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Exact solution for an exchange impurity in a one-dimensional correlated host

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Abstract. The one-dimensional t–J model at the supersymmetric point, $J = 2t$, with a magnetic impurity of arbitrary spin S is studied exactly using the Bethe *ansatz* technique. The impurity interacts by spin exchange with the electrons on neighbouring sites of a lattice without destroying the integrability. The discrete Bethe *ansatz* equations diagonalizing the model, and the thermodynamic equations are derived. The impurity free energy is obtained for arbitrary band filling as a function of temperature and external magnetic field. The impurity can localize up to one itinerant hole, and has in general mixed-valent properties.

1. Introduction

During the last decade the Hubbard and t–J models have received great attention in the context of the high-T_c cuprate superconductors [1]. The Hubbard model for a strong Coulomb repulsion reduces to the t–J model with small J and excluded multiple-electron occupation of each site. 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 CuO_2 plane) can also be reduced to an effective one-band t–J model [2]. Hence, the t–J model can be considered with t and J as independent parameters which may have comparable values.

The one-dimensional t–J model has been investigated by numerous methods, e.g., with a variational *ansatz* for the Luttinger liquid [3], by cluster diagonalization using the Lanczos method [4], Monte Carlo simulations [5], and the Bethe *ansatz* [6, 7]. The one-dimensional t–J model is only integrable for $J = \pm 2t$. The necessary condition for the integrability is the factorization of the many-electron scattering matrix into two-particle scattering matrices (the Yang–Baxter triangular relation), which imposes conditions on the scattering process. Only for $J = \pm 2t$ [6, 7] are the sets of wavenumbers of the incoming and outgoing particles identical, leading to a graded permutation superalgebra [6, 8–10], i.e. the spin of the electrons and the charge holes play a similar role. The integrability of the supersymmetric model was first stated by Lai [11] and Sutherland [6], and has subsequently been rediscovered by other authors [7, 12, 13].

Impurities play an important role in correlated electron compounds, in particular in one dimension, since even a small number 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 non-interacting metals (e.g. in the Kondo

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effect, the Anderson impurity model, and the multichannel Kondo problem; see references [14–17]), there are only a few exceptions of integrable models with interactions containing impurities. Andrei and Johannesson [18] incorporated a magnetic impurity of arbitrary spin into the isotropic spin-$\frac{1}{2}$ Heisenberg chain. The interaction between the impurity and the neighbouring 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 [19, 20]. 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 [17, 20]. It has been argued [21] that these low-temperature properties of the impurity correspond to non-generic fixed points. The peculiarities, however, do not arise from integrability [22]. Other authors [23] proposed different models involving non-magnetic impurities, which do not introduce backward scattering.

Interactions among the conduction electrons of the host are particularly important in one dimension, where the properties change from those of a normal Fermi liquid to those of a Luttinger liquid [24]. In reference [25] it was shown, using Abelian bosonization and renormalization-group calculations, that for Luttinger liquids with magnetic impurity the Kondo temperature depends on the exchange coupling in a power-law fashion, but if the coupling is sufficiently strong, there is a crossover to the usual exponential dependence. Using the poor man's scaling method, it was argued in [26] that in Luttinger liquids at low temperatures the impurity spin is screened completely (for $S = \frac{1}{2}$), like in the Kondo effect for an ordinary Fermi liquid, and that the exchange coupling with the impurity flows to the strong-coupling regime for both antiferromagnetic and ferromagnetic interactions. Recently, in reference [27], it was shown using non-Abelian bosonization and boundary conformal field theory that the Kondo interaction corresponds to equal forward and backward scattering, and that there are two types of scaling fixed point: either a local Fermi liquid, or a non-Fermi liquid displaying critical behaviour.

In this paper we consider a magnetic impurity embedded into the supersymmetric t–J model. There is more than one example of magnetic impurity that can be devised without spoiling the integrability. In a previous contribution we presented the solution of the supersymmetric t–J model with an undercompensated Anderson-like mixed-valent impurity [28]. Here we consider a Kondo-like magnetic impurity embedded in the supersymmetric t–J model. The Bethe *ansatz* equations automatically ensure the integrability of the model. The impurity consists of a spin S on a given link, which by construction interacts only with electrons on both neighbouring sites via spin exchange. This coupling gives rise to underscreening of an effective spin $S + \frac{1}{2}$ to an effective spin S. The impurity is driven by the interactions of the host, and is hence quite different from an ordinary Kondo impurity. The effective impurity spin $S + \frac{1}{2}$ arises from the 'attractive' interactions in the host t–J model [7], where the ground state consists of a Dirac sea for electrons in singlet pairs. Since in the t–J host there are both charge and spin interactions, the charge of the impurity also interacts with the t–J host (in contrast to the case of a non-interacting host). This gives rise to intermediate-valence behaviour of the impurity [16]. Charge and spin fluctuations of the impurity, however, occur on different energy scales. The impurity takes one electron from the host, hence producing a hole in the Dirac sea. This destroys one gapless singlet pair giving rise to one energy scale which is specific to the host. The second energy scale is the usual Kondo temperature. Close to integer valence, two fixed points play a role for the spin degrees of freedom: (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 scattering matrices and the discrete Bethe *ansatz* equations diagonalizing the lattice gas with impurity are introduced in section 2. The monodromy matrix and details of the diagonalization of the transfer matrix are sketched in appendix A. In appendix B the impurity Hamiltonian is constructed for the lattice and for the continuum limit. In section 3 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 section 4, and concluding remarks follow in section 5.

