Open su(4)-invariant spin ladder with boundary defects

Yupeng Wang

Department of Physics, Florida State University, Tallahassee, Florida 32306
and Institute of Physics, Chinese Academy of Sciences, Beijing 100080, People's Republic of China

P. Schlottmann

Department of Physics, Florida State University, Tallahassee, Florida 32306

(Received 16 March 2000)

The integrable su(4)-invariant spin-ladder model with a boundary defect is studied using the Bethe ansatz method. The exact phase diagram for the ground state is given and the boundary quantum critical behavior is discussed. It consists of a gapped phase in which the rungs of the ladder form singlet states and a gapless Luttinger liquid phase. It is found that in the gapped phase the boundary bound state corresponds to an unscreened local moment, while in the Luttinger liquid phase the local moment is screened at low temperatures in analogy to the Kondo effect.

I. INTRODUCTION

Spin-ladder systems are an active field of research in condensed matter physics experimentally realized in some quasi-one-dimensional materials.[1] The simplest example is the two-leg isotropic spin-1/2 ladder that has a gapped ground state. Generalizations of ladders to more legs and couplings beyond nearest-neighbor exchanges show a remarkably rich behavior and can interpolate among a variety of systems.[2-4] For instance, a dimerized phase driven by biquadratic interactions was predicted in Ref. 2 and then demonstrated in a generalized spin-ladder model[3] by constructing the exact ground state and studying elementary excitations. Recently, a modulation structure induced by frustration was reported in a two-leg spin ladder.[5] Quantum phase transitions from a gapped phase to a gapless phase were theoretically predicted and experimentally studied in the Heisenberg ladder system $Cu_2(C_5H_{12}N_2)_2Cl_4$ in the presence of a magnetic field.[6]

Solutions of integrable models provide a useful starting point for the understanding of more general correlated many-body systems. A few integrable spin-ladder models have recently been proposed.[7-10] For instance the integrable su(4)-invariant spin ladder[7] represents a special case of the Nersesyan-Tsvelik model.[2] This model was recently generalized to the multileg case[11] and hole doping of the ladder was also studied.[12] In general some four-spin interaction terms must be included in integrable models (required by the integrability), which could be either related to spin-phonon mediated interactions or in the hole-doped phase they could be generated by the Coulomb repulsion between the holes moving in the spin correlated background.[2] The importance of a biquadratic interaction for properties of CuO_2 plaquettes was pointed out in Ref. 13 and its effect on excitations in a spin ladder was studied in Ref. 3. Some experiments indeed revealed that such multispin interactions are realized in solid films of ^3He absorbed on graphite,[14] in a two-dimensional Wigner solid of electrons formed in a Si inversion layer,[15] in bcc solid ^3He,[16] and in heavy fermion systems.

Impurities always play a relevant role in low-dimensional systems. This is especially the case in Luttinger liquids, where an impurity may drive the system to a strong coupling fixed point,[17] which corresponds to an open boundary condition at the impurity site for low-energy excitations. Therefore, the boundary impurity is of particular interest in quasi-one-dimensional systems. Typical examples are the spin chain with boundary magnetic fields,[18,19] or equivalently two-dimensional classical statistical systems with boundary fields,[19,20] and a quantum impurity coupled to a one-dimensional strongly correlated electron host.[21,22]

In this paper we study the open su(4)-invariant spin ladder with a boundary defect. Boundary effects can arise, for example, if (i) the transverse coupling at the boundary is different from that in the bulk or if (ii) the rung-rung coupling at the boundary is different from that in the bulk. We will consider the following two model Hamiltonians:

Model I,

$$H = \frac{1}{4} \sum_{j=1}^{N-1} (1 + \vec{\sigma}_j \cdot \vec{\sigma}_{j+1})(1 + \vec{\tau}_j \cdot \vec{\tau}_{j+1}) + \frac{1}{4} J \sum_{j=2}^{N} \vec{\sigma}_j \cdot \vec{\tau}_j$$
$$+ \frac{1}{4} J' \vec{\sigma}_1 \cdot \vec{\tau}_1, \tag{1}$$

Model II,

$$H = \frac{1}{4} \sum_{j=2}^{N-1} (1 + \vec{\sigma}_j \cdot \vec{\sigma}_{j+1})(1 + \vec{\tau}_j \cdot \vec{\tau}_{j+1}) + \frac{1}{4} J \sum_{j=1}^{N} \vec{\sigma}_j \cdot \vec{\tau}_j$$
$$+ \frac{1}{4} U(1 + \vec{\sigma}_1 \cdot \vec{\sigma}_2)(1 + \vec{\tau}_1 \cdot \vec{\tau}_2), \tag{2}$$

where $\vec{\sigma}_j$ and $\vec{\tau}_j$ are Pauli matrices acting on the site j of the upper leg and lower leg, respectively, and J represents the transverse rung coupling constant in the bulk, while J' is the coupling at the boundary rung. U denotes the rung-rung coupling strength between the first and second rungs. Without the boundary defects (i.e., $J' = J$, $U = 1$), the model is exactly solvable with periodic boundary conditions.[7] In Sec. II we show that model I is integrable for arbitrary J', obtain the corresponding Bethe ansatz solution, and discuss the physi-

cal consequences of the boundary bound state. In Sec. III the exact solution of model II is presented for arbitrary U. Conclusions follow in Sec. IV.

