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## Models of impurities in valence-bond spin chains and ladders

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**Abstract.** We present the class of models of a nonmagnetic impurity in an S = 1/2 generalized ladder with an Affleck–Kennedy–Lieb–Tasaki-type (AKLT-type) valence-bond ground state, and of an S = 1/2 impurity in the S = 1 AKLT chain. The ground state in the presence of impurity can be found exactly. The recently studied phenomenon of local enhancement of antiferromagnetic correlations around the impurity is absent for this family of models.

Over the last decade, low-dimensional spin systems, particularly the Heisenberg spin chains and ladders, have continued to attract considerable attention [1, 2]. The interest in spin ladders is particularly stimulated by the hope of getting some insight into the physics of metal oxide superconductors; in support of this hope, superconductivity in the ladder compound  $Sr_{0.4}Ca_{13.6}Cu_{24}O_{41.84}$  subjected to hole doping and under high pressure was recently reported [3]. It is now well established that 'standard' (i.e., with only 'leg' and 'rung' exchange couplings)  $S = \frac{1}{2}$  isotropic spin ladders have a disordered gapped ground state when the number of legs is even, while odd-legged ladders have quasi-long-range-ordered gapless ground states. On the other hand, 'generalized' ladders including other couplings can serve as interesting toy models with a rich behaviour which is often very different from that of 'standard' models [4–9].

Recently, interesting experimental results on ladders doped with nonmagnetic impurities (Zn substituted for Cu) have been obtained [10]: surprisingly, the antiferromagnetic (AF) order was found to be stabilized by the doping; a similar behaviour has also been observed for spin–Peierls chains [11]. A number of numerical studies [12, 13] indicated that local AF correlations near a nonmagnetic impurity are enhanced compared to the case for a system without vacancies. It has been suggested that this phenomenon, as well as several other similar effects in one- and two-dimensional antiferromagnets [14], can be explained on a common basis using the so-called 'pruned' resonating-valence-bond (RVB) picture [13]. Nonmagnetic impurity affects the formation of instant singlet bonds for spins which are located in the immediate vicinity, making some of the bonds geometrically impossible and thus enhancing the other bonds. This explanation is thought to be rather general and does not depend much on the interaction details.

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In this paper I show that for certain models of nonmagnetic impurities in generalized S = 1/2 spin ladders with exact matrix-product ground states of the type considered by us recently [6, 9], local AF correlations are partly or completely insensitive to the presence of impurity.



Figure 1. Nonmagnetic impurity in the generalized S = 1/2 spin ladder as described by the Hamiltonian (1). The Vs denote the biquadratic couplings.

Consider the model of a vacancy in the generalized S = 1/2 ladder with additional diagonal and biquadratic interactions, described by the following Hamiltonian:

$$\widehat{H} = \sum_{i} \widehat{h}_{i,i+1} + \widehat{h}_{-1,1} \tag{1}$$

where

$$\begin{split} \widehat{h}_{ij} &= \frac{1}{2} J_R(S_{1i} \cdot S_{2i} + S_{1,i+1} \cdot S_{2,i+1}) + J_L^{ij}(S_{1i} \cdot S_{1j} + S_{2i} \cdot S_{2j}) \\ &+ J_D^{ij}(S_{1i} \cdot S_{2j} + S_{2i} \cdot S_{1j}) \\ &+ V_{LL}^{ij}(S_{1i} \cdot S_{1j})(S_{2i} \cdot S_{2j}) + V_{DD}^{ij}(S_{1i} \cdot S_{2j})(S_{2i} \cdot S_{1j}). \end{split}$$

Here the indices 1 and 2 distinguish lower and upper legs, and *i* labels rungs (see figure 1), and the terms involving the vacancy site  $S_{2,0}$  are implicitly assumed to be missing in  $\hat{h}_{0,1}$  and  $\hat{h}_{-1,0}$ . The 'bulk' couplings  $J_R$ ,  $J_L^{i,i+1} = J_D^{i,i+1} = 1$ , and  $V_{LL}^{i,i+1} = V_{DD}^{i,i+1} = 4/5$  do not depend on *i*,  $J_R$  is a free parameter, and we have introduced the extra 'edge' interaction between the rungs -1 and 1 across the vacancy to make the problem solvable.

