Anderson-like impurity in the one-dimensional *t-J* model: Formation of local states and magnetic behavior

Holger Frahm and Guillaume Palacios
Institut für Theoretische Physik, Universität Hannover, Appelstrasse 2, 30167 Hannover, Germany
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We consider an integrable model describing an Anderson-like impurity coupled to an open *t-J* chain. Both the hybridization (i.e., its coupling to bulk chain) and the local spectrum can be controlled without breaking the integrability of the model. As the hybridization is varied, holon and spinon bound states appear in the many body ground state. Based on the exact solution we study the state of the impurity and its contribution to thermodynamic quantities as a function of an applied magnetic field. Kondo behavior in the magnetic response of the impurity can be observed provided that its parameters have been adjusted properly to the energy scales of the holon and spinon excitations of the one-dimensional bulk.

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I. INTRODUCTION

The possibility of controlled embedding of quantum impurities, i.e., local scatterers with internal degrees of freedom, into nanofabricated devices has led to new manifestations of Kondo physics, e.g., in quantum dot systems or atoms deposited on metallic surfaces.[1] In these systems many parameters of the impurity, such as its internal spectrum, its coupling to the metallic environment and the properties of the latter can be tuned within the experiment. Investigating the effects of these parameters on observable quantities leads to various new questions: originally, most of the theoretical work on the quantum impurity problems has neglected the effect of electronic correlations in the host system.[2] If the latter is one dimensional, however, any interaction leads to non-Fermi-liquid behavior. The low energy regime is then described by a Tomonaga Luttinger liquid (TLL) characterized by continuously varying exponents of its ground state correlation functions.[3] As a consequence, the local density of states vanishes as a power law in such a system. Therefore it is to be expected that the critical properties of the impurity will be strongly affected. This problem of a quantum impurity coupled to a TLL has been the subject of intense studies in recent years—both analytically based on field theoretical methods and numerically. These studies indicate that depending on the coupling parameters different nontrivial fixed points at intermediate or strong coupling can be realized which determine the observables accessible to experiments (see, e.g., Refs. 4–8).

This picture of the low energy behavior of these systems has to be supported by methods which do not rely on the analysis at weak coupling, e.g., exact solutions as for the Kondo and Anderson impurity problem in a Fermi liquid.[9] For results which cover the full range of experimentally available parameters specific realizations of quantum impurity models have to be studied. An approach which allows one to make contact to the universal low energy behavior identified using the methods mentioned above is based on integrable lattice models. Starting, e.g., from the Bethe ansatz solvable supersymmetric *t-J* model for electrons on a one-dimensional lattice or variations thereof one can consider different representations of the graded Lie algebra $gl(2|1)$ for the spectrum of electronic states on bulk and impurity sites without destroying integrability.[10–13] The physical properties of these impurities can be tuned by variation of the representation [which may depend on a continuous parameter for $gl(2|1)$] and by a shift in the spectral parameter which directly enters the coupling between the impurity and the host system.

The resulting Hamiltonian of models constructed along these lines takes a particularly simple form when such impurities are combined with open boundaries.[14–16] In this paper we shall consider the system introduced in Ref. 17, based on the supersymmetric *t-J* chain with open boundary conditions. The Hamiltonian of this model is

$$\mathcal{H} = -\mathcal{P}\left(\sum_{j=2}^{L}\sum_{\sigma} c_{j,\sigma}^{\dagger}c_{j+1,\sigma} + c_{j+1,\sigma}^{\dagger}c_{j,\sigma}\right)\mathcal{P} + 2\sum_{j=2}^{L}\left[\vec{S}_j\vec{S}_{j+1} - \frac{n_j n_{j+1}}{4} + \frac{1}{2}(n_j + n_{j+1})\right] - HS^z - \mu N + \mathcal{H}_b, \tag{1}$$

where $\mathcal{P}$ projects out double occupancies on the bulk sites ($j=2$ to $L+1$) and $\vec{S}_j = \Sigma_{\alpha\beta} c_{j,\alpha}^{\dagger}\vec{\sigma}_{\alpha\beta}c_{j,\beta}$, $n_j = \Sigma_{\sigma} c_{j,\sigma}^{\dagger}c_{j,\sigma}$ are the electronic spin and number operators on site j. The magnetization of the system is controlled by the field H and we consider the system at fixed hole concentration $\delta = 1 - \Sigma_j n_j / L$ (alternatively one may use a grand canonical approach to control δ by variation of the chemical potential μ). The impurity is added at the boundary (site 1) of this chain, its internal spectrum and coupling to the bulk is determined by

$$\mathcal{H}_b = \frac{4}{4t^2 + (\alpha+2)^2}\left[\alpha n_2 + 2\vec{S}_1\vec{S}_2 - \frac{n_1 n_2}{2} + n_1 + n_2 - \sum_{\sigma}(Q_{2,\sigma}^{\dagger}Q_{1,\sigma} + Q_{1,\sigma}^{\dagger}Q_{2,\sigma})\right], \tag{2}$$

where $Q_{2,\sigma} = |0\rangle\langle\sigma|_2$ and $Q_{1,\sigma} = \sqrt{\alpha+1}\,|0\rangle\langle\sigma|_1 - 2\sigma\sqrt{\alpha}\,|\bar{\sigma}\rangle\langle 2|_1$ are generalized electron annihilation operators for sites 1 and 2. The parameter $\alpha > 0$ labels the four-dimensional representation of $gl(2|1)$ used in the construction of Eq. (2) and controls the internal spectrum of the impurity. The terms in Eq. (2) describe exchange and Coulomb interaction between the electrons on site 1 and those in the chain as well as a term allowing for the hopping of electrons between the bulk and the impurity. Comparing this model with that of the single-impurity Anderson model, $V_0 \equiv \frac{4}{4t^2+(\alpha+2)^2}$ can be identified with a hybridization coupling. Since we consider an open chain, the parameter t can be either real positive or purely imaginary, thereby allowing to cover the entire range $-\infty < V_0 < \infty$ for this coupling between the bulk and the impurity site. Note that additional parameters can be introduced into the model by adding static boundary fields.[17] For generic parameters, however, the $1/L$ contributions of the impurity, boundary and boundary fields to the thermodynamic properties are additive in the integrable model. Since the t-J model with open boundaries and boundary fields has already been studied in great detail[18] we restrict our analysis to the impurity contributions to the magnetization and the susceptibilities. These are functions of the bulk density of holes δ, the magnetic field H and the parameters controlling the impurity, i.e., α and V_0. Furthermore we consider only the ground state properties of the system to avoid the subtleties arising in the analysis of systems with open boundaries at finite temperatures.[19]

In the following section we identify the configuration of the impurity in the ground state of the many particle system as a function of these parameters. Then we study the magnetic susceptibility and occupation of the impurity at zero magnetic field where we derive analytic expressions near half filling ($\delta=0$) which are complemented by numerical results for general δ. Based on these results we identify the relevant energy scales in the system which allow for a quantitative study of the properties of the system in an external magnetic field.

II. FORMATION OF BOUND STATES

A. Bethe ansatz equations

The spectrum of the model (1) has already been obtained by means of the algebraic Bethe ansatz technique.[17] An eigenstate with $N_e=N_\uparrow+N_\downarrow$ electrons is characterized by the roots of the Bethe ansatz equations (BAEs)

$$[e_1(\lambda_j)]^{2L} = \prod_{k\neq j}^{M_s} e_2(\lambda_j-\lambda_k)e_2(\lambda_j+\lambda_k)\prod_{\beta=1}^{M_c} e_{-1}(\lambda_j-\vartheta_\beta) \times e_{-1}(\lambda_j+\vartheta_\beta), \quad j=1,\ldots,M_s,$$

$$e_\alpha(\vartheta_\gamma+t)e_\alpha(\vartheta_\gamma-t) = \prod_{k=1}^{M_s} e_{-1}(\vartheta_\gamma-\lambda_k)e_{-1}(\vartheta_\gamma+\lambda_k), \quad \gamma=1,\ldots,M_c. \tag{3}$$

Here $e_n(x)=\frac{x+in/2}{x-in/2}$. The $M_s=L+1-N_\uparrow$ spin rapidities λ_j parametrize magnetic excitations starting from the completely filled state with maximum polarization (one electron per bulk site, two electrons on the impurity site with $N_\uparrow=L+1$, $N_\downarrow=1$) and the $M_c=L+2-N_e$ charge rapidities ϑ_γ describe holes added to this state. The phases e_α in the second set of these equations are due to the presence of the impurity (2), similarly as in Ref. 10. The energy of the corresponding Bethe state is then given by the expression

$$E = V_0(\alpha+2)+2(L-1)-\sum_{j=1}^{M_s}\frac{1}{\lambda_j^2+\frac{1}{4}}+\left(\mu-\frac{H}{2}\right)M_c + HM_s-\mu(L+2)-\frac{H}{2}L. \tag{4}$$

