_0^2 - 1)}{2J_1 \Delta_0^4 E_{\text{bound}}}. \tag{29}$$

For calculation of $I$ we note that according to (18) the pole $z = -(J_1 + \sqrt{J_1^2 - J_2^2})/J_2$ lies outside the unit circle. Therefore only residues in the poles $z = 0$, $z = \sqrt{J_1^2 - J_2^2}/J_2$, and one of the appropriate points $1/\Delta_0$ (for $|\Delta_0| > 1$) or $\Delta_0$ (for $|\Delta_0| < 1$) give contributions to $I$. Performing the calculations one can obtain

$$\varepsilon_{\text{scatt}} = \frac{3J_6^2}{8J_1 \Delta_0^2}\left(1 - \frac{J_2|\Delta_0^2 - 1| + 2\Delta_0 \sqrt{J_1^2 - J_2^2}}{2[2\Delta_0 J_1 + (\Delta_0^2 + 1)J_2]^{\frac{3}{2}}} \right). \tag{31}$$

Then according to (16)

$$\rho = \rho_{\text{bound}} + \rho_{\text{scatt}} + o(J_6^2), \tag{32}$$

where

$$\rho_{\text{scatt}} = \frac{3J_6^2}{4\Delta_0 J_1 + (\Delta_0^2 + 1)J_2^2} \times \left[ \frac{(\Delta_0^2 + 1)J_1 + 2\Delta_0 J_2}{\sqrt{J_1^2 - J_2^2}} - |\Delta_0^2 - 1| \right],$$

$$\rho_{\text{bound}} = 6\Theta(\Delta_0^2 - 1)\frac{(\Delta_0^2 - 1)J_2^2}{\Delta_0^2 E_{\text{bound}}}. \tag{33}$$
The denominators $\sqrt{J_t^2 - J_r^2} \propto \sqrt{\varepsilon}$ and $E_{\text{bound}}^2$ in (33) describe the ground state (1) destruction caused by condensation of scattering and bound singlet pairs.

IV. COMPARISON WITH NUMERICAL RESULTS

Here we compare the DMRG data for the case

$$0 \leq J_r \leq 2, \quad J_t = 1, \quad J_{rr} = J_{dd} = 0, \quad (34)$$

(also in Ref. 11 was taken $J_{\text{norm}} = 0$, so we had to shift the data for $\varepsilon$ with the corresponding results obtained analytically with the use of the perturbative formulas (21), (29), (31) and (32), (33)). It is more instructive to do it in the case of maximal dimerization (considered in Ref. 11) namely for $J_r = 2$.

For $J_d = 0$ the Ref. 11 gives $\rho = 0.11, \varepsilon = 0.11$ (our results: $\rho = 0.22, \varepsilon = 0.14$). For $J_d = 0.2$, $\rho = 0.10$ and $\varepsilon = 0.08$ (our results: $\rho = 0.14, \varepsilon = 0.09$). For $J_d = 0.4, \rho = 0.07$ and $\varepsilon = 0.05$ (our results: $\rho = 0.09, \varepsilon = 0.05$). For $J_d = 0.6, \rho = 0.04$ and $\varepsilon = 0.03$ (our results: $\rho = 0.04, \varepsilon = 0.03$). For $J_d = 0.8$, $\rho = 0.01$ and $\varepsilon < 0.01$ (our results: $\rho = 0.01, \varepsilon = 0.007$). Comparing numerical and analytic results one may conclude that the suggested perturbative approach works better for frustrated ladders. Really at $J_d = 0.8$ even for $J_r = 1.6$ the numerical result $\rho = 0.03$ coincides with the theoretical one. Also for $J_d = 0.8$ and $J_r = 1.5$ in the both approaches $\varepsilon = 0.02$.

A discrepancy between the numerical data and analytical predictions for non frustrated spin ladders indicates that besides dynamics of single rungs their properties are governed by creation-annihilation processes. However the latter may be suppressed by strong antiferromagnetic rung coupling.

V. SUMMARY

In this paper the perturbative formulas for the gas parameter (Eqs. (32), (33)) and ground state energy energy per rung (Eqs. (21), (29), (31)) were obtained for spin ladders belonging to the rung-dimerized phase. At strong diagonal frustration as well as at rather strong antiferromagnetic rung coupling the result agrees with the previous DMRG calculations. In this region the conditions (20) are satisfied so one may conclude that the system really lies in the rung-dimerized phase.

It will be interesting to compare the analytical and numerical approaches more precisely and in a wider range of the coupling parameters including four-spin terms.

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