

Entanglement Spectra of Heisenberg Ladders of higher Spin

John Schliemann¹ and Andreas M. Läuchli²

¹Institute for Theoretical Physics, University of Regensburg, D-93040 Regensburg, Germany

²Institut für Theoretische Physik, Universität Innsbruck, A-6020 Innsbruck, Austria

E-mail: john.schliemann@physik.uni-regensburg.de

Abstract. We study the entanglement spectrum of Heisenberg spin ladders of arbitrary spin length S in the perturbative regime of strong rung coupling. For isotropic spin coupling the the entanglement spectrum is, within first order perturbation theory, always proportional to the energy spectrum of the single chain with a proportionality factor being also independent of S . A more complicated situation arises for anisotropic ladders of higher spin $S \geq 1$ since here even the unperturbed ground state has a nontrivial entanglement spectrum. Finally we discuss related issues in dimerized spin chains.

1. Introduction

Quantum entanglement has by now developed to a key ingredient and tool of quantum many body physics[1, 2]. More recently, the notion of the *entanglement spectrum* has provided a novel conceptual input to the field leading to new insights in the properties of various systems[3]. These comprise quantum Hall monolayers at fractional filling [3, 4, 5, 6, 7, 8, 9, 10, 11, 12, 13, 14, 15], quantum Hall bilayers at filling factor $\nu = 1$ [16], spin systems of one [17, 18, 19, 20, 21, 22, 23] and two [24, 25, 26, 27] spatial dimensions, and topological insulators [28, 29]. Other topics recently covered include rotating Bose-Einstein condensates [30], coupled Tomonaga-Luttinger liquids [31], and systems of Bose-Hubbard[32] and complex paired superfluids[33].

In Ref. [21] Poilblanc reported the observation that chain-chain entanglement spectra in two-leg spin-1/2 ladders are remarkably similar to the *energy* spectrum of a single spin-1/2 Heisenberg chain. Furthermore, the effective inverse temperature fitted to the data was found to depend on the ratio of the leg to the rung couplings and vanishes in the limit of strong rung coupling. Subsequently, one of the present authors observed a similarly striking resemblance between the entanglement spectra of quantum Hall bilayers at $\nu = 1$ and the energy spectrum of a single physical layer at half filling.[16]

In the case of isotropic spin-1/2 ladders the above observations were explained only shortly later by Peschel and Chung [22] and by the present authors [23] via first-order

perturbation theory around the limit of strong rung coupling. Moreover, as shown in Ref. [23], an anisotropic spin-1/2 ladder will in general lead to an entanglement Hamiltonian with renormalized anisotropy, and in second order perturbation theory further corrections to the entanglement Hamiltonian occur.

In the present paper we extend the above results for isotropic Heisenberg ladders to the case of arbitrary spin length S . We find that the entanglement spectrum is still, within first order perturbation theory, proportional to the energy spectrum of the single chain. This is an remarkable result since important features of the latter spectra, such as presence or absence of an excitation gap over the ground state, depend crucially on the spin length.[34, 35, 36] Furthermore, the proportionality factor (effective temperature) between the entanglement spectrum and the single-chain energy spectrum spectrum turns out to be independent of the spin length.

Moreover, we also investigate $S = 1$ ladders with uniaxial anisotropy. Here we encounter the situation that already the unperturbed ground state is not fully entangled leading to a zero-order reduced density operator which is, differently from the $S = 1/2$ case studied earlier[23], not proportional to the unit matrix.

This paper is organized as follows. In section 2 we analyze the entanglement spectrum of isotropic Heisenberg ladders of arbitrary spin length within first and second order perturbation theory around the limit of strong rung coupling. In first order, the entanglement spectrum is found to be proportional to the energy spectrum of the single chain, and the proportionality factor turns out to be independent of S . Our analytical findings are compared with results of exact numerical diagonalizations of small systems. Section 3 deals with spin ladders with anisotropic couplings and exemplifies the case of spin length $S = 1$. Technically complicated details pertaining to sections 2 and 3 are deferred to the appendices. In section 4 we remark on related observations in dimerized spin chains of higher spin length. We close with a summary and an outlook in section 5.

2. Isotropic Heisenberg ladder of arbitrary spin

We consider the Hamiltonian $\mathcal{H} = \mathcal{H}_0 + \mathcal{H}_1$ of an isotropic spin ladder of arbitrary spin length with

$$\mathcal{H}_0 = J_r \sum_i \vec{S}_{2i} \vec{S}_{2i+1}, \quad (1)$$

$$\mathcal{H}_1 = J_l \sum_i \left(\vec{S}_{2i} \vec{S}_{2i+2} + \vec{S}_{2i-1} \vec{S}_{2i+1} \right) \quad (2)$$

describing the coupling along the rungs and legs, respectively. The sites on, say, the first (second) leg are denoted by even (odd) labels such that the i -th rung consists of sites $2i$ and $2i + 1$. All spin- S operators are taken to be dimensionless such that J_r, J_l have dimension of energy. The following considerations apply to finite systems with periodic boundary conditions as well as to those of infinite size. Let us now treat \mathcal{H}_1 as a perturbation to \mathcal{H}_0 with antiferromagnetic coupling, $J_r > 0$. It is expected in

general that the ground state of two leg spin S ladders are gapped for finite $J_r > 0$ and J_l . For $S = 1$ for example this has been verified numerically in Ref. [37]. The perturbative expansion around the strong rung coupling limit is therefore an expansion into an extended phase. The unperturbed ground state reads

$$|0\rangle = \bigotimes_i |s_i\rangle, \quad (3)$$

where the singlet state on each rung is given by, using obvious notation,

$$|s_i\rangle = \sum_{m=-S}^S \frac{(-1)^{S-m}}{\sqrt{2S+1}} |m\rangle_{2i} | -m\rangle_{2i+1}. \quad (4)$$