The ground state and the low-energy magnetic and charged excitations (spinons and holons) of the t-J model with open boundary conditions without boundary fields or an impurity—similar to the model with periodic boundary conditions—are described by positive rapidities $\{\lambda_j,\vartheta_\gamma\}$ solving the BAE (3). Sufficiently strong boundary magnetic fields or potentials lead to the formation of boundary bound states in the spectrum of the system. In terms of the many-particle Bethe states this is reflected by the appearance of isolated, purely imaginary roots to the BAE.[20–22] Note that a necessary condition for such roots is the existence of singularities in the boundary phase shifts to compensate divergencies appearing in the scattering phases for imaginary rapidities. A similar mechanism for the creation of bound states has been found to exist in integrable impurity problems,[23] although it has not been studied systematically so far. For the present model with the impurity described by Eq. (2) bound states appear for a sufficiently strong hybridization V_0. This regime is reached by choosing $t=i\tau$ purely imaginary ($\tau>0$ without loss of generality). In the presence of a particular solution with an imaginary root $\mathrm{Im}(\vartheta_{\gamma_0})>0$, the right-hand side of the second set of equations in Eq. (3) vanishes in the thermodynamic limit ($M_s\to\infty$ with $M_{s,c}/L$ kept fixed). Therefore, ϑ_γ has to be exponentially close to a zero of $e_\alpha(\vartheta_\gamma+t)e_\alpha(\vartheta_\gamma-t)=e_{\alpha+2\tau}(\vartheta_\gamma)e_{\alpha-2\tau}(\vartheta_\gamma)$, i.e., $\vartheta_{\gamma_0}=-i(\alpha/2\pm\tau)$. This bound state solution appears for $\tau>\alpha/2\equiv\tau_0$. Increasing τ further eventually leads to the appearance of additional imaginary roots in the ground state configuration. The analysis of this sequence of bound states suggests a division of the V_0-α parameter space of the impurity into four regions labeled by an index (R) counting the number of bound state solutions present in the ground state of the system (see Fig. 1). R runs from 0 [the region described by the BAE (3)] to III (a region with three bound states).

(I) $\tau_0<\tau<(\alpha+1)/2\equiv\tau_1$. As seen above, a complex root $\vartheta_{M_c}=i(\tau-\alpha/2)$ appears in the set of the charge rapidities $\{\vartheta_\gamma\}$ for $\tau>\alpha/2$. Explicitly taking into account this root, describing a bound state in the holon sector, and rearranging the equations we end up with a set of modified BAEs:

$$e_1^{2L}(\lambda_j) = e_{-(2\tau+1-\alpha)}(\lambda_j)e_{2\tau-1-\alpha}(\lambda_j)\prod_{k\neq j}^{M_s} e_2(\lambda_j-\lambda_k)e_2(\lambda_j+\lambda_k) \times\prod_{\beta=1}^{M_c-1} e_{-1}(\lambda_j-\vartheta_\beta)e_{-1}(\lambda_j+\vartheta_\beta), \quad j=1,\ldots,M_s,$$

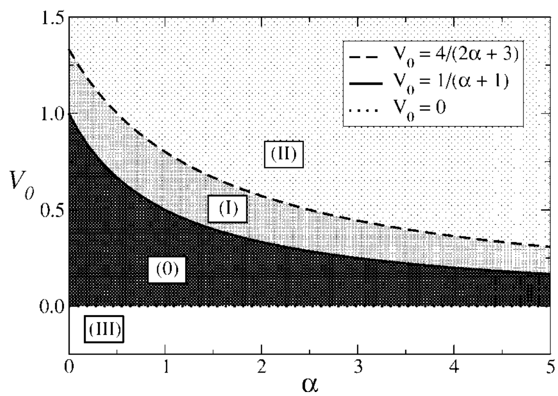

FIG. 1. Spectrum of impurity bound states in the V_0-α parameter space.

$$e_{\alpha+2\tau}(\vartheta_\gamma)e_{\alpha-2\tau}(\vartheta_\gamma)=\prod_{k=1}^{M_s} e_{-1}(\vartheta_\gamma-\lambda_k)e_{-1}(\vartheta_\gamma+\lambda_k),$$

$$\gamma=1,\ldots,M_c-1. \tag{5}$$

(II) $\tau_1<\tau<\alpha/2+1\equiv\tau_2$. Increasing τ even further, we will generate a new bound state, this time, in the spin sector. We associate to this bound state, the complex spin rapidity $\lambda_{M_s}=i[\tau-(\alpha+1)/2]$. Once again, the BAE have to be changed in consequence:

$$e_1^{2L}(\lambda_j)=e_{-(2\tau-\alpha-3)}(\lambda_j)e_{2\tau-1-\alpha}(\lambda_j)\prod_{k\neq j}^{M_s-1} e_2(\lambda_j-\lambda_k)e_2(\lambda_j+\lambda_k)$$

$$\times\prod_{\beta=1}^{M_c-1} e_{-1}(\lambda_j-\vartheta_\beta)e_{-1}(\lambda_j+\vartheta_\beta),\quad j=1,\ldots,M_s-1,$$

$$e_{\alpha+2\tau}(\vartheta_\gamma)=e_{2\tau-2-\alpha}(\vartheta_\gamma)\prod_{k=1}^{M_s-1} e_{-1}(\vartheta_\gamma-\lambda_k)e_{-1}(\vartheta_\gamma+\lambda_k),$$

$$\gamma=1,\ldots,M_c-1. \tag{6}$$

From Eq. (4) we see that the contribution of this 'spinon bound state' to the energy of this Bethe state will be

$$E_{M_s}=[(\tau-\alpha/2)(1-\tau+\alpha/2)]^{-1}. \tag{7}$$

(III) $\tau>\tau_2$. For $\tau>\alpha/2+1$, a third bound state is created. Another purely imaginary root, $\vartheta_{M_c-1}=i(\tau-\alpha/2-1)$, will coexist with a set of real rapidities in the charge sector and with the root of region (I). The new BAEs in this region are

$$e_1^{2L}(\lambda_j)=\prod_{k\neq j}^{M_s-1} e_2(\lambda_j-\lambda_k)e_2(\lambda_j+\lambda_k)$$

$$\times\prod_{\beta=1}^{M_c-2} e_{-1}(\lambda_j-\vartheta_\beta)e_{-1}(\lambda_j+\vartheta_\beta),$$

$$j=1,\ldots,M_s-1,$$

$$e_{\alpha+2\tau}(\vartheta_\gamma)=e_{2\tau-2-\alpha}(\vartheta_\gamma)\prod_{k=1}^{M_s-1} e_{-1}(\vartheta_\gamma-\lambda_k)e_{-1}(\vartheta_\gamma+\lambda_k),$$

$$\gamma=1,\ldots,M_c-2. \tag{8}$$

The bound states in this sector, consisting of two charge and one spin rapidity can be interpreted as a singlet with vanishing charge bound to the impurity.

Increasing τ beyond $\alpha/2+1$ does not lead to additional bound states as expected for an impurity with a single orbital allowing for occupation of at most two charges. Therefore, we conclude that the maximum number of bound states allowed to develop themselves upon variation of the hybridization at the boundary impurity site is three—two holons and one spinon.