II. SOLUTION OF MODEL I

A. Bethe ansatz formulation

The quantum states of a single rung are $|\sigma_j^z, \tau_j^z\rangle$. It is convenient to define

$$|0\rangle = \frac{1}{\sqrt{2}}(|\uparrow,\downarrow\rangle - |\downarrow,\uparrow\rangle),$$

$$|1\rangle = |\uparrow,\uparrow\rangle, \quad |3\rangle = |\downarrow,\downarrow\rangle,$$

$$|2\rangle = \frac{1}{\sqrt{2}}(|\uparrow,\downarrow\rangle + |\downarrow,\uparrow\rangle), \tag{3}$$

which satisfy the orthogonality relation $\langle\alpha|\beta\rangle = 0$. For simplicity we have omitted the rung index j and obviously, the first state denotes a singlet rung and the latter three the triplet states. We introduce the Hubbard operators

$$X^{\alpha\beta} = |\alpha\rangle\langle\beta|, \quad \alpha,\beta = 0,1,2,3, \tag{4}$$

and rewrite Hamiltonian (1) as

$$H = \sum_{j=1}^{N-1} \sum_{\alpha,\beta=0}^{3} X_j^{\alpha\beta} X_{j+1}^{\beta\alpha} - J \sum_{j=2}^{N} X_j^{00} - J' X_1^{00}$$
$$+ \frac{1}{4}J(N-1) + \frac{1}{4}J', \tag{5}$$

and the total number of α rungs can be expressed as $N_\alpha = \sum_{j=1}^{N} X_j^{\alpha\alpha}$. In this way we have reduced model I to an su(4)-invariant spin chain with an effective splitting or, equivalently, to an su(4)-invariant t-J model[23,24] with a finite chemical potential and a boundary potential. Both the effective chemical potential J and the boundary field J' lift the su(4) symmetry of the Hamiltonian. The Hamiltonian (5) can be diagonalized via either the algebraic Bethe ansatz[18,20,21] or the coordinate Bethe ansatz.[25] As the pseudovacuum, we choose the state in which all rungs are in a singlet,

$$|\Omega\rangle \equiv |0_1\rangle \otimes |0_2\rangle \otimes \cdots \otimes |0_N\rangle. \tag{6}$$

The Bethe wave functions can be constructed as

$$|\Psi\rangle = \sum_{\{j_m,\alpha_m\}} \Psi_{\alpha_1,\ldots,\alpha_{M_1}}(j_1,\ldots,j_{M_1}) X_{j_1}^{\alpha_1 0} \cdots X_{j_{M_1}}^{\alpha_{M_1} 0} |\Omega\rangle, \tag{7}$$

where Ψ is an amplitude, the sum over j_m runs from 1 to N, and the sum over α_m from 1 to 3. The elimination of the "unwanted" terms from $H|\Psi\rangle$ yields the standard nested Bethe ansatz equations (BAE):

$$\left(\frac{\lambda_j - \frac{i}{2}}{\lambda_j + \frac{i}{2}}\right)^{2N} = -\frac{\lambda_j - \frac{i}{2}\eta}{\lambda_j + \frac{i}{2}\eta} \prod_{r=\pm} \prod_{l\neq j}^{M_1} \frac{\lambda_j - r\lambda_l - i}{\lambda_j - r\lambda_l + i}$$
$$\times \prod_{\alpha=1}^{M_2} \frac{\lambda_j - r\mu_\alpha + \frac{i}{2}}{\lambda_j - r\mu_\alpha - \frac{i}{2}},$$

$$\prod_{r=\pm} \prod_{\beta\neq\alpha}^{M_2} \frac{\mu_\alpha - r\mu_\beta - i}{\mu_\alpha - r\mu_\beta + i} = \prod_{r=\pm} \prod_{j=1}^{M_1} \frac{\mu_\alpha - r\lambda_j - \frac{i}{2}}{\mu_\alpha - r\lambda_j + \frac{i}{2}}$$
$$\times \prod_{\delta=1}^{M_3} \frac{\mu_\alpha - r\nu_\delta - \frac{i}{2}}{\mu_\alpha - r\nu_\delta + \frac{i}{2}},$$

$$\prod_{r=\pm} \prod_{\gamma\neq\delta}^{M_3} \frac{\nu_\delta - r\nu_\gamma - i}{\nu_\delta - r\nu_\gamma + i} = \prod_{r=\pm} \prod_{\alpha=1}^{M_2} \frac{\nu_\delta - r\mu_\alpha - \frac{i}{2}}{\nu_\delta - r\mu_\alpha + \frac{i}{2}}, \tag{8}$$

where the parameter η is determined by J and J' via

$$J - J' - 1 = \frac{1+\eta}{1-\eta}, \tag{9}$$

and $M_1 = N_1 + N_2 + N_3$, $M_2 = N_2 + N_3$ and $M_3 = N_3$. Here λ_j, μ_α, and ν_δ represent the rapidities of the flavor waves. The energy spectrum of the Hamiltonian (1) is given by

$$E = -\sum_{j=1}^{M_1} \left(\frac{1}{\lambda_j^2 + \frac{1}{4}} - J\right) - \frac{3}{4}JN - \frac{3}{4}(J'-J) + N - 1. \tag{10}$$

B. Ground-state properties

For the periodic boundary conditions all the rapidities are real in the ground state. For $J=4$ the system has a quantum critical point.[7] When $J>4$, the ground state is the pseudovacuum $|\Omega\rangle$, i.e., all rungs are in the singlet state. For $J<4$, on the other hand, there is a continuum of excitations given by a Luttinger liquid of in general three components.

