

## Integrable supersymmetric $t$ - $J$ model with magnetic impurity

P. Schlottmann

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

A. A. Zvyagin

*B. I. Verkin Institute for Low Temperature Physics and Engineering, Ukrainian National Academy of Sciences, 47 Lenin Avenue, Kharkov 310164, Ukraine*

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We consider the one-dimensional  $t$ - $J$  model, which consists of spin-1/2 electrons on a lattice with nearest neighbor hopping  $t$  constrained by the excluded multiple occupancy of the lattice sites and spin-exchange  $J$  between neighboring sites. The model is integrable at the supersymmetric point,  $J=2t$ . We extend the model by introducing an impurity of arbitrary spin  $S$  that interacts with the electrons on the neighboring sites without destroying the integrability. The lattice model is defined by the scattering matrices via the quantum inverse scattering method. The interaction Hamiltonian between the impurity and the itinerant electrons is only explicitly constructed in the continuum limit. The discrete Bethe ansatz equations diagonalizing the model are derived and the solutions are classified according to the string hypothesis. The thermodynamic Bethe ansatz equations are derived and the impurity free energy is obtained for arbitrary bandfilling as a function of temperature and external magnetic field. The properties of the impurity depend on one coupling parameter. The impurity can localize up to one itinerant electron and has in general mixed valent properties. The integer valent low  $T$  small  $H$  fixed point of the impurity corresponds to an asymptotically free spin  $S$ , while if either  $T$  or  $H$  (or both) become large the impurity behaves like an asymptotically free spin  $(S+\frac{1}{2})$ . [S0163-1829(97)03605-9]

### I. INTRODUCTION

The Hubbard and  $t$ - $J$  models are frequently invoked as models for highly correlated electrons, in particular for the high- $T_c$  cuprate superconductors,<sup>1-3</sup> but as well for heavy fermion systems.<sup>4,5</sup> On one hand, the Hubbard model in the limit of a strong Coulomb repulsion reduces to the  $t$ - $J$  model. The strong on-site correlations limit the site occupations to at most one electron. States with double occupation are energetically unfavorable and can be projected out, so that there are then three states per site, in contrast to four states for the Hubbard model. Virtual transitions to states with doubly occupied sites give rise to an exchange interaction between electrons on nearest neighbor sites via a canonical transformation.<sup>6-8</sup> The validity of this transformation is restricted to small exchange constants or large  $U$  and three site interactions (correlated hopping) are usually neglected. On the other hand, the low-energy excitations of the three-band Hubbard model (two oxygen  $p$  states and one copper  $3d$  orbital per unit cell of the  $\text{CuO}_2$  plane) can also be reduced to an effective one-band  $t$ - $J$  model.<sup>9-12</sup> In this context, which does not involve the canonical transformation, one arrives at the  $t$ - $J$  model without actually going through the traditional Hubbard model and  $J/t$  is not restricted to be small. In fact  $t$  and  $J$  are comparable energies and we may consider them as independent parameters not related to  $t^2/U$ .

The phase diagram of the one-dimensional  $t$ - $J$  model has been investigated by numerous methods, e.g., with a variational ansatz for the Luttinger liquid,<sup>13,14</sup> by cluster diagonalization using Lanczos method,<sup>15,16</sup> and Monte Carlo simulations.<sup>17,18</sup> Variational studies strongly depend on the

trial wave function and exact diagonalizations are limited by the relatively small cluster sizes. The most reliable results are probably those obtained by variational Monte Carlo simulations,<sup>17</sup> which are less limited by the size of the system. The zero-temperature phase diagram as a function of  $J/t$  and band filling  $n$  shows three qualitatively different phases: (i) a Luttinger liquid ground state, which may have an effective repulsive or attractive long-range interaction, (ii) a spin gap phase, and (iii) a phase separated ground state in which all electrons (and all holes) are clustered together.<sup>15</sup>

Unfortunately, the one-dimensional  $t$ - $J$  model is not integrable for all ratios of  $t/J$ . The necessary condition for the integrability is the factorization of the many-electron scattering matrix into two-particle scattering matrices (Yang-Baxter triangular relation). The Yang-Baxter relation imposes conditions on the scattering matrix that are only satisfied for  $J=\pm 2t$ .<sup>4,19</sup> At this special point in a scattering process the sets of wave numbers of the incoming and outgoing particles are identical, leading to permutation symmetry. The spin of the electrons and the charge ‘holes’ play a very similar role forming a graded superalgebra.<sup>19-22</sup> The integrability of the supersymmetric model was first stated by Lai<sup>23</sup> and Sutherland<sup>19</sup> and has subsequently been rediscovered by other authors.<sup>4,24,25</sup> Asymptotically exact results can also be extracted from the Bethe ansatz for small deviations from supersymmetry and low electron concentrations.<sup>26</sup>

Impurities play a very important role in correlated electron compounds, since even a small amount of defects may change the properties of the system. Unfortunately, an impurity introduced into an integrable system usually destroys the integrability. Besides magnetic impurities in noninteracting metals (e.g., the Kondo effect, the Anderson impurity model,

and the multichannel Kondo problem, see Refs. 27–30), there are only a few exceptions for integrable models with interactions containing impurities. Andrei and Johannesson<sup>31</sup> incorporated a magnetic impurity of arbitrary spin into the isotropic spin- $\frac{1}{2}$  Heisenberg chain. The interaction between the impurity and the neighboring lattice sites has to be of a special form to preserve the integrability. These results were then extended to the Babujian-Takhtajan spin chain of spin  $S'$  and an arbitrary impurity of spin  $S$ .<sup>32,33</sup> The properties of isolated impurities are analogous to those of the multichannel Kondo problem, i.e., the underscreened, spin-compensated and overscreened situations have to be distinguished.<sup>30,33</sup> It has been argued<sup>34</sup> that these low-temperature properties of the impurity correspond to nongeneric fixed points. The peculiarities, however, do not arise from integrability.<sup>35</sup> Other authors<sup>36</sup> proposed a different, nonmagnetic impurity, model based on the Heisenberg chain, which lacks of backward scattering. Within the context of the  $t$ - $J$  model Bares<sup>37</sup> extended the ideas of Andrei and Johannesson<sup>31</sup> to introduce an integrable nonmagnetic impurity which does not change the marginal Fermi liquid properties. Another avenue is pursued by Pfannmüller and Frahm,<sup>38</sup> who consider a fusion procedure for different representations of the  $gl(2,1)$  superalgebra.

In this paper we consider a *magnetic* impurity embedded into the supersymmetric  $t$ - $J$  model. The Bethe ansatz equations automatically ensure the integrability of the model. The model is defined by the scattering matrices via the quantum inverse scattering method. The Hamiltonian and other conserved currents can in principle be constructed from the transfer matrix. The impurity consists of a spin  $S$  on a given link  $m$ , which by construction interacts only with both neighboring sites. The impurity can absorb (and release it again) one conduction electron and form an effective spin  $S + \frac{1}{2}$ . The impurity has therefore intermediate valence character, which can be changed as a function of a model parameter. The model is structurally similar to the generalization of the Anderson impurity to two magnetic configurations, which was found to be integrable some time ago.<sup>29,39,40</sup> Close to integer valence two fixed points play a role: (i) at low  $T$  and small fields the impurity behaves like an asymptotically free spin  $S$  and (ii) if either  $T$  or  $H$  (or both) are large the fixed point corresponds to the asymptotic freedom of a spin  $S + \frac{1}{2}$ . There is a smooth crossover between these regimes at intermediate  $T$  and  $H$ .

The rest of the paper is organized as follows. The vertex weights, the monodromy matrix, the diagonalization of the transfer matrix, and the discrete Bethe ansatz equations are introduced in Sec. II. These equations define the lattice model and determine the properties of the impurity. In Sec. II we also explicitly construct the interaction Hamiltonian between the impurity and the correlated itinerant electrons for the continuum limit. In Sec. III we classify the solutions of the Bethe ansatz equations according to the string hypothesis and derive the thermodynamic Bethe ansatz equations. The thermodynamic properties of the impurity are studied in Sec. IV and a summary with concluding remarks follows in Sec. V.

## II. TRANSFER MATRIX AND THE BETHE ANSATZ EQUATIONS

We begin this section by briefly restating the results for the supersymmetric  $t$ - $J$  model we need here. Then we intro-

duce the impurity scattering matrix, construct the monodromy matrix, and derive the discrete Bethe ansatz equations for the lattice model. Finally, we present the interaction Hamiltonian between the impurity and the correlated itinerant electrons, which we construct in the continuum limit (but not for the lattice).