In the absence of the vacancy, the model (1) describes the generalized Bose–Gayen model as introduced in reference [9], at the special value of the leg/diagonal coupling ratio of 1. For  $J_R > 8/5$  its ground state is a product of singlet bonds along the ladder rungs, and we will be interested in the interval  $J_R < 8/5$ , where the ground state coincides with that of the effective S = 1 Affleck–Kennedy–Lieb–Tasaki (AKLT) chain [15], whose S = 1 spins are formed by the triplet degrees of freedom of the rungs [9]. This effective AKLT ground state can be conveniently written in the form of the so-called matrix-product state [16, 17]:

$$\Psi_0 = \operatorname{tr}\left(\prod_i \mathbf{g}_i\right) \qquad \mathbf{g}_i = \frac{1}{\sqrt{3}} \begin{bmatrix} |t_0\rangle_i & -\sqrt{2}|t_+\rangle_i \\ \sqrt{2}|t_-\rangle_i & -|t_0\rangle_i \end{bmatrix}$$
(2)

where  $|t_{\mu}\rangle_i$ ,  $\mu = 0, \pm 1$ , are the triplet states of the *i*th rung. The ground-state energy per rung is [9]

$$E_0 = -13/10 + J_R/4.$$

We will look for the wave function of the ground state in the presence of the impurity in the form of the following matrix product:

$$\Psi_0^{\rm imp} = \operatorname{tr}(\mathbf{g}_{-N} \cdots \mathbf{g}_{-1} \mathbf{G}_0 \mathbf{g}_1 \cdots \mathbf{g}_N) \tag{3}$$

where the matrix  $\mathbf{G}_0$  corresponding to the unpaired spin at the 0th rung is chosen on the basis of the requirement that  $\Psi_0^{\text{imp}}$  has both the total spin and its *z*-projection equal to 1/2; the most general form of  $\mathbf{G}_0$  is [18]

$$\mathbf{G}_{0} = \frac{1}{\sqrt{3+x^{2}}} \begin{bmatrix} (x-1)|\uparrow\rangle & 0\\ -2|\downarrow\rangle & (x+1)|\uparrow\rangle \end{bmatrix}$$
(4)

where x is a free parameter. Physically, the wave function  $\Psi_0^{\text{imp}}$  describes a superposition  $(x/\sqrt{3})\Psi_{1/2}^{0,1/2} + \Psi_{1/2}^{1,1/2}$ , where  $\Psi_{j_{\text{tot}}}^{j_{\text{lad}},1/2}$  denotes a wave function with the total spin  $j_{\text{tot}}$  composed from the states of the unpaired spin 1/2 and the states of the rest of the ladder having total spin  $j_{\text{lad}}$ ; in  $\Psi_{1/2}^{0,1/2}$  the unpaired spin is completely decoupled from the rest of the ladder (which is in the effective AKLT state with one valence bond across the impurity), while in  $\Psi_{1/2}^{1,1/2}$  it is coupled with the edge Kennedy–Tasaki triplet [19] into the state with  $j_{\text{tot}} = 1/2$ ; see figure 2.



**Figure 2.** A schematic valence-bond representation of the wave functions  $\Psi_{1/2}^{0,1/2}$  and  $\Psi_{1/2}^{1,1/2}$  contained in (3); solid and dashed lines denote singlet and triplet valence-bond links, respectively. Solid ovals indicate that the spins on each rung are coupled into effective triplets; the dashed oval in the bottom panel denotes that the triplet valence bond and the unpaired spin are coupled into a spin-1/2 state.

Furthermore, the Hamiltonian (1) conserves parity with respect to the mirror transformation  $i \mapsto -i$ , and one can see that  $\Psi_{1/2}^{1,1/2}$  and  $\Psi_{1/2}^{0,1/2}$  have different parities. The solution with completely decoupled unpaired spins is not very interesting, so we will look for a ground-state wave function of the form (3), (4) with x = 0. Following the approach outlined in reference [17], we demand that the local Hamiltonian  $\hat{h}_{imp}$ , defined as (recall that the terms with  $S_{2,0}$  should be dropped)

$$\widehat{h}_{\rm imp} = \widehat{h}_{-1,0} + \widehat{h}_{0,1} + \widehat{h}_{-1,1} - \varepsilon_0 \tag{5}$$

(where  $\varepsilon_0$  is a free parameter), annihilates all states contained in the matrix product  $\mathbf{g}_{-1}\mathbf{G}_0\mathbf{g}_{+1}$ , and that all other eigenstates of  $\hat{h}_{imp}$  have positive energies. These conditions are sufficient for  $\Psi_0^{imp}$  to be the ground state of  $\hat{H}$ . The construction routine is well described in the literature [17, 6, 9], so I only address it briefly here.