The boundary defect may change the phase diagram close to the end point of the ladder. In particular, imaginary solutions of the BAE arising from the boundary scattering matrix [first factor on the right-hand side of the first set of Eqs. (8)] correspond to wave functions that fall off exponentially from the boundary. In fact, $\lambda = i\eta/2$ is always a solution of the BAE in the thermodynamic limit $N\to\infty$ for $\eta>0$ and $\eta\neq1$ [$\eta=1$ is a singular point of Eq. (9), which corresponds to $J'=\pm\infty$]. This imaginary mode represents the boundary bound state corresponding to a triplet rung. A careful analysis of the energy carried by the imaginary mode yields that

the boundary bound state is not always stable (occupied) in the ground state. We limit ourselves to the situation of anti-ferromagnetic coupling ($J>0$). From Eq. (10) we have that the energy of the imaginary mode is

$$\epsilon_b = J - \frac{4}{1-\eta^2}. \tag{11}$$

The boundary bound state is stable if $\epsilon_b<0$. Otherwise the imaginary mode represents an excited state. We have to distinguish the cases $J>4$ from $J<4$. (i) For $J>4$, there is a critical line given by

$$\eta_c = \sqrt{1 - \frac{4}{J}}, \tag{12}$$

which separates the spin singlet rung ground state ($0<\eta<\eta_c$ and $\eta>1$) from the spin triplet ground state ($\eta_c<\eta<1$) at the boundary of the ladder. For $0<\eta<\eta_c$ and $\eta>1$ we have $\epsilon_b>0$, while for $\eta_c<\eta<1$ ϵ_b is negative and the boundary bound state is filled. (ii) For $0<J<4$ the bulk corresponds to a three-component Luttinger liquid with real λ, μ, and ν modes. Here the boundary bound state is stable in the whole parameter region $0<\eta<1$, but it is empty if $\eta>1$. The boundary triplet state for $0<\eta<1$ is coupled to the continuum giving rise to a Kondo-like screening.

Consider now the response of the system to an external magnetic field h. The magnetic field couples to the ladder via the Zeeman effect, i.e. the Hamiltonian has an extra term $-h\Sigma_{j=1}^N(X_j^{11}-X_j^{33})$. The critical line $J=4$ separating the gapped and gapless regions is now shifted to $J-h=4$. The bound-state energy is also reduced by h. Hence, for $J-h>4$, the critical line Eq. (12) is now given by $\eta_c=\sqrt{1-4/(J-h)}$. The threefold degeneracy of the triplet rung state at the boundary is lifted by the field, so that an arbitrarily small field induces a finite magnetization ±1 (depending on the direction of the field) due to the stabilization of the bound state. Therefore, the boundary quantum phase transition at $\eta=\eta_c$ is of first order and the susceptibility is divergent at $T=0$, following a Curie law.

To summarize, the boundary phase diagram for $J>h$ is shown in Fig. 1(a) and consists of seven regions. For $J-h>4$ the bulk is gapped and we have argued that for $\eta<0$ there is no bound state and the rungs all form singlets. For $0<\eta<\eta_c$ the bound state is not stable and all rungs are in singlet states. For $\eta_c<\eta<1$ there is a triplet state at the boundary (the triplet wave function falls off exponentially into the bulk of the ladder), and finally for $\eta>1$ the bound state is again unstable. For $J-h<4$ the bulk is a Luttinger liquid, without a bound state for $\eta<0$, with a stable bound state for $0<\eta<1$, and with an unstable bound state for $\eta>1$. Below we show that a Kondo-like screening occurs for $0<\eta<1$.

It is also interesting to study the situation for $h-J>0$. The bulk is then always a Luttinger liquid and only four cases for the boundary bound state have to be distinguished [see Fig. 1(b)]. We assume here that $h-J$ is sufficiently small so that the spin ladder is not spin polarized. If $\eta<0$ there is no bound state, for $0<\eta<1$ the bound state is filled with a predominantly spin-up triplet state (the Kondo screening is quenched by the magnetic field), for $1<\eta<\eta_c$ there is an empty bound state, and for $\eta>\eta_c$ the bound state is again stable (with magnetic field quenched Kondo screening).
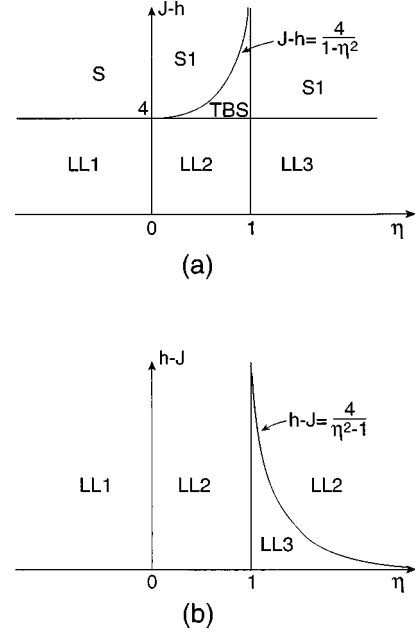