2. Construction of the Bethe *ansatz* equations

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

$$H_0 = -t\sum_{i\sigma} P(c^{\dagger}_{i\sigma}c_{i+1\sigma} + c^{\dagger}_{i+1\sigma}c_{i\sigma})P + J\sum_i \left(\boldsymbol{S}_i\cdot\boldsymbol{S}_{i+1} - \frac{1}{4}n_i n_{i+1}\right) \qquad (1)$$

where $c^{\dagger}_{i\sigma}$ creates an electron of spin σ at site i, P is a projector that excludes the multiple occupancy of each site, $\boldsymbol{S}_i = c^{\dagger}_{i\sigma}\boldsymbol{S}_{\sigma\sigma'}c_{i\sigma'}$ are the spin-$\frac{1}{2}$ operators, $n_i = \sum_\sigma c^{\dagger}_{i\sigma}c_{i\sigma}$ is the number operator for site i, and J is the antiferromagnetic exchange coupling. The hopping t can be equated to 1.

Model (1) is only integrable for $J = 2t$, i.e. at the supersymmetric point [6, 11]. The scattering matrix for two electrons with wavenumbers k_1 and k_2 then takes the form [7]

$$\hat{X}(k_1,k_2) = \frac{(p_1-p_2)\hat{I} + \mathrm{i}\hat{P}}{p_1-p_2+\mathrm{i}} \qquad (2)$$

where $p = \frac{1}{2}\cot(k/2)$, and $\hat{I}$ and $\hat{P}$ are the identity and permutation operators, respectively. This scattering matrix satisfies the triangular Yang–Baxter relation, which, together with the excluded multiple occupancy of sites, provides necessary and sufficient conditions for the integrability of (1).

We introduce the impurity via its scattering matrix with the itinerant electrons. If the integrability of the supersymmetric t–J model is to be preserved, the impurity scattering matrix $\hat{S}$ has to satisfy the triangular Yang–Baxter relation with $\hat{X}$ [15, 16] (see appendix A). As already mentioned in section 1, the impurity scattering matrix following from the Yang–Baxter relations is not unique, i.e. more than one impurity form can be constructed without destroying the integrability [28].

In this paper we consider the impurity scattering matrix [29]

$$S^{\sigma\sigma'}_{MM'}(p-p_0) = a(p-p_0)\frac{(p-p_0+\mathrm{i}/2)\delta_{\sigma\sigma'}\delta_{MM'} + \mathrm{i}\hat{\sigma}_{\sigma\sigma'}\hat{S}_{MM'}}{p-p_0+\mathrm{i}} \qquad (3)$$

where the $\hat{\sigma}$ are the Pauli matrices, $\hat{S}$ the impurity spin matrices, M is the spin component of the impurity, the unprimed (primed) indices refer to the incoming (outgoing) states, and $a(p) = [(p^2+1)/(p^2+(S+\frac{1}{2})^2)]^{1/2}$. Here $S \neq 0$ is the spin of the impurity, $|M| \leqslant S$, and p_0 is a parameter controlling the impurity characteristics.

Consider now N_e itinerant electrons and the impurity in a box of N_a sites. Periodic boundary conditions imposed on a given electron require it to interchange position with all of the other electrons, each interchange involving a two-particle scattering matrix. Hence, when the particle is back at the original position, we obtain an operator consisting of a

product of $N_e - 1$ electron–electron scattering matrices, $\hat{X}$, and one scattering matrix due to the impurity, $\hat{S}$:

$$\hat{T}_j(p_j) = \hat{X}^{-1}_{j,j+1}(p_j - p_{j+1}) \cdots \hat{X}^{-1}_{j,N_e}(p_j - p_{N_e}) \times \hat{S}^{-1}_j(p_j - p_0)\hat{X}^{-1}_{j,1}(p_j - p_1) \cdots \hat{X}^{-1}_{j,j-1}(p_j - p_{j-1}). \tag{4}$$

One such operator (the transfer matrix) is obtained for each electron, i.e. $j = 1, \ldots, N_e$, and all N_e operators are to be diagonalized simultaneously (see appendix A). The corresponding eigenvalues are $\exp(\mathrm{i}k_j N_a) = [(p_j + \mathrm{i}/2)/(p_j - \mathrm{i}/2)]^{N_a}$. Due to the spin degree of freedom, the diagonalization of the operators $\hat{T}_j$ leads to a new eigenvalue problem that can be solved in terms of a second (nested) Bethe *ansatz*. Each Bethe *ansatz* gives rise to a set of rapidities, $\{p_j\}$, $j = 1, \ldots, N_e$, for the charges, and a further set, $\{\Lambda_\alpha\}$, $\alpha = 1, \ldots, M^*$, for the spins (M^* is the number of down-spin electrons), which satisfy the discrete Bethe *ansatz* equations for the t–J model with impurity:

$$\exp\{-\mathrm{i}\arctan[2(p_j - p_0)/(2S+1)] + \mathrm{i}\arctan(p_j - p_0)\}\left[\frac{p_j + \mathrm{i}/2}{p_j - \mathrm{i}/2}\right]^{N_a} = \prod_{\beta=1}^{M^*} \frac{p_j - \Lambda_\beta + \mathrm{i}/2}{p_j - \Lambda_\beta - \mathrm{i}/2} \qquad j = 1, \ldots, N_e \tag{5}$$

$$\frac{\Lambda_\alpha - p_0 + \mathrm{i}S}{\Lambda_\alpha - p_0 - \mathrm{i}S} \prod_{j=1}^{N_e} \frac{\Lambda_\alpha - p_j + \mathrm{i}/2}{\Lambda_\alpha - p_j - \mathrm{i}/2} = -\prod_{\beta=1}^{M^*} \frac{\Lambda_\alpha - \Lambda_\beta + \mathrm{i}}{\Lambda_\alpha - \Lambda_\beta - \mathrm{i}} \qquad \beta = 1, \ldots, M^*. \tag{6}$$

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 [7]

$$E = -2N_e + 2\sum_{j=1}^{N_e} \frac{1/2}{p_j^2 + 1/4}. \tag{7}$$

If $S = \frac{1}{2}$, equations (5) and (6) correspond to the Bethe *ansatz* equations of the standard supersymmetric t–J model for $N_e + 1$ particles and M^* flipped spins. The additional charge has rapidity p_0, which is not determined selfconsistently. Hence, the 'additional electron' is distinguishable from the remaining ones.

