Models of impurities in valence bond spin chains and ladders

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We present the class of models of a nonmagnetic impurity in an AKLT-type valence bond ground state, and of a $S = \frac{1}{2}$ impurity in the $S = 1$ AKLT chain. The ground state in presence of impurity can be found exactly. 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 of researchers. The interest to spin ladders is particularly stimulated by the hope to get 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$_{11.84}$ in presence of hole doping and high pressure was recently reported. It is now well established that “regular” (i.e., with only “leg” and “rung” exchange couplings) $S = \frac{1}{2}$ isotropic spin ladders have a disordered gapped ground state. On the other hand, “generalized” ladders including other couplings can serve as interesting toy models with a rich behavior which is often very different from that of “regular” models.

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

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

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

\[
\hat{H} = \sum_i \hat{h}_{i,i+1} + \hat{h}_{-1,1},
\]

where

\[
\hat{h}_{ij} = \frac{1}{2} J_R (S_{1i} S_{2i} + S_{1,i+1} S_{2,i+1}) + J_L^{ij} (S_{1i} S_{1j} + S_{2i} S_{2j}) + J_D^{ij} (S_{1i} S_{2j} + S_{2i} S_{1j}) + V_{LL}^{ij} (S_{1i} S_{1j})(S_{2i} S_{2j}) + V_{DD}^{ij} (S_{1i} S_{2j})(S_{2i} S_{1j}),
\]

here the indices 1 and 2 distinguish lower and upper legs, and $i$ labels rungs (see Fig. 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 $J_R$, $J_L^{ij+1} = J_D^{ij+1} = 1$, and $V_{LL}^{ij+1} = V_{DD}^{ij+1} = \frac{1}{4}$ 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 absence of the vacancy the model describes the generalized Bose-Gayen model as introduced in Ref. at the special value of the leg/diagonal coupling ratio equal to 1. At $J_R > \frac{3}{4}$ its ground state is a product of singlet bonds along the ladder rungs, and we will be interested in the interval $J_R < \frac{3}{4}$, where the ground state coincides with that of the effective $S = 1$ Affleck-Kennedy-Lieb-Tasaki (AKLT) chain whose $S = 1$ spins are formed by the triplet degrees of freedom of the rung. This effective AKLT ground state can be conveniently written in a form of the so-called matrix product state:

\[
\Psi_0 = \text{tr}(\prod_i g_i), \quad g_i = \frac{1}{\sqrt{3}} \begin{bmatrix} t_0 \langle i \rangle & -\sqrt{2} t_+ \langle i \rangle & -\sqrt{2} t_- \langle i \rangle \\ t_+ \langle i \rangle & -|t_0\rangle \langle i | & -\sqrt{2} |t_-\rangle \langle i | \\ t_- \langle i \rangle & -\sqrt{2} |t_+\rangle \langle i | & -|t_0\rangle \langle i |
\end{bmatrix},
\]

where $|t_\mu\rangle$, $\mu = 0, \pm 1$ are the triplet states of the $i$-th rung. The ground state energy per rung is

\[
E_0 = -\frac{13}{10} + J_R/4.
\]

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

\[
\Psi_0^{\text{imp}} = \text{tr}(g_{-N} \cdots g_{-1} G_0 g_1 \cdots g_N),
\]

where the matrix $G_0$ corresponding to the unpaired spin at the 0-th rung is chosen from 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 $G_0$ is:

$$G_0 = \frac{1}{\sqrt{3 + x^2}} \left[ \begin{array}{cc} (x - 1) \uparrow & 0 \\ -2 \downarrow & (x + 1) \uparrow \end{array} \right],$$

(4)

$x$ being a free parameter. Physically, the wave function $\Psi_0^{\text{imp}}$ describes a superposition $(x/\sqrt{3})\Psi_{1/2}^{0,1/2} + \Psi_{1/2}^{1/2}$, where $\Psi_{1/2}^{\text{tot}}$ 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 $j_{\text{tot}}$ 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 $\Psi_{1/2}^{1/2}$ it is coupled with the edge Kennedy-Tasaki triplet into the state with $j_{\text{tot}} = 1/2$, see Fig. 2.

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

$$\hat{h}_{\text{imp}} = \hat{h}_{-1,0} + \hat{h}_{0,1} + \hat{h}_{-1,1} - \varepsilon_0,$$

(5)

where $\varepsilon_0$ is a free parameter, annihilates all states contained in the matrix product $g_{-1}G_0g_{+1}$, and that all other eigenstates of $\hat{h}_{\text{imp}}$ have positive energies. These conditions are sufficient for $\Psi_0^{\text{imp}}$ to be the ground state of $\hat{H}$. The construction routine is well described in literature so that I only briefly address it here.