B. Continuum limit: Equations for the densities

The analysis of the BAE is simplified by doubling of the real roots of the BAE with positive and negative ones identified, i.e., $\lambda_{-j}=-\lambda_j$ and $\vartheta_{-\gamma}=-\vartheta_\gamma$. In the thermodynamic limit, the real roots $\{\lambda_j\}$ ($\{\vartheta_\gamma\}$) form continuous distributions which are conveniently described in terms of their densities $\rho_s(\lambda)$ $[\rho_c(\vartheta)]$. Those densities obey the following coupled, but linear, integral equations:

$$\begin{pmatrix}\rho_s(\lambda)\\ \rho_c(\vartheta)\end{pmatrix}=\begin{pmatrix}2a_1(\lambda)\\ 0\end{pmatrix}+\frac{1}{L}\begin{pmatrix}\hat{\rho}_s^{(R)}(\lambda)+\hat{\rho}_s^{(b)}(\lambda)\\ \hat{\rho}_c^{(R)}(\vartheta)+\hat{\rho}_c^{(b)}(\vartheta)\end{pmatrix}+\begin{pmatrix}-\int_{-A}^{A}a_2 & \int_{-B}^{B}a_1\\ \int_{-A}^{A}a_1 & 0\end{pmatrix}*\begin{pmatrix}\rho_s(\lambda)\\ \rho_c(\vartheta)\end{pmatrix}. \tag{9}$$

[the driving terms $\hat{\rho}_{s,c}^{(i)}(\lambda)$ at order $1/L$ are defined below in Eqs. (13) and (14)]. Here we have introduced $a_y(x)=\frac{1}{2\pi}\frac{y}{y^2/4+x^2}$ and $\int_{-k}^{k}f*g$ denotes the convolution $\int_{-k}^{k}dyf(x-y)g(y)$. The boundaries of integration A and B for the spin and charge sector, respectively, are fixed by the conditions

$$\int_{-A}^{A}d\lambda\rho_s(\lambda)=\frac{2[M_s-\theta(\tau-\tau_1)]+1}{L},$$

$$\int_{-B}^{B}d\vartheta\rho_c(\vartheta)=\frac{2[M_c-\theta(\tau-\tau_0)-\theta(\tau-\tau_2)]+1}{L}, \tag{10}$$

where $\theta(x)$ is the Heaviside step function and τ_k are the thresholds for the appearance of bound states identified above. Note that the boundaries of integration A and B are completely fixed through Eq. (10) by bulk quantities (i.e., total densities of spin σ electrons). Alternatively, they can be specified in a grand canonical approach by the conjugate potentials, i.e., the chemical potential μ and the magnetic field H. In this case the ground state is obtained by filling all modes with negative dressed energies $\varepsilon_s(\lambda)$ and $\varepsilon_c(\vartheta)$ solving the integral equations

$$\begin{pmatrix}\varepsilon_s(\lambda)\\ \varepsilon_c(\vartheta)\end{pmatrix}=\begin{pmatrix}-2\pi a_1(\lambda)+H\\ \mu-\dfrac{H}{2}\end{pmatrix}+\begin{pmatrix}-\int_{-A}^{A}a_2 & \int_{-B}^{B}a_1\\ \int_{-A}^{A}a_1 & 0\end{pmatrix}*\begin{pmatrix}\varepsilon_s(\lambda)\\ \varepsilon_c(\vartheta)\end{pmatrix} \qquad (11)$$

with $\varepsilon_s(\pm A)=0$ and $\varepsilon_c(\pm B)=0$. The unpolarized ground state for vanishing magnetic field, for example, corresponds to $A=\infty$.

Since Eq. (9) is a linear system of integral equations, the generic solution for both spin and charge densities is of the form

$$\rho=\rho_\infty+\frac{1}{L}(\rho_{\mathrm{imp}}+\rho_b). \qquad (12)$$

The first term in Eq. (12) is the bulk density obtained by solving Eq. (9) with $L=\infty$. The remaining two terms of order $1/L$ are the contributions due to the presence of the impurity and due to the openness of the chain, respectively.

Depending on the region fixed by the parameters α and t (or τ) the driving terms $\hat{\rho}_{s,c}^{(R)}$ in the integral equations (9) are obtained from the discrete BAEs (3), (5), (6), or (8) as

$$\hat{\rho}_s^{(R)}(\lambda)=\begin{cases}0, & R=0,\\ a_{2\tau+1-\alpha}(\lambda)+a_{1+\alpha-2\tau}(\lambda), & R=\mathrm{I},\\ -a_{3+\alpha-2\tau}(\lambda)-a_{2\tau-\alpha-1}(\lambda), & R=\mathrm{II},\\ 0, & R=\mathrm{III}\end{cases} \qquad (13)$$

for the spin sector and

$$\hat{\rho}_c^{(R)}(\vartheta)=\begin{cases}a_\alpha(\vartheta+t)+a_\alpha(\vartheta-t), & R=0,\ (t=i\tau\in\mathbb{R}),\\ a_{\alpha+2\tau}(\vartheta)+a_{\alpha-2\tau}(\vartheta), & R=0\ (\tau=-it\in\mathbb{R}),\\ a_{\alpha+2\tau}(\vartheta)+a_{\alpha-2\tau}(\vartheta), & R=\mathrm{I},\\ a_{\alpha+2\tau}(\vartheta)+a_{2+\alpha-2\tau}(\vartheta) & R=\mathrm{II},\mathrm{III}\end{cases} \qquad (14)$$

for the charge sector. The contributions due to the boundaries can be calculated with the driving terms $\hat{\rho}_s^{(b)}(\lambda)=a_2(\lambda)$ and $\hat{\rho}_c^{(b)}(\vartheta)=-a_1(\vartheta)$. As a consequence of the decomposition (12), the bulk, impurity and boundary contributions to any thermodynamic quantity can be studied separately. For instance, the ground state energy per site is formally

$$\frac{E_0}{L}=\epsilon_\infty+\frac{\epsilon_{\mathrm{imp}}+\epsilon_b}{L}. \qquad (15)$$

From this, magnetization, density of electrons and the corresponding susceptibilities are obtained by taking the appropriate derivatives with respect to the conjugate fields. The focus of this paper is on the characterization of the impurity. Therefore, we will concentrate on the contributions to these quantities which are determined by Eqs. (13) and (14). The finite size contributions of the boundaries are of purely geometric nature and have been studied by Eßler.[18]

C. The impurity's ground state

So far, we have distinguished four regions of the α–τ parameter space of the impurity, characterized by different possible bound state configurations. Each of theses regions is described by a different set of BAE. Before studying how the properties of the system are affected by the presence of the impurity, the configuration corresponding to the true ground state has to be identified. For this, the impurity's contribution to the energy has to be computed using the applicable sets of BAE in the vicinity of the transition lines $\tau=\tau_k$. The formal expression for this contribution in terms of the densities is

$$\begin{aligned}\epsilon_{\mathrm{imp}}=&(\alpha+2)V_0-2-\pi\int_{-A}^{A}d\lambda\rho_s^{(R)}(\lambda)a_1(\lambda)+\left(\mu-\frac{H}{2}\right)\\ &\times\left(\frac{1}{2}\int_{-B}^{B}d\vartheta\rho_c^{(R)}(\vartheta)+\theta(\tau-\tau_0)+\theta(\tau-\tau_2)\right)\\ &+H\left(\frac{1}{2}\int_{-A}^{A}d\lambda\rho_s^{(R)}(\lambda)+\theta(\tau-\tau_1)\right)-2\mu.\end{aligned} \qquad (16)$$

Here, we want to concentrate on the case $H=0$: for small magnetic fields (i.e., $A\gg1$), a convenient treatment of the integral equations (9) is obtained by rewriting the one for ρ_s as follows:

$$\rho_s^{(R)}=\frac{\hat{\rho}_s^{(R)}}{1+a_2}+\left(\int_{-\infty}^{-A}+\int_{A}^{\infty}\right)\frac{a_2}{1+a_2}*\rho_s^{(R)}+\int_{-B}^{B}\frac{a_1}{1+a_2}*\rho_c^{(R)}. \qquad (17)$$

Now, at $H=0$ ($A\to\infty$), the densities are given in terms of the solution to a scalar integral equation for the density $\rho_c^{(R)}$ of charge rapidities

$$\rho_s^{(R)}=\hat{\rho}_{s,H=0}^{(R)}+\int_{-B}^{B}G_0*\rho_c^{(R)},$$

$$\rho_c^{(R)}=\hat{\rho}_{c,H=0}^{(R)}+\int_{-B}^{B}G_1*\rho_c^{(R)}. \qquad (18)$$

The driving terms at zero field are

$$\hat{\rho}_{s,H=0}^{(R)}(\lambda)=\begin{cases}0, & R=0,\\ G_{2\tau-\alpha}(\lambda)+G_{\alpha-2\tau}(\lambda), & R=\mathrm{I},\\ -G_{2+\alpha-2\tau}(\lambda)-G_{2\tau-\alpha-2}(\lambda), & R=\mathrm{II},\\ 0, & R=\mathrm{III}\end{cases} \qquad (19)$$

and

$$\hat{\rho}^{(R)}_{c,H=0}(\vartheta) = \begin{cases} \hat{\rho}_c^{(0)}, & R=0, \\ \hat{\rho}_c^{(\mathrm{I})} + G_{2\tau-\alpha+1}(\vartheta) + G_{\alpha-2\tau+1}(\vartheta), & R=\mathrm{I}, \\ \hat{\rho}_c^{(\mathrm{II})} - G_{3+\alpha-2\tau}(\vartheta) - G_{2\tau-\alpha-1}(\vartheta), & R=\mathrm{II}, \\ \hat{\rho}_c^{(\mathrm{III})} & R=\mathrm{III} \end{cases} \tag{20}$$

for all four regions. The functions $\hat{\rho}_c$ have been defined above in Eq. (14) and

$$G_\beta(x) = \int_{-\infty}^{\infty} \frac{d\omega}{2\pi} \exp(-i\omega x) \frac{\exp(-\beta|\omega/2|)}{2\cosh(\omega/2)}. \tag{21}$$

Now, we can express the impurity's contribution (16) to the energy in terms of the solution to the integral equation (18).