If we suppress the charge fluctuations in equations (5) and (6), i.e. equating p_j to zero for all j on the right-hand side of (5) and on the left-hand side of (6), and with $p_0 = 1/J$ (J is the Kondo coupling), we essentially (there are two partial waves) recover the Bethe *ansatz* equations of the standard Kondo problem. The Hamiltonian describing the interaction of the impurity with the itinerant electrons is derived in appendix B.

3. Thermodynamic Bethe *ansatz* equations

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, (5) and (6). The structure of the solutions of the Bethe *ansatz* equations is determined by the host (the supersymmetric t–J model) and can be taken over from reference [7]. The classification of states is also similar to that of the fermion gas with an attractive δ-function potential [30, 31], and the $j = 1/2$ Anderson impurity in the $U \to \infty$ limit [32]. In fact, the t–J host also corresponds to an infinite on-site repulsion of electrons (excluded multiple occupation of each site).

In the thermodynamic limit the rapidities are classified according to (i) $N_e - 2M^{*\prime}$ real charge rapidities, corresponding to unpaired propagating electrons, (ii) $2M^{*\prime}$ complex charge rapidities, representing bound or spin-paired electron states, of the form $p_\alpha^\pm = \Lambda'_\alpha \pm \mathrm{i}/2$, where Λ'_α is a real spin rapidity, $\alpha = 1, \ldots, M^{*\prime}$, and (iii) M_n^* strings of complex spin rapidities (bound spin states) of length $n-1$, $n = 1, \ldots, \infty$, of the form

$$\Lambda_{\alpha,n}^\mu = \Lambda_{\alpha,n} + \mathrm{i}\mu/2 \qquad \mu = -(n-1), -(n-3), \ldots, n-1 \tag{8}$$

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

$$M^{*\prime} + \sum_{n=1}^{\infty} n M_n^* = M^*.$$

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 the above solutions into the discrete Bethe *ansatz* equations, we obtain after Fourier transforming and some algebra [7]

$$\hat\sigma_{m+1,h}(\omega) + \hat\sigma_{m-1,h}(\omega) + \delta_{m,2S}\mathrm{e}^{\mathrm{i}p_0\omega}/(2\pi N_a) = 2\cosh\left(\frac{1}{2}\omega\right)[\hat\sigma_m(\omega) + \hat\sigma_{m,h}(\omega)] \qquad m \geqslant 1 \tag{9}$$

$$\hat\sigma_{1,h}(\omega) + \hat\sigma'_h(\omega) + 1 = 2\cosh\left(\frac{1}{2}\omega\right)[\hat\rho(\omega) + \hat\rho_h(\omega)] \tag{10}$$

$$\mathrm{e}^{-(1/2)|\omega|}\hat\sigma'_h(\omega) + \mathrm{e}^{-(1/2)|\omega|} + \mathrm{e}^{\mathrm{i}p_0\omega}[\mathrm{e}^{-(S+1/2)|\omega|} - \mathrm{e}^{-|\omega|} - \mathrm{e}^{-(S-1/2)|\omega|} - 1]/(4\pi N_a) = 2\cosh\left(\frac{1}{2}\omega\right)[\hat\sigma'(\omega) + \hat\sigma'_h(\omega)] + \hat\rho(\omega) \tag{11}$$

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 [7]

$$\begin{aligned} E/N_a &= -2N_e/N_a + 2\pi\int \mathrm{d}p\ \rho(p)a_1(p) + 2\pi\int \mathrm{d}\Lambda\ \sigma'(\Lambda)a_2(\Lambda) \\ N_e/N_a &= \int \mathrm{d}p\ \rho(p) + 2\int \mathrm{d}\Lambda\ \sigma'(\Lambda) \\ S_z/N_a &= S/N_a + \frac{1}{2}\int \mathrm{d}p\ \rho(p) - \sum_{n=1}^{\infty} n\int \mathrm{d}\Lambda\ \sigma_n(\Lambda) \end{aligned} \tag{12}$$

where $a_n(x) = (1/\pi)[2n/(4x^2 + n^2)]$.

The above equations are valid quite generally for all states. We now restrict ourselves to thermal equilibrium by minimizing the free-energy functional with respect to the density functions, subject to (9)–(11) and the constraints of constant number of electrons and constant magnetization (the corresponding Lagrange multipliers are the chemical potential μ and the magnetic field H). We introduce an energy function for each class of rapidities, defined as

$$\begin{aligned} &\rho_h/\rho = \exp(\varepsilon(p)/T) \qquad \sigma'_h/\sigma' = \exp(\psi(\Lambda)/T) \\ &\sigma_{n,h}/\sigma_n = \exp(\varphi_n(\Lambda)/T) = \eta_n(\Lambda) \qquad \varphi_0 \equiv -\varepsilon \end{aligned} \tag{13}$$

which satisfy the following integral equations [7]:

$$\varepsilon(p) = 2\pi G_0(p) + TG_0 \star \ln[(1 + \mathrm{e}^{\psi/T})/(1 + \eta_1)] \tag{14}$$

$$\psi(\Lambda) = -2 + 2\pi G_1(\Lambda) - \mu + TG_1 \star \ln(1 + \mathrm{e}^{\psi/T}) + TG_0 \star \ln(1 + \mathrm{e}^{-\varepsilon/T}) \tag{15}$$

$$\varphi_n(\Lambda) = TG_0 \star \ln[(1 + \eta_{n+1})(1 + \eta_{n-1})] \tag{16}$$

