On the ground state energy scaling in quasi-rung-dimerized spin ladders

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On the basis of periodic boundary conditions we study perturbatively a large \( N \) asymptotics (\( N \) is the number of rungs) for the ground state energy density and gas parameter of a spin ladder with slightly destroyed rung-dimerization. Exactly rung-dimerized spin ladder is treated as the reference model. Explicit perturbative formulas are obtained for three special classes of spin ladders.

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I. INTRODUCTION

Phase structure of frustrated spin ladders and spin ladders with four-spin terms has been intensively studied in the last decade both theoretically and numerically. Among other phases the mathematically most simple one and at the same time, probably, the one most interesting for physical applications is the so called rung-singlet (or rung-dimerized) phase. Within it the ground state may be well approximated by an infinite tensor product of rung-dimers (singlet pairs)

\[ |0\rangle_{r-d} = \otimes_n |0\rangle_n. \]  

This state will be an exact ground state only for rather big antiferromagnetic rung-coupling and under a special condition on the coupling constants. The latter has no physical background and thus there are absolutely no grounds to assume its relevance for real compounds. Nevertheless it is a common opinion that for rather big antiferromagnetic rung coupling a spin ladder should still remain in the rung-singlet phase. This means that all physical properties of such a ladder may be obtained perturbatively on the basis of the "bare" ground state \( |1\rangle \) and its excitations. Together with verification by machinery calculations this approach should give a comprehensive description of the rung-singlet phase. A machinery calculation will provide excellent tests for suggested formulas and hence they should be good governing parameters for a perturbation theory based on the gas approximation. Perturbative expressions for \( \rho \) and \( E \) were derived in Ref. 12. In the present paper assuming periodic boundary conditions we obtain in three special cases the corresponding extrapolation formulas for \( \rho_N \) and \( E_N \).

The two formulas

\[ E_N = E_\infty + (-1)^N A e^{-N/N_0}, \]

\[ E_N = E_\infty - A N^2, \]

\((A, N_0)\) are free parameters) have already been suggested correspondingly for open and periodic boundary conditions. The expression \( (4) \) was implied ad hoc, while Eq. \((5)\) follows from conformal theory argumentation. The perturbative formulas obtained below for three special classes of spin ladders have a rather different form

\[ E_N = E_\infty + (A + (-1)^{N} B)e^{-(N-1)/N_0}. \]

II. DESCRIPTION OF THE MODEL

We shall use an equivalent representation

\[ \hat{H} = \hat{H}_0 + J_0 \hat{V}, \]
of the spin ladder Hamiltonian $J^4_6, 12$. Here $J_6$ is a perturbation parameter and

$$\hat{H}_0 = \sum_{n=1}^{N} J_1 Q_n + J_2 (\Psi_n \cdot \Psi_{n+1} + \bar{\Psi}_n \cdot \bar{\Psi}_{n+1})$$

$$\hat{V} = \sum_{n=1}^{N} V_{n,n+1},$$

$V_n = S_{1,n} + S_{2,n}, \quad Q_n = \frac{1}{2} S^2_{n},$

$V_{n,n+1} = \Psi_n \cdot \Psi_{n+1} + \Psi_n \cdot \Psi_{n+1},$

\begin{equation}
(\Psi_{i,n} \text{ for } i = 1, 2 \text{ are spin-1/2 operators associated with } n\text{-th rung}). \text{ The local operators}
\end{equation}

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

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

may be interpreted as (neither Bose nor Fermi) creation-annihilation operators for rung-triplets. Namely

$$\Psi^a_n |0\rangle_n = |1\rangle_n^a, \quad \bar{\Psi}^a_n |1\rangle_n^b = 0,$$

$$\bar{\Psi}^a_n |0\rangle_n = 0, \quad \Psi^a_n |1\rangle_n^b = \delta_{ab} |0\rangle_n.$$  