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 $g_{-1}G_0g_{+1}$ contains only states of the following three multiplets:

$$\Psi_{j,m}^{1/2} = \psi_{j,m}^{111}, \quad \Psi_{j,m}^{2} = \psi_{j,m}^{110}, \quad \Psi_{j,m}^{3} = \psi_{j,m}^{112},$$

(6)

where $\Psi_{S_A,S_B,SA,B}$ 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 $-1$th, $0$th and $1$th rung and the $[-1, 1]$ block, respectively. The local Hamiltonian $\hat{h}_{\text{imp}}$ should annihilate the states $|j, m\rangle$, so that it can be generally written as a projector onto the subspace of the remaining seven multiplets,

$$\Psi_{j,m}^{1/2} = \frac{1}{\sqrt{2}}(\psi_{j,m}^{101} + \psi_{j,m}^{011}), \quad \Psi_{j,m}^{2} = \psi_{j,m}^{000}, \quad \Psi_{j,m}^{3} = \frac{1}{\sqrt{2}}(\psi_{j,m}^{010} - \psi_{j,m}^{011}),$$

(7)

$$\Psi_{j,m}^{1} = \frac{1}{\sqrt{2}}(\psi_{j,m}^{101} + \psi_{j,m}^{011}), \quad \Psi_{j,m}^{2} = \psi_{j,m}^{111}, \quad \Psi_{j,m}^{3} = \frac{1}{\sqrt{2}}(\psi_{j,m}^{101} - \psi_{j,m}^{011}).$$

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

$$\hat{h}_{\text{imp}} = \sum_{j = 1/2, 3/2} \sum_{m = -j}^{j} \lambda_j^{(i)}|\Psi_{jm}\rangle\langle\Psi_{jm}|,$$

(8)

where all $\lambda_j^{(i)}$ should be positive to ensure that $|\Psi_0\rangle$ is the ground state. Demanding further that this structure is compatible with the particular form of the Hamiltonian $H$, one arrives at the following family of solutions for the coupling constants and the parameter $\varepsilon_0$:

$$J_{L}^{1,1} = \lambda_{1/2}^{(1)}/2 + (1 + J_R)/4, \quad V_{L}^{1,1} = J_R + 2\lambda_{1/2}^{(1)} - 1,$$

$$J_{D}^{1,1} = (1 - \lambda_{1/2}^{(1)}/2 - J_R/4, \quad V_{L}^{1,1} = -2\lambda_{1/2}^{(1)} - J_R, \quad \varepsilon_0 = -19/16 + J_R/4,$$

(9)

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

$$\lambda_{1/2}^{(2)} = 1 - J_R, \quad \lambda_{1/2}^{(3)} = 1/2 - (\lambda_{1/2}^{(1)} + J_R)/2, \quad \lambda_{3/2}^{(1)} = 3/2 + \lambda_{1/2}^{(1)}, \quad \lambda_{3/2}^{(2)} = 3/2, \quad \lambda_{3/2}^{(3)} = 2/5 - (\lambda_{1/2}^{(1)} + J_R)/5, \quad \lambda_{5/2} = 5/2.$$

(10)

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 $\hat{h}_{\text{imp}}$ require that

$$J_R \leq 1/2 - \lambda_{1/2}^{(1)}, \quad \lambda_{1/2}^{(1)} \geq 0.$$  

(11)

The most symmetric solution from the above family is achieved by setting $\lambda_{1/2}^{(1)} = (1 - 2J_R)/4$, $J_R \leq 1/2$, then $J_{L}^{1,1} = J_R^{1,1} = 3/8$ and $V_{L}^{1,1} = V_{D}^{1,1} = -1/2$.