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

$$\lim_{n\to\infty} \frac{1}{n}\varphi_n(\Lambda) = H. \tag{17}$$

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

$$\begin{aligned} F_{tJ}/N_a &= -T\int \mathrm{d}p\ a_1(p)\ln(1+\mathrm{e}^{-\varepsilon(p)/T}) - T\int \mathrm{d}\Lambda\ a_2(\Lambda)\ln(1+\mathrm{e}^{-\psi(\Lambda)/T}) \\ &= -\psi(0) - 2\mu - 2 \end{aligned} \tag{18}$$

$$\begin{aligned} F_{imp} = -\frac{T}{2}\int \mathrm{d}\Lambda\ &[G_{2S+1}(\Lambda - p_0) - G_2(\Lambda - p_0) - G_{2S-1}(\Lambda - p_0) - G_0(\Lambda - p_0)] \\ &\times \ln(1+\mathrm{e}^{\psi(\Lambda)/T}) - T\int \mathrm{d}\Lambda\ G_0(\Lambda - p_0)\ln(1+\mathrm{e}^{\varphi_{2S}(\Lambda)/T}) \end{aligned} \tag{19}$$

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

If the temperature is much larger than the bandwidth, i.e. $T \gg 2$, we can neglect the independent (driving) terms in equations (14)–(16), so the potentials ε, ψ, and φ_n do not depend on p and Λ, and satisfy [7, 30]

$$\begin{aligned} &1 + \eta_n = \left\{\sinh\left[(nH/2T) + x\right]/\sinh(H/2T)\right\}^2 \\ &\mathrm{e}^{2\varepsilon/T} = (1+\mathrm{e}^{\psi/T})/(1+\eta_1) \\ &\mathrm{e}^{2(\psi+\mu)/T} = (1+\mathrm{e}^{-\varepsilon/T})(1+\mathrm{e}^{\psi/T}) \end{aligned} \tag{20}$$

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

$$\mathrm{e}^{2x} = \mathrm{e}^{2H/T}[1+\mathrm{e}^{-(H+2\mu)/2T}]/[1+\mathrm{e}^{(H-2\mu)/2T}]. \tag{21}$$

The free energy of the host corresponds to the three degrees of freedom per site of a hole and a spin $\frac{1}{2}$, $F_{tJ}/N_a = -T\ln[1 + 2\mathrm{e}^{\mu/T}\cosh(H/2T)]$, where μ is measured from the bottom of the band. The free energy of the impurity is discussed in section 4.

The ground-state integral equations are obtained from equations (14)–(16) in the limit $T \to 0$. The energy potentials φ_n are positive over the entire Λ range for all $n \geqslant 1$, so string states are not occupied as $T \to 0$. Only the ε-band (unpaired electrons) and the ψ-band (spin-paired electrons) are populated. The zeros of the potentials define the Fermi points, $\varepsilon(\pm B) = 0$ and $\psi(\pm Q) = 0$. Both integration limits, B and Q, are functions of μ and H. In the limit $T \to 0$, equations (14) and (15) yield [7]

$$\varepsilon(p) = -2 + 2\pi a_1(p) - \frac{1}{2}H - \mu - \int_{|\Lambda|>Q} \mathrm{d}\Lambda\ a_1(p-\Lambda)\psi(\Lambda) \tag{22}$$

$$\begin{aligned} \psi(\Lambda) = -4 + 2\pi a_2(\Lambda) - 2\mu &- \int_{|\Lambda'|>Q} \mathrm{d}\Lambda'\ a_2(\Lambda - \Lambda')\psi(\Lambda') \\ &- \int_{|p|>B} \mathrm{d}p\ a_1(\Lambda - p)\varepsilon(p). \end{aligned} \tag{23}$$

Similar equations determine the density functions. The energy, the number of electrons,

and the magnetization of the host are given by

$$E/N_a = -2N_e/N_a + 2\pi \int_{|p|>B} \mathrm{d}p\ \rho(p)a_1(p) + 2\pi \int_{|\Lambda|>Q} \mathrm{d}\Lambda\ \sigma'(\Lambda)a_2(\Lambda)$$
$$N_e/N_a = \int_{|p|>B} \mathrm{d}p\ \rho(p) + 2\int_{|\Lambda|>Q} \mathrm{d}\Lambda\ \sigma'(\Lambda) \tag{24}$$
$$S_z/N_a = S/N_a + \frac{1}{2}\int_{|p|>B} \mathrm{d}p\ \rho(p).$$

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 [7]. The ground-state properties of the impurity are discussed in section 4.

4. Properties of the impurity

On the one hand, in the continuum limit the impurity scattering matrix, equation (3), is that of the single-channel Kondo problem of spin S [29]. On the other hand, the impurity is driven by the host, i.e. by the supersymmetric t–J model, through the energy potentials $\psi(\Lambda)$ and $\varphi_{2S}(\Lambda)$. Hence, some impurity properties are then expected to be different from those of the standard Kondo problem. In particular, the t–J model correlates spins and charges, so in contrast to the case for the ordinary Kondo problem, our impurity also couples to the charges. The impurity then acquires some mixed-valent character, corresponding to two magnetic configurations [33, 34]. Except for in special limits, the integral equations for the energy potentials of the t–J model cannot be solved analytically. We therefore limit ourselves to discussing the high-temperature limit and the ground-state properties of the impurity.

In the high-temperature limit the leading contribution corresponds to constant energy potentials, independent of Λ and p, and the impurity free energy (19) is given by

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

Expressing $\mathrm{e}^{\psi/T}$ and $\mathrm{e}^{\varphi_{2S}/T}$ using equations (20) and (21), the zero-field impurity free energy can be written approximately as

$$F_{imp} = -T\ln[(2S + 1 + f)f] \tag{25}$$

where $f = [1 + \exp(g(p_0) - \mu)/T)]^{-1}$ is the Fermi function, and μ is measured from the bottom of the conduction band. This expression 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 exact expression for the function $g(p_0)$ is complicated, but it 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 favoured for $\mu \to 0$, i.e. for low electron densities, while close to half-filling, $\mu = 2\ln(2)$, the configuration of spin $S + \frac{1}{2}$ is favoured.