(0) $t=i\tau$ real and $0<\tau<\tau_0$. In the absence of bound state, the $1/L$ correction to the ground state energy reads

$$\epsilon_{\mathrm{imp}}^{(0)} = E_b + \frac{1}{2}\int_{-B}^{B} \mathrm{d}\vartheta[\mu - 2\pi G_1(\vartheta)]\rho_c^{(0)}(\vartheta), \tag{22}$$

where $E_b = V_0(\alpha+2) - 2(\mu+1)$.

(I) $\tau_0<\tau<\tau_1$. As we have seen previously, in region (I) a first bound state is created in the charge sector. The energy contribution due to the impurity now becomes

$$\epsilon_{\mathrm{imp}}^{(\mathrm{I})} = E_b - \pi[G_{2\tau-\alpha+1}(0) + G_{\alpha-2\tau+1}(0)] + \frac{1}{2}\int_{-B}^{B} d\vartheta[\mu - 2\pi G_1(\vartheta)]\rho_c^{(I)}(\vartheta) + \mu. \tag{23}$$

Here ρ_c has to be evaluated with the appropriate driving term (20) for region I. The additional chemical potential is due to the charge in the bound state and the terms containing the G functions are the consequence of the rearrangement of the rapidities in the spin sector.

(II) $\tau_1<\tau<\tau_2$. In region II, two bound states are possible. Using the appropriate driving terms in Eq. (18), the $1/L$ correction to the energy becomes

$$\epsilon_{\mathrm{imp}}^{(\mathrm{II})} = E_b + \pi[G_{3+\alpha-2\tau}(0) + G_{2\tau-\alpha-1}(0)] + \frac{1}{2}\int_{-B}^{B} d\vartheta[\mu - 2\pi G_1(\vartheta)]\rho_c^{(II)}(\vartheta) + \mu + E_{M_s}. \tag{24}$$

The extra term E_{M_s} is the energy contribution (7) of the spin bound state.

(III) $\tau>\tau_2$. In region (III), ϵ_{imp} takes the form

$$\epsilon_{\mathrm{imp}}^{(\mathrm{III})} = E_b + \frac{1}{2}\int_{-B}^{B} d\vartheta[\mu - 2\pi G_1(\vartheta)]\rho_c^{(\mathrm{III})}(\vartheta) + 2\mu + E_{M_s}. \tag{25}$$

The proper ground state configuration is the one which minimizes the impurity contribution to the energy as given in Eqs. (22)–(25). In Fig. 2, we present numerical data for ϵ_{imp}, for fixed $\alpha=1$ and bulk hole concentration $\delta=0.2$, as a function of the hybridization V_0 (note that $\epsilon_{\mathrm{imp}}^{(R)}$ can be continued to regions with larger R, describing a configuration where an allowed bound state is not occupied). From these numerical data we conclude that as far as the ground state of the impurity is concerned, three intervals in the hybridization have to be distinguished (see also Fig. 1).

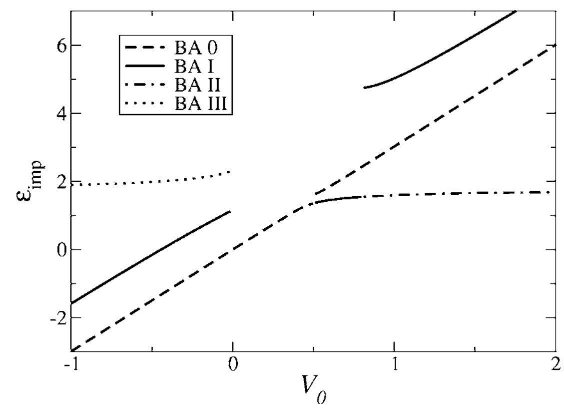

FIG. 2. Impurity contribution to the ground state energy for different bound state configurations as a function of the hybridization V_0 for bulk hole concentration of $\delta=0.2$. The impurity parameter is fixed to $\alpha=1$. Note that the Bethe ansatz for the configuration $R=$I and II gives identical results for $\varepsilon_{\mathrm{imp}}$ at negative V_0.

$V_0<1/(\alpha+1)$ (real t and $\tau=-it\in[0,\tau_0]\cup[\tau_2,\infty]$). For attractive ($V_0<0$) and weakly repulsive ($V_0>0$) hybridization the bound states identified above are not occupied, hence the ground state is described by Eqs. (9) with $R=0$.

$1/(\alpha+1)<V_0<4/(2\alpha+3)$ (i.e., $\tau_0<\tau<\tau_1$). In this interval the holon bound state is occupied in the ground state configuration which is described by Eq. (9) with the driving terms for $R=$I.

$V_0>4/(2\alpha+3)$ (i.e., $\tau_1<\tau<\tau_2$). For strong repulsive coupling between the impurity and the host the ground state is obtained using the configuration from $R=$II, i.e., with the holon *and* the spinon bound state occupied.

Note that the charge $Q=0$ singlet bound state of region III is never present in the ground state of the system. In the following we continue to label our results by the index $R=0$–III, the relation to the physical ground state as a function of V_0, however, is given by the classification above.

III. ZERO-FIELD SUSCEPTIBILITY AND OCCUPATION OF THE IMPURITY

A. Analytical results close to half filling

In this section, we will explicitly calculate the magnetization of the impurity in a small field. With our parameterization of the BAE's roots, the impurity contribution to the magnetization is given by

$$M_{\mathrm{imp}} = \frac{1}{4}\int_{-B}^{B} \mathrm{d}\vartheta \rho_c^{(R)}(\vartheta) + \frac{1}{2}[\theta(\tau-\tau_0) + \theta(\tau-\tau_2)] - \frac{1}{2}\int_{-A}^{A} \mathrm{d}\lambda \rho_s^{(R)}(\lambda) - \theta(\tau-\tau_1). \tag{26}$$

Proceeding as for Eq. (17), we can rewrite this expression for the impurity's magnetization as an integral over the spin density only:

$$M_{\mathrm{imp}} = \frac{1}{2}\int_A^\infty d\lambda \rho_s^{(R)}(\lambda) - \theta(\tau-\tau_1) + \frac{1}{2}[\theta(\tau-\tau_0)+\theta(\tau-\tau_2)]. \tag{27}$$

Introducing $g(z)=\rho_s^{(R)}(A+z)$ in the integral equation (17), we obtain the following equation for the unknown function g:

$$g(z) = \hat{\rho}_{s,H=0}^{(R)}(A+z) + \int_0^\infty dz' G_1(z-z')g(z') + \int_0^\infty dz' G_1(2A + z + z')g(z') + \int_{-B}^{B} dz' G_0(z-z'+A)\rho_c^{(R)}(z'). \tag{28}$$

For small magnetic fields corresponding to large values of A this equation can be solved by iteration using Wiener-Hopf methods. Following Ref. 24, we expand $g=g_1+g_2+\cdots$, where

$$g_1(z) = g_0^{(R)}(A+z) + C_{\alpha,\tau}^{(R)}G_0(A+z) + \int_0^\infty dz' G_1(z-z')g_1(z'), \tag{29}$$

$$g_n(z) = \int_0^\infty dz' G_1(2A+z+z')g_{n-1}(z') + \int_0^\infty dz' G_1(z-z')g_n(z'), \quad n>1. \tag{30}$$

Here $g_0^{(R)}=\hat{\rho}_{s,H=0}^{(R)}$ and we have used that, for $A\gg B$,

$$\int_{-B}^{B} dz' G_0(A+z-z')\rho_c^{(R)}(z') \approx G_0(A+z)\int_{-B}^{B} dz' e^{\pi z'}\rho_c^{(R)}(z') \tag{31}$$

to define the number $C_{\alpha,\tau}^{(R)} \equiv \int_{-B}^{B} dz' e^{\pi z'}\rho_c^{(R)}(z')$ which is given in terms of $\rho_c^{(R)}$ alone.