FIG. 1. Boundary phase diagram of the two-leg su(4)-invariant spin ladder with different transverse coupling at the first rung (model I) for (a) $J-h>0$ and (b) $h-J>0$. The interaction strength at the first rung is parametrized by η defined in Eq. (9). Quantum critical behavior with mean-field exponents is obtained along the line $J-h=4$. Several phases are possible at the boundary. In S all rungs are in a singlet state and there is no boundary bound state. In $S1$ the ground state consists of singlet rungs but there is an empty boundary bound state. TBS (triplet bound state) refers to a phase in which the boundary bound-state is stable, i.e., there is a boundary triplet state with wave function falling off exponentially into the bulk. LL1, LL2 and LL3 refer to a Luttinger liquid with no boundary bound state, with a stable boundary bound state (triplet state), and with an unstable boundary bound state, respectively. In (b) we assumed that $h-J$ is sufficiently small so that the ladder is not spin polarized.

The thermodynamics of the boundary defect can also be derived from the BAE, Eq. (8), following the standard method.[26,27] The thermodynamic BAE allow us to study the boundary quantum critical behavior. The boundary defect induces a "ghost spin" η. However, unlike in su(2)-invariant models,[22] the ghost spin does not lead to an anomalous remnant entropy because the su(4) symmetry in the present model is already lifted by the finite J.

C. The quantum critical line $J=4$

Along the quantum critical line $J=4$, the boundary defect can show critical behavior as the bulk does.[7] We now consider the case $\eta>1$. In zero magnetic field, the ground state of the bulk consists only of singlet rungs. In a weak magnetic field some triplet rungs with $S^z=1$ appear in the ground state, while N_2 and N_3 still remain equal to zero, since the energy of the state $|2\rangle$ is unchanged and that of the state $|3\rangle$ is increased ($h>0$). We denote with $\rho(\lambda)$ the distribution of real λ modes, including the boundary-defect contribution. From the BAE, Eq. (12), we obtain

$$\rho(\lambda) + \int_{-\Lambda}^{\Lambda} d\lambda' a_2(\lambda-\lambda')\rho(\lambda') = a_1(\lambda) - \frac{1}{2N}a_\eta(\lambda), \tag{13}$$

where $a_n(\lambda) = n/2\pi[\lambda^2 + (n/2)^2]$ and $\Lambda^2 = 1/(4-h) - 1/4$. For $h \ll 1$, we have $\Lambda \approx \sqrt{h}/4$ and Eq. (13) can be solved by iteration,

$$\rho(\lambda) = \left(\frac{2}{\pi} - \frac{1}{\pi \eta N} \right) \left(1 - \frac{2\Lambda}{\pi} \right) + \cdots, \qquad (14)$$

with the ground-state energy given by

$$E = \int_{-\Lambda}^{\Lambda} d\lambda \left(4 - \frac{1}{\lambda^2 + \frac{1}{4}} - h \right) \rho(\lambda) - \frac{3}{4} J N$$

$$- \frac{3}{4}(J' - J) + N - 1. \qquad (15)$$

Combining Eqs. (14) and (15) we obtain the susceptibility of the system

$$\chi = -\frac{\partial^2 E}{\partial h^2} = \left(\frac{2}{\pi} - \frac{1}{\pi \eta N} \right) \left(\frac{1}{4} h^{-1/2} - \frac{1}{3\pi} \right) + O(h^{1/2}). \qquad (16)$$

The susceptibility diverges with the square root of the field as a consequence of the van Hove singularity of the empty λ band. The boundary bound state removes one degree of freedom from the bulk, so that its contribution to the susceptibility is negative. This result is not surprising, since in this case J' is much larger than J. Consequently the boundary rung is in a tight singlet and hence insensitive to the field, so that the whole susceptibility is reduced.

Similar arguments indeed yield a positive boundary susceptibility for $\eta < 0$. As discussed before, in the region $0 < \eta < 1$, a stable boundary bound-state occurs and a small field already induces a finite magnetization.

With a simple scaling approach we find that the low-temperature specific heat and the magnetic susceptibility of the boundary defect at the line $J = 4$ behaves as

$$\delta C(T) \sim T^{1/2}, \quad \delta \chi(T) \sim T^{-1/2}. \qquad (17)$$

Such a result can also be predicted by a simple spin-wave theory with a dispersion relation $\epsilon(k) \sim k^2$ or alternatively exactly via the low-temperature expansion of the thermodynamic BAE.[28,29] The boundary critical exponents in Eqs. (16) and (17) are exactly the same as for the bulk.[7]

D. Kondo effect in the gapless phase

In the gapless phase, $0 < J < 4$, the system is a three-component Luttinger liquid. In the sense of the su(4) t-J model, the triplet rungs are considered spin-1 hard-core bosons. The λ rapidities represent the charge sector, while the μ and ν rapidities parametrize the spin degrees of freedom, which have su(3) invariance.

As discussed above [see Fig. 1(a)] a stable boundary bound state only exists at low temperatures for $0 < \eta < 1$. The boundary bound state corresponds to a local moment with spin 1. The boundary coupling J' does not break the su(3) invariance of the hard-core bosons and the boundary local moment is spin compensated in analogy to the Kondo effect.