In order to compute the ground state in first-order perturbation theory in \mathcal{H}_1 , let us first consider the states

$$\vec{S}_{2i}|s_i\rangle = -\vec{S}_{2i+1}|s_i\rangle \quad (5)$$

which transform under general $SU(2)$ -rotations generated by $\vec{S}_{2i} + \vec{S}_{2i+1}$ as triplets. Thus, as a special case of the Wigner-Eckart theorem, the states $S_{2i}^{\pm}|s_i\rangle$ and $S_{2i}^z|s_i\rangle$ are proportional to the triplet components $|t_i^{\pm}\rangle$ and $|t_i^z\rangle$, respectively, which are obtained readily by expliciting Eqs. (4),(5) and normalizing the results,

$$|t_i^1\rangle = -\sqrt{\frac{3}{2}} \sum_{m=-S}^{S-1} \left[\frac{(-1)^{S-m} \sqrt{S(S+1) - m(m+1)}}{\sqrt{S(S+1)(2S+1)}} \right. \\ \left. \times |m+1\rangle_{2i} | -m\rangle_{2i+1} \right], \quad (6)$$

$$|t_i^0\rangle = \sum_{m=-S}^S \frac{\sqrt{3}(-1)^{S-m} m}{\sqrt{S(S+1)(2S+1)}} |m\rangle_{2i} | -m\rangle_{2i+1}, \quad (7)$$

$$|t_i^{-1}\rangle = -\sqrt{\frac{3}{2}} \sum_{m=-S}^{S-1} \left[\frac{(-1)^{S-m} \sqrt{S(S+1) - m(m+1)}}{\sqrt{S(S+1)(2S+1)}} \right. \\ \left. \times |m\rangle_{2i} | -(m+1)\rangle_{2i+1} \right]. \quad (8)$$

Considering now two neighboring rungs, the state

$$\vec{S}_{2i}\vec{S}_{2i+2}|s_i\rangle|s_{i+1}\rangle = \vec{S}_{2i+1}\vec{S}_{2i+3}|s_i\rangle|s_{i+1}\rangle \quad (9)$$

transforms as a singlet under arbitrary rotations and, according to the above finding, must be composed of triplet states on each rung. In other words, this state is proportional to (cf. again Eq. (4))

$$\frac{1}{\sqrt{3}} \left(|t_i^1\rangle|t_{i+1}^{-1}\rangle - |t_i^0\rangle|t_{i+1}^0\rangle + |t_i^{-1}\rangle|t_{i+1}^1\rangle \right). \quad (10)$$

Indeed, a direct calculation yields the following matrix elements,

$$\langle t_i^{\pm 1} | \langle t_{i+1}^{\mp 1} | \vec{S}_{2i} \vec{S}_{2i+2} | s_i \rangle | s_{i+1} \rangle = -\frac{1}{3} S(S+1), \quad (11)$$

$$\langle t_i^0 | \langle t_{i+1}^0 | \vec{S}_{2i} \vec{S}_{2i+2} | s_i \rangle | s_{i+1} \rangle = \frac{1}{3} S(S+1). \quad (12)$$

Note that the norm $\|\vec{S}_{2i}\vec{S}_{2i+2}|s_i\rangle|s_{i+1}\rangle\|^2 = (S(S+1))^2/3$ equals the sum of the squares of the above three scalar products, in accordance with the previous arguments.

With these results, the correction to the ground state within first order perturbation theory can be formulated as

$$|1\rangle = \frac{J_l}{3J_r} S(S+1) \sum_i \left[\left(\cdots |t_i^1\rangle |t_{i+1}^{-1}\rangle \cdots \right) - \left(\cdots |t_i^0\rangle |t_{i+1}^0\rangle \cdots \right) + \left(\cdots |t_i^{-1}\rangle |t_{i+1}^1\rangle \cdots \right) \right] \quad (13)$$

where the dots denote singlet states on each rung not explicitly specified. The reduced density operator is obtained by tracing out one of the legs from $\rho^{(1)} = (|0\rangle + |1\rangle)(\langle 0| + \langle 1|)$ and is given within first order in J_l/J_r by

$$\rho_{\text{red}}^{(1)} = \frac{1}{(2S+1)^L} \left(1 - \frac{2J_l}{J_r} \sum_i \vec{S}_i \vec{S}_{i+1} \right) \quad (14)$$

with L being the number of rungs. Again within first order perturbation theory, this result can be formulated as

$$\rho_{\text{red}}^{(1)} = \frac{1}{Z} \exp\left(-\mathcal{H}_{\text{ent}}^{(1)}\right) \quad (15)$$

with $Z = \text{tr} \exp(-\mathcal{H}_{\text{ent}}^{(1)})$ being a partition function with respect to the entanglement Hamiltonian

$$\mathcal{H}_{\text{ent}}^{(1)} = \frac{2J_l}{J_r} \sum_i \vec{S}_i \vec{S}_{i+1}. \quad (16)$$

Remarkably, the prefactor

$$\beta = \frac{2J_l}{J_r}, \quad (17)$$

which can also be viewed as a formal inverse temperature, is independent of the spin length S . Fig. 1 shows the full entanglement spectrum of a $S = 1$ spin ladder obtained via numerical diagonalization in a wide range of J_l/J_r . As seen in the right panel, in the limit of small J_l/J_r the entanglement spectrum compares excellently to the energy spectrum of a single Heisenberg chain, as predicted by perturbation theory.