The field dependence of the free energy at high T is also given by equations (19), (20), and (21). Again the exact expression is tedious, so we limit ourselves to presenting

an approximate one, which includes the field dependence and interpolates between the two configurations:

$$F_{imp} = -T \ln\{\mathcal{Z}_{(S+1/2)} + \exp[(g(p_0) - \mu)/T]\mathcal{Z}_S\} \tag{26}$$

where $\mathcal{Z}_S = \sinh[(2S+1)H/2T]/\sinh(H/2T)$ is the partition function of a free spin S in a magnetic field. 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 [35]. The Curie constant and the entropy under the Schottky peak depend on the valence admixture, i.e. the parameter $g(p_0) - \mu$.

To discuss the ground-state properties of the impurity, we observe that equations (9)–(11) 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 non-zero rapidity distributions in the ground state. In the limit $T \to 0$, the densities for the impurity satisfy

$$\rho_{i,h}(p) + \rho_i(p) + \int_{|\Lambda|>Q} \mathrm{d}\Lambda\ a_1(p-\Lambda)\sigma_i'(\Lambda) = \frac{1}{2}[a_{2S+1}(p-p_0) - a_2(p-p_0)] \tag{27}$$

$$\sigma_{i,h}'(\Lambda) + \sigma_i'(\Lambda) + \int_{|\Lambda'|>Q} \mathrm{d}\Lambda'\ a_2(\Lambda-\Lambda')\sigma_i'(\Lambda') + \int_{|p|>B} \mathrm{d}p\ a_1(\Lambda-p)\rho_i(p)$$
$$= \frac{1}{2}[a_{2S+2}(\Lambda-p_0) - a_{2S}(\Lambda-p_0) - a_1(\Lambda-p_0) - a_3(\Lambda-p_0)] \tag{28}$$

and the impurity energy, magnetization, and valence are given by

$$E_{imp} = 2\pi \int_{|p|>B} \mathrm{d}p\ \rho_i(p)a_1(p) + 2\pi \int_{|\Lambda|>Q} \mathrm{d}\Lambda\ \sigma_i'(\Lambda)a_2(\Lambda)$$
$$M_{imp} = S + \frac{1}{2}\int_{|p|>B} \mathrm{d}p\ \rho_i(p) \tag{29}$$
$$n_{imp} = \int_{|p|>B} \mathrm{d}p\ \rho_i(p) + 2\int_{|\Lambda|>Q} \mathrm{d}\Lambda\ \sigma_i'(\Lambda).$$

The integral equations are coupled Fredholm ones, and differ from the single Wiener–Hopf equation of the standard Kondo impurity [14, 15, 29]. This is the consequence of the charges coupling to the impurity via the correlations in the host, and the fact that there are two Fermi points (forward- and backward-moving particles). 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. for $B \to \infty$, only one integral equation remains. Analytical results can be obtained in the limits of low electron density ($Q \to \infty$) and low hole density ($Q \to 0$). 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 the bound itinerant electron) of the impurity is ($S > 0$)

$$n_{imp} = -\frac{1}{2\pi}\frac{Q}{Q^2 - p_0^2} \tag{30}$$

where we have 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

$$n_{imp} = -1 + \mathcal{O}(Q). \tag{31}$$

Hence, in this limit we introduced one localized hole into the host (one electron of the host is localized at the impurity). Corrections for small Q (low hole concentration) reduce the valence of holes proportionally to Q. Hence, as a function of band filling, the valence smoothly varies between 0 ($N_e \to 0$) and -1 ($N_e \to N_a$). The fact that the impurity has a negative charge density is a novel feature, not common to other impurity models. It is an essential property of the supersymmetric t–J model, for which there is an effective attraction that causes gapless singlet pairs. This effect appears to be reversed at high temperatures, where n_{imp} grows monotonically with the electron density.

For $S = \frac{1}{2}$, the impurity corresponds to adding one unbound electron to the system, which produces a negative 'driving term' in equation (28). Thus, in this case the negative valence of the impurity is similar to the parity effect, i.e. the difference between the behaviours for even and odd numbers of electrons (see also equations (5) and (6)).

The ground-state magnetization is obtained following standard procedures (see reference [16]) from equations (27) and (28). Using equation (28), we express σ' as a function of the remaining quantities and insert it into (27). We obtain a Fredholm integral equation for ρ with two kinds of driving terms, namely, independent terms depending on p_0 and a term involving σ'_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 integral equation for the 'Kondo'-like spin excitations is

$$\rho_{i,h}(p) + \rho_i(p) - \int_{|p'|>B} \mathrm{d}p'\ G_1(p-p')\rho_i(p') = G_{2S}(p-p_0) \tag{32}$$

where we may assume that p_0 is positive and large. Equation (32) is of the Fredholm type and can then be reduced to a hierarchical sequence of Wiener–Hopf integral equations. The leading contribution is just (32) 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 $(1/\pi)\ln(H/T_K)$, where T_K plays the role of a 'Kondo' temperature. The solution of the Wiener–Hopf equation yields [16]

$$M_{imp} = S\left[1 + \frac{1}{2}\mathcal{L}^{-1} - \frac{1}{4}\ln(\mathcal{L})/\mathcal{L}^2 + \cdots\right] \qquad H \ll T_K \qquad S \neq 0 \tag{33}$$

$$M_{imp} = \left(S + \frac{1}{2}\right)\left[1 - \frac{1}{2}\mathcal{L}^{-1} - \frac{1}{4}\ln(\mathcal{L})/\mathcal{L}^2 + \cdots\right] \qquad H \gg T_K \tag{34}$$

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 (the logarithms characterize asymptotic freedom) to the itinerant electrons. For intermediate fields, the magnetization smoothly interpolates between these two limits. Corrections of higher logarithmic order to (33) and (34) require the solution of other equations in the hierarchical sequence of Wiener–Hopf equations, but these contributions are non-universal.