The leading behavior of the impurity magnetization for large A is now obtained from Eq. (29): using the results (A5) and (A6) from Appendix A we find

$$M_{\mathrm{imp}} = \begin{cases} \dfrac{e^{-\pi A}}{\sqrt{2\pi e}}\, C_{\alpha,\tau}^{(0)} & R=0, \\ \dfrac{e^{-\pi A}}{\sqrt{2\pi e}}\left(C_{\alpha,\tau}^{(I)} + 2\cos\left(\dfrac{\pi(2\tau-\alpha)}{2}\right)\right) + 1/2, & R=\mathrm{I}, \\ \dfrac{e^{-\pi A}}{\sqrt{2\pi e}}\left(C_{\alpha,\tau}^{(II)} + 2\cos\left(\dfrac{\pi(2\tau-\alpha)}{2}\right)\right) - 1/2, & R=\mathrm{II}. \end{cases} \tag{32}$$

Here the dependence of M_{imp} on the density of electrons in the host is completely given through the constants $C_{\alpha,\tau}$. The zero field limit of these quantities is given in terms of the solution to the integral equation (18) for $\rho_c^{(R)}$. In general this equation has to be solved numerically. For $B\ll 1, |2\tau-\alpha|$ (i.e., close to half filling and the impurity sufficiently far away from the threshold for the holon bound state), however, it can be solved by iteration. Doing so, we obtain at first order in B the following expressions for $C_{\alpha,\tau}$:

$$C_{\alpha,\tau}^{(R)} = 2B\begin{cases} \dfrac{4\alpha}{\pi(\alpha^2-4\tau^2)}, & R=0, \\ \dfrac{4\alpha}{\pi(\alpha^2-4\tau^2)} + G_{2\tau+1-\alpha}(0) + G_{1+\alpha-2\tau}(0), & R=\mathrm{I}, \\ \dfrac{4(1+\alpha)}{\pi(2+\alpha-2\tau)(\alpha+2\tau)} - G_{3+\alpha-2\tau}(0) - G_{2\tau-\alpha-1}(0), & R=\mathrm{II}. \end{cases} \tag{33}$$

At the threshold, $\tau=\tau_0=\alpha/2$, the leading contribution to $C_{\alpha,\tau_0}^{(0)}$, $C_{\alpha,\tau_0}^{(I)}$ at small hole concentration are ± 1 independent of δ.

Finally, the boundaries of integration, A and B, have to be expressed in terms of physical quantities, namely, the concentration $\delta=M_c/L$ of holes (doping) in the bulk and the magnetic field using the relations (10) and (11). Again, restricting ourselves to the regime close to half filling we have $\pi\delta=2B\ln 2$. To express A in terms of the magnetic field one has to enforce $\varepsilon_s(A)=0$. A Wiener-Hopf analysis of the integral equations (11) gives[18]

$$\pi A = -\ln(H/H_0) + \frac{1}{4\ln H}, \quad H_0 = \sqrt{(2\pi/e)}(2\pi - C) \tag{34}$$

with $C=\int_{-B}^{B} d\vartheta e^{\pi\vartheta}\varepsilon_c(\vartheta)$, here ε_c is the dressed energy of the holes given by Eq. (11). Close to half filling $C\ll 2\pi$ and $H_0\approx(2\pi)^{3/2}/\sqrt{e}$. Using Eqs. (33) and (34) the low-field magnetization is found to be linear in H. Thus we obtain for the impurity contribution to the zero field magnetic susceptibility close to half filling $\delta\ll 1, |2\tau-\alpha|$:

$$(0):\quad \chi_{\text{imp}} = \frac{1}{\pi^2}\frac{\alpha\delta}{(\alpha^2-4\tau^2)\ln 2} + \mathcal{O}(\delta^2), \tag{35}$$

$$(\mathrm{I}):\quad \chi_{\text{imp}} = \frac{1}{2\pi^2}\left[\frac{\pi\delta}{2\ln 2}\left(\frac{4\alpha}{\pi(\alpha^2-4\tau^2)} + G_{2\tau+1-\alpha}(0) + G_{1+\alpha-2\tau}(0)\right) + \cos\left(\frac{\pi(2\tau-\alpha)}{2}\right)\right] + \mathcal{O}(\delta^2), \tag{36}$$

$$(\mathrm{II}):\quad \chi_{\text{imp}} = \frac{1}{2\pi^2}\left[\frac{\pi\delta}{2\ln 2}\left(\frac{4(1+\alpha)}{\pi(2+\alpha-2\tau)(\alpha+2\tau)} - G_{3+\alpha-2\tau}(0) - G_{2\tau-\alpha-1}(0)\right) + \cos\left(\frac{\pi(2\tau-\alpha)}{2}\right)\right] + \mathcal{O}(\delta^2). \tag{37}$$

Finally, we can compute the change in the number of electrons due to the presence the impurity which is obtained from Eq. (10) to be

$$D_{\text{imp}} = 2 - \frac{1}{2}\int_{-B}^{B} d\vartheta \rho_c^{(R)}(\vartheta) - \theta(\tau-\tau_0) - \theta(\tau-\tau_2). \tag{38}$$

Again this expression can be calculated at zero field, close to half-filling and away from the holon bound state threshold ($B \ll 1, |2\tau-\alpha|$) giving

$$D_{\text{imp}} = \begin{cases} 2 - \dfrac{\pi\delta}{\ln 2}\dfrac{2\alpha}{\pi(\alpha^2-4\tau^2)}, & R=0, \\ 1 - \dfrac{\pi\delta}{2\ln 2}\left(\dfrac{4\alpha}{\pi(\alpha^2-4\tau^2)} + G_{2\tau+1-\alpha}(0) + G_{1+\alpha-2\tau}(0)\right), & R=\mathrm{I}, \\ 1 - \dfrac{\pi\delta}{2\ln 2}\left(\dfrac{4(1+\alpha)}{\pi(2+\alpha-2\tau)(\alpha+2\tau)} - G_{3+\alpha-2\tau}(0) - G_{2\tau-\alpha-1}(0)\right), & R=\mathrm{II}. \end{cases} \tag{39}$$

B. Numerical results for arbitrary doping

For finite density of holes (B finite) the integral equations (18) and (11) for the charge components of the densities and dressed energies have to be solved numerically. In Figs. 3–5, we present results of this analysis for the zero field susceptibility and occupation of the impurity for different doping as a function of the hybridization V_0. Note that for general filling factors, the constant C in the definition (34) of H_0 is no longer negligible, thus

$$\chi_{\text{imp}}(H=0) = \frac{1}{2\pi(2\pi-C)}\begin{cases} C_{\alpha,\tau}^{(0)}, & R=0, \\ C_{\alpha,\tau}^{(I)} + 2\cos\left(\dfrac{\pi(2\tau-\alpha)}{2}\right), & R=\mathrm{I}, \\ C_{\alpha,\tau}^{(II)} + 2\cos\left(\dfrac{\pi(2\tau-\alpha)}{2}\right), & R=\mathrm{II}. \end{cases} \tag{40}$$

First notice that the $\alpha=0$ case where the doubly occupied state decouples from the remaining three electronic impurity states $|0\rangle$, $|\sigma\rangle$ is special: here, for $V_0<1$, the impurity is doubly occupied $D_{\text{imp}}\equiv 2$. Therefore the impurity does not contribute to the magnetic susceptibility of the system, i.e., $\chi_{\text{imp}}=0$. For $V_0>1$ (regions I and II), the occupation is less than 2 due to the filled holon bound state and there is a small finite impurity contribution to the susceptibility.