In summary, the entanglement spectrum within first order perturbation theory perfectly matches the energy spectrum of a single spin chain. This observation has already been made in Refs. [22, 23] for $S = 1/2$ and is generalized here to arbitrary spin length. The latter result might be considered as somewhat unexpected since important features of energy spectra of spin chains, such as presence or absence of an excitation gap over the ground state, depend crucially on the spin length.[34, 35, 36]

The contributions of second order in J_l/J_r require lengthier calculations which are outlined in the appendix. The final result for the reduced density in up to second order is

$$\rho_{\text{red}}^{(2)} = \frac{1}{(2S+1)^L} \left[1 - \frac{2J_l}{J_r} \sum_i \vec{S}_i \vec{S}_{i+1} + \frac{1}{2} \left(\frac{2J_l}{J_r} \right)^2 \left[\left(\sum_i \vec{S}_i \vec{S}_{i+1} \right)^2 + \frac{2}{5} S(S+1) \sum_i \vec{S}_i \vec{S}_{i+2} \right] \right]$$

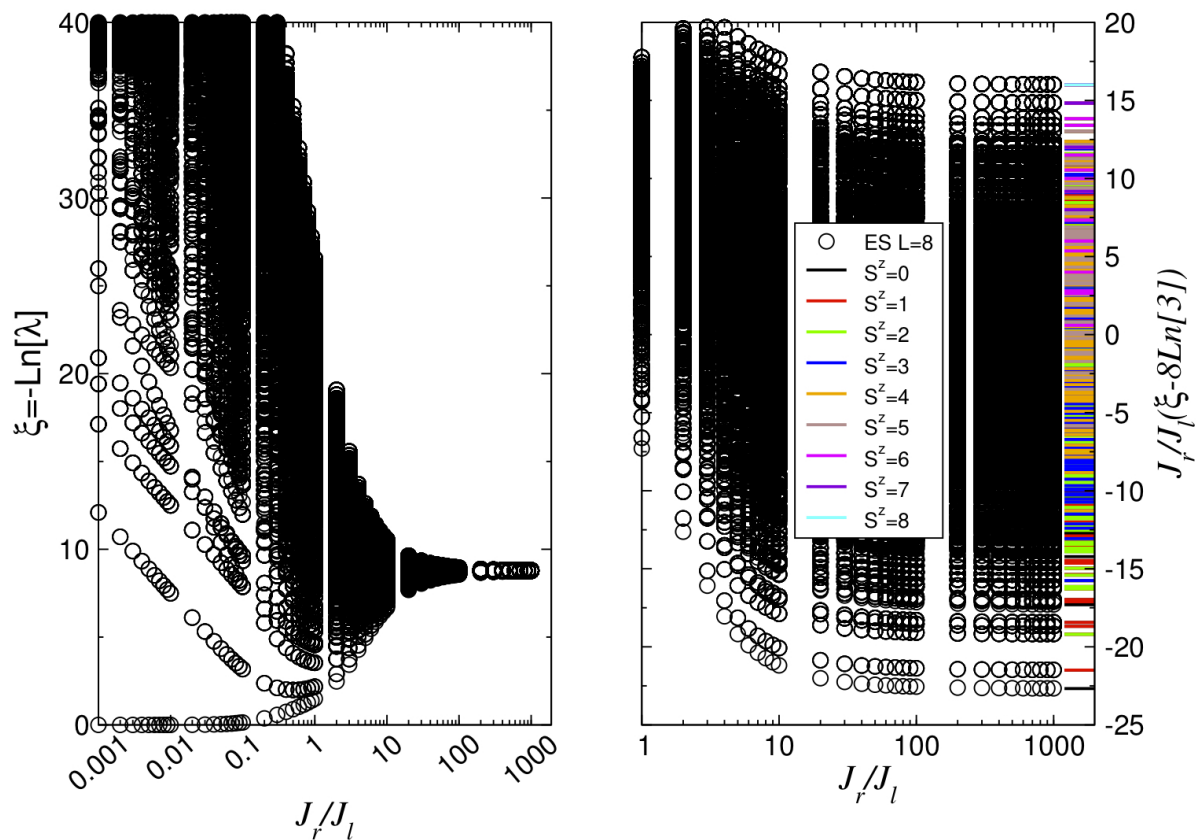


Figure 1. (Color online) The entanglement spectrum of a $S = 1$ spin ladder with $L = 8$ rungs as a function of J_l/J_r obtained via numerical diagonalization. In the right panel we have linearly rescaled the data in order to compare it directly with the spectrum shown on the very right of a single spin $S = 1$ chain of eight sites labeled by the z -component of the total spin. The energies have been multiplied by 2, according to Eq. (16).

$$\begin{aligned}
 & -\frac{1}{10} \sum_i \left((\vec{S}_i \vec{S}_{i+1}) (\vec{S}_{i+1} \vec{S}_{i+2}) + (\vec{S}_{i+1} \vec{S}_{i+2}) (\vec{S}_i \vec{S}_{i+1}) \right) \\
 & -\frac{1}{6} \sum_i \left((\vec{S}_i \vec{S}_{i+1})^2 + 2\vec{S}_i \vec{S}_{i+1} \right) - \frac{5}{18} (S(S+1))^2 L \Big], \quad (18)
 \end{aligned}$$

which can, within the same order, be reformulated as

$$\rho_{\text{red}}^{(2)} = \frac{1}{Z} \exp(-\mathcal{H}_{\text{ent}}^{(2)}) \quad (19)$$

with $Z = \text{tr} \exp(-\mathcal{H}_{\text{ent}}^{(2)})$ and

$$\begin{aligned}
 \mathcal{H}_{\text{ent}}^{(2)} = & \frac{2J_l}{J_r} \sum_i \vec{S}_i \vec{S}_{i+1} - \left(\frac{J_l}{J_r} \right)^2 \left[\frac{4}{5} S(S+1) \sum_i \vec{S}_i \vec{S}_{i+2} \right. \\
 & - \frac{1}{5} \sum_i \left((\vec{S}_i \vec{S}_{i+1}) (\vec{S}_{i+1} \vec{S}_{i+2}) + (\vec{S}_{i+1} \vec{S}_{i+2}) (\vec{S}_i \vec{S}_{i+1}) \right) \\
 & \left. - \frac{1}{3} \sum_i \left((\vec{S}_i \vec{S}_{i+1})^2 + 2\vec{S}_i \vec{S}_{i+1} \right) + \frac{1}{9} (S(S+1))^2 L \right]. \quad (20)
 \end{aligned}$$

For the case $S = 1/2$ the second-order entanglement Hamiltonian simplifies to

$$\mathcal{H}_{\text{ent}}^{(2)} = \frac{2J_l}{J_r} \sum_i \vec{S}_i \vec{S}_{i+1} - \frac{1}{2} \left(\frac{J_l}{J_r} \right)^2 \sum_i (\vec{S}_i \vec{S}_{i+2} - \vec{S}_i \vec{S}_{i+1}) \quad (21)$$

as already given in Ref. [23]. We note that the constant term in the Hamiltonian (20) is strictly speaking arbitrary since it is always canceled against contributions to the partition function. In Eq. (20) this constant was adjusted such that $\text{tr}(\mathcal{H}_{\text{ent}}^{(2)}) = 0$.