### A. Supersymmetric $t$ - $J$ model

The one-dimensional  $t$ - $J$  model is defined by the Hamiltonian

$$H_0 = -t \sum_{i\sigma} P(c_{i\sigma}^\dagger c_{i+1\sigma} + c_{i+1\sigma}^\dagger c_{i\sigma}) P + J \sum_i \left( \mathbf{S}_i \mathbf{S}_{i+1} - \frac{1}{4} n_i n_{i+1} \right), \quad (2.1)$$

where  $c_{i\sigma}^\dagger$  creates an electron of spin  $\sigma$  at site  $i$ ,  $P$  is a projector that excludes the multiple occupancy of each site,  $\mathbf{S}_i = c_{i\sigma}^\dagger \mathbf{S}_{\sigma\sigma'} c_{i\sigma'}$  are the spin- $\frac{1}{2}$  operators and  $n_i = \sum_\sigma c_{i\sigma}^\dagger c_{i\sigma}$  is the number operator for site  $i$ . Here  $J$  is the exchange coupling (assumed antiferromagnetic) and without loss of generality  $t$  can be equated to 1.

Model (2.1) is only integrable for  $J = 2t$ , i.e., at the supersymmetric point.<sup>19,23</sup> The scattering matrix for two electrons with wave numbers  $k_1$  and  $k_2$  then takes the form<sup>4</sup>

$$\hat{X}(k_1, k_2) = \frac{(p_1 - p_2) \hat{I} + i \hat{P}}{p_1 - p_2 + i}, \quad (2.2)$$

where  $p = \frac{1}{2} \cot(k/2)$ ,  $\hat{I} = \delta_{\sigma_1 \sigma'_1} \delta_{\sigma_2 \sigma'_2}$  and  $\hat{P} = \delta_{\sigma'_1 \sigma_2} \delta_{\sigma'_2 \sigma_1}$  are the identity and permutation operators for the spin indices, respectively. Here unprimed (primed) spin indices refer to states before (after) scattering. It is easy to verify that the two-electron scattering matrix satisfies the Yang-Baxter triangular relation

$$X_{\sigma_2 \sigma'_2}^{\sigma_1 \sigma'_1}(p_1 - p_2) X_{\sigma_3 \sigma'_3}^{\sigma'_1 \sigma''_1}(p_1 - p_3) X_{\sigma'_3 \sigma''_3}^{\sigma'_2 \sigma''_2}(p_2 - p_3) = X_{\sigma_3 \sigma'_3}^{\sigma_2 \sigma'_2}(p_2 - p_3) X_{\sigma'_3 \sigma''_3}^{\sigma_1 \sigma'_1}(p_1 - p_3) X_{\sigma'_2 \sigma''_2}^{\sigma'_1 \sigma''_1}(p_1 - p_2), \quad (2.3)$$

where repeated indices are summed over. Relation (2.3), in addition to the excluded multiple occupancy of sites, are necessary and sufficient conditions for the integrability of Eq. (2.1).

The energy is determined by the wave numbers; for a particle of wavenumber  $k$  we have<sup>4</sup>

$$E = -2 \cos(k) = -2 + 2 \frac{1/2}{p^2 + 1/4}. \quad (2.4)$$

### B. Impurity scattering matrix

We introduce the impurity via its scattering matrix with the itinerant electrons. If the integrability of the model is to be preserved, the impurity scattering matrix  $\hat{S}$  has to satisfy the following triangular Yang-Baxter relation<sup>28,29</sup>

$$\begin{aligned}
& X_{\sigma_2 \sigma_2'}^{\sigma_1 \sigma_1'}(p_1 - p_2) S_{MM'}^{\sigma_1' \sigma_1''}(p_1 - p_0) S_{M'M''}^{\sigma_2' \sigma_2''}(p_2 - p_0) \\
&= S_{MM'}^{\sigma_2 \sigma_2'}(p_2 - p_0) S_{M'M''}^{\sigma_1 \sigma_1'}(p_1 - p_0) X_{\sigma_2 \sigma_2'}^{\sigma_1' \sigma_1''}(p_1 - p_2), \quad (2.5)
\end{aligned}$$

where the sum over repeated indices is implicit. The index  $M$  refers to the spin component of the magnetic impurity. In principle, there is not a unique impurity scattering matrix satisfying Eq. (2.5), i.e., there is more than one impurity form that could be constructed without destroying the integrability of the supersymmetric  $t$ - $J$  model.

In this paper we consider the impurity scattering matrix

$$\begin{aligned}
S_{MM'}^{\sigma \sigma'}(p - p_0) &= \delta_{\sigma \sigma'} \delta_{MM'} + (M \sigma | M + \sigma)(M' \sigma' | M' + \sigma') \\
&\times \frac{i(2S + 1)}{p - p_0 - i(2S + 1)/2} P_{MM'}^{\sigma \sigma'}, \quad (2.6)
\end{aligned}$$

where again the unprimed (primed) indices refer to the incoming (outgoing) states and  $P_{MM'}^{\sigma \sigma'} = \delta_{\sigma \sigma'} \delta_{MM'} + \delta_{-\sigma \sigma'} \delta_{M'M+2\sigma}$ . Here  $S$  is the spin of the impurity and necessarily  $|M| \leq S$ . The Clebsch-Gordan coefficient  $(M \sigma | M + \sigma)$ , which is actually a shorthand notation for

$$(SM; \frac{1}{2} \sigma | S \frac{1}{2}(S + \frac{1}{2})M + \sigma), \quad (2.7)$$

selects the way the impurity interacts with the itinerant electrons. The impurity is then capable of temporarily absorbing the spin of one conduction electron to form an effective spin  $(S + \frac{1}{2})$ , i.e., it exists in two different spin configurations. This is characteristic of intermediate valence systems, where actual states are the linear superposition of two electronic configurations of the ions.<sup>29,39,40</sup> Here  $p_0$  is the parameter that controls the degree of ‘‘valence admixture.’’ Note that both, Eqs. (2.2) and (2.6), are unitary.

### C. Monodromy matrix and Bethe ansatz equations

The monodromy matrix<sup>28,29</sup> is defined as

$$\begin{aligned}
& L_{\{\sigma_1' \dots \sigma_N' M'\} \tau'}^{\{\sigma_1 \dots \sigma_N M\} \tau}(\alpha; \alpha_1, \dots, \alpha_{N+1}) \\
&= X_{\sigma_1' \sigma_1}^{\tau' \mu_1}(\alpha_1 - \alpha) X_{\sigma_2' \sigma_2}^{\mu_1 \mu_2}(\alpha_2 - \alpha) \dots X_{\sigma_N' \sigma_N}^{\mu_{N-1} \mu_N}(\alpha_N - \alpha) \\
&\times S_{M'M}^{\mu_N \tau}(\alpha_{N+1} - \alpha), \quad (2.8)
\end{aligned}$$

with the implicit summation over all the  $\mu_j$  indices. With respect to the indices  $\tau$  and  $\tau'$  the monodromy matrix forms a  $2 \times 2$  matrix, which we will denote  $\hat{L}_\tau^{\tau'}(\alpha)$  omitting the spin indices and the parameters  $\alpha_j$ .