Using the standard matrix product technique, it is easy to calculate the spin correlation functions and distribution of the excess spin in the state $|\Psi_0\rangle$. The mean value of $S_1^z$ at each site is given by

$$\langle S_{1,0}^z \rangle = -1/6, \quad \langle S_{1,1}^z \rangle = \langle S_{2,1}^z \rangle = 2/9 \left( \left( \frac{1}{3} \right)^{2|\downarrow| - 1} \right),$$

(12)

here $|\downarrow| \geq 1$. Following Ref. 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 absence of the vacancy. Quite surprisingly, one finds that the AF correlations are not at all affected by the presence of a vacancy.
\[\langle S_{1,0}^\alpha S_{1,1}^\alpha \rangle = \langle S_{1,n}^\alpha S_{1,n+1}^\alpha \rangle = (-1)^i \cdot 3^{-|i|-1} = \langle S_{2,n}^\alpha S_{2,n+1}^\alpha \rangle \]

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

One can then consider the AF correlations along the legs are not affected, except for the correlations involving the unpaired spin \(S_{1,0}\), which are enhanced for \(u\) being in the interval between \(-x\) and \((x - 3)/(1 + x)\) and suppressed otherwise. In valence-bond-model types the decay of all correlations is purely exponential for all distances, and presence of the impurity can only change the prefactor in front of the exponent; accidentally, for the chosen ansatz 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:

\[\langle S_{1,1}^\alpha \rangle = \frac{2(x - 1)}{1 - u(3 + x^2)}, \quad \langle S_{2,1}^\alpha \rangle = \frac{2(x - \sigma)}{(u + \sigma)(3 + x^2)}, \quad \sigma \equiv \text{sgn}(i), \quad |i| \geq 1.\]

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

\[\hat{H} = \sum_{i \geq 1} (\hat{h}_{i,i+1} + \hat{h}_{i-1,i}) + \hat{h}_{\text{imp}},\]

\[\hat{h}_{\text{imp}} = (J_+ S_1 + J_- S_{-1}) \cdot \tau + J'(S_{-1} \cdot S_1) - \varepsilon_0 + (S_{-1} \cdot S_1)\{V_+ S_1 + V_- S_{-1} \cdot \tau\} + V' (S_1 \cdot S_1)^2,\]

where \(\hat{h}_{i,i+1} = S_i \cdot S_{i+1} + \frac{1}{2}(S_i \cdot S_j)^2\) is the local Hamiltonian of the AKLT chain in the bulk, and \(\hat{h}_{\text{imp}}\) describes the interaction induced by presence of the impurity spin \(\tau\), see Fig. 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 \(\Psi_0\), \(\Psi_1\), one can repeat the entire construction routine as described above for the ladder, and obtain the following family of Hamiltonians for which \(\Psi_0\) is the exact ground state:

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

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

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

\[V' = -(15 + x^2)\lambda_{3/2} + 5\lambda_{5/2}/18,\]

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

Here \(\lambda_{3/2} \geq 0, \lambda_{5/2} \geq 0\) are the eigenvalues of \(\hat{h}_{\text{imp}}\) corresponding to the multiplets

\[\Psi_{\frac{3}{2},m} = (5 + x^2)^{-1/2}(\psi_{\frac{112}{2},m} - \sqrt{3}\psi_{\frac{111}{2},m}), \quad \Psi_{\frac{5}{2},m} = \psi_{\frac{112}{2},m},\]

respectively. For \(x \neq 0, \infty\) the Eqs. \(\frac{6}{10}\) describe models with an asymmetric impurity. Again, as in case of the ladder, one can straightforwardly check that the "edge" spin correlation function in presence of the impurity \(\langle S_{1,1}^\alpha S_{1,1}^\alpha \rangle\) 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 bi quadratic terms involving the impurity spin \(\tau\):

\[J_\pm = J, \quad J' = -V' = \frac{1}{4}J, \quad V_\pm = 0.\]

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

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spin ladder as described by the Hamiltonian (1). $V$'s denote the biquadratic couplings.

\[
\hat{h}_{ij} = J^R_2 \begin{pmatrix}
1 & J^{ij}_D \\
J^{ij}_D & 1
\end{pmatrix} + V^R_{LL} + V^R_{DD}
\]

FIG. 1. Nonmagnetic impurity in the generalized $S = \frac{1}{2}$ spin ladder as described by the Hamiltonian (1). $V$'s denote the biquadratic couplings.

\[
\Psi^{0,1/2} = \begin{pmatrix}
\cdots \\
\bullet \\
\cdots
\end{pmatrix}
\]

\[
\Psi^{1,1/2} = \begin{pmatrix}
\cdots \\
\bullet \\
\cdots
\end{pmatrix}
\]

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

\[
S_{-2} \quad S_{-1} \quad \tau \quad S_{1} \quad S_{2}
\]

\[+V' \bullet \quad +V_+ \bullet \quad +V_+ \bullet \quad +V_+ \bullet \]

FIG. 3. $S = \frac{1}{2}$ impurity in the $S = 1$ AKLT chain as described by the Hamiltonian (13). $\tau$ is the impurity spin, and $V$'s indicate the biquadratic couplings.