The 'Kondo' limit corresponds to the suppression of the charge (valence) fluctuations of the impurity. Charge fluctuations are described by the energy potential $\psi(\Lambda)$, so equation (14) can be replaced by

$$\varepsilon(p) = \epsilon_F \mathrm{e}^{-\pi|p|} - TG_0 \star \ln(1+\eta_1) \tag{35}$$

where we kept only the low-lying excitations, given by large $|p|$, and ϵ_F is an energy scale of the order of the band half-width. The coupled integral equations (16) and (35) are very similar to those of the ordinary Kondo problem, except that there are two Fermi points in

the Dirac sea of spin rapidities, in contrast to the case of the Kondo problem for free host electrons which involves only one partial wave [14, 15]. The impurity free energy due to spin fluctuations is given by the term of (19) involving φ_{2S}. This term contains the only p_0-dependence in the problem. Assuming that p_0 is positive and large (the Kondo limit), $p_0 = 1/J$ plays the role of the Kondo coupling. 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.

The magnetic susceptibility shows Kondo logarithms in both the high- and low-temperature limits [14, 15]:

$$\chi = (\mu^2/3T)\left[1 - \mathcal{L}_T{}^{-1} + \frac{1}{2}\ln|\mathcal{L}_T|/\mathcal{L}_T{}^2 + \cdots\right] \tag{36}$$

where $\mathcal{L}_T = \ln(T_K/T)$ and μ is the effective magnetic moment, which takes different forms in the two limits, i.e., $\mu^2 = S(S+1)$ as $T \to 0$ and $\mu^2 = (S+\frac{1}{2})(S+\frac{3}{2})$ as $T \to \infty$. Hence, as seen already for the ground state, the impurity spin is only partially compensated at low T.

5. Conclusions

In this paper we have considered a magnetic impurity embedded into a one-dimensional lattice with strongly interacting electrons. The integrable model providing the background of itinerant electrons is the supersymmetric t–J model. The translational invariance is broken by introducing an additional spin S, but the integrability is preserved by construction. We introduced an impurity scattering matrix, equation (3), 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, provides the necessary and sufficient conditions for the integrability of the t–J model with impurity. The interaction of the itinerant electrons with the impurity is via an exchange interaction with the two neighbouring sites of the impurity.

We derived the Bethe *ansatz* equations, diagonalizing the t–J model with impurity, classified all of 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.

Due to the interactions among the host electrons, the impurity is in a mixed-valent state resulting from the superposition of the spin-S and spin-$(S+\frac{1}{2})$ configurations. This is seen both from the high-temperature free energy of the impurity and from the ground-state properties. The degree of admixture is a function of the parameter p_0 (related to the exchange coupling with the impurity) and the chemical potential. At high T and for a given p_0, the fraction of localized electron at the impurity increases monotonically with 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, i.e. the impurity absorbs a fraction of an electron and creates a hole in the Dirac sea of the host. This implies a negative impurity charge density, a unique feature of our model. Such behaviour is due to the 'attractive' nature of the interactions in the host (the supersymmetric t–J model), for which electrons paired into singlets determine the low-temperature properties of the model.

In the limit of large $|p_0|$ and for a given finite electron density at low temperatures, the impurity can be mapped onto the single-orbital channel Kondo problem of spin $S+\frac{1}{2}$. This mapping is only approximate, because of the correlations among the conduction electrons, and the interaction between impurity and itinerant electrons not being a contact potential for

the lattice problem. Hence, on the one hand charge fluctuations are present, and on the other hand the impurity is scattered not only 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 impact on the impurity properties if T_K is much smaller than the bandwidth.

Thus, in the Kondo limit the impurity is (under)compensated, i.e. it has an effective spin S in a small field at low temperatures. The field and/or the temperature (if it is 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 $S+\frac{1}{2}$; and at higher T ($\approx T_K$) the broad structure of the Kondo resonance gives rise to the second peak [35]. At larger fields, the two energy scales are no longer separated, and the two peaks merge into one.

It was mentioned in section 2 that the electron–impurity scattering matrix satisfying the triangular Yang–Baxter relation is not uniquely defined. In reference [28] we considered a different impurity embedded into the supersymmetric t–J chain. The corresponding scattering matrix is (instead of (3))

$$S^{\sigma\sigma'}_{MM'}(p-p_0)=\delta_{\sigma\sigma'}\delta_{MM'}+(M\sigma|M+\sigma)(M'\sigma'|M'+\sigma')\frac{\mathrm{i}(2S+1)}{p-p_0-\mathrm{i}(2S+1)/2}P^{\sigma\sigma'}_{MM'} \tag{37}$$

where $P^{\sigma\sigma'}_{MM'}=\delta_{\sigma\sigma'}\delta_{MM'}+\delta_{-\sigma\sigma'}\delta_{M'M+2\sigma}$. The Clebsch–Gordan coefficient $(M\sigma|M+\sigma)$, which is a shorthand notation for

$$\left(SM;\frac{1}{2}\sigma\middle|S\frac{1}{2}\left(S+\frac{1}{2}\right)M+\sigma\right) \tag{38}$$

selects the way in which 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. Hence, the impurity has intermediate valence already, without correlations in the host [16, 36, 37]. This impurity is then quite different from the one considered in the present paper.