From the Yang-Baxter relations it follows that the monodromy matrix satisfies the identity<sup>28,29</sup>

$$\begin{aligned}
& X_{\tau_2 \tau_2'}^{\tau_1 \tau_1'}(\alpha - \alpha') \hat{L}_{\tau_3}^{\tau_1'}(\alpha') \hat{L}_{\tau_3}^{\tau_2'}(\alpha) \\
&= \hat{L}_{\tau_2}^{\tau_2}(\alpha) \hat{L}_{\tau_1}^{\tau_1'}(\alpha') X_{\tau_2 \tau_2'}^{\tau_1' \tau_3}(\alpha - \alpha'), \quad (2.9)
\end{aligned}$$

where the sum over repeated indices is implicit. Using that  $\hat{X}(\alpha) \hat{X}(-\alpha) = \hat{\mathbf{1}}$ , we multiply Eq. (2.9) from the left by  $X_{\tau_3 \tau_3'}^{\tau_3 \tau_3'}(\alpha' - \alpha)$  and sum over the indices  $\tau_1$  and  $\tau_2$  to obtain

$$\begin{aligned}
& \delta_{\tau_3 \tau_3'} \delta_{\tau_3' \tau_2'} \hat{L}_{\tau_1}^{\tau_1'}(\alpha') \hat{L}_{\tau_2}^{\tau_2'}(\alpha) = \sum_{\tau_1 \tau_2} X_{\tau_3 \tau_3'}^{\tau_3 \tau_3'}(\alpha' - \alpha) \hat{L}_{\tau_2}^{\tau_2'}(\alpha) \\
&\times \hat{L}_{\tau_1}^{\tau_1'}(\alpha') X_{\tau_2 \tau_2'}^{\tau_1' \tau_3}(\alpha - \alpha'). \quad (2.10)
\end{aligned}$$

Summing over  $\tau_1'$ ,  $\tau_2'$ ,  $\tau_3$ , and  $\tau_3'$  the left-hand side is just  $\hat{T}(\alpha') \hat{T}(\alpha)$ , where  $\hat{T}(\alpha) = \sum_\tau \hat{L}_\tau^\tau(\alpha)$  is known as the transfer matrix. The right-hand side corresponds to the trace of a product of operators. Using the invariance of the trace under a cyclic permutation of these operators and taking into account that  $\hat{X}$  is unitary, we obtain  $\hat{T}(\alpha) \hat{T}(\alpha')$ . Hence, transfer matrices at different  $\alpha$  values commute and can all be diagonalized simultaneously.

Consider now  $N_e$  itinerant electrons and the impurity in a box of  $N_a$  sites with periodic boundary conditions. Periodic boundary conditions imposed on a given electron means that it has to interchange position with all other electrons. Each shifting through (permutation) involves a two-particle scattering matrix, such that when the particle is back at the original position we obtained an operator that consists of a product of  $(N_e - 1)$  electron-electron scattering matrices,  $\hat{X}$ , and one scattering matrix due to the impurity,  $\hat{S}$ , i.e.,

$$\begin{aligned}
\hat{T}_j(k_j) &= \hat{X}_{j,j+1}^{-1}(p_j - p_{j+1}) \dots \hat{X}_{j,N}^{-1}(p_j - p_N) \hat{S}_j^{-1}(p_j - p_0) \\
&\times \hat{X}_{j,1}^{-1}(p_j - p_1) \dots \hat{X}_{j,j-1}^{-1}(p_j - p_{j-1}). \quad (2.11)
\end{aligned}$$

The periodic boundary condition for each electron gives rise to one such operator, i.e.,  $j = 1, \dots, N_e$ , and the  $N_e$  operators have to be diagonalized simultaneously. The corresponding eigenvalues are  $\exp(ik_j N_a)$  or expressed in terms of the rapidity  $p_j$

$$\left[ \frac{p_j + i/2}{p_j - i/2} \right]^{N_a}. \quad (2.12)$$

With  $\alpha_{N+1} = p_0$ ,  $\alpha_l = p_l$  for  $l = 1, \dots, N_e$  and  $\alpha = p_j$ ,  $j = 1, \dots, N_e$ , Eq. (2.11) is just the trace over the monodromy matrix, which as shown above can be diagonalized simultaneously for all values of the spectral parameter.

The four components of the monodromy matrix with respect to the indices  $\tau$  and  $\tau'$  are denoted by<sup>28</sup>

$$\hat{L}_1^1 = \hat{A}, \quad \hat{L}_2^1 = \hat{B}, \quad \hat{L}_1^2 = \hat{C}, \quad \hat{L}_2^2 = \hat{D}, \quad (2.13)$$

so that the diagonalization of  $\hat{T}(\alpha)$  corresponds diagonalizing  $\hat{A}(\alpha) + \hat{D}(\alpha)$ . The operators  $\hat{A}$ ,  $\hat{B}$ ,  $\hat{C}$ , and  $\hat{D}$  obey commutation relations which are obtained from Eq. (2.9) by explicitly using the two-electron scattering matrix, (2.2). The procedure is tedious and the results are similar to those derived in Refs. 28 and 29, so that they will not be repeated here. We denote with  $\Omega_0$  the state of maximum spin (usually called the vacuum state), i.e., the state in which all electron spins point upward and the impurity spin is in the state

$M=S$ . The  $\hat{C}$  operator acts like a ‘‘spin-raising’’ operator and when applied to  $\Omega_0$  it yields zero. The diagonal operators satisfy

$$\hat{A}(\alpha)\Omega_0 = \Lambda_A(\alpha)\Omega_0, \quad \hat{D}(\alpha)\Omega_0 = \Lambda_D(\alpha)\Omega_0,$$

$$\Lambda_A(\alpha) = \frac{\alpha_{N+1} - \alpha + i(2S+1)/2}{\alpha_{N+1} - \alpha - i(2S+1)/2}, \quad (2.14)$$

$$\Lambda_D(\alpha) = \frac{\alpha_{N+1} - \alpha - i(2S-1)/2}{\alpha_{N+1} - \alpha - i(2S+1)/2} \prod_{j=1}^{N_e} \frac{\alpha_j - \alpha}{\alpha_j - \alpha + i}.$$

On the other hand,  $\hat{B}$  has properties like a ‘‘spin-lowering’’ operator, such that the vector

$$\Omega(\alpha'_1, \dots, \alpha'_{M^*}) = \prod_{\beta=1}^{M^*} \hat{B}(\alpha'_\beta)\Omega_0 \quad (2.15)$$

corresponds to  $M^*$  flipped spins and has a spin projection equal to  $\frac{1}{2}N_e - M^* + S$ .

The Bethe ansatz equations are the conditions on the set of parameters  $\alpha'_1, \dots, \alpha'_{M^*}$  under which the vector (2.15) is an eigenvector of  $\hat{A}(\alpha) + \hat{D}(\alpha)$ . We apply  $\hat{A}(\alpha) + \hat{D}(\alpha)$  to  $\Omega(\alpha'_1, \dots, \alpha'_{M^*})$  and commute  $(\hat{A} + \hat{D})$  through all the  $\hat{B}$  operators. Two types of terms arise, namely, (i) terms that reproduce the vector (2.15) and (ii) terms of the form

$$\sum_{\gamma=1}^{M^*} \Lambda_\gamma(\alpha, \{\alpha'_\beta\}) \prod_{\beta=1, \beta \neq \gamma}^{M^*} \hat{B}(\alpha'_\beta)\hat{B}(\alpha)\Omega_0, \quad (2.16)$$

which are usually referred to as ‘‘unwanted’’ terms. The actual expression of  $\Lambda_\gamma(\alpha, \{\alpha'_\beta\})$  is obtained by making use of the commutation relations of the operators (2.13). Hence, the vector (2.15) is an eigenvector of  $(\hat{A} + \hat{D})$  only if  $\Lambda_\gamma(\alpha, \{\alpha'_\beta\}) = 0$  for each  $\gamma$ . This leads to the following condition on the set of parameters  $\{\alpha'_\beta\}$ :

$$\frac{\alpha_{N+1} - \alpha'_\gamma + i(2S+1)/2}{\alpha_{N+1} - \alpha'_\gamma - i(2S-1)/2} \prod_{j=1}^{N_e} \frac{\alpha_j - \alpha'_\gamma + i}{\alpha_j - \alpha'_\gamma} = - \prod_{\beta=1}^{M^*} \frac{\alpha'_\gamma - \alpha'_\beta - i}{\alpha'_\gamma - \alpha'_\beta + i}. \quad (2.17)$$

The eigenvalue of  $(\hat{A} + \hat{D})$ , i.e., the amplitude multiplying the term of type (i) that reproduces the vector (2.15), is again obtained using the commutation relations of the operators (2.13)

$$\Lambda_A(\alpha) \prod_{\beta=1}^{M^*} \frac{\alpha - \alpha'_\beta + i}{\alpha - \alpha'_\beta} + \Lambda_D(\alpha) \prod_{\beta=1}^{M^*} \frac{\alpha - \alpha'_\beta - i}{\alpha - \alpha'_\beta}. \quad (2.18)$$

With  $\alpha_{N+1} = p_0$ ,  $\alpha_l = p_l$  for  $l=1, \dots, N_e$ ,  $\alpha = p_j$ , setting  $\alpha'_\beta = \Lambda_\beta + i/2$  and using Eq. (2.12), we obtain the discrete Bethe ansatz equations<sup>29</sup> for the  $t$ - $J$  model with impurity

$$\frac{p_j - p_0 + i(2S+1)/2}{p_j - p_0 - i(2S+1)/2} \left[ \frac{p_j + i/2}{p_j - i/2} \right]^{N_e} = \prod_{\beta=1}^{M^*} \frac{p_j - \Lambda_\beta + i/2}{p_j - \Lambda_\beta - i/2},$$

$$j=1, \dots, N_e, \quad (2.19)$$

$$\frac{\Lambda_\alpha - p_0 + iS}{\Lambda_\alpha - p_0 - iS} \prod_{j=1}^{N_e} \frac{\Lambda_\alpha - p_j + i/2}{\Lambda_\alpha - p_j - i/2} = - \prod_{\beta=1}^{M^*} \frac{\Lambda_\alpha - \Lambda_\beta + i}{\Lambda_\alpha - \Lambda_\beta - i},$$

$$\beta=1, \dots, M^*. \quad (2.20)$$

In each equation the first factor on the left-hand side arises from the impurity. The remaining factors correspond to the supersymmetric  $t$ - $J$  model without impurity. The energy of the system is given by Eq. (2.4) summed over all  $j$  and the magnetization is  $S_z = \frac{1}{2}N_e - M^* + S$ .