From (8) and (9) readily follows that

$$[\hat{H}_0, \hat{Q}] = 0,$$

where the operator

$$\hat{Q} = \sum_n Q_n,$$

according to relations

$$Q_n |0\rangle_n = 0, \quad Q_m |1\rangle_n = \delta_{mn} |1\rangle_n,$$

has a sense of the number operator for rung-triplets $6, 12$. For rather big $J_1$ (for example necessary to be $J_1 > J_2$) vector (1) is the zero energy ($\hat{H}_0 |0\rangle_{r-d} = 0$) ground state for $\hat{H}_0$, whose physical Hilbert space splits into a direct sum $6, 12$.

$$\mathcal{H} = \bigoplus_{m=0}^{\infty} \mathcal{H}^m, \quad \hat{Q}|\mathcal{H}^m = m.$$  

The subspace $\mathcal{H}^0$ is generated by the single vector (1). According to (2), (3) and (8)

$$\rho_N = \frac{\partial E_N}{\partial J_1}.$$  

Since $\hat{V} : |0\rangle_{r-d} \rightarrow \mathcal{H}^2$, a perturbative treatment of the term $J_6 V$ gives

\begin{equation}
E_N = -\frac{J^2_6}{N} \sum_{|\mu\rangle \in \mathcal{H}^2} \frac{|\langle \mu | \hat{V} |0\rangle_{r-d}|^2}{E(\mu)} + o(J^2_6),
\end{equation}

where all the states $|\mu\rangle$ in the sum have zero total spin and quasimomentum. In the $N \rightarrow \infty$ limit $12$

$$E_{\infty} = -\Theta(\Delta^2_0 - 1) \frac{3J^2_6(\Delta^2_0 - 1)}{\Delta_0 E_{\text{bound}}}$$

$$-\frac{3J^2_6}{4J_2 \Delta_0} \left(1 - \frac{J_3 |\Delta^2_0 - 1| + 2\Delta_0 \sqrt{J^2_4 - J^2_2}}{2\Delta_0 |J_1 + (\Delta^2_0 + 1)J_2|}\right),$$

where $\Theta(x) = 1$ for $x > 0$ and $\Theta(x) = 0$ for $x \leq 0$ and

$$\Delta_0 = J_3 - 2J_4 + 4J_5,$$

$$E_{\text{bound}} = 4J_1 + 2J_2 \left(\Delta_0 + \frac{1}{\Delta_0}\right).$$

\section*{III. A FINITE-N TWO-PARTICLE PROBLEM}

A zero total spin and quasimomentum two-magnon state has the following general form,

$$|2-\text{magn}| = \sum_{1 \leq m < n \leq N} a(n - m)|1\rangle_n|1\rangle_m...|1\rangle_n...$$  

The dimension of the corresponding Hilbert space is $N/2$ for even $N$ and $(N-1)/2$ for odd. The wave function $a(n)$ should be normalised

$$\sum_{n=1}^{N-1} (N-n)|a(n)|^2 = \sum_{m<n} |a(n-m)|^2 = \frac{1}{3},$$

and satisfy the periodicity condition $a(n-m) = a(n + N - n)$ or shortly

$$a(n) = a(N - n).$$

Performing a substitution $n \rightarrow N - n$ and using (23) one can obtain from (22)