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Appendix A. The monodromy matrix and diagonalization of the transfer matrix

The two-electron scattering matrix (2) satisfies the triangular Yang–Baxter relation

$$\begin{aligned}&X^{\sigma_1\sigma_1'}_{\sigma_2\sigma_2'}(p_1-p_2)X^{\sigma_1'\sigma_1''}_{\sigma_3\sigma_3'}(p_1-p_3)X^{\sigma_2'\sigma_2''}_{\sigma_3'\sigma_3''}(p_2-p_3)\\&\qquad=X^{\sigma_2\sigma_2'}_{\sigma_3\sigma_3'}(p_2-p_3)X^{\sigma_1\sigma_1'}_{\sigma_3'\sigma_3''}(p_1-p_3)X^{\sigma_1'\sigma_1''}_{\sigma_2'\sigma_2''}(p_1-p_2)\end{aligned} \tag{A1}$$

with the identity and permutation operators given by $\hat{I}=\delta_{\sigma_1\sigma_1'}\delta_{\sigma_2\sigma_2'}$ and $\hat{P}=\delta_{\sigma_1'\sigma_2}\delta_{\sigma_2'\sigma_1}$. Unprimed (primed) spin indices refer to states before (after) scattering. Similarly, the electron–impurity scattering matrix satisfies

$$\begin{aligned}&X^{\sigma_1\sigma_1'}_{\sigma_2\sigma_2'}(p_1-p_2)S^{\sigma_1'\sigma_1''}_{MM'}(p_1-p_0)S^{\sigma_2'\sigma_2''}_{M'M''}(p_2-p_0)\\&\qquad=S^{\sigma_2\sigma_2'}_{MM'}(p_2-p_0)S^{\sigma_1\sigma_1'}_{M'M''}(p_1-p_0)X^{\sigma_1'\sigma_1''}_{\sigma_2'\sigma_2''}(p_1-p_2).\end{aligned} \tag{A2}$$

Equations (A1) and (A2) are the necessary and sufficient conditions for the integrability [15, 16].

The monodromy matrix [15, 16] is defined as

$$L^{\{\sigma_1',\ldots,\sigma_{N_e+1}'\}\tau'}_{\{\sigma_1,\ldots,\sigma_{N_e+1}\}\tau}(\alpha;\alpha_1,\ldots,\alpha_{N_e+1}) = X^{\tau'\mu_1}_{\sigma_1'\sigma_1}(\alpha_1-\alpha)X^{\mu_1\mu_2}_{\sigma_2'\sigma_2}(\alpha_2-\alpha)\cdots X^{\mu_{N_e-1}\mu_{N_e}}_{\sigma_{N_e}'\sigma_{N_e}}(\alpha_{N_e}-\alpha)S^{\mu_{N_e}\tau}_{MM'}(\alpha_{N_e+1}-\alpha) \tag{A3}$$

with implicit summation over all of the μ_j-indices. With respect to the indices τ and τ', the monodromy matrix forms a 2×2 matrix, which we denote as $\hat{L}^{\tau'}_{\tau}(\alpha)$ (omitting the spin indices and parameters α_j) or in terms of the components [15]

$$\hat{L}^1_1=\hat{A} \qquad \hat{L}^1_2=\hat{B} \qquad \hat{L}^2_1=\hat{C} \qquad \hat{L}^2_2=\hat{D}. \tag{A4}$$

The trace of $\hat{L}^{\tau'}_{\tau}(\alpha)$ is the transfer matrix, $\hat{T}(\alpha)=\sum_\tau \hat{L}^{\tau}_{\tau}(\alpha)=\hat{A}(\alpha)+\hat{D}(\alpha)$. It is straightforward to prove that transfer matrices for different values of the spectral parameter α commute and can all be diagonalized simultaneously [15, 16].

The operators $\hat{A}$, $\hat{B}$, $\hat{C}$ and $\hat{D}$ obey commutation relations which are obtained from equations (A1) and (A2) by explicitly using the two-electron scattering matrix, equation (2). The results are similar to those for other models [15, 16], and will not be repeated here. The vacuum state Ω_0 is the state of maximum spin (all electron spins point upward and the impurity is in the state $M=S$). The $\hat{C}$-operator acts like a 'spin-raising' operator, and when applied to Ω_0 it yields zero. On the other hand, $\hat{B}$ has the properties of a 'spin-lowering' operator, so the vector

$$\Omega(\alpha_1',\ldots,\alpha_{M^*}')=\prod_{\beta=1}^{M^*}\hat{B}(\alpha_\beta')\Omega_0 \tag{A5}$$

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 $\alpha_1',\ldots,\alpha_{M^*}'$ under which the vector (A5) is an eigenvector of $\hat{A}(\alpha)+\hat{D}(\alpha)$. Applying $\hat{A}(\alpha)+\hat{D}(\alpha)$ to $\Omega(\alpha_1',\ldots,\alpha_{M^*}')$ and commuting $\hat{A}+\hat{D}$ through all the $\hat{B}$-operators, two types of term arise, namely: (i) those reproducing the vector (A5); and (ii) 'unwanted' terms of different form. Hence, the vector (A5) is an eigenvector of $\hat{A}+\hat{D}$ only if the coefficients of the 'unwanted' terms vanish. This leads to the following condition on the set of parameters $\{\alpha_\beta'\}$:

$$\frac{\alpha_{N_e+1}-\alpha_\gamma+\mathrm{i}(2S+1)/2}{\alpha_{N_e+1}-\alpha_\gamma-\mathrm{i}(2S-1)/2}\prod_{j=1}^{N_e}\frac{\alpha_j-\alpha_\gamma'+\mathrm{i}}{\alpha_j-\alpha_\gamma'}=-\prod_{\beta=1}^{M^*}\frac{\alpha_\gamma'-\alpha_\beta'-\mathrm{i}}{\alpha_\gamma'-\alpha_\beta'+\mathrm{i}} \tag{A6}$$

for $\gamma=1,\ldots,M^*$.