#### D. Impurity Hamiltonian

Our model is defined by the scattering matrices, (2.2) and (2.6), via the quantum inverse scattering method. By construction of the transfer matrix the impurity spin interacts only with the two nearest neighbor sites, i.e., we can assume the impurity on a given link and interacting with the sites joined by the link. The Hamiltonian and higher conserved currents, which describe the interaction between the impurity and the itinerant electrons can be obtained by differentiating the logarithm of the transfer matrix  $\hat{T}(\alpha)$  with respect to the spectral parameter  $\alpha$ . The first derivative determines the Hamiltonian of the lattice interacting with the impurity. This procedure is tedious and has explicitly been carried out for the Heisenberg antiferromagnet with impurity<sup>32</sup> in terms of reduced tensor operators for the lattice and impurity spins. This leads to complicated expressions and little understanding. To gain some insight into the physics of the impurity and its interaction with the conduction electrons, it is instructive to derive the Hamiltonian in the continuum limit of the model, i.e., in the limit where the lattice constant tends to zero. This situation is considerably simpler. All properties derived in this paper, except for this subsection, are valid for the lattice model.

In the continuum limit we can linearize the kinetic energy in the momentum around the Fermi level and restrict ourselves to low-energy excitations. Assume the two Fermi points are given by  $\pm k_{\text{FS}}$  related to  $\pm p_{\text{FS}}$  by  $p_{\text{FS}} = \frac{1}{2} \cot(k_{\text{FS}}/2)$ . Denoting  $v = [2 \sin(k_{\text{FS}}/2)]^{-2}$  the group velocity of the electrons we have that the scattering matrices take the form

$$\hat{X}(k_1 - k_2) = \frac{(k_1 - k_2)\hat{I} - iv^{-1}\hat{P}}{k_1 - k_2 - iv^{-1}}, \quad (2.21)$$

$$S_{MM'}^{\sigma\sigma'}(k - \epsilon) = \delta_{\sigma\sigma'} \delta_{MM'} - (M\sigma | M + \sigma)(M'\sigma' | M' + \sigma')$$

$$\times \frac{iv^{-1}(2S+1)}{k - \epsilon + iv^{-1}(2S+1)/2} P_{MM'}^{\sigma\sigma'}. \quad (2.22)$$

Identifying  $v^{-1} = V^2/(2S+1)$  these scattering matrices are exactly those of a mixed valence impurity with two magnetic configurations of spins  $S$  and  $S + \frac{1}{2}$  hybridized via electron of spin  $\frac{1}{2}$ .<sup>29,39,40</sup> Here  $\epsilon$  is related to  $p_0$  and represents the en-

ergy difference between the two configuration relative to the Fermi level. The two partial waves in one dimension, e.g., forward and backward moving electrons, can be transformed into even and odd parity states about the impurity site. Since odd parity states do not interact with the impurity in the continuum limit (contact potential), they can be disregarded. Hence, actually only even parity states play a role in the continuum limit. Allowing for a rescaling of the length of the box, the continuum limit Hamiltonian for the impurity placed at the origin can be written as<sup>41,42</sup>

$$H_{\text{imp}} = \epsilon \sum_{M_1} |S_1 M_1\rangle \langle S_1 M_1| + V \sum_{\sigma M M_1} (M \sigma | M_1) \int dx \delta(x) \times [c_{\sigma}^{\dagger}(x) |SM\rangle \langle S_1 M_1| + |S_1 M_1\rangle \langle SM| c_{\sigma}(x)], \quad (2.23)$$

where the bra and ket denote the impurity states,  $S_1 = S + \frac{1}{2}$  and  $M_1 = M + \sigma$  is the corresponding  $z$  projection. The completeness condition for the impurity requires

$$\sum_{M_1} |S_1 M_1\rangle \langle S_1 M_1| + \sum_M |SM\rangle \langle SM| = 1. \quad (2.24)$$

There is a fundamental difference between the impurity embedded in the noninteracting gas of electrons<sup>29,39,40</sup> and in the correlated electron gas discussed here. In the former case the properties of the impurity are determined as a function of two parameters, namely,  $\epsilon$  and  $V$ , so that charge and spin-fluctuations can occur on different energy scales. The impurity in the correlated gas of electrons has only one free parameter,  $p_0$ , while the second parameter is fixed by the condition of integrability. The degree of charge fluctuations, however, strongly depends on the parameter  $p_0$ , and for large  $|p_0|$  the Kondo limit is obtained.

Note that with minor modifications to the impurity scattering matrix (2.6) the model can also be defined for  $S_1 = S - \frac{1}{2}$ . In the case of the mixed-valent Anderson model embedded into a gas of uncorrelated electrons, this is straightforwardly achieved by interchanging electrons and holes. The case is more subtle for correlated electrons, where the case  $S_1 = S - \frac{1}{2}$  requires an independent and new solution.

In contrast to the continuum limit the impurity interaction on the lattice has additional complications. Since the interaction is no longer a contact potential, both partial waves (even and odd parity states) play a role in the interaction. Furthermore, the sign of the parameter  $p_0$  is important, in particular if finite size effects are considered. It gives rise to an effective mesoscopic momentum, i.e., to a persistent charge current.

### III. THERMODYNAMICS

In this section we first classify the possible states of the system according to the string hypothesis, then we derive the thermodynamic Bethe ansatz equations, and finally we briefly discuss the high-temperature and  $T \rightarrow 0$  (ground state) limits of the thermodynamic equations.

#### A. Classification of states

Each eigenstate of the system is specified by two sets of rapidities,  $\{p_j\}$  and  $\{\Lambda_{\alpha}\}$ , for the charges and the spins, respectively, which satisfy the discrete Bethe ansatz equations,

(2.19) and (2.20). The structure of the solutions of the Bethe ansatz equations is determined by the host (supersymmetric  $t$ - $J$  model), rather than by the impurity, and can be taken over from Ref. 4. The classification of states is also similar to that of the fermion gas with attractive  $\delta$ -function potential<sup>43,44</sup> and the  $j=1/2$  Anderson impurity in the  $U \rightarrow \infty$  limit.<sup>45</sup>

In the thermodynamic limit the rapidities are classified according to (i)  $(N_e - 2M^{*'})$  real charge rapidities, corresponding to unpaired propagating electrons, (ii)  $2M^{*'}$  complex charge rapidities, representing bound or spin-paired electron states, of the form

$$p_{\alpha}^{\pm} = \Lambda'_{\alpha} \pm i/2, \quad (3.1)$$

where  $\Lambda'_{\alpha}$  is a real spin rapidity,  $\alpha = 1, \dots, M^{*'}$ , and (iii)  $M_n^*$  strings of complex spin rapidities (bound spin states) of length  $(n-1)$ ,  $n = 1, \dots, \infty$ , of the form

$$\Lambda_{\alpha,n}^{\mu} = \Lambda_{\alpha,n} + i\mu/2, \quad \mu = -(n-1), -(n-3), \dots, (n-1), \quad (3.2)$$

where again  $\Lambda_{\alpha,n}$  is a real parameter. The integers  $M^{*'}$  and  $M_n^*$  satisfy the relation

$$M^{*'} + \sum_{n=1}^{\infty} n M_n^* = M^*. \quad (3.3)$$

Distribution functions for the rapidities and their ‘holes’ are now introduced for each class, i.e.,  $\rho(p)$  and  $\rho_h(p)$  for the real charge rapidities,  $\sigma'(\Lambda)$  and  $\sigma'_h(\Lambda)$  for the spin-paired states and  $\sigma_n(\Lambda)$  and  $\sigma_{n,h}(\Lambda)$  for the strings of  $n$  spin rapidities. Inserting Eqs. (3.1) and (3.2) into the discrete Bethe ansatz equations, we obtain after Fourier transforming and some algebra<sup>4</sup>