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The states of the [-1, 0, 1] block can be classified into multiplets  $\Psi_{jm}$ , where *j* is the total spin of the block and *m* is its *z*-projection. In total, there are ten multiplets (five with j = 1/2, four with j = 3/2, and one with j = 5/2); one can however straightforwardly check that the matrix product  $\mathbf{g}_{-1}\mathbf{G}_0\mathbf{g}_{+1}$  contains only states of the following three multiplets:

$$\Psi_{1/2,m}^{g,1} = \psi_{1/2,m}^{111} \qquad \Psi_{1/2,m}^{g,2} = \psi_{1/2,m}^{110} \qquad \Psi_{3/2,m}^{g} = \psi_{3/2,m}^{112}.$$
(6)

Here  $\psi_{jm}^{S_A,S_B,S_{AB}}$  denotes the state of the [-1, 0, 1] block with the total spin j,  $S_A$ ,  $S_B$ , and  $S_{AB}$  being the total momenta of the -1 and +1 rungs and the [-1, 1] block, respectively. The local Hamiltonian  $\hat{h}_{imp}$  should annihilate the states (6), so it can be generally written as a projector onto the subspace of the remaining seven multiplets:

$$\Psi_{1/2,m}^{e,1} = \frac{1}{\sqrt{2}} (\psi_{1/2,m}^{101} + \psi_{1/2,m}^{011}) \qquad \Psi_{1/2,m}^{e,2} = \psi_{1/2,m}^{000}$$

$$\Psi_{1/2,m}^{e,3} = \frac{1}{\sqrt{2}} (\psi_{1/2,m}^{101} - \psi_{1/2,m}^{011}) \qquad \Psi_{3/2,m}^{e,2} = \psi_{3/2,m}^{111}$$

$$\Psi_{3/2,m}^{e,3} = \frac{1}{\sqrt{2}} (\psi_{3/2,m}^{101} + \psi_{3/2,m}^{011}) \qquad \Psi_{5/2,m}^{e,2} = \psi_{5/2,m}^{112}.$$
(7)

We make a further simplification—assuming that  $\hat{h}_{imp}$  does not mix the above multiplets; hence,

$$\widehat{h}_{\rm imp} = \sum_{j=1/2,3/2,5/2} \sum_{i} \sum_{m=-j}^{J} \lambda_{j}^{(i)} |\Psi_{jm}^{e,i}\rangle \langle \Psi_{jm}^{e,i}|$$
(8)

where all  $\lambda_j^{(i)}$  should be positive to ensure that (3) is the ground state. Demanding further that this structure is compatible with the particular form of the Hamiltonian (1), one arrives at the following family of solutions for the coupling constants and the parameter  $\varepsilon_0$ :

$$J_{L}^{-1,1} = \lambda_{1/2}^{(1)}/2 + (1+J_{R})/4 \qquad V_{LL}^{-1,1} = J_{R} + 2\lambda_{1/2}^{(1)} - 1$$
  
$$J_{D}^{-1,1} = (1-\lambda_{1/2}^{(1)})/2 - J_{R}/4 \qquad V_{DD}^{-1,1} = -2\lambda_{1/2}^{(1)} - J_{R} \qquad (9)$$

$$\varepsilon_0 = -19/16 + J_R/4$$

where  $\lambda_{1/2}^{(1)}$  plays the role of a free parameter, and the expressions for the other eigenvalues are

$$\lambda_{1/2}^{(2)} = 1 - J_R \qquad \qquad \lambda_{1/2}^{(3)} = 1/4 - (\lambda_{1/2}^{(1)} + J_R)/2 \lambda_{3/2}^{(1)} = 3/2 + \lambda_{1/2}^{(1)} \qquad \qquad \lambda_{3/2}^{(2)} = 3/2$$
(10)  
$$\lambda_{3/2}^{(3)} = 2/5 - (\lambda_{1/2}^{(1)} + J_R)/5 \qquad \qquad \lambda_{5/2} = 5/2.$$

The parameter  $\varepsilon_0$  has the meaning of a ground-state energy of the [-1, 0, 1] block; thus the states with and without a vacancy differ in energy by the value  $\varepsilon_0 - 2E_0$ . The conditions of positivity of  $\hat{h}_{imp}$  require that

$$J_R \leqslant \frac{1}{2} - \lambda_{1/2}^{(1)} \qquad \lambda_{1/2}^{(1)} \geqslant 0.$$
(11)