3. Ladders with anisotropic couplings

The case of uniaxially anisotropic $S = 1/2$ spin ladders was already treated within first-order perturbation theory in the couplings along the legs in Refs. [22, 23]. As an important feature, the unperturbed ground state on each rung remains, for not too large anisotropy, the fully entangled singlet state. This is no longer the case for larger spins since the anisotropic contribution to the Hamiltonian couples the singlet to all higher multiplets with even total spin. To give a specific example, let us consider the anisotropic rung Hamiltonian

$$\mathcal{H}_0 = J_r \sum_i \left(S_{2i}^x S_{2i+1}^x + S_{2i}^y S_{2i+1}^y + \Delta S_{2i}^z S_{2i+1}^z \right) \quad (22)$$

for $S = 1$. Here the ground state on rung i is given by

$$|g_i\rangle = \alpha_- |s_i\rangle - \frac{\delta}{|\delta|} \alpha_+ |q_i^0\rangle \quad (23)$$

$$= \frac{1}{\sqrt{3}} \left(\left(\alpha_- - \frac{\delta}{|\delta|} \frac{\alpha_+}{\sqrt{2}} \right) [|1\rangle_{2i} | -1\rangle_{2i+1} + | -1\rangle_{2i} |1\rangle_{2i+1}] \right. \\ \left. - \left(\alpha_- + \frac{\delta}{|\delta|} \sqrt{2} \alpha_+ \right) |0\rangle_{2i} |0\rangle_{2i+1} \right) \quad (24)$$

with

$$\alpha_{\pm} = \sqrt{\frac{1}{2} \left(1 \mp \frac{3/2 - (1 - \Delta)/6}{\sqrt{2 + \Delta^2/4}} \right)}, \quad (25)$$

$\delta = 1 - \Delta$, and the quintuplet component $|q_i^0\rangle$ being defined in Eq. (A.6). This ground state leads to the unperturbed reduced density matrix

$$\rho_{\text{red}}^{(0)} = \prod_i \frac{1}{3} \left(\left(\alpha_- + \frac{\delta}{|\delta|} \sqrt{2} \alpha_+ \right)^2 - 3 \left(\frac{\delta}{|\delta|} \sqrt{2} \alpha_- \alpha_+ + \frac{1}{2} \alpha_+^2 \right) S_i^z S_i^z \right), \quad (26)$$

which is obviously not proportional to the unity operator but contains for $\Delta \neq 1$ anisotropic spin couplings of arbitrary range. In linear order in the deviation δ from isotropy we have $\alpha_+ \approx \sqrt{2}|\delta|/9$, $\alpha_- \approx 1$, and therefore

$$\rho_{\text{red}}^{(0)} = \frac{1}{3L} \left(1 - \frac{2\delta}{3} \sum_i \left(S_i^z S_i^z - \frac{2}{3} \right) \right) + \mathcal{O}(\delta^2), \quad (27)$$

or

$$\rho_{\text{red}}^{(0)} = \frac{1}{Z} \exp(-\mathcal{H}_{\text{ent}}^{(0)}) + \mathcal{O}(\delta^2) \quad (28)$$

with $Z = \text{tr} \exp(-\mathcal{H}_{\text{ent}}^{(0)})$ and

$$\mathcal{H}_{\text{ent}}^{(0)} = \frac{2\delta}{3} \sum_i \left(S_i^z S_i^z - \frac{2}{3} \right) \quad (29)$$

Moreover, a more tedious calculation outlined in Appendix B yields the following result for the reduced density matrix in first order in J_l/J_r and δ ,

$$\begin{aligned} \rho_{\text{red}}^{(1)} = \frac{1}{3^L} \left\{ 1 - \frac{2\delta}{3} \sum_i \left(S_i^z S_i^z - \frac{2}{3} \right) \right. \\ \left. - \frac{2J_l}{J_r} \left[\sum_i \left(\vec{S}_i \vec{S}_{i+1} + \frac{\delta}{3} \left(2 \left(S_i^x S_{i+1}^x + S_i^y S_{i+1}^y \right) - S_i^z S_{i+1}^z \right) \right) \right. \right. \\ \left. \left. - \frac{\delta}{3} \left(\left(\sum_i \left(S_i^z S_i^z - \frac{2}{3} \right) \right) \left(\sum_i \vec{S}_i \vec{S}_{i+1} \right) \right. \right. \right. \\ \left. \left. \left. + \left(\sum_i \vec{S}_i \vec{S}_{i+1} \right) \left(\sum_i \left(S_i^z S_i^z - \frac{2}{3} \right) \right) \right) \right] \right\} \quad (30) \end{aligned}$$