$$\sum_{n=1}^{N-1} n |a(N-n)|^2 = \sum_{n=1}^{N-1} n |a(n)|^2 = \frac{1}{3},$$

Together (22) and (24) result in

$$\sum_{n=1}^{N-1} |a(n)|^2 = \frac{2}{3N}.\tag{25}$$

The Schrödinger equation gives

$$4J_1a(n) + 2J_2[a(n-1) + a(n+1)] = Ea(n),$$

for $1 < n < N - 1$ and

$$2(2J_1 + J_2 \Delta_0)a(1) + 2J_2 a(2) = Ea(1),\tag{27}$$

for $n = 1$. 
General solution of the system (26), (27) has the form
\[
a(n, z) = \frac{1}{\sqrt{Z(z)}} \left[ \left( 1 - \frac{\Delta_0}{z} \right) z^n - \frac{1}{z^n} \left( 1 - \Delta_0 z \right) \right],
\]
and dispersion
\[
E(z) = 4J_1 + 2J_2 \left( z + \frac{1}{z} \right).
\]
The normalization constant \( Z(z) \) ensures condition (25). The parameter \( z \) corresponds to relative quasimomentum of magnon pair and satisfy an equation
\[
z^{N-1} = \frac{\Delta_0 z - 1}{z - \Delta_0} = -z \frac{\Delta_0 - 1/z}{\Delta_0 - z}.
\]
The latter is invariant under complex conjugation and a duality symmetry
\[
z \rightarrow \frac{1}{z},
\]
which according to (28) is related to multiplication of the wave function on (-1). Hence for even \( N \) the roots of (30) are joined in dual pairs, while for odd \( N \) there is an additional autodual root \( z = -1 \).

In the three special cases \( \Delta_0 = -1, \Delta_0 = 1 \) and \( \Delta_0 = 0 \) Eq. (30) may be solved explicitly. Denoting the corresponding solutions as \( u_j, v_j \) and \( w_j \) respectively one has
\[
u_j = e^{(j+1)i\pi/(N-1)}, \quad j = 0, ..., N-2, \quad (\Delta_0 = -1),
\]
\[
v_j = e^{2ji\pi/(N-1)}, \quad j = 0, ..., N-2, \quad (\Delta_0 = 1),
\]
\[
w_j = e^{(2j+1)i\pi/N}, \quad j = 0, ..., N-1, \quad (\Delta_0 = 0).
\]

Taking into account that all the roots (32) lie in a unite circle one may readily get
\[
Z(z) = 3N(N-1)(1 - \Delta_0 z)(1 - \frac{\Delta_0}{z}), \quad \Delta_0 = \pm 1,
\]
\[
Z(z) = 3N^2, \quad \Delta = 0,
\]
and then
\[
|a(n, z)|^2 = \frac{1}{3N(N-1)} \left[ 2 + \Delta_0 \left( z^{2n-1} + \frac{1}{z^{2n-1}} \right) \right], \quad \Delta_0 = \pm 1,
\]
\[
|a(n, z)|^2 = \frac{1}{3N^2} \left( 2 - z^{2n} - \frac{1}{z^{2n}} \right), \quad \Delta_0 = 0.
\]

IV. EXACT RESULTS AT \( \Delta_0 = 0 \) AND \( \Delta_0 = \pm 1 \)

Let \( |z| \) be the state related to wave function (28). From (9) and (21) follows that
\[
|\langle z|\hat{V}|0\rangle_{\tau - a}|^2 = 9N^2|a(1, z)|^2.
\]

For the evaluation of \( E_N \) one has to perform in (17) a summation over all duality pairs of roots. Since both the roots in a pair give the same contribution this is equivalent to inserting the factor 1/2 before summation over all roots. Hence (17) and (35) result in
\[
E_N(\Delta_0) = -\frac{3}{4} J_0^2 G_N(\Delta_0) + o(J_0^2),
\]
where
\[
G_N(-1) = \frac{1}{N-1} \sum_{j=0}^{N-2} \frac{2 - (u_j + 1/u_j)}{2J_1 + 2J_2(u_j + 1/u_j)} = \frac{1}{J_2(N-1)} \sum_{j=0}^{N-2} \left[ -1 + \frac{J_1 + J_2}{\sqrt{J_1^2 - J_2^2}} \left( \frac{J_- - u_j}{J_- - u_j} - \frac{J_+}{J_+ - u_j} \right) \right],
\]
\[
G_N(1) = \frac{1}{N-1} \sum_{j=0}^{N-2} \frac{2 + (v_j + 1/v_j)}{2J_1 + 2J_2(v_j + 1/v_j)} = \frac{1}{J_2(N-1)} \sum_{j=0}^{N-2} \left[ 1 - \frac{J_1 - J_2}{\sqrt{J_1^2 - J_2^2}} \left( \frac{J_- - v_j}{J_- - v_j} - \frac{J_+}{J_+ - v_j} \right) \right],
\]
\[
G_N(0) = \frac{1}{N} \sum_{j=0}^{N-1} \frac{2w_j^2 - w_j^4 - 1}{w_j(J_2 w_j^2 - 2J_1 w_j + J_2)} = \frac{2}{J_2 N} \sum_{j=0}^{N-1} \left[ J_1 - \frac{J_2}{2} \left( w_j + \frac{1}{w_j} \right) - \sqrt{J_1^2 - J_2^2} \left( \frac{J_-}{J_- - w_j} - \frac{J_+}{J_+ - w_j} \right) \right],
\]
\[
J_\pm = -J_1 \pm \sqrt{J_1^2 - J_2^2}.
\]