The most symmetric solution from the above family is achieved by setting  $\lambda_{1/2}^{(1)} = (1 - 2J_R)/4$  and  $J_R \leq 1/2$ ; then

$$J_L^{-1,1} = J_D^{-1,1} = 3/8$$
  $V_{LL}^{-1,1} = V_{DD}^{-1,1} = -1/2.$ 

Using the standard matrix-product technique, it is easy to calculate the spin-correlation functions and distribution of the excess spin in the state (3). The mean value of  $S^z$  at each site is given by

$$\langle S_{1,0}^{z} \rangle = -\frac{1}{6} \qquad \langle S_{1,i}^{z} \rangle = \langle S_{2,i}^{z} \rangle = \frac{2}{9} \left( -\frac{1}{3} \right)^{|i|-1}.$$
 (12)

Here  $|i| \ge 1$ . Following reference [13], we calculate the spin-correlation functions along the ladder legs, with the starting site being next to the vacancy, and compare them to the correlations in the absence of the vacancy. Quite surprisingly, one finds that the AF correlations are not at all affected by the presence of a vacancy:

$$\langle S_{1,0}^{\alpha} S_{1,i}^{\alpha} \rangle = \langle S_{2,1}^{\alpha} S_{2,i+1}^{\alpha} \rangle = (-1)^{|i|} 3^{-|i|-1} = \langle S_{1,n}^{\alpha} S_{1,n+i}^{\alpha} \rangle_{w/o} = \langle S_{2,n}^{\alpha} S_{2,n+i}^{\alpha} \rangle_{w/o}.$$
(13)

Here  $\alpha = x, y, z$ , 'w/o' in the second line means 'without vacancy', and  $|i| \ge 1$ . Note that, despite the presence of the excess spin, the spin correlations remain *isotropic*.

One can show that the above features (insensitivity of AF correlations to the presence of a vacancy and their isotropic character) survive also in more complicated matrix-product-solvable models: the *ansatz* (3), (4) can obviously be used in its most general form, with the 'bulk' matrices  $\mathbf{g}_i$  including singlet degrees of freedom of the ladder rungs [20]:

$$\mathbf{g}_i \mapsto \mathbf{g}_i(u) = \frac{1}{\sqrt{3+u^2}} \begin{bmatrix} u|s\rangle_i + |t_0\rangle_i & -\sqrt{2}|t_+\rangle_i \\ \sqrt{2}|t_-\rangle_i & u|s\rangle_i - |t_0\rangle_i \end{bmatrix}.$$

Then generally the Hamiltonian (1) will not be invariant under the parity transformation  $i \rightarrow -i$ , so the matrix (4) can also be used in its general form with arbitrary x. (The corresponding family of impurity models with exact ground states can be obtained for this general *ansatz*, in exactly the same way as we did above; however, the resulting model Hamiltonians are extremely cumbersome and therefore we do not present those solutions here.) For such a state, the above formula for the correlations will change as follows:

$$\langle S_{1,1}^{\alpha} S_{1,i+1}^{\alpha} \rangle = \langle S_{2,1}^{\alpha} S_{2,i+1}^{\alpha} \rangle = \langle S_{1,n}^{\alpha} S_{1,n+i}^{\alpha} \rangle_{w/o} = \langle S_{2,n}^{\alpha} S_{2,n+i}^{\alpha} \rangle_{w/o} = q^{|i|} / (u^{2} + 3)$$

$$\langle S_{1,0}^{\alpha} S_{1,i}^{\alpha} \rangle = \frac{(1+x)q^{|i|}}{(1-u)(3+x^{2})} \qquad q = \frac{u^{2} - 1}{u^{2} + 3}.$$
(14)

One can see that the AF correlations along the legs are not affected, except the correlations involving the unpaired spin  $S_{1,0}$ , which are enhanced if u is in the interval between -x and (x-3)/(1+x) and suppressed otherwise. In valence-bond-type models, the decay of all of the correlations is purely exponential for all distances, and the presence of the impurity can only change the prefactor, in front of the exponent; coincidentally, for the chosen *ansatz* (3), (4) the changes coming from the excess spin and 'distortions' due to the presence of a vacancy completely compensate each other. The spin excess distribution is also modified and is generally asymmetric:

$$\langle S_{1,i}^z \rangle = \frac{2(\sigma x - 1)q^{|i|}}{(1 - \sigma u)(3 + x^2)} \qquad \langle S_{2,i}^z \rangle = \frac{2(x - \sigma)q^{|i|}}{(u + \sigma)(3 + x^2)} \langle S_{1,0}^z \rangle = \frac{(x^2 - 1)}{2(3 + x^2)} \qquad \sigma \equiv \operatorname{sgn}(i) \qquad |i| \ge 1.$$

Finally, one can observe that the model of a vacancy in the S = 1/2 ladder can be reformulated as a model of the S = 1/2 impurity in the S = 1 AKLT chain. Consider the model described by the following Hamiltonian:



Figure 3. S = 1/2 impurity in the S = 1 AKLT chain as described by the Hamiltonian (15).  $\tau$  is the impurity spin, and the Vs indicate the biquadratic couplings.

$$\widehat{H} = \sum_{i \ge 1} (\widehat{h}_{i,i+1}^{\text{AKLT}} + \widehat{h}_{-i,-i-1}^{\text{AKLT}}) + \widehat{h}_{\text{imp}}$$
(15)

where

$$\begin{split} \widehat{h}_{\text{imp}} &= (J_{+}S_{1} + J_{-}S_{-1}) \cdot \tau + J'(S_{-1} \cdot S_{1}) - \varepsilon_{0} \\ &+ (S_{-1} \cdot S_{1}) \big\{ (V_{+}S_{1} + V_{-}S_{-1}) \cdot \tau \big\} + V'(S_{-1} \cdot S_{1})^{2}. \end{split}$$

Here

$$\widehat{h}_{i,j}^{\text{AKLT}} = S_i \cdot S_j + \frac{1}{3} (S_i \cdot S_j)^2$$

is the local Hamiltonian of the AKLT chain in the bulk, and  $\hat{h}_{imp}$  describes the interaction induced by the presence of the impurity spin  $\tau$  (see figure 3), the parameter  $\varepsilon_0$  being just a constant energy shift having the meaning of the ground-state energy of the  $[-1, \tau, 1]$  block. Using the *ansatz* (3), (4), one can repeat the entire construction routine as described above for the ladder, and obtain the following family of Hamiltonians for which  $\Psi_0^{imp}$  is the exact ground state:

$$J_{\pm} = \{5(3 - x^2)/9 \pm 2x\}\lambda_{3/2} + 5\lambda_{5/2}/9$$

$$J' = -(5 + x^2)\lambda_{3/2}/3 + 5\lambda_{5/2}/6$$

$$V_{\pm} = \{-5(3 + x^2)/9 \pm 4x/3\}\lambda_{3/2} + 5\lambda_{5/2}/9$$

$$V' = -(15 + x^2)\lambda_{3/2}/9 + 5\lambda_{5/2}/18$$

$$\varepsilon_0 = (30 - 2x^2)\lambda_{3/2}/9 + 5\lambda_{5/2}/9.$$
(16)

Here  $\lambda_{3/2} \ge 0$ ,  $\lambda_{5/2} \ge 0$  are the eigenvalues of  $\hat{h}_{imp}$  corresponding to the multiplets

$$\Psi^{e}_{3/2,m} = (5+x^2)^{-1/2} (x\psi^{112}_{3/2,m} - \sqrt{5}\psi^{111}_{3/2,m}) \qquad \Psi^{e}_{5/2,m} = \psi^{112}_{5/2,m}$$

respectively. For  $x \neq 0$ ,  $\infty$  the equations (16) describe models with an asymmetric impurity. Again, as in case of the ladder, one can straightforwardly check that the 'edge' spincorrelation function in the presence of the impurity  $\langle S_1^{\alpha} S_i^{\alpha} \rangle$  just coincides with that in the bulk, independently of the value of x. The above family contains two interesting solutions. One is achieved by setting x = 0,  $\lambda_{5/2} = 3\lambda_{3/2}$  and describes the simple symmetric model without biquadratic terms involving the impurity spin  $\tau$ :

$$J_{\pm} = J$$
  $J' = -V' = \frac{1}{4}J$   $V_{\pm} = 0.$  (17)

Another solution corresponds to  $\lambda_{3/2} = 0$ ; then the ground state of the model is twofold degenerate since the even- and odd-parity wave functions  $\Psi_0^{imp}(x = 0)$  and  $\Psi_0^{imp}(x = \infty)$  are eigenstates with the same energy.

In conclusion, I have presented two model families describing impurities in antiferromagnetic (AF) spin chains and ladders which admit exact solutions for the ground state. Those models exhibit an interesting property of insensitivity of local AF correlations to the presence of impurity, in contrast to the usual behaviour expected for standard models with only nearest-neighbour bilinear exchange [13]. It should be remarked that there is no contradiction between the results of reference [13] and those of the present paper, because the models considered are very different; however, our results imply that the effect of impurity-induced local enhancement of AF correlations, despite its generality, can be sensitive to the details of local interaction near the impurity. For instance, an essential ingredient of all of the models considered in the present paper is rather strong interaction of next-nearest neighbours across the impurity (roughly, its strength is in the range from one quarter to one half of the nearest-neighbour exchange).

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