$$\hat{\sigma}_{m+1,h}(\omega) + \hat{\sigma}_{m-1,h}(\omega) + \delta_{m,2S} e^{ip_0\omega} / (2\pi N_a) = 2 \cosh\left(\frac{1}{2}\omega\right) [\hat{\sigma}_m(\omega) + \hat{\sigma}_{m,h}(\omega)], \quad m \geq 1, \quad (3.4)$$

$$\hat{\sigma}_{1,h}(\omega) + \hat{\sigma}'_h(\omega) + 1 = 2 \cosh\left(\frac{1}{2}\omega\right) [\hat{\rho}(\omega) + \hat{\rho}_h(\omega)], \quad (3.5)$$

$$e^{-(1/2)|\omega|} \hat{\sigma}'_h(\omega) + e^{-(1/2)|\omega|} + e^{[ip_0\omega - (S+1/2)|\omega|]} / (2\pi N_a) = 2 \cosh\left(\frac{1}{2}\omega\right) [\hat{\sigma}'(\omega) + \hat{\sigma}'_h(\omega)] + \hat{\rho}(\omega), \quad (3.6)$$

where  $\hat{\rho}(\omega) \equiv \hat{\sigma}_{0,h}(\omega)$ . The terms proportional to  $1/N_a$  are due to the impurity scattering matrix. The energy, the total number of electrons and the magnetization are given by<sup>4</sup>

$$E/N_a = -2N_e/N_a + 2 \int dp \rho(p) \frac{1/2}{p^2 + 1/4} + 2 \int d\Lambda \sigma'(\Lambda) \frac{1}{\Lambda^2 + 1}, \quad N_e/N_a = \int dp \rho(p) + 2 \int d\Lambda \sigma'(\Lambda), \quad (3.7)$$

$$S_z/N_a = S/N_a + \frac{1}{2} \int dp \rho(p) - \sum_{n=1}^{\infty} n \int d\Lambda \sigma_n(\Lambda).$$

### B. Thermal equilibrium

The above equations are valid quite generally for all states. We now restrict ourselves imposing thermal equilibrium by minimizing the free energy functional with respect to the density functions subject to Eqs. (3.4)–(3.6) and the constraints of constant number of electrons and constant magnetization (the corresponding Lagrange multipliers are the chemical potential  $\mu$  and the magnetic field  $H$ ). We introduce an energy function for each class of rapidities through

$$\begin{aligned} \rho_h/\rho &= \exp[\varepsilon(p)/T], & \sigma'_h/\sigma' &= \exp[\psi(\Lambda)/T], \\ \sigma_{n,h}/\sigma_n &= \exp[\varphi_n(\Lambda)/T] = \eta_n(\Lambda), & \varphi_0 &\equiv -\varepsilon. \end{aligned} \quad (3.8)$$

which satisfy the following integral equations<sup>4</sup>

$$\varepsilon(p) = J\pi G_0(p) + TG_0 \star \ln[(1 + e^{\psi/T})/(1 + \eta_1)], \quad (3.9)$$

$$\begin{aligned} \psi(\Lambda) &= -2 + J\pi G_1(\Lambda) - \mu + TG_1 \star \ln(1 + e^{\psi/T}) \\ &+ TG_0 \star \ln(1 + e^{-\varepsilon/T}), \end{aligned} \quad (3.10)$$

$$\varphi_n(\Lambda) = TG_0 \star \ln[(1 + \eta_{n+1})(1 + \eta_{n-1})], \quad (3.11)$$

where the last equation holds for  $n = 1, \dots, \infty$ , the *star* denotes convolution,  $\eta_0 = e^{-\varepsilon/T}$ , and  $G_l(\Lambda)$  is the Fourier transform of  $\exp(-|\omega|/2)/2 \cosh(\omega/2)$ . The field dependence is introduced via the field boundary condition,

$$\lim_{n \rightarrow \infty} \frac{1}{2} \varphi_n(\Lambda) = H. \quad (3.12)$$

By differentiating Eqs. (3.9)–(3.11) with respect to  $J$ , we obtain from similarity with Eqs. (3.4)–(3.6) that the relation between energy potentials and density functions is

$$\sigma_{n,h} = -[\partial \varphi_n / \partial(\pi J)] / (1 + e^{-\varphi_n/T}), \quad (3.13)$$

$$\rho = [\partial \varepsilon / \partial(\pi J)] / (1 + e^{\varepsilon/T}), \quad (3.14)$$

$$\sigma'_h = [\partial \psi / \partial(\pi J)] / (1 + e^{-\psi/T}). \quad (3.15)$$

The complementary functions can be obtained with the aid of Eq. (3.8).

An alternative set of integral equations, equivalent to Eqs. (3.9)–(3.11), is the following<sup>4</sup>

$$\begin{aligned} \varepsilon(p) &= -2 + 2\pi a_1(p) - \frac{1}{2}H - \mu + Ta_1 \star \ln(1 + e^{-\psi/T}) \\ &- T \sum_{n=1}^{\infty} a_n \star \ln(1 + \eta_n^{-1}), \end{aligned} \quad (3.16)$$

$$\begin{aligned} \psi(\Lambda) &= -4 + 2\pi a_2(\Lambda) - 2\mu + Ta_2 \star \ln(1 + e^{-\psi/T}) \\ &+ Ta_1 \star \ln(1 + e^{-\varepsilon/T}), \end{aligned} \quad (3.17)$$

$$\begin{aligned} \ln[1 + \eta_n(\Lambda)] &= (nH/T) + a_n \star \ln(1 + e^{-\varepsilon/T}) \\ &+ \sum_{m=1}^{\infty} A_{nm} \star \ln(1 + \eta_m^{-1}), \end{aligned} \quad (3.18)$$

where

$$a_n(\Lambda) = (n/2\pi) / [\Lambda^2 + (n/2)^2] \quad (3.19)$$

and  $A_{nm}(\Lambda)$  is the Fourier transform of

$$\coth(\frac{1}{2}|\omega|) [e^{-|n-m||\omega|/2} - e^{-(n+m)|\omega|/2}]. \quad (3.20)$$

The equilibrium free energy of the system is the sum of the free energies of the supersymmetric  $t$ - $J$  model and the impurity

$$\begin{aligned} F_{tJ}/N_a &= -\psi(0) - 2\mu - 2 = -T \int dp a_1(p) \ln(1 + e^{-\varepsilon(p)/T}) \\ &- T \int d\Lambda a_2(\Lambda) \ln(1 + e^{-\psi(\Lambda)/T}), \end{aligned} \quad (3.21)$$

$$\begin{aligned} F_{\text{imp}} &= -T \int d\Lambda G_{2S+1}(\Lambda - p_0) \ln(1 + e^{\psi(\Lambda)/T}) \\ &- T \int d\Lambda G_0(\Lambda - p_0) \ln(1 + e^{\varphi_{2S}(\Lambda)/T}), \end{aligned} \quad (3.22)$$

where the impurity energy is defined up to a temperature independent function of  $p_0$ .

In the following subsections we consider the  $T \rightarrow \infty$  and  $T \rightarrow 0$  limits of these equations.

### C. High-temperature limit

If the temperature is much larger than the bandwidth, i.e.,  $T \gg 2$ , we can neglect the independent (driving) terms in Eqs. (3.9)–(3.11), so that the potentials  $\varepsilon$ ,  $\psi$ , and  $\varphi_n$  do not depend on the variables  $p$  and  $\Lambda$ . Equations (3.9)–(3.11) reduce to a system of algebraic equations, which has the following solution.<sup>4,40,43</sup>

$$\begin{aligned} 1 + \eta_n &= [\sinh(nH/2T + x) / \sinh(H/2T)]^2, \\ e^{2\varepsilon/T} &= (1 + e^{\psi/T}) / (1 + \eta_1), \end{aligned} \quad (3.23)$$

$$e^{2(\psi+\mu)/T} = (1 + e^{-\varepsilon/T}) (1 + e^{\psi/T}),$$

where  $\eta_0 = e^{-\varepsilon/T}$  and

$$e^{2x} = e^{2H/T} [1 + e^{-(H+2\mu)/2T}] / [1 + e^{(H-2\mu)/2T}]. \quad (3.24)$$

The free energy of the host corresponds to the three degrees of freedom per site (a hole and a spin 1/2)

$$F_{tJ}/N_a = -T \ln[1 + 2e^{\mu/T} \cosh(H/2T)], \quad (3.25)$$

where  $\mu$  is measured from the bottom of the band. The free energy of the impurity is discussed in Sec. IV.