For $\alpha>0$, evaluation of Eq. (38) can result in $D_{\text{imp}}>2$. This appears counterintuitive since the impurity (2) does not allow for an occupation with more than two particles, i.e., $\langle n_1\rangle \le 2$. In the contribution D_{imp} of the impurity to the number of electrons in the system, however, *all* L^0 contributions including the host polarization resulting from charges on the impurity site are taken into account. Hence $D_{\text{imp}}>\langle n_1\rangle$ becomes possible as a consequence of the attractive interaction between the impurity and the bulk electrons for $V_0<0$. Note, that the difference $D_{\text{imp}}|_{V_0=-\infty} - D_{\text{imp}}|_{V_0=+\infty}$ approaches 2, showing the depletion of the impurity orbital at large positive V_0. For small hole concentration δ we had found above that the impurity occupation changes at the threshold for the formation of the holon bound state $V_0 \gtrsim 1/(\alpha+1)$. For finite δ this resonance moves to smaller values of V_0, determined by the condition that the (real) impurity parameter t is of the order of the boundary B which is given by the bulk hole concentration through Eq. (9). Below this value of the hybridization, i.e., for $t \gtrsim B$ the impurity is doubly occupied and essentially decoupled from the host.

The same shift is observed in the resonance of the impurity contribution to the zero-field susceptibility which moves from the threshold for the holon bound state towards smaller values of V_0 as the hole concentration is increased. This reso-

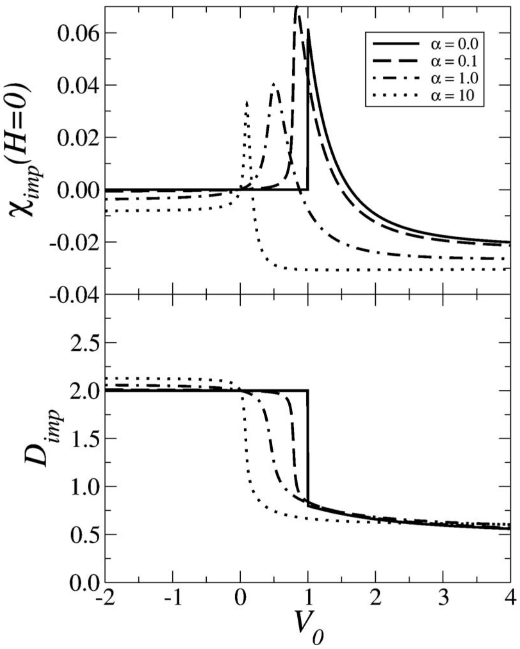

FIG. 3. Zero field susceptibility χ_{imp} (upper panel) and electron number D_{imp} on the impurity site (lower panel) for bulk doping $\delta=0.2$ as a function of V_0.

nance is the response of the unpaired electron on the impurity site which appears when $D_{\mathrm{imp}} \approx 1$. Although still limited by fluctuations in the impurity's occupation the susceptibility at the resonance grows strongly with δ. This is shown in Fig. 6 where the maximum of $\chi_{\mathrm{imp}}(H=0)$ as a function of V_0 is given for different values of the impurity parameter α as a function of the hole concentration in the bulk t-J chain. For $\delta \to 0$ the susceptibility approaches that of the bulk system while it diverges for $\delta \to 1$, i.e., vanishing bulk density of electrons. In this limit the remaining electron on the impurity site is essentially an uncoupled local moment.

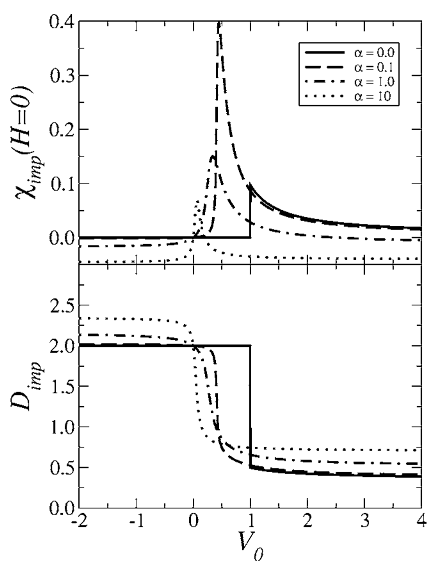

FIG. 4. Same as Fig. 3 for δ=0.5.

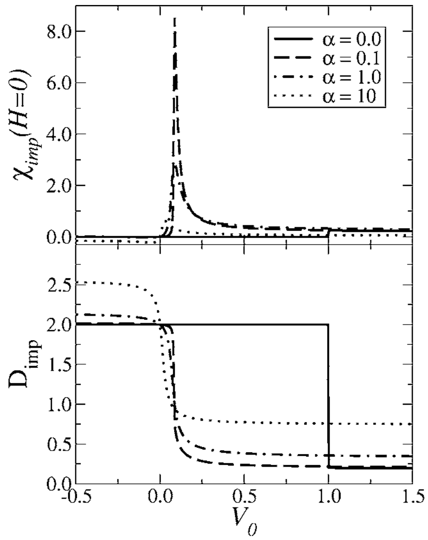

FIG. 5. Same as Fig. 3 for δ=0.8.

IV. IMPURITY IN A MAGNETIC FIELD

As we have seen above the magnetic behavior of the impurity is most interesting in the regime of weak coupling V_0 parametrized by real values of t. This parameter introduces a scale where the response of the impurity to external fields is expected to change. In the present problem where the impurity site is coupled to the t–J chain with separated spin and charge degrees of freedom this response will depend on the relation of this scale to the typical energies in these sectors as well. First, using the relation (34), we obtain the Kondo field determining the scale where the susceptibility of an impurity coupled to the spin degrees of freedom changes as

$$H_K \sim H_0 \exp(-\pi t) \approx H_0 \exp\left(-\frac{\pi}{\sqrt{V_0}}\right) \tag{41}$$

for large t corresponding to $V_0 \ll 1$. Note that the dependence of H_K on the hybridization is exponential and not a power-law as found for a Kondo impurity in a TLL.[4,5] This reflects the absence of backscattering in the integrable impurity model considered here.

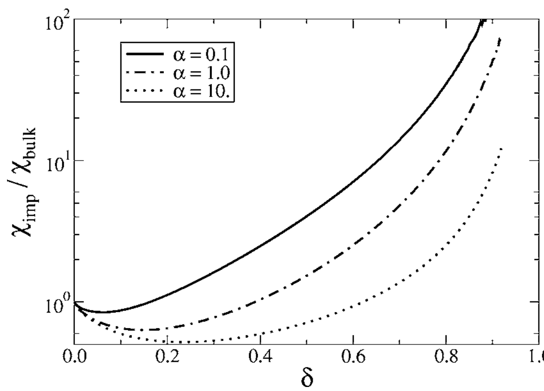

FIG. 6. Maximum value of $\chi_{\mathrm{imp}}(H=0)$ as a function of δ. For small δ this maximum appears close to the threshold for the creation of the holon bound state $V_0 = 1/(\alpha+1)$.

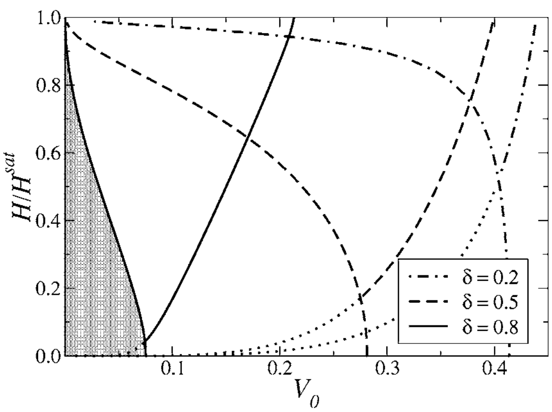

FIG. 7. Relevant energy scales for the impurity problem as a function of the hybridization V_0 for $\alpha=1$: for fixed hole concentration δ (e.g., full lines for $\delta=0.8$) the impurity is decoupled from the host for magnetic fields below the left line (shaded area). Above this threshold (or at sufficiently large V_0) the Kondo scale H_K (right branch of full line) becomes visible in the impurity's response to the external field. The dotted lines indicate the continuation of the Kondo scale H_K (41) into the decoupled region.

On the other hand, as seen from the BAE (3), the primary effect of the impurity (2) is to induce a phase shift in the charge sector. Hence, the hybridization has to exceed a minimal value below which the impurity is doubly occupied and will not contribute to the magnetic response of the system (this is different from the Anderson impurity model considered by Bortz *et al.* where the local orbital can be populated by at most one electron[13]). Finally, for the impurity to be visible in the *magnetic* response, spin and charge sectors have to be coupled at the scale introduced by the hybridization. This coupling is determined by the relative size of the impurity parameter t and that of the host parameters A, B. Note that the latter are functions of the magnetic field: we have already used that $A\to\infty$ while B approaches a finite constant for $H\to 0$. On the other hand, the system becomes completely polarized for $H=H^{\text{sat}}=4\cos^2(\pi\delta/2)$. In this limit $A\to A^{\text{sat}}=\frac{1}{2}\sqrt{4/H^{\text{sat}}-1}=\frac{1}{2}\tan(\pi\delta/2)$ while $B\to\infty$. Therefore, depending on the relative size of A and B two scenarios can be distinguished for fixed hole concentration δ in the bulk.