In (37) we used for calculations the formulas
\[
\sum_{j=0}^{N-2} \frac{1}{J - u_j} = \frac{(N-1)J^{N-2}}{J^{N-1} + 1},
\]
\[
\sum_{j=0}^{N-2} \frac{1}{J - v_j} = \frac{(N-1)J^{N-2}}{J^{N-1} + (-1)^N J N^{-1}},
\]
which may be proved according to the following argumentation. The sums in (39) are fractions whose numerator and denominator are symmetric polynomials with respect to $u_j, v_j$ and $w_j$ respectively. However according to (30) all these polynomials except
\[
u_0 \ldots u_{N-2} = (-1)^{N-1}, \quad v_0 \ldots v_{N-2} = 1,
\]
\[
w_0 \ldots w_{N-1} = (-1)^N
\]
are equal to zero.

From equality $J_+ J_- = 1$ readily follows
\[
\frac{J_{+}^{N-1}}{J_{+}^{N-1} + 1} - \frac{J_{-}^{N-1}}{J_{-}^{N-1} + (-1)^{N-1}} = 1 - \frac{(-J_+)^{N-1}}{1 + (-J_+)^{N-1}}.
\]

Using (41) one may readily reduce Eqs. (37) to the form
\[
G_N(-1) = \frac{1}{J_2} \left[ \sqrt{\frac{1 + J_2}{J_1}} \cdot \frac{1 - J_+^{N-1}}{1 + J_+^{N-1}} - 1 \right],
\]
\[
G_N(1) = \frac{1}{J_2} \left[ 1 - \sqrt{\frac{J_1 - J_2}{J_1 + J_2}} \cdot \frac{1 - (-J_+)^{N-1}}{1 + (-J_+)^{N-1}} \right],
\]
\[
G_N(0) = \frac{2}{J_2} \left[ \frac{J_1}{J_2} - \sqrt{\frac{J_1^2 - J_2^2}{J_2^2}} \cdot \frac{1 - J_+^N}{1 + J_+^N} \right].
\] (42)

It may be readily observed that the corresponding values for $E_{\infty}(\Delta_0)$ agree with Eq. (18). The scaling law has the form (6) with
\[
A(-1) = 0, \quad B(-1) = -\frac{3J_0^2}{2J_2} \sqrt{\frac{J_1 + J_2}{J_1 - J_2}},
\]
\[
A(1) = \frac{3J_0^2}{2J_2} \sqrt{\frac{J_1 - J_2}{J_1 + J_2}}, \quad B(1) = 0, \quad A(0) = 0, \quad B(0) = \frac{3J_0^2}{J_2^2} \sqrt{\frac{J_1^2 - J_2^2}{J_1^2 + J_2^2}},
\] (43)

at $J_2 > 0$ and
\[
A(-1) = -\frac{3J_0^2}{2J_2} \sqrt{\frac{J_1 + J_2}{J_1 - J_2}}, \quad B(-1) = 0, \quad A(1) = 0, \quad B(1) = \frac{3J_0^2}{2J_2^2} \sqrt{\frac{J_1 - J_2}{J_1 + J_2}}, \quad A(0) = \frac{3J_0^2}{J_2^2} \sqrt{\frac{J_1^2 - J_2^2}{J_1^2 + J_2^2}}, \quad B(0) = 0, \quad (44)
\]
at $J_2 < 0$. In both the cases
\[
N_0 = \frac{1}{\ln |J_2| - \ln (J_1 - \sqrt{J_1^2 - J_2^2})}.
\] (45)

The corresponding formulas for $\rho_N$ have the similar form and may be readily obtained from (16).

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