To show this we explicitly consider the imaginary mode $i\eta/2$ in the BAE, which then become

$$\left(\frac{\lambda_j - \frac{i}{2}}{\lambda_j + \frac{i}{2}} \right)^{2N} = -\frac{\lambda_j - \frac{i}{2}\eta}{\lambda_j + \frac{i}{2}\eta} \frac{\lambda_j - i\left(1 - \frac{\eta}{2}\right)}{\lambda_j + i\left(1 - \frac{\eta}{2}\right)} \frac{\lambda_j - i\left(1 + \frac{\eta}{2}\right)}{\lambda_j + i\left(1 + \frac{\eta}{2}\right)} \prod_{r=\pm} \prod_{l \neq j}^{M_1 - 1} \frac{\lambda_j - r\lambda_l - i}{\lambda_j - r\lambda_l + i} \prod_{\alpha=1}^{M_2} \frac{\lambda_j - r\mu_\alpha + \frac{i}{2}}{\lambda_j - r\mu_\alpha - \frac{i}{2}},$$

$$\prod_{r=\pm} \prod_{\beta \neq \alpha}^{M_2} \frac{\mu_\alpha - r\mu_\beta - i}{\mu_\alpha - r\mu_\beta + i} = \prod_{r=\pm} \frac{\mu_\alpha - \frac{i}{2}(1 + r\eta)}{\mu_\alpha + \frac{i}{2}(1 + r\eta)} \prod_{j=1}^{M_1 - 1} \frac{\mu_\alpha - r\lambda_j - \frac{i}{2}}{\mu_\alpha - r\lambda_j + \frac{i}{2}} \prod_{\delta=1}^{M_3} \frac{\mu_\alpha - r\nu_\delta - \frac{i}{2}}{\mu_\alpha - r\nu_\delta + \frac{i}{2}},$$

$$\prod_{r=\pm} \prod_{\gamma \neq \delta}^{M_3} \frac{\nu_\delta - r\nu_\gamma - i}{\nu_\delta - r\nu_\gamma + i} = \prod_{r=\pm} \prod_{\alpha=1}^{M_2} \frac{\nu_\delta - r\mu_\alpha - \frac{i}{2}}{\nu_\delta - r\mu_\alpha + \frac{i}{2}}. \qquad (18)$$

For large N the solutions of the BAE, Eq. (18), are strings of arbitrary length for all three sets of rapidities. We introduce the usual densities of λ, μ, ν strings $\rho_{1,n}(\lambda)$, $\rho_{2,n}(\mu)$, $\rho_{3,n}(\nu)$, and their respective hole densities $\rho_{1,n}^h(\lambda)$, $\rho_{2,n}^h(\mu)$, $\rho_{3,n}^h(\nu)$. In the thermodynamic limit these densities satisfy the following integral equations:[30]

$$\rho_{1,n}^h(\lambda) + \sum_m A_{mn} \rho_{1,m}(\lambda) = \sum_m B_{mn} \rho_{2,m}(\lambda) + a_n(\lambda),$$

$$\rho_{2,n}^h(\lambda) + \sum_m A_{mn} \rho_{2,m}(\lambda) = \sum_m B_{mn}(\rho_{1,m}(\lambda) + \rho_{3,m}(\lambda)), \qquad (19)$$

$$\rho_{3,n}^h(\lambda) + \sum_m A_{mn}\rho_{3,m}(\lambda) = \sum_m B_{mn}\rho_{2,m}(\lambda),$$

where we neglected the boundary driving terms which are of order N^{-1}. Here

$$A_{mn} = [m+n] + 2[m+n-2] + \cdots + 2[|m-n|+2]$$
$$+ [|m-n|],$$

$$B_{mn} = \sum_{l=1}^{\min\{m,n\}} [m+n-2l+1],$$

and $[n]$ is the integral operator with kernel $a_n(\lambda)$ and $a_0(\lambda)$ is the δ-function.

The free-energy functional is given by

$$F/N = \sum_{r,n} \int d\lambda \{ \epsilon_{r,n}\rho_{r,n}(\lambda) - T[\rho_{r,n}(\lambda)$$
$$+ \rho_{r,n}^h(\lambda)]\ln[\rho_{r,n}(\lambda) + \rho_{r,n}^h(\lambda)] + T\rho_{r,n}(\lambda)\ln\rho_{r,n}(\lambda)$$
$$+ T\rho_{r,n}^h(\lambda)\ln\rho_{r,n}^h(\lambda)\}, \qquad (20)$$

where $\epsilon_{1,n} = -2\pi a_n(\lambda) + n(J-h)$, $\epsilon_{2,n} = \epsilon_{3,n} = nh$. Minimizing Eq. (20) with respect to the densities and taking into account the relations (19), we obtain[30,31]

$$\ln(1+\eta_{r,n}) = \frac{\epsilon_{r,n}}{T} + \sum_{m,s} A_{mn}^{rs} \ln(1+\eta_{s,m}^{-1}), \quad r,s = 1,2,3 \qquad (21)$$

with $A_{mn}^{rs} = A_{mn}\delta_{r,s} - B_{mn}(\delta_{r,s+1}+\delta_{r,s-1})$, $\eta_{r,n} = \rho_{r,n}^h/\rho_{r,n}$, and $\eta_{0,n}^{-1} = \eta_{4,n}^{-1} \equiv 0$. An equivalent set of integral equations is

$$\ln\eta_{r,n} = G*[\ln(1+\eta_{r,n+1}) + \ln(1+\eta_{r,n-1})]$$
$$- G*[\ln(1+\eta_{r+1,n}^{-1}) + \ln(1+\eta_{r-1,n}^{-1})],$$