(i) For sufficiently weak hybridization, corresponding to large t such that $t=B>A$ at some value $H=H_B$ of the magnetic field, the impurity is decoupled from the (charge degrees of the) host at the Kondo scale (41). In this case the impurity contribution χ_{imp} to the susceptibility will exhibit a resonance at $H=H_B>H_K$ while being suppressed below H_B.

(ii) If the impurity and the host are already coupled at the Kondo scale, i.e., $t=A<B$, Kondo-like behavior of the susceptibility can be observed where the susceptibility approaches some nonuniversal finite value as $H\to 0$.

Finally, for V_0 large enough for $H_K>H^{\text{sat}}$ corresponding to $t<A^{\text{sat}}$ (or t purely imaginary) no resonance is present in the susceptibility due to the finite bandwidth of the lattice model.

In Fig. 7 the regions corresponding to these scenarios are shown for various values of the hole concentration δ. By numerical integration of the Bethe ansatz equations (9) the occupation of the impurity in these regions is determined.

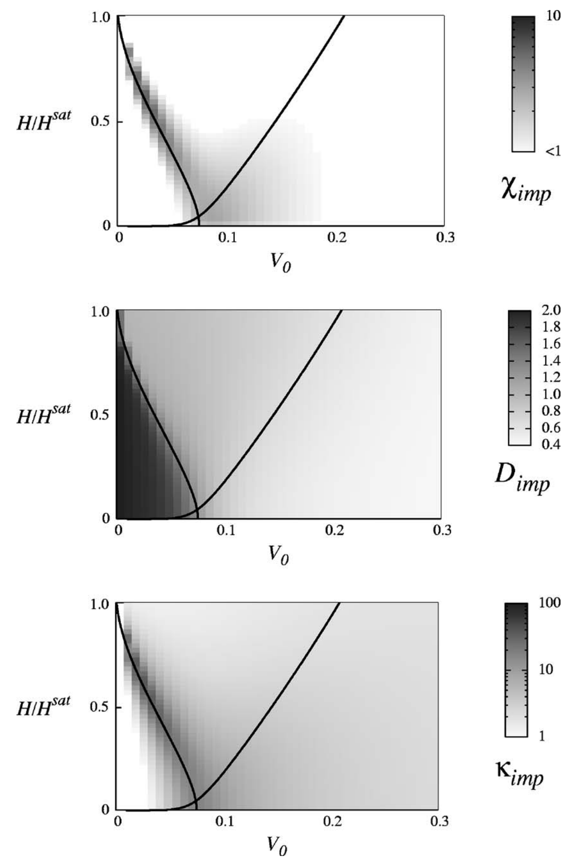

FIG. 8. (a) Susceptibility χ_{imp}, (b) electronic occupation D_{imp}, and (c) charge compressibility κ_{imp} (normalized to its bulk value) of the impurity as a function of the hybridization and magnetic field for $\delta=0.8$ and $\alpha=1$ (phase boundaries from Fig. 7 are superimposed). Note the logarithmic scale used for the shading of the susceptibilities.

Fluctuations in the densities are measured by the impurity contribution to the magnetic susceptibility χ_{imp} and charge compressibility $\kappa_{\text{imp}}=\partial D_{\text{imp}}/\partial\mu$ of the system. Just as the corresponding bulk quantities these thermodynamic coefficients are conveniently computed based on their representation in terms of the dressed charge matrix (see Appendix B). In Fig. 8 our numerical results on these quantities as a function of the hybridization and the magnetic field are shown for hole concentration $\delta=0.8$. For intermediate values of the hybridization $0.1\lesssim V_0\lesssim 0.2$ the coupling of the impurity to the holon excitations is effective. For small magnetic fields below the Kondo scale H_K the impurity contribution to the susceptibility takes a nonuniversal value χ_0 characteristic for the strong coupling regime of an Anderson impurity. Above H_K the field dependence is that of a local moment with logarithmic deviations from full polarization (see Fig. 9). The emergence of universal Kondo-like behavior $\chi_{\text{imp}}=f(H/H_K)/2\pi H_K$ for smaller hybridization $V_0\lesssim 0.1$ is suppressed by the decoupling of the impurity from the host. Here the double occupancy of the impurity for small fields and the formation of a local moment with an impurity occupation close to 1 appearing for fields $H\gtrsim H_B\gg H_K$ are clearly visible. In the vicinity of the transition between these regions the occupation and magnetization of the impurity

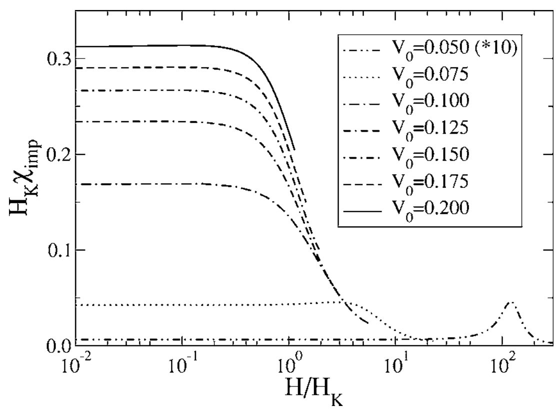

FIG. 9. Magnetic field dependence of the impurity susceptibility for $\delta=0.8$, $\alpha=1$ and various values of the hybridization: for $V_0 \gtrsim 0.1$ the transition between the strong coupling behavior for small fields and the formation of a local moment above $H\approx H_K$ is clearly seen. At smaller values of V_0 the susceptibility is strongly suppressed due to the decoupling of the doubly occupied impurity from the host (data for $V_0=0.05$ are enhanced by a factor of 10).

fluctuate strongly, as shown by the resonances in the susceptibilities (Fig. 8). Finally, for larger values of $V_0 \gtrsim 0.2$, the occupation of the impurity decreases well below 1 and the susceptibilities are approximately constant over the entire range of the external field $0 < H < H^{\text{sat}}$.

V. SUMMARY AND CONCLUSION

We have studied the properties of an Anderson-type impurity embedded into a supersymmetric *t-J* chain with open boundaries. Within this model the hybridization coupling V_0 of the impurity to the holons in the 1D host can be tuned freely while preserving the integrability. Upon variation of V_0 the nature of the many-particle ground state changes due to the appearance of a sequence of bound states in the holon and spinon sectors. From our analysis of the contribution of the impurity to the electronic density and magnetization of the system and the corresponding susceptibilities at vanishing magnetic field we have identified two regimes: for attractive or weakly repulsive hybridization the impurity is doubly occupied with vanishing fluctuations. Here the impurity and the host are effectively decoupled due to a mismatch of V_0 and the relevant scales in the holon sector. For strong hybridization one holon and one spinon bound state are occupied. Between these regions the susceptibility exhibits a sharp resonance which diverges as the density of bulk electrons tends to 0. In a magnetic field exceeding the characteristic scale for excitations in the spinon sector $H \gtrsim H_K$ a third region appears for intermediate values of the hybridization: this regime is characterized by the formation of a local moment with small corrections to full polarization. In this range of V_0 the field dependence of the susceptibility approaches the characteristic Kondo scaling behavior until the decoupling of the impurity from the holon sector sets in.

Note that the zero field analysis of Sec. III can be extended to small magnetic fields. This will lead to additional logarithmic corrections to the thermodynamic quantities. In the response of the Hamiltonian (1) they will be hidden by the ones due to the presence of open boundaries.[18]

The model considered in this paper can be generalized in a number of ways. As discussed in the Introduction, the boundary impurity can be combined with a local potential or magnetic field which by itself will generate a sequence of bound states in the holon and spinon sector. Fine-tuning the parameters describing the impurity and those of the boundary field, part of the impurity spectrum can be projected out from the Hilbert space.[25] This procedure leads, e.g., to exactly solvable models for a true Kondo spin S or an impurity coupled only to one spin channel of the host electrons (see also Refs. 15 and 16). While the projection onto a subset of impurity states is well understood on the level of the Hamiltonian and its construction it is an open problem, how the corresponding spectra (which will differ for different choices of the projected subset) are to be computed. In particular the role of the bound states in these sectors needs further investigation which is left for future work.