Again, the presence of an only incompletely entangled unperturbed ground state leads to a considerably more complicated entanglement spectrum compared to isotropic spin ladders. Let us therefore return to the case of an isotropic Heisenberg Hamiltonian (1) along the runs for again arbitrary spin length S . As a perturbation we introduce the bilinear Hamiltonian

$$\mathcal{H}_1 = J_l \sum_i \left(S_{2i}^\alpha A_{\alpha\beta} S_{2i+2}^\beta + S_{2i-1}^\alpha A_{\alpha\beta} S_{2i+1}^\beta \right) \quad (31)$$

describing an arbitrarily anisotropic coupling between next neighbors encoded, using sum convention, in the matrix A . Using the relations

$$S_{2i}^\pm |s_i\rangle = -S_{2i+1}^\pm |s_i\rangle = \mp \sqrt{\frac{2}{3}} S(S+1) |t_i^{\pm 1}\rangle, \quad (32)$$

$$S_{2i}^z |s_i\rangle = -S_{2i+1}^z |s_i\rangle = \sqrt{\frac{1}{3}} S(S+1) |t_i^z\rangle \quad (33)$$

and

$$\text{tr}_{2i+1} |t_i^{\pm 1}\rangle \langle s_i| = \frac{\mp \sqrt{3/2}}{\sqrt{S(S+1)(2S+1)}} S_{2i}^\pm, \quad (34)$$

$$\text{tr}_{2i+1} |t_i^z\rangle \langle s_i| = \frac{\sqrt{3}}{\sqrt{S(S+1)(2S+1)}} S_{2i}^z \quad (35)$$

it is easy to see that the reduced density matrix in first order in J_l/J_r is of the form (15) with

$$\mathcal{H}_{\text{ent}}^{(1)} = \frac{2J_l}{J_r} \sum_i S_i^\alpha A_{\alpha\beta} S_{i+1}^\beta. \quad (36)$$

Thus, the entanglement Hamiltonian in lowest nontrivial order perfectly reproduces the functional form of the perturbation along the legs. This result is easily generalized to the case of bilinear couplings of longer range, or spatially inhomogeneous couplings (with

the matrix A depending on lattice indices). The above finding (36) can be seen as the consequence of conditions already formulated in Ref. [22]: (i) full entanglement of the unperturbed ground state, and (ii) the perturbation couples only to a single energy level (here the triplet) of the unperturbed Hamiltonian.

4. Dimerized spin chains

The above observation that spin ladders with isotropic couplings have perturbative entanglement spectra allowing for simple interpretations, can be generalized to spin systems of other geometry. As an example, let us consider a dimerized spin- S chain (as opposed to a spin ladder) described by $\mathcal{H} = \mathcal{H}_0 + \mathcal{H}_1$ with

$$\mathcal{H}_0 = J_0 \sum_i \vec{S}_{2i} \vec{S}_{2i+1}, \quad (37)$$

$$\mathcal{H}_1 = J_1 \sum_i \vec{S}_{2i-1} \vec{S}_{2i}. \quad (38)$$

For simplicity and definiteness we assume a even number L of lattice sites with periodic boundary conditions. Thus, the ground state $|G_0\rangle$ ($|G_1\rangle$) of \mathcal{H}_0 (\mathcal{H}_1) consists of singlets coupling each even (odd) lattice site to the site with next higher label. Considering now \mathcal{H}_1 as a perturbation to \mathcal{H}_0 and tracing out all, say, odd lattice sites, one readily obtains a first-order reduced density matrix of the form (15) with

$$\mathcal{H}_{\text{ent}}^{(1)} = \frac{J_1}{J_0} \sum_i \vec{S}_{2i} \vec{S}_{2i+2}. \quad (39)$$

Here the missing factor of 2 compared to Eq. (16) just reflects that we consider here a single spin chain and not two-leg ladder.

Moreover, it is also instructive to study a general linear combination of the above two singlet states,

$$|\psi\rangle = (\cos(\theta/2)|G_0\rangle + \sin(\theta/2)e^{i\varphi}|G_1\rangle) \quad (40)$$

with two real parameters θ , φ . For $S = 1/2$ such states span the ground state space of the Majumdar-Ghosh spin chain.[38] Tracing out again the odd-labeled sites from $\rho = |\psi\rangle\langle\psi|$ leads to

$$\rho_{\text{red}} = \frac{1}{(2S+1)^{L/2}} \left(1 + \frac{1}{2} \sin\theta (e^{i\varphi} T^+ + e^{-i\varphi} T) \right) \quad (41)$$

where the operator

$$T = \bigotimes_{i=1}^{L/2} \left(\sum_{m=-S}^S |m\rangle_{2i+2} \langle m|_{2i} \right) \quad (42)$$

translates all spin states by one lattice site of the reduced chain. Thus, the eigenstates $|k\rangle$ of ρ_{red} fulfill $T|k\rangle = e^{ik}|k\rangle$ where the wave number k is restricted to integer multiple of $4\pi/L$ by the boundary conditions. In particular, the levels of the entanglement spectrum read as a function of k

$$\xi(k) = -\ln(1 + \sin\theta \cos(\varphi - k)) + \frac{L}{2} \ln(2S+1). \quad (43)$$

5. Conclusions and outlook

We have analyzed the entanglement spectrum of Heisenberg spin ladders of arbitrary spin length S in the perturbative regime of strong rung coupling. For isotropic spin coupling the the entanglement spectrum turns out, within first order perturbation theory, to be proportional to the energy spectrum of the single chain with the proportionality factor being independent of S . Additional corrections are obtained in second order perturbation theory which are also fully evaluated. A more complicated situation arises for anisotropic ladders of higher spin $S \geq 1$ since here even the unperturbed ground state has a nontrivial entanglement spectrum. Finally we have discussed related issues in dimerized spin chains.