$$\ln\eta_{r,1} = -\frac{2\pi}{T}G(\lambda)\delta_{r,1} + G*\ln(1+\eta_{r,2})$$
$$- G*[\ln(1+\eta_{r+1,1}^{-1}) + \ln(1+\eta_{r-1,1}^{-1})],$$

$$\lim_{n\to\infty}\frac{\ln\eta_{1,n}}{n} = \frac{J-h}{T}, \quad \lim_{n\to\infty}\frac{\ln\eta_{2,n}}{n} = \lim_{n\to\infty}\frac{\ln\eta_{3,n}}{n} = \frac{h}{T} \equiv 2x_0, \qquad (22)$$

where $*$ denotes convolution and $G(\lambda) = [2\cosh(\pi\lambda)]^{-1}$. The equilibrium free energy is

$$F/N = -T\sum_n [n]\ln(1+\eta_{1,n}^{-1}).$$

At low T the exchange J gives rise to a Fermi surface for the charges, which are only significantly populated in the interval $|\lambda| < \Lambda = \sqrt{1/J - 1/4}$, but are unoccupied for $|\lambda| > \Lambda$. The low-energy spin excitations, on the other hand, take place at very large rapidities (for $h=0$ the spin Fermi surface is at ∞). Hence, at low T the charge and spin sectors are well separated and only weakly coupled. Assuming complete decoupling of the spin and charge sectors, a solution of Eq. (22) can be easily obtained for large n,

$$\eta_{2,n} = \eta_{3,n} = \frac{\sinh(nx_0)\sinh(n+1)x_0}{\sinh x_0 \; \sinh(2x_0)} - 1. \qquad (23)$$

Although the boundary bound state has also some charge fluctuations (triplet-singlet rung admixture), these do not affect the dynamics of the spin (weak coupling of spin and charge sectors). We can then limit ourselves to the spin degrees of freedom of the bound state. Its contribution to the free energy is

$$F_{bs} = -\frac{1}{2}T\sum_{n=1}^{\infty} \int d\lambda \left[a_n\left(\lambda - \frac{i}{2}\eta\right) \right.$$
$$\left. + a_n\left(\lambda + \frac{i}{2}\eta\right) \right] \ln[1+\eta_{2,n}^{-1}] \qquad (24)$$

or, equivalently,

$$F_{bs} = F_{bs}^0 - \frac{1}{2}T\sum_{r=\pm}\sum_{q=1}^{2} \int d\lambda G_q(\lambda + ir\eta/2)\ln[1+\eta_{q+1,1}], \qquad (25)$$

where F_{bs}^0 the ground-state energy of the local moment and

$$G_q(\lambda) = \frac{\sin[\pi(1-q/3)]}{\cosh(2\pi\lambda/3) + \cos[\pi(1-q/3)]}.$$

Substituting Eq. (23) into Eq. (25) we readily obtain that the residual entropy of the magnetic moment is exactly zero, which means that the boundary bound state is fully screened by the Kondo effect. These results are analogous to those of a Coqblin-Schrieffer impurity embedded into the same host.[32]

III. SOLUTION OF MODEL II

To show that model II is integrable we rewrite the Hamiltonian (2) as

$$H = H_0 + H_1,$$

$$H_0 = \sum_{j=2}^{N-1} P_{jj+1} + UP_{12},$$

$$H_1 = -J\sum_{j=1}^{N} X_j^{00} + \frac{1}{4}NJ, \qquad (26)$$

where $P_{ij} = (1+\vec{\sigma}_i\cdot\vec{\sigma}_j)(1+\vec{\tau}_i\cdot\vec{\tau}_j)/4$ is the permutation operator between rung i and rung j. Obviously, $[H_0,H_1]=0$, which means that they can be diagonalized simultaneously. We define the Lax operators

$$S_{ij}(\lambda) \equiv \lambda - iP_{ij}, \qquad (27)$$

which satisfy the Yang-Baxter relations[33]

$$S_{ij}(\lambda-\mu)S_{ik}(\lambda)S_{jk}(\mu) = S_{jk}(\mu)S_{ik}(\lambda)S_{ij}(\lambda-\mu). \qquad (28)$$

As shown in Refs. 18 and 22, the monodromy matrix

$$T_\tau(\lambda) \equiv S_{N\tau}(\lambda)S_{N-1\tau}(\lambda)\cdots S_{2\tau}(\lambda)S_{1\tau}(\lambda-ic)S_{1\tau}(\lambda$$
$$+ ic)S_{2\tau}(\lambda)\cdots S_{N-1\tau}(\lambda)S_{N\tau}(\lambda) \qquad (29)$$

satisfies the reflection Yang-Baxter equation

$$S_{\tau\tau'}(\lambda-\mu)T_{\tau}(\lambda)S_{\tau\tau'}(\lambda+\mu)T_{\tau'}(\mu)$$

$$=T_{\tau'}(\mu)S_{\tau\tau'}(\lambda+\mu)T_{\tau}(\lambda)S_{\tau\tau'}(\lambda-\mu), \qquad (30)$$

where c is an arbitrary constant and τ and τ' are indices of the four-dimensional auxiliary space. From Eq. (30) we have

$$[t(\lambda),t(\mu)]=0 \qquad (31)$$

with $t(\lambda)\equiv tr_{\tau}T_{\tau}(\lambda)$. Therefore, $t(\lambda)$ serves as the generating functional of a variety of conserved quantities. H_0 is