### D. Ground state equations

The ground state integral equations are obtained from Eqs. (3.11), (3.16), and (3.17) in the limit  $T \rightarrow 0$ . From Eq.

(3.11) it follows that the energy potentials  $\varphi_n$  are positive over the entire  $\Lambda$  range for all  $n \geq 1$ . Hence, as  $T \rightarrow 0$  the string states are not occupied. Only the  $\varepsilon$  band (unpaired electrons) and the  $\psi$  band (spin-paired electrons) are populated. We separate these energy potentials into their positive and negative parts, i.e.,  $\varepsilon(p) = \varepsilon^+(p) + \varepsilon^-(p)$ ,  $\psi(\Lambda) = \psi^+(\Lambda) + \psi^-(\Lambda)$ , so that the terms with “+” supraindex are positive (empty states or holes) and those with “-” are negative (occupied states or particles). The zeroes of the potentials define the integration limits,  $\varepsilon(\pm B) = 0$  and  $\psi(\pm Q) = 0$ . Both,  $B$  and  $Q$ , are functions of  $\mu$  and  $H$ . In the limit  $T \rightarrow 0$ , Eqs. (3.16) and (3.17) yield<sup>4</sup>

$$\varepsilon(p) = -2 + 2\pi a_1(p) - \frac{1}{2}H - \mu - \int_{|\Lambda| > Q} d\Lambda a_1(p - \Lambda) \psi(\Lambda), \quad (3.26)$$

$$\begin{aligned} \psi(\Lambda) = & -4 + 2\pi a_2(\Lambda) - 2\mu \\ & - \int_{|\Lambda'| > Q} d\Lambda' a_1(\Lambda - \Lambda') \psi(\Lambda') \\ & - \int_{|p| > B} dp a_1(\Lambda - p) \varepsilon(p). \end{aligned} \quad (3.27)$$

Similar equations, which can be obtained using Eqs. (3.14) and (3.15), determine the density functions.

The energy, the number of electrons and magnetization of the host are given by

$$\begin{aligned} E/N_a = & -2N_e/N_a + 2\pi \int_{|p| > B} dp \rho(p) a_1(p) \\ & + 2\pi \int_{|\Lambda| > Q} d\Lambda \sigma'(\Lambda) a_2(\Lambda), \\ N_e/N_a = & \int_{|p| > B} dp \rho(p) + 2 \int_{|\Lambda| > Q} d\Lambda \sigma'(\Lambda), \quad (3.28) \\ S_z/N_a = & S/N_a + \frac{1}{2} \int_{|p| > B} dp \rho(p). \end{aligned}$$

In zero magnetic field we have  $B = \infty$  and the unpaired electron band is empty. As a function of field  $B$  decreases monotonically. In zero field the number of electrons in the system is a decreasing function of the parameter  $Q$ .<sup>4</sup>

The ground state properties of the impurity are discussed in Sec. IV.

#### IV. PROPERTIES OF THE IMPURITY

In this section we present results for the impurity embedded in the supersymmetric  $t$ - $J$  lattice, first in the high-temperature limit, then the ground state properties, and finally the Kondo limit. It is evident from Eq. (3.22) that the impurity is driven by the host, i.e., the supersymmetric  $t$ - $J$  model, through the energy potentials  $\psi(\Lambda)$  and  $\varphi_{2S}(\Lambda)$ . Some impurity properties are then expected to be different from those of the mixed-valent impurity with two magnetic configurations embedded in a noninteracting electron gas. Except for special limits the integral equations for the energy

potentials of the  $t$ - $J$  model cannot be solved analytically and a solution has to be obtained numerically.

#### A. High-temperature limit

In the high-temperature limit the leading contribution is obtained by assuming the energy potentials constant, i.e., independent of  $\Lambda$  and  $p$ . The impurity free energy (3.22) is then approximately given by

$$F_{\text{imp}} = -\frac{1}{2} T \ln[(1 + e^{\psi(p_0)/T})(1 + e^{\varphi_{2S}(p_0)/T})] \quad (4.1)$$

and by using Eqs. (3.23) and (3.24) this reduces to

$$F_{\text{imp}} = -T \ln(\mathcal{Z}_{(S+1/2)} + \exp\{[g(p_0) - \mu]/T\} \mathcal{Z}_S), \quad (4.2)$$

where  $\mu$  is measured from the bottom of the conduction band and

$$\mathcal{Z}_S = \frac{\sinh[(2S+1)H/2T]}{\sinh(H/2T)} \quad (4.3)$$

is the partition function of a free spin  $S$  in a magnetic field. Expression (4.2) corresponds to an impurity with two coexisting configurations, one of spin  $(S + \frac{1}{2})$  and the other of spin  $S$ . The degree of admixture of the two configurations is a function of  $p_0$  via the function  $g(p_0)$ , which is even in  $p_0$  and monotonically decreasing for  $p_0 > 0$  with  $g(p_0 = \pm \infty) = 0$ . The function  $g(p_0)$  can be approximated by  $2\pi G_1(p_0)$ . The properties of the impurity depend on the band filling through the chemical potential. For a given intermediate  $p_0$  the spin  $S$  configuration is favored for  $\mu \rightarrow 0$ , i.e., for low electron densities where the impurity is unlikely to localize an electron, while close to half-filling,  $\mu = 2 \ln(2)$ , the configuration of spin  $(S + \frac{1}{2})$  is favored, since the impurity can bind one itinerant electron. Next to leading corrections to Eq. (4.2) can be obtained following the procedure outlined in Ref. 40.

For a fixed field the specific heat of the impurity as a function of  $T$  displays a Schottky anomaly and the zero-field susceptibility follows a Curie law.<sup>46</sup> The Curie constant and the entropy under the Schottky peak depends on the admixture, i.e., the parameter  $[g(p_0) - \mu]$ .

#### B. Ground state integral equations

Equations (3.4)–(3.6) are linear in the densities and have driving terms arising from the itinerant electrons and from the impurity. Hence, the density functions can be separated into a host and an impurity contribution. Since the impurity is driven by the itinerant electrons, only  $\rho_i(p)$  for  $|p| > B$  and  $\sigma'_i(\Lambda)$  for  $|\Lambda| > Q$  are nonzero rapidly distributions in the groundstate. In the limit  $T \rightarrow 0$  the impurity density functions satisfy

$$\begin{aligned} \rho_{i,h}(p) + \rho_i(p) + \int_{|\Lambda| > Q} d\Lambda a_1(p - \Lambda) \sigma'_i(\Lambda) \\ = a_{2S+1}(p - p_0), \end{aligned} \quad (4.4)$$

$$\begin{aligned} \sigma'_{i,h}(\Lambda) + \sigma'_i(\Lambda) + \int_{|\Lambda'|>Q} d\Lambda' a_2(\Lambda - \Lambda') \sigma'_i(\Lambda') \\ + \int_{|p|>B} dp a_1(\Lambda - p) \rho_i(p) = a_{2S+2}(p - p_0), \end{aligned} \quad (4.5)$$

and the impurity energy, magnetization and valence are given by

$$\begin{aligned} E_{\text{imp}} &= 2\pi \int_{|p|>B} dp \rho_i(p) a_1(p) \\ &+ 2\pi \int_{|\Lambda|>Q} d\Lambda \sigma'_i(\Lambda) a_2(\Lambda), \\ M_{\text{imp}} &= S + \frac{1}{2} \int_{|p|>B} dp \rho_i(p), \\ n_{\text{imp}} &= \int_{|p|>B} dp \rho_i(p) + 2 \int_{|\Lambda|>Q} d\Lambda \sigma'_i(\Lambda). \end{aligned} \quad (4.6)$$

The integral equations are of the Fredholm type and differ from those of the corresponding Anderson impurity, which are coupled Wiener-Hopf equations.<sup>40</sup> Note that the impurity density functions are not symmetric in their argument, the asymmetry being introduced by  $p_0$  in the driving terms. Without loss of generality we can symmetrize them by considering the half-sum for  $\pm p_0$ .