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Appendix A. Second-order contribution to the ground state and the reduced density matrix of isotropic spin ladders

Defining the two-rung singlet state

$$\sigma_{ij}^{(1)} = \frac{1}{\sqrt{3}} \left(|t_i^1\rangle |t_j^{-1}\rangle - |t_i^0\rangle |t_j^0\rangle + |t_i^{-1}\rangle |t_j^1\rangle \right) \quad (\text{A.1})$$

the first-order contribution can be formulated as

$$|1\rangle = \frac{J_l}{\sqrt{3}J_r} S(S+1) \sum_i \left(\cdots \sigma_{i,i+1}^{(1)} \cdots \right). \quad (\text{A.2})$$

The second-order correction to a non-degenerate state $|0\rangle$ is given by the general expression (using obvious notation)

$$\begin{aligned} |2\rangle = & \sum_{\alpha \neq 0} |\alpha\rangle \frac{\langle 0 | \mathcal{H}_1 | 0 \rangle \langle \alpha | \mathcal{H}_1 | 0 \rangle}{(E_0 - E_\alpha)^2} - \frac{1}{2} |0\rangle \sum_{\alpha \neq 0} \frac{\langle 0 | \mathcal{H}_1 | \alpha \rangle \langle \alpha | \mathcal{H}_1 | 0 \rangle}{(E_0 - E_\alpha)^2} \\ & + \sum_{\alpha \neq 0 \neq \beta} |\alpha\rangle \frac{\langle \alpha | \mathcal{H}_1 | \beta \rangle \langle \beta | \mathcal{H}_1 | 0 \rangle}{(E_0 - E_\alpha)(E_0 - E_\beta)}. \end{aligned} \quad (\text{A.3})$$

The first term of the above r.h.s. does not contribute in the present case, and in the second term again only triplet excitations on the rungs occur which can be evaluated using the matrix elements calculated previously. The last contribution is more complicated since here (for $S > 1/2$) also quintuplet excitations on a given rung come into play. The components of such a quintuplet on rung i read explicitly

$$\begin{aligned} |q_i^2\rangle &= Q(S) \sum_{m=-S+1}^{S-1} \left[(-1)^{S-m} \sqrt{S(S+1) - m(m-1)} \right. \\ &\quad \left. \cdot \sqrt{S(S+1) - m(m+1)} |m+1\rangle_{2i} - |m+1\rangle_{2i+1} \right], \quad (\text{A.4}) \\ |q_i^1\rangle &= Q(S) \sum_{m=-S}^{S-1} \left[(-1)^{S-m} \sqrt{S(S+1) - m(m+1)} \right. \end{aligned}$$

$$\cdot (2m+1)|m+1\rangle_{2i} - m\rangle_{2i+1}], \quad (\text{A.5})$$

$$|q_i^0\rangle = Q(S) \sqrt{\frac{2}{3}} \sum_{m=-S}^S [(-1)^{S-m} (S(S+1) - 3m^2) |m\rangle_{2i} - m\rangle_{2i+1}] \quad (\text{A.6})$$

$$|q_i^{-1}\rangle = Q(S) \sum_{m=-S}^{S-1} [(-1)^{S-m} \sqrt{S(S+1) - m(m+1)} \cdot (2m+1)|m\rangle_{2i} - m-1\rangle_{2i+1}], \quad (\text{A.7})$$

$$|q_i^{-2}\rangle = Q(S) \sum_{m=-S+1}^{S-1} [(-1)^{S-m} \sqrt{S(S+1) - m(m-1)} \cdot \sqrt{S(S+1) - m(m+1)} |m-1\rangle_{2i} - m-1\rangle_{2i+1}], \quad (\text{A.8})$$

where

$$Q(S) = \frac{-\sqrt{15/2}}{\sqrt{S(S+1)(2S+1)(2S+3)(2S-1)}} \quad (\text{A.9})$$

The highest-weight state $|q_i^2\rangle$ of the above multiplet is again readily obtained by, e.g., applying S_{2i}^+ on $|t_i^1\rangle$ and normalizing the result. Now in order to compute the second-order correction to the ground state one needs to evaluate expressions of the form

$$(\vec{S}_{2i}\vec{S}_{2i+2} + \vec{S}_{2i+1}\vec{S}_{2i+3}) (\cdots \sigma_{j,j+1}^{(1)} \cdots). \quad (\text{A.10})$$

If the rungs involved do not overlap, i.e. $|i-j| > 1$, we just obtain another independent singlet $\sigma_{i,i+1}^{(1)}$ composed of triplets on rungs i and $i+1$. In the remaining cases one finds, after somewhat tedious calculations, the following expansions,

$$\begin{aligned} & (\vec{S}_{2i-2}\vec{S}_{2i} + \vec{S}_{2i-1}\vec{S}_{2i+1}) (\cdots \sigma_{i,i+1}^{(1)} \cdots) \\ &= -\frac{\sqrt{2}}{3} \sqrt{S(S+1)(2S+3)(2S-1)} (\cdots \sigma_{i-1,i,i+1} \cdots) \\ & \quad + \frac{2}{3} S(S+1) (\cdots \sigma_{i-1,i+1}^{(1)} \cdots), \end{aligned} \quad (\text{A.11})$$

$$\begin{aligned} & (\vec{S}_{2i}\vec{S}_{2i+2} + \vec{S}_{2i+1}\vec{S}_{2i+3}) (\cdots \sigma_{i,i+1}^{(1)} \cdots) \\ &= -\frac{1}{\sqrt{15}} (2S+3)(2S-1) (\cdots \sigma_{i,i+1}^{(2)} \cdots) \\ & \quad - (\cdots \sigma_{i,i+1}^{(1)} \cdots) - \frac{2}{\sqrt{3}} S(S+1) |0\rangle. \end{aligned} \quad (\text{A.12})$$

Here we have introduced two further types of singlet states,

$$\begin{aligned} \sigma_{ij}^{(2)} &= \frac{1}{\sqrt{5}} (|q_i^2\rangle |q_j^{-2}\rangle - |q_i^1\rangle |q_j^{-1}\rangle + |q_i^0\rangle |q_j^0\rangle \\ & \quad - |q_i^{-1}\rangle |q_j^1\rangle + |q_i^{-2}\rangle |q_j^2\rangle), \end{aligned} \quad (\text{A.13})$$

$$\sigma_{ijk} = \frac{1}{\sqrt{3}} (|\tau_{ij}^1\rangle |t_k^{-1}\rangle - |\tau_{ij}^0\rangle |t_k^0\rangle + |\tau_{ij}^{-1}\rangle |t_k^1\rangle) \quad (\text{A.14})$$