related to $t(\lambda)$ as

$$H_0=\frac{i}{8(1-c^2)}(-1)^{N+1}\frac{dt(\lambda)}{d\lambda}\bigg|_{\lambda=0}, \qquad (32)$$

provided that $U=1/(1-c^2)$. Hence, H_0 and Hamiltonian (2) are integrable in the sense of the algebraic Bethe ansatz. Following the standard procedure we readily obtain the BAE of model II,

$$\left(\frac{\lambda_j-\frac{i}{2}}{\lambda_j+\frac{i}{2}}\right)^{2(N-1)}=\frac{\lambda_j+i\left(c+\frac{1}{2}\right)}{\lambda_j-i\left(c+\frac{1}{2}\right)}\frac{\lambda_j-i\left(c-\frac{1}{2}\right)}{\lambda_j+i\left(c-\frac{1}{2}\right)}\prod_{r=\pm}\prod_{l\neq j}^{M_1}\frac{\lambda_j-r\lambda_l-i}{\lambda_j-r\lambda_l+i}\prod_{\alpha=1}^{M_2}\frac{\lambda_j-r\mu_\alpha+\frac{i}{2}}{\lambda_j-r\mu_\alpha-\frac{i}{2}},$$

$$\prod_{r=\pm}\prod_{\beta\neq\alpha}^{M_2}\frac{\mu_\alpha-r\mu_\beta-i}{\mu_\alpha-r\mu_\beta+i}=\prod_{r=\pm}\prod_{j=1}^{M_1}\frac{\mu_\alpha-r\lambda_j-\frac{i}{2}}{\mu_\alpha-r\lambda_j+\frac{i}{2}}\prod_{\delta=1}^{M_3}\frac{\mu_\alpha-r\nu_\delta-\frac{i}{2}}{\mu_\alpha-r\nu_\delta+\frac{i}{2}},$$

$$\prod_{r=\pm}\prod_{\gamma\neq\delta}^{M_3}\frac{\nu_\delta-r\nu_\gamma-i}{\nu_\delta-r\nu_\gamma+i}=\prod_{r=\pm}\prod_{\alpha=1}^{M_2}\frac{\nu_\delta-r\mu_\alpha-\frac{i}{2}}{\nu_\delta-r\mu_\alpha+\frac{i}{2}} \qquad (33)$$

with the energy eigenvalues given by

$$E=-\sum_{j=1}^{M_1}\left(\frac{1}{\lambda_j^2+\frac{1}{4}}-J\right)-\frac{3}{4}JN+U+N-2. \qquad (34)$$

The Hamiltonian (32) is only Hermitian if the parameter c is either real or imaginary. For imaginary c, $U<1$, and the first rung is weakly coupled to the bulk. For real c (we can consider $c>0$ because $\pm c$ yields the same U) the imaginary mode $\lambda_b=i(c-1/2)$ is a solution of the BAE, Eq. (33), in the thermodynamic limit $N\to\infty$ for $c>1/2$. This bound state again corresponds to a triplet boundary bound state, i.e., its wave function falls off exponentially with the distance from the boundary. The energy of the bound state is $\epsilon_b=J-1/(c-c^2)$, which can be stable only if $\epsilon_b<0$, i.e., in the region $1/2<c<1$. This corresponds to $U>1$ for which the first rung is strongly coupled to the bulk. For $c>1$, i.e. $U<0$, the bound state has positive energy and is empty. The first rung is then ferromagnetically coupled to the ladder.

As in the case of model I, there is a critical line for $J>4$ given by

$$J_c=\frac{1}{(c-c^2)}, \qquad (35)$$

which separates the region of an occupied (stable) and empty (unstable) bound state. Hence, when $J>J_c$ the ground state is a spin singlet, while for $4<J<J_c$ and $1/2<c<1$ the boundary bound state is stable in the ground state.

In summary, the physical properties of the two models are very similar. The main difference can be understood in terms of the number of ''ghost spin'' solutions (number of bound state solutions) of the BAE,[22] which correspond to images of the real local moment. In the Kondo regime for $J<4$ there are two ''ghost spins,'' $c+1/2$ and $c-1/2$, in the spin sector of the second model, while there is only one in model I. This can be read off from the impurity factors in the BAE's Eqs. (8) and (33). Since the effects of the ghost spin contributions are additive, the physics in both situations is very similar.

IV. CONCLUSIONS

We studied two models for boundary defects of the open two-leg su(4)-invariant spin ladder. In model I the transverse coupling at the boundary rung is different from the bulk, while in model II the coupling of the first rung to the ladder is different from the rung-rung coupling in the bulk. The two models under consideration are integrable and we obtained the exact solution by means of Bethe's ansatz. Depending on the model parameters three situations may arise in the thermodynamic limit: (i) there is no imaginary mode solution of the BAE and hence the states of the first rung are part of the

continuum of the bulk, (ii) an imaginary boundary mode exists, but corresponds to a positive energy ϵ_b, i.e. the state is empty, and (iii) an imaginary boundary mode with negative energy exists. In case (ii) the boundary bound state does not affect the ground-state properties, but does contribute to the finite T thermodynamics. The situation (iii) is the most interesting one, since a spin-1 boundary bound state is filled in the ground state. The boundary phase diagram of model I is shown in Figs. 1(a) and 1(b).