In the absence of a magnetic field, i.e.,  $B \rightarrow \infty$ , only one integral equation remains. Analytical results can be obtained in the limits of low electron density ( $Q \rightarrow \infty$ ) and low ‘‘hole’’ density ( $Q \rightarrow 0$ ). For large  $Q$  the Fredholm integral equation can be transformed into a hierarchical sequence of Wiener-Hopf integral equations. The leading contribution to the valence (fraction of bound itinerant electron) of the impurity is

$$n_{\text{imp}} = \frac{2S+2}{2\pi} \frac{Q}{Q^2 - p_0^2}, \quad (4.7)$$

where we assumed that  $Q \gg |p_0|$ . On the other hand, if the electron band is filled,  $Q=0$ , the integral equation can be solved by Fourier transformation and

$$n_{\text{imp}} = 1 - \mathcal{O}(Q). \quad (4.8)$$

Hence, in this limit we have one localized conduction electron. Corrections for small  $Q$  (low hole concentration) reduce the valence proportionally to  $Q$ . Hence, as a function of band filling the valence smoothly varies between 0 ( $N_e \rightarrow 0$ ) and 1 ( $N_e \rightarrow N_d$ ).

### C. Ground state magnetization

The ground state magnetization is obtained following standard procedures (see Refs. 29 and 40) from Eqs. (4.4) and (4.5). From Eq. (4.5) we express  $\sigma'$  as a function of the remaining quantities and insert it into Eq. (4.4). We obtain a Fredholm integral equation for  $\rho$  with two kinds of driving terms, namely, independent terms depending on  $p_0$  and a term involving  $\sigma'_h$ . The magnetization is then the sum of two

contributions, the magnetization due to the internal degrees of freedom of the impurity and the magnetization arising from the valence admixture. Since the magnetic field is usually much smaller than the bandwidth, the latter contribution is small and linear in the field and will be neglected here. The Fredholm equation for the ‘‘Kondo’’-like spin excitations is

$$\begin{aligned} \rho_{i,h}(p) + \rho_i(p) - \int_{|p'|>B} dp' G_1(p - p') \rho_i(p') \\ = G_{2S}(p - p_0), \end{aligned} \quad (4.9)$$

where we may assume that  $p_0$  is positive and large. Equation (4.9) can then be reduced to a hierarchical sequence of Wiener-Hopf integral equations. The leading contribution is given by Eq. (4.9) with the integration range restricted to positive  $p'$  larger than  $B$ . The equation then depends only on the parameter  $p_0 - B$  which we parametrize by  $(1/\pi) \ln(H/T_K)$ , where  $T_K$  plays the role of a ‘‘Kondo’’ temperature. The solution of the Wiener-Hopf equation yields<sup>40</sup>

$$\begin{aligned} M_{\text{imp}} &= S \left[ 1 + \frac{1}{2} \mathcal{L}^{-1} - \frac{1}{4} \ln(\mathcal{L}) / \mathcal{L}^2 + \dots \right], \\ H &\ll T_K, \end{aligned} \quad (4.10)$$

$$\begin{aligned} M_{\text{imp}} &= (S + \frac{1}{2}) \left[ 1 - \frac{1}{2} \mathcal{L}^{-1} - \frac{1}{2} \ln(\mathcal{L}) / \mathcal{L}^2 + \dots \right], \\ H &\gg T_K, \end{aligned} \quad (4.11)$$

where  $\mathcal{L} = |\ln(H/T_K)|$ . Hence, in a small field the impurity has an asymptotically free spin  $S$ , while in strong magnetic fields the effective spin is  $(S + \frac{1}{2})$  weakly coupled (logarithm characterize asymptotic freedom) to the itinerant electrons. For intermediate fields the magnetization smoothly interpolates between these two limits. Higher order corrections to Eqs. (4.10) and (4.11) require the solution of other equations in the hierarchical sequence of Wiener-Hopf equations.

If  $S=0$ , on the other hand, the ground state is a singlet and the small-field magnetization is proportional to the field. Equation (4.10) is not valid for this case, although Eq. (4.11) is still applicable.

### D. ‘‘Kondo’’ limit

In order to obtain the ‘‘Kondo’’ limit we must suppress the valence fluctuations. Charge fluctuation are described by the energy potential  $\psi(\Lambda)$ , so that Eq. (3.9) can be replaced by

$$\varepsilon(p) = \epsilon_F e^{-\pi|p|} - T G_0 \star \ln(1 + \eta_1), \quad (4.12)$$

where we kept only the low-lying excitations, given by large  $|p|$ , and  $\epsilon_F$  is an energy scale of the order of the band half-width. The coupled integral equations (3.11) and (4.12) are very similar to those of the Kondo problem, except that there are two Fermi points in the Dirac sea of spin rapidities, in contrast to the Kondo problem which involves only one partial wave.<sup>27,28</sup> The impurity free energy due to spin fluctuations is given by the term of Eq. (3.22) involving  $\varphi_{2S}$ . This term contains the only  $p_0$  dependence in the problem. Again



we assume that  $p_0$  is positive and large (Kondo limit). The interference of the two Fermi points (backward scattering of spin waves) is then not very important for the impurity properties and can be neglected. Redefining the integration variables,  $p = \frac{1}{2}[\lambda - (2/\pi)\ln(\epsilon_F/T)]$  and  $\Lambda = \frac{1}{2}[\lambda - (2/\pi)\ln(\epsilon_F/T)]$  and denoting

$$\tilde{\eta}_1(\lambda) = e^{-\varepsilon(p)/T}, \quad \tilde{\eta}_{n+1}(\lambda) = \eta_n(\Lambda) = e^{\varphi_n(\Lambda)/T}, \quad (4.13)$$

we obtain from Eqs. (3.11) and (4.12) the thermodynamic Bethe ansatz equations for the single orbital channel Kondo problem and the impurity free energy is now given by<sup>27-29,40</sup>

$$F_{\text{imp}} = -\frac{1}{4}T \int d\lambda \ln[1 + \tilde{\eta}_{2S+1}(\lambda)] \times \{\cosh[\frac{1}{2}\pi\lambda - \ln(T/T_K)]\}^{-1}, \quad (4.14)$$

where  $p_0 = (1/\pi)\ln(\epsilon_F/T_K)$ . Equation (4.14) is the free energy of the Kondo exchange model for arbitrary spin  $(S + \frac{1}{2})$ .

For  $S \neq 0$  the magnetic susceptibility shows Kondo logarithms in both the high- and low-temperature limits

$$\chi = (\mu^2/3T)[1 - \mathcal{L}^{-1} + \frac{1}{2}\ln|\mathcal{L}/\mathcal{L}^2 + \dots|], \quad (4.15)$$

where  $\mathcal{L} = \ln(T_K/T)$  and  $\mu$  is the effective magnetic moment, which is different in the two limits, i.e.,  $\mu^2 = S(S+1)$  as  $T \rightarrow 0$  and  $\mu^2 = (S + \frac{1}{2})(S + \frac{3}{2})$  as  $T \rightarrow \infty$ . Hence, as seen already for the ground state the impurity spin is only partially compensated at low  $T$ . If  $S = 0$ , on the other hand, the ground state is a singlet and the susceptibility is finite.

## V. CONCLUDING REMARKS

Impurities are expected to play a relevant role in highly correlated electrons and may alter the properties of the system. In this paper we pursued the exact solution of a *magnetic* impurity embedded into a one-dimensional lattice with strongly interacting electrons. The model has one free parameter,  $p_0$ , that tunes the properties of the impurity. In contrast, the same impurity in a host without correlations has two parameters, such that charge and spin fluctuations can be varied independently. The absence of backward scattering (condition for the integrability) makes this impurity problem probably nongeneric, in the sense that away from supersymmetry and for a different impurity-lattice coupling the low-temperature properties of the impurity may change. Exact solutions, even for simplified systems, may provide insights and a testing ground for approximations intended for more complicated problems.

In contrast to other proposed integrable impurity systems<sup>36,37</sup> we consider here a *magnetic* impurity, i.e., break the translational invariance by introducing an additional spin  $S$  into the lattice. The integrable model providing the background of itinerant electrons is the supersymmetric  $t$ - $J$  model. Its integrability was shown long ago<sup>19,23</sup> and its properties were studied in Refs. 4 and 24, including ground state properties, thermodynamics, and excitation spectrum. We

constructed an impurity scattering matrix, Eq. (2.6) that obeys the triangular Yang-Baxter relations with the scattering matrix of the supersymmetric  $t$ - $J$  model. This, together with the excluded multiple occupation of the lattice sites, is the necessary and sufficient condition for the integrability of the  $t$ - $J$  model with impurity. The scattering matrices also define the Hamiltonian and higher conserved currents via the quantum inverse scattering method.