$$= \frac{1}{\sqrt{3}} (|t_i^1\rangle |\tau_{kj}^{-1}\rangle - |t_i^0\rangle |\tau_{kj}^0\rangle + |t_i^{-1}\rangle |\tau_{kj}^1\rangle), \quad (\text{A.15})$$

where

$$|\tau_{ij}^1\rangle = \sqrt{\frac{1}{10}}|t_i^1\rangle|q_j^0\rangle - \sqrt{\frac{3}{10}}|t_i^0\rangle|q_j^1\rangle + \sqrt{\frac{3}{5}}|t_i^{-1}\rangle|q_j^2\rangle \quad (\text{A.16})$$

$$|\tau_{ij}^0\rangle = \sqrt{\frac{3}{10}}|t_i^1\rangle|q_j^{-1}\rangle - \sqrt{\frac{2}{5}}|t_i^0\rangle|q_j^0\rangle + \sqrt{\frac{3}{10}}|t_i^{-1}\rangle|q_j^1\rangle \quad (\text{A.17})$$

$$|\tau_{ij}^{-1}\rangle = \sqrt{\frac{3}{5}}|t_i^1\rangle|q_j^{-2}\rangle - \sqrt{\frac{3}{10}}|t_i^0\rangle|q_j^{-1}\rangle + \sqrt{\frac{1}{10}}|t_i^{-1}\rangle|q_j^0\rangle \quad (\text{A.18})$$

are the components of a two-rung triplet state composed of a triplet on rung i and a quintuplet on rung j . Summing up, the second-order correction to the ground state can be written as

$$\begin{aligned} |2\rangle = & - \left(\frac{J_l}{J_r}\right)^2 \frac{(S(S+1))^2}{6} L|0\rangle \\ & + \left(\frac{J_l}{J_r}\right)^2 \left[\frac{(S(S+1))^2}{6} \sum_{|i-j|>1} (\cdots \sigma_{i,i+1}^{(1)} \cdots \sigma_{j,j+1}^{(1)} \cdots) \right. \\ & + \frac{2\sqrt{2}}{15\sqrt{3}} (S(S+1))^{3/2} \sqrt{(2S+3)(2S-1)} \sum_i (\cdots \sigma_{i-1,i,i+1} \cdots) \\ & - \frac{2(S(S+1))^2}{3\sqrt{3}} \sum_i (\cdots \sigma_{i,i+2}^{(1)} \cdots) \\ & + \frac{1}{18\sqrt{5}} S(S+1)(2S+3)(2S-1) \sum_i (\cdots \sigma_{i,i+1}^{(2)} \cdots) \\ & \left. + \frac{1}{2\sqrt{3}} \sum_i (\cdots \sigma_{i,i+1}^{(1)} \cdots) \right], \quad (\text{A.19}) \end{aligned}$$

where the first line on the r.h.s results from the second term in Eq. (A.3), and all other contributions stem from the second line there. With these results at hand, the second-order correction to the reduced density matrix is given by the sum of the expressions

$$\text{tr}_{\text{1leg}} (|1\rangle\langle 1|) = \left(\frac{J_l}{J_r}\right)^2 \frac{1}{(2S+1)^L} \left(\sum_i \vec{S}_i \vec{S}_{i+1} \right)^2, \quad (\text{A.20})$$

$$\begin{aligned} \text{tr}_{\text{1leg}} (|0\rangle\langle 2| + |2\rangle\langle 0|) = & \left(\frac{J_l}{J_r}\right)^2 \frac{1}{(2S+1)^L} \left[\left(\sum_i \vec{S}_i \vec{S}_{i+1} \right)^2 \right. \\ & - \frac{1}{5} \sum_i \left((\vec{S}_i \vec{S}_{i+1}) (\vec{S}_{i+1} \vec{S}_{i+2}) + (\vec{S}_{i+1} \vec{S}_{i+2}) (\vec{S}_i \vec{S}_{i+1}) \right) \\ & - \frac{1}{3} \sum_i \left((\vec{S}_i \vec{S}_{i+1})^2 + 2\vec{S}_i \vec{S}_{i+1} \right) \\ & \left. + \frac{4}{5} S(S+1) \sum_i \vec{S}_i \vec{S}_{i+2} - \frac{5}{9} (S(S+1))^2 L \right], \quad (\text{A.21}) \end{aligned}$$

which lead to Eq. (18). The above considerations refer explicitly to the case $S > 1/2$ due to the presence of the quintuplets which are absent for $S = 1/2$. In the second-order correction to the ground state rungs with such states occur in the second and the fourth

line of Eq. (A.19). The corresponding contributions to the reduced density matrix read

$$\left(\frac{J_l}{J_r}\right)^2 \frac{4/5}{(2S+1)^L} \left[\sum_i \left((\vec{S}_i \vec{S}_{i+1}) (\vec{S}_{i+1} \vec{S}_{i+2}) + (\vec{S}_{i+1} \vec{S}_{i+2}) (\vec{S}_i \vec{S}_{i+1}) \right) - \frac{2}{3} S(S+1) \sum_i \vec{S}_i \vec{S}_{i+2} \right], \quad (\text{A.22})$$

$$\left(\frac{J_l}{J_r}\right)^2 \frac{2/3}{(2S+1)^L} \sum_i \left((\vec{S}_i \vec{S}_{i+1})^2 + \frac{1}{2} \vec{S}_i \vec{S}_{i+1} - \frac{1}{3} (S(S+1))^2 \right), \quad (\text{A.23})$$

respectively, and vanish for $S = 1/2$ due to elementary identities of Pauli matrices. As a result, the $S = 1/2$ reduced density matrix in up to second order in J_l/J_r is given by

$$\rho_{\text{red}}^{(2)} = \frac{1}{2^L} \left[1 - \frac{2J_l}{J_r} \sum_m \vec{S}_m \vec{S}_{m+1} + \frac{1}{2} \left(\frac{2J_l}{J_r}\right)^2 \left[\left(\sum_i \vec{S}_i \vec{S}_{i+1} \right)^2 - \frac{3}{16} L + \frac{1}{4} \sum_i (\vec{S}_i \vec{S}_{i+2} - \vec{S}_i \vec{S}_{i+1}) \right] \right], \quad (\text{A.24})$$

which was already found in Ref. [23].