ACKNOWLEDGMENTS

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APPENDIX A: SOLUTION OF THE INTEGRAL EQUATIONS (30)

The integral equations (30) are of Wiener-Hopf (WH) type

$$g(z) = g_0(z) + \int_0^\infty dz' G_1(z-z') g_1(z') \tag{A1}$$

and can be solved using standard techniques based on the factorization of the Fourier transformed kernel $G_1(\omega)$

$$[1 - G_1(\omega)]^{-1} = G^+(\omega) G^-(\omega), \quad \lim_{\omega\to\infty} G^\pm(\omega) = 1 \tag{A2}$$

into functions $G^\pm(\omega)$ which are analytic for $\text{Im}(\omega) > 0$ (<0), respectively. For the *t-J* model these techniques have been applied before[18,26] and the factorization of the kernel is known to be

$$G^-(\omega) = G^+(-\omega) = \frac{\sqrt{2\pi}}{\Gamma\left(\frac{1}{2} + i\frac{\omega}{2\pi}\right)} \left(\frac{i\omega}{2\pi e}\right)^{i\omega/2\pi}. \tag{A3}$$

In Eqs. (29) and (30) for $n=1$ and 2 three different driving terms g_0 need to be considered. (a) The case $g_0(z) = G_0(A+z)$ already appears in the calculation of bulk quantities such as the dressed energies for the *t-J* model. Following Refs. 18 and 26 we find for g

$$g_a^+(\omega) = iG^+(\omega) G^-(-i\pi) \frac{e^{-\pi A}}{\omega + i\pi}. \tag{A4}$$

Using the explicit expressions (A3) we obtain

$$\int_0^\infty dz g_a(z) = g_a^+(\omega=0) = \sqrt{\frac{2}{e\pi}} e^{-\pi A}, \tag{A5}$$

which will be necessary to compute the impurity's magnetization.

(b) The second type of driving term, according to Eq. (19), is $g_0(z)=G_\beta(z+A)+G_{-\beta}(z+A)$. The analysis of the WH equation is completely analogous to the first case and we find

$$g_b^+(\omega) = 2iG^+(\omega)G^-(-i\pi)\frac{e^{-\pi A}}{\omega+i\pi}\cos\left(\frac{\pi\beta}{2}\right) = 2\cos\left(\frac{\pi\beta}{2}\right) g_a^+(\omega). \tag{A6}$$

(c) Finally, the driving term in Eq. (30) for the subleading contribution g_2 is proportional to $g_0(z) = \int_0^\infty dz' G_1(2A+z+z')g_a(z')$. Following Ref. 18, we perform a Laplace tansform of $g_0(z)$ to obtain

$$g_0(z) \simeq \frac{1}{4\pi}\int_0^\infty dx e^{-2Ax} e^{-|z|x} g_a^+(ix)(x+\cdots), \tag{A7}$$

where we have used the asymptotic expansion of the function $G_1(z) \sim 1/4\pi z^2 + \mathcal{O}(z^{-4})$. Now the solution of the Wiener-Hopf equation is given by

$$g_c^+(\omega) \simeq G^+(\omega)\frac{i}{4\pi}\int_0^\infty \mathrm{d}x e^{-2Ax}(x+\cdots)\frac{G^+(ix)g_a^+(ix)}{\omega+ix}. \tag{A8}$$

The presence of the rapidly decaying factor $\exp(-2Ax)$ (remember that $A \gg 1$ at small field) in the integrand suggests the following expansion around $x=0$:

$$g_a^+(ix)G^+(ix)(x+\cdots) \sim 2\frac{e^{-\pi A}}{\sqrt{e\pi}}x + \mathcal{O}(x^2). \tag{A9}$$

From this expression we obtain

$$\int_0^\infty dz g_c(z) = g_c^+(\omega=0) = \sqrt{\frac{2}{e\pi}}\frac{e^{-\pi A}}{4\pi A} + \mathcal{O}\left(\frac{1}{A^2}\right). \tag{A10}$$

APPENDIX B: EXPRESSIONS FOR THE SUSCEPTIBILITIES

For the numerical analysis of the susceptibilities in a finite magnetic field it is convenient to use their expressions in terms of the so-called dressed charge matrix.[27–29] This quantity is as the solution of the Bethe ansatz integral equations

$$\begin{pmatrix} \xi_{ss}(\lambda) & \xi_{cs}(\lambda) \\ \xi_{sc}(\vartheta) & \xi_{cc}(\vartheta) \end{pmatrix} = \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix} + \begin{pmatrix} -\int_{-A}^{A} a_2 & \int_{-B}^{B} a_1 \\ \int_{-A}^{A} a_1 & 0 \end{pmatrix} * \begin{pmatrix} \xi_{ss}(\lambda) & \xi_{cs}(\lambda) \\ \xi_{sc}(\vartheta) & \xi_{cc}(\vartheta) \end{pmatrix}. \tag{B1}$$

The magnetic susceptibility at fixed μ is obtained by first taking the derivatives of the magnetization as obtained from Eq. (10) with respect to the boundaries of integration A and B. Then, starting from the conditions $\varepsilon_s(A)=0=\varepsilon_c(B)$, one obtains two equations for their derivatives $\partial A/\partial H$ and $\partial B/\partial H$ which are then solved in terms of ξ at the boundaries of integration

$$\begin{pmatrix} Z_{ss} & Z_{cs} \\ Z_{sc} & Z_{cc} \end{pmatrix} = \begin{pmatrix} \xi_{ss}(A) & \xi_{cs}(A) \\ \xi_{sc}(B) & \xi_{cc}(B) \end{pmatrix}. \tag{B2}$$

This approach leads to the following expression for the bulk magnetic susceptibility at fixed chemical potential:[28]

$$\chi_{\mathrm{bulk}}\Big|_\mu = \frac{1}{4\pi}\left(\frac{(Z_{cc}-2Z_{sc})^2}{v_c} + \frac{(Z_{cs}-2Z_{ss})^2}{v_s}\right), \tag{B3}$$

where and $v_s=\varepsilon_s'(A)/\pi\rho_s(A)$, $v_c=\varepsilon_c'(B)/\pi\rho_c(B)$ are the spinon and holon Fermi velocities, respectively. The impurity contribution to the magnetic susceptibility is obtained analogously starting from Eq. (26) as[10]

$$\chi_{\mathrm{imp}}\Big|_\mu = \frac{1}{4\pi}\left(\frac{(Z_{cc}-2Z_{sc})^2 f_c}{v_c} + \frac{(Z_{cs}-2Z_{ss})^2 f_s}{v_s}\right), \tag{B4}$$

with $f_s=\rho_s^{(R)}(A)/\rho_s(A)$ and $f_c=\rho_c^{(R)}(B)/\rho_c(B)$.

In this paper we work at fixed (bulk) hole concentration $\delta=\int_{-B}^{B} d\vartheta \rho_{\infty,c}(\vartheta)$. Using $\partial\delta/\partial H$ together with the expression of the chemical potential entering Eqs. (11) in terms of the independent variables H and δ the bulk susceptibility is found to be (see also Refs. 27 and 29)

$$\chi_{\mathrm{bulk}}\Big|_\delta = \frac{(\det Z)^2}{\pi}\frac{1}{v_c Z_{cs}^2 + v_s Z_{cc}^2}. \tag{B5}$$

Again, it is straightforward to compute the impurity contribution to the susceptibility within this approach giving

$$\chi_{\mathrm{imp}}\Big|_\delta = \frac{\det Z}{\pi}\frac{1}{v_c Z_{cs}^2 + v_s Z_{cc}^2}\left\{ f_s Z_{cc}\left(Z_{ss} - \frac{1}{2}Z_{cs}\right) - f_c Z_{cs}\left(Z_{sc} - \frac{1}{2}Z_{cc}\right)\right\}. \tag{B6}$$

To measure the valence fluctuations on the impurity site one has to consider the charge compressibility. Again, the bulk and impurity contributions to $\kappa=\partial N_e/\partial\mu$ are conveniently expressed in terms of the dressed charge matrix[10,27–29]

$$\kappa_{\mathrm{bulk}}\Big|_H = \frac{Z_{cc}^2}{\pi v_c} + \frac{Z_{cs}^2}{\pi v_s},$$

$$\kappa_{\mathrm{imp}}\Big|_H = \frac{Z_{cc}^2}{\pi v_c}f_c + \frac{Z_{cs}^2}{\pi v_s}f_s. \tag{B7}$$

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