The interaction of the itinerant electrons with the impurity is via an effective hybridization with the two neighboring sites to the impurity. The impurity of spin  $S$  is capable of localizing one itinerant electron. The Clebsch-Gordan coefficient selects the coupling of the conduction electron spin to the impurity to form a total spin  $(S + \frac{1}{2})$ .

We derived the Bethe ansatz equations diagonalizing the  $t$ - $J$  model with impurity, classified all the states according to the string hypothesis, obtained the thermodynamic equations including the free energy of the impurity, and discussed the high-temperature and ground state properties.

At high temperatures the impurity is in a mixed valent state resulting from the superposition of the spin  $S$  and spin  $(S + \frac{1}{2})$  configurations. The susceptibility is Curie-like and in a magnetic field the specific heat as a function of temperature displays the expected Schottky anomaly. The degree of admixture is a function of the parameter  $p_0$  (related to the energy difference between the two configurations) and the chemical potential. For a given  $p_0$  the fraction of localized electron (valence) increases monotonically with the band filling. The variation of the valence with the band filling is more dramatic at low temperatures, where its range is from 0 to 1.

In the limit of large  $|p_0|$  and for a given finite electron density, the impurity has an effective spin  $(S + \frac{1}{2})$  at low temperatures. We have shown how this situation can be mapped onto the single orbital channel Kondo problem of spin  $(S + \frac{1}{2})$ . This mapping is only approximate, because the interaction between impurity and itinerant electrons is not a contact potential for the lattice problem; hence, the impurity is not only scattered by the even parity states (about the impurity site), but also by the odd parity states. Consequently, backward scattering across the spin rapidity Fermi surface cannot be neglected, but as argued, it does not have a dramatic effect on the impurity properties.

Hence, in the Kondo limit the impurity is undercompensated, i.e., it has an effective spin  $S$  in a small field at low temperatures. The field and/or the temperature (if larger than  $T_K$ ) break up the partial screening and the effective spin  $(S + \frac{1}{2})$  is recovered. The susceptibility follows a Curie law with a temperature dependent Curie constant. In a small magnetic field the specific heat has two peaks, one is the Schottky peak at  $T \approx H$  arising from the underscreened spin  $S$  and at higher  $T$  ( $\approx T_K$ ) the broad structure of the Kondo resonance gives rise to the second peak.<sup>46</sup> At larger fields, the two energy scales are no longer separated, and both peaks merge into one.

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- <sup>1</sup> P. W. Anderson, *Science* **235**, 1196 (1987).
- <sup>2</sup> F. C. Zhang and T. M. Rice, *Phys. Rev. B* **37**, 3759 (1988).
- <sup>3</sup> C. Gros, R. Joynt, and T. M. Rice, *Phys. Rev. B* **36**, 381 (1987).
- <sup>4</sup> P. Schlottmann, *Phys. Rev. B* **36**, 5177 (1987).
- <sup>5</sup> P. Schlottmann, *Physica B* **171**, 30 (1991).
- <sup>6</sup> W. Brinkman and T. M. Rice, *Phys. Rev. B* **2**, 1324 (1970).
- <sup>7</sup> W. Kohn, *Phys. Rev.* **133A**, 171 (1964).
- <sup>8</sup> C. Gros, *Ann. Phys. (N.Y.)* **189**, 53 (1989).
- <sup>9</sup> H. Eskes and G. A. Sawatzky, *Phys. Rev. Lett.* **61**, 1415 (1988).
- <sup>10</sup> A. K. McMahan, R. M. Martin, and S. Satpathy, *Phys. Rev. B* **38**, 6650 (1989).
- <sup>11</sup> M. S. Hybertsen, M. Schlüter, and N. E. Christensen, *Phys. Rev. B* **39**, 9028 (1989).
- <sup>12</sup> M. S. Hybertsen, E. B. Stechel, M. Schlüter, and D. R. Jennison, *Phys. Rev. B* **41**, 11 068 (1990).
- <sup>13</sup> C. S. Hellberg and E. J. Mele, *Phys. Rev. Lett.* **67**, 2080 (1991).
- <sup>14</sup> H. Yokoyama and M. Ogata, *Phys. Rev. Lett.* **67**, 3610 (1991).
- <sup>15</sup> M. Ogata, M. U. Luchini, S. Sorella, and F. F. Assaad, *Phys. Rev. Lett.* **66**, 2388 (1991).
- <sup>16</sup> K. Hallberg and C. A. Balseiro, *Solid State Commun.* **82**, 523 (1992).
- <sup>17</sup> C. S. Hellberg and E. J. Mele, *Phys. Rev. B* **48**, 646 (1993).
- <sup>18</sup> H. Yokoyama and H. Shiba, *J. Phys. Soc. Jpn.* **57**, 2482 (1988).
- <sup>19</sup> B. Sutherland, *Phys. Rev. B* **12**, 3795 (1975).
- <sup>20</sup> P. A. Bares, G. Blatter, and M. Ogata, *Phys. Rev. B* **44**, 130 (1991).
- <sup>21</sup> S. Sarkar, *J. Phys. A* **24**, 5775 (1991).
- <sup>22</sup> F. H. L. Essler and V. E. Korepin, *Phys. Rev. B* **46**, 9147 (1992).
- <sup>23</sup> C. K. Lai, *J. Math. Phys.* **15**, 167 (1974).
- <sup>24</sup> P. A. Bares and G. Blatter, *Phys. Rev. Lett.* **64**, 2567 (1990).
- <sup>25</sup> S. Sarkar, *J. Phys. A* **23**, L409 (1990).
- <sup>26</sup> P. Schlottmann, *Phys. Rev. B* **41**, 4164 (1990).
- <sup>27</sup> N. Andrei, K. Furuya, and J. Lowenstein, *Rev. Mod. Phys.* **55**, 331 (1983).
- <sup>28</sup> A. M. Tsvelick and P. B. Wiegmann, *Adv. Phys.* **32**, 453 (1983).
- <sup>29</sup> P. Schlottmann, *Phys. Rep.* **181**, 1 (1989).
- <sup>30</sup> P. Schlottmann and P. D. Sacramento, *Adv. Phys.* **42**, 641 (1993).
- <sup>31</sup> N. Andrei and H. Johannesson, *Phys. Lett. A* **100**, 108 (1984).
- <sup>32</sup> K. Lee and P. Schlottmann, *Phys. Rev. B* **37**, 379 (1988).
- <sup>33</sup> P. Schlottmann, *J. Phys. Condens. Matter* **3**, 6617 (1991).
- <sup>34</sup> E. Sorensen, S. Eggert, and I. Affleck, *J. Phys. A* **26**, 6757 (1993).
- <sup>35</sup> P. Schlottmann, *Phys. Rev. B* **49**, 9202 (1994).
- <sup>36</sup> A. Punnoose, H.-P. Eckle, and R. Römer (unpublished).
- <sup>37</sup> P. A. Bares (unpublished).
- <sup>38</sup> M. Pfannmüller and H. Frahm (unpublished).
- <sup>39</sup> C. R. Proetto, A. A. Aligia, and C. A. Balseiro, *Phys. Lett.* **107A**, 93 (1985); *Phys. Rev. B* **31**, 6143 (1985); *Z. Phys. B* **59**, 413 (1985).
- <sup>40</sup> P. Schlottmann, *Z. Phys. B* **59**, 391 (1985).
- <sup>41</sup> J. Mazzaferro, C. A. Balseiro, and B. Alascio, *Phys. Rev. Lett.* **47**, 274 (1981).
- <sup>42</sup> P. Schlottmann, in *Valence Instabilities*, edited by P. Wachter and H. Boppert (North-Holland, Amsterdam, 1982), p. 471.
- <sup>43</sup> M. Takahashi, *Prog. Theor. Phys.* **46**, 1388 (1971).
- <sup>44</sup> C. K. Lai, *Phys. Rev. Lett.* **26**, 1472 (1971); *Phys. Rev. A* **8**, 2567 (1973).
- <sup>45</sup> P. Schlottmann, *Z. Phys. B* **52**, 127 (1983).
- <sup>46</sup> A. A. Aligia, C. A. Balseiro, C. R. Proetto, and P. Schlottmann, *Z. Phys. B* **62**, 311 (1986); *J. Magn. Magn. Mater.* **63&64**, 231 (1987).