Appendix B. First-order perturbation theory for anisotropic ladders

We now consider an Hamiltonian of the form (22) acting with amplitude J_l (cf. Eq. (2)) as a perturbation along the legs. Its action on the each rung pair is given by

$$\begin{aligned} & (S_{2i}^x S_{2i+2}^x + S_{2i}^y S_{2i+2}^y + \Delta S_{2i}^z S_{2i+2}^z \\ & + S_{2i+1}^x S_{2i+3}^x + S_{2i+1}^y S_{2i+3}^y + \Delta S_{2i+1}^z S_{2i+3}^z) |g_i\rangle |g_{i+1}\rangle \\ & = \frac{4}{3} \Delta^2 \left(\alpha_- - \frac{\delta}{|\delta|} \frac{\alpha_+}{\sqrt{2}} \right)^2 |t_i^0\rangle |t_{i+1}^0\rangle \\ & - \frac{1}{3} \left(2\alpha_- + \frac{\delta}{|\delta|} \frac{\alpha_+}{\sqrt{2}} \right)^2 (|t_i^1\rangle |t_{i+1}^{-1}\rangle + |t_i^{-1}\rangle |t_{i+1}^1\rangle) \\ & + \frac{3}{2} \alpha_+^2 (|q_i^1\rangle |q_{i+1}^{-1}\rangle + |q_i^{-1}\rangle |q_{i+1}^1\rangle). \end{aligned} \quad (\text{B.1})$$

Remarkably, no coupling to the excited rung eigenstates

$$|e_i\rangle = \alpha_+ |s_i\rangle + \frac{\delta}{|\delta|} \alpha_- |q_i^0\rangle \quad (\text{B.2})$$

occurs, which are the other orthogonal states spanned by $|s_i\rangle$ and $|q_i^0\rangle$. Now the first-order correction to the ground state is readily obtained as

$$\begin{aligned} |1\rangle & = \frac{J_l}{J_r} \frac{2\Delta^2/3}{E_g + 2 - \Delta} \left(\alpha_- - \frac{\delta}{|\delta|} \frac{\alpha_+}{\sqrt{2}} \right)^2 \sum_i (\cdots |t_i^0\rangle |t_{i+1}^0\rangle \cdots) \\ & - \frac{J_l}{J_r} \frac{1/6}{E_g + 1} \left(2\alpha_- + \frac{\delta}{|\delta|} \frac{\alpha_+}{\sqrt{2}} \right)^2 \sum_i (\cdots [|t_i^1\rangle |t_{i+1}^{-1}\rangle + |t_i^{-1}\rangle |t_{i+1}^1\rangle] \cdots) \\ & + \frac{J_l}{J_r} \frac{3/4}{E_g - 1} \alpha_+^2 \sum_i (\cdots [|q_i^1\rangle |q_{i+1}^{-1}\rangle + |q_i^{-1}\rangle |q_{i+1}^1\rangle] \cdots) \end{aligned} \quad (\text{B.3})$$

where the dots denote states $|g_j\rangle$ (cf. Eq. (23)) on all rungs j not explicitly specified, and

$$E_g = -\frac{1}{2} + \frac{1-\Delta}{2} - \sqrt{2 + \frac{\Delta^2}{4}} \quad (\text{B.4})$$

such that the ground state energy on each unperturbed rung is $J_r E_g$. With these results at hand it is straightforward to compute the reduced density matrix within first order in J_l/J_r . For general anisotropy, however, the resulting expressions are rather cumbersome and difficult to interpret. We therefore concentrate here on the linear order in $\delta = 1 - \Delta$,

$$\begin{aligned} |1\rangle = & -\frac{J_l}{J_r} \frac{2}{3} \left(1 - \frac{5}{9}\delta\right) \sum_i \left(\cdots |t_i^0\rangle |t_{i+1}^0\rangle \cdots\right) \\ & + \frac{J_l}{J_r} \frac{2}{3} \left(1 + \frac{7}{9}\delta\right) \sum_i \left(\cdots \left[|t_i^1\rangle |t_{i+1}^{-1}\rangle + |t_i^{-1}\rangle |t_{i+1}^1\rangle\right] \cdots\right) + \mathcal{O}(\delta^2) \end{aligned} \quad (\text{B.5})$$

where on each unspecified rung we have states of the form

$$|g_i\rangle = |s_i\rangle - \frac{\sqrt{2}\delta}{9} |q_i^0\rangle + \mathcal{O}(\delta^2) \quad (\text{B.6})$$

which also build up the unperturbed ground state. Note that in linear order in δ no contribution to $|1\rangle$ from quintuplets occurs. Finally, tracing out one of the legs leads one finds for the reduced density matrix

$$\begin{aligned} \rho_{\text{red}}^{(1)} = & \frac{1}{3L} \left\{ 1 - \frac{2\delta}{3} \sum_i \left(S_i^z S_i^z - \frac{2}{3} \right) \right. \\ & - \frac{2J_l}{J_r} \sum_i \left[\vec{S}_i \vec{S}_{i+1} \left(1 - \frac{2\delta}{3} \sum_{j \neq i, i+1} \left(S_j^z S_j^z - \frac{2}{3} \right) \right) \right. \\ & \left. \left. + \frac{8\delta}{9} \left(S_i^x S_{i+1}^x + S_i^y S_{i+1}^y \right) - \frac{7\delta}{9} S_i^z S_{i+1}^z \right] \right\} \\ & + \mathcal{O}(\delta^2). \end{aligned} \quad (\text{B.7})$$

Using the identities $S^z S^z S^\pm + S^\pm S^z S^z = S^\pm$ and $(S^z)^3 = S^z$ for $S = 1$ operators leads to the more symmetric form (30).

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