The su(4)-invariant two-leg ladder has a critical line at $J = 4$. For $J > 4$ all the rungs of the bulk are in the singlet state, while for $J < 4$ the system is a Luttinger liquid of in general three components. For $J > 4$ a stable boundary bound state carries a magnetic moment (triplet state with wave function that falls off exponentially into the bulk), while in all other cases the boundary rung is in its singlet state. For $J < 4$, on the other hand, a stable boundary bound state carries a Kondo compensated (screened by the spin degrees of freedom in the Luttinger liquid) magnetic moment of spin-1, i.e., ultimately the ground state is a singlet. An unstable bound state just removes one degree of freedom from the Luttinger liquid. Both models considered here display similar properties at the boundary.

[1] E. Dagotto and T.M. Rice, Science **271**, 618 (1996).

[2] A.A. Nersesyan and A.M. Tsvelik, Phys. Rev. Lett. **78**, 3939 (1997).

[3] A.K. Kolezhuk and H.-J. Mikeska, Int. J. Mod. Phys. B **12**, 2325 (1998); Phys. Rev. Lett **80**, 2709 (1998); S. Brehmer, H.-J. Mikeska, M. Müller, N. Nagaosa, and S. Uchida, Phys. Rev. B **60**, 329 (1999).

[4] I. Bose and S. Gayen, Phys. Rev. B **48**, 10 653 (1993); A Gosh and I. Bose, *ibid.* **55**, 3613 (1997).

[5] Y. Wang, Int. J. Mod. Phys. B **13**, 3323 (1999).

[6] G. Chaboussant, Y. Fegot-Revurat, M.-H. Julien, M. E. Hanson, C. Berthier, M. Horvatić, L. P. Levy, and O. Piovesana, Phys. Rev. Lett. **80**, 2713 (1998).

[7] Y. Wang, Phys. Rev. B **60**, 9236 (1999).

[8] H. Frahm and C. Rödenbeck, J. Phys. A **30**, 4467 (1997).

[9] N. Muramoto and M. Takahashi, J. Phys. Soc. Jpn. **68**, 2098 (1999).

[10] S. Albeverio, S.M. Fei, and Y. Wang, Europhys. Lett. **47**, 364 (1999).

[11] M.T. Batchelor and M. Maslen, J. Phys. A **32**, L337 (1999).

[12] H. Frahm and A. Kundu, J. Phys.: Condens. Matter **11**, L557 (1999).

[13] Y. Honda, Y. Kuramoto, and T. Watanabe, Phys. Rev. B **47**, 11 329 (1993).

[14] K. Ishida, M. Morishita, K. Yawata, and H. Fukuyama, Phys. Rev. Lett. **79**, 3451 (1997); M. Roger, C. Bäuerle, Yu. M. Bunkov, A.-S. Chen, and H. Godfrin, *ibid.* **80**, 1308 (1998).

[15] T. Okamoto and S. Kawaji, Phys. Rev. B **57**, 9097 (1998).

[16] For a review, see D.D. Osheroff, J. Low Temp. Phys. **87**, 297 (1992).

[17] C.L. Kane and M.P.A. Fisher, Phys. Rev. Lett. **68**, 1220 (1992); E. Sørensen, S. Eggert, and I. Affleck, J. Phys. A **26**, 6757 (1993).

[18] E.K. Sklyanin, J. Phys. A **21**, 2375 (1988).

[19] F. C. Alcaraz, M. N. Barber, M. T. Batchelor, R. J. Baxter, and G. R. W. Quispel, J. Phys. A **20**, 6397 (1987).

[20] C.M. Yung and M.T. Batchelor, Nucl. Phys. B **453**, 552 (1995).

[21] A. Foerster and M. Karowski, Nucl. Phys. B **396**, 611 (1993); **408**, 512 (1993).

[22] Y. Wang, Phys. Rev. B **56**, 14 045 (1997); Y. Wang and U. Eckern, *ibid.* **59**, 6400 (1999); J. Dai, Y. Wang, and U. Eckern, *ibid.* **60**, 6594 (1999); J. Dai and Y. Wang, *ibid.* **60**, 12 309 (1999).

[23] B. Sutherland, Phys. Rev. B **12**, 3795 (1975).

[24] P. Schlottmann, Phys. Rev. B **36**, 5177 (1987).

[25] Y. Wang, J. Dai, Z. Hu, and F.-C. Pu, Phys. Rev. Lett. **79**, 1901 (1997).

[26] C.N. Yang and C.P. Yang, J. Math. Phys. **10**, 1115 (1969).

[27] M. Takahashi, Prog. Theor. Phys. **46**, 401 (1971); **46**, 1388 (1971).

[28] P. Schlottmann, Phys. Rev. B **33**, 4880 (1986).

[29] Y. Wang and J. Dai, Phys. Rev. B **59**, 13 561 (1999).

[30] H. Johannesson, Phys. Lett. A **116**, 133 (1986).

[31] N. Andrei, K. Furuya, and J.H. Lowenstein, Rev. Mod. Phys. **55**, 331 (1983); A.M. Tsvelik, and P.B. Wiegmann, Adv. Phys. **32**, 453 (1983).

[32] P. Schlottmann, J. Phys.: Condens. Matter **10**, 2525 (1998).

[33] C.N. Yang, Phys. Rev. Lett. **10**, 1312 (1967).