The eigenvalue of the vector (A5) applied to $\hat{A}+\hat{D}$ is then

$$a(\alpha_{N_e+1}-\alpha)\frac{\alpha_{N_e+1}-\alpha+\mathrm{i}(2S+1)/2}{\alpha_{N_e+1}-\alpha+\mathrm{i}}\prod_{\beta=1}^{M^*}\frac{\alpha-\alpha_\beta'+\mathrm{i}}{\alpha-\alpha_\beta'} + a(\alpha_{N_e+1}-\alpha)\frac{\alpha_{N_e+1}-\alpha-\mathrm{i}(2S-1)/2}{\alpha_{N_e+1}-\alpha+\mathrm{i}}\prod_{j=1}^{N_e}\frac{\alpha_j-\alpha}{\alpha_j-\alpha+\mathrm{i}}\prod_{\beta=1}^{M^*}\frac{\alpha-\alpha_\beta'-\mathrm{i}}{\alpha-\alpha_\beta'}. \tag{A7}$$

With $\alpha_{N_e+1}=p_0$, $\alpha_l=p_l$ for $l=1,\ldots,N_e$, $\alpha=p_j$, and setting $\alpha_\beta'=\Lambda_\beta+\mathrm{i}/2$ in (A6) and (A7), we obtain the discrete Bethe *ansatz* equations for the model.

Appendix B. The impurity Hamiltonian

By construction of the transfer matrix, the impurity spin interacts only with the two nearest-neighbour sites. The Hamiltonian describing the interaction between the impurity and the itinerant electrons is obtained by differentiating the logarithm of the transfer matrix $\hat{T}(\alpha)$ with respect to α at the point $\alpha = 0$, and has the form $H_{t-J,imp} = H_0 + H_{imp}$, where H_0 is given by equation (1). Here the impurity is situated at the site $N_a + 1$. H_0 can conveniently be written in terms of Hubbard operators as [8, 10] $H_0 = \sum_{n=1}^{N_a-1} H_{n,n+1}$, where

$$H_{n,n+1} = -\sum_{\sigma,\tau=\pm1} (X_n^{\sigma,0} X_{n+1}^{0,\sigma} + X_n^{0,\sigma} X_{n+1}^{\sigma,0} - X_n^{\sigma,\tau} X_{n+1}^{\tau,\sigma} + X_n^{0,0} X_{n+1}^{0,0}). \tag{B8}$$

For the impurity Hamiltonian we obtain

$$\begin{aligned} H_{imp} = {} & h_1(S, p_0)(H_{N_a,N_a+1} + H_{N_a+1,1}) + h_2(S, p_0) H_{N_a,1} \\ & + \mathrm{i}\, h_3(S, p_0)[(H_{N_a,N_a+1} + H_{N_a+1,1}), H_{N_a,1}] \end{aligned} \tag{B9}$$

where

$$\begin{aligned} H_{N_a,N_a+1} &= -\sum_{\sigma,M} (X_{N_a}^{\sigma,0} X_{N_a+1}^{0,M} + X_{N_a}^{0,\sigma} X_{N_a+1}^{M,0} - X_{N_a}^{\sigma,M} X_{N_a+1}^{M,\sigma} + X_{N_a}^{0,0} X_{N_a+1}^{0,0}) \\ H_{N_a+1,1} &= -\sum_{\sigma,M} (X_{N_a+1}^{\sigma,0} X_1^{0,M} + X_{N_a+1}^{0,\sigma} X_1^{M,0} - X_{N_a+1}^{\sigma,M} X_1^{M,\sigma} + X_{N_a+1}^{0,0} X_1^{0,0}). \end{aligned} \tag{B10}$$

Here $X^{a,b} = |a\rangle\langle b|$ are the Hubbard operators ($a, b = 0, \pm1$ for host electrons, and $a, b = 0, -S, \ldots, S$, $|M| \leqslant S$ for the impurity), and the square bracket in (B9) denotes the commutator. Note that both host and impurity states are restricted to only one particle (or hole) at each site. $h_1(S, p_0)$ and $h_2(S, p_0)$ are even functions of p_0, and $h_3(S, p_0)$ is an odd function of p_0. The impurity Hamiltonian breaks the parity and the time-reversal symmetries separately, but, of course, PT is conserved. The sign of the parameter p_0 is important, in particular if finite-size effects are considered, since it gives rise to a mesoscopic momentum.

It is instructive to study the continuum limit of the model, i.e. the limit where the lattice constant tends to zero. We can then linearize the kinetic energy in the momentum around the Fermi level and restrict ourselves to low-energy excitations. Assume that the two Fermi points are given by $\pm k_{FS}$, related to $\pm p_{FS}$ by $p_{FS} = \frac{1}{2}\cot(k_{FS}/2)$. Using the notation $v = [2\sin(k_{FS}/2)]^{-2}$ for the group velocity of the electrons, we have that the scattering matrices take the form

$$\hat{X}(k_1 - k_2) = \frac{(k_1 - k_2)\hat{I} - \mathrm{i}v^{-1}\hat{P}}{k_1 - k_2 - \mathrm{i}v^{-1}} \tag{B11}$$

$$S_{MM'}^{\sigma\sigma'}(k - \epsilon) = a(p - p_0)\frac{[(2k - 2\epsilon - \mathrm{i})/2]\delta_{\sigma\sigma'}\delta_{MM'} - \mathrm{i}v^{-1}\hat{\sigma}_{\sigma\sigma'}\hat{S}_{MM'}}{k - \epsilon - \mathrm{i}v^{-1}}. \tag{B12}$$

Identifying $v^{-1} = V^2/(2S + 1)$, these scattering matrices are those of a mixed-valence impurity with two magnetic configurations of spins S and $S + \frac{1}{2}$ hybridized via an electron of spin $\frac{1}{2}$ [16]. Here ϵ is related to p_0, and represents the energy difference between the two configurations relative to the Fermi level. The two partial waves in one dimension, i.e. 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 (the 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 [33, 34]

$$H_{imp} = \epsilon \sum_{M} |SM\rangle\langle SM| + V \sum_{\sigma M_1 M} \int \mathrm{d}x\ \delta(x)[c_\sigma^\dagger(x)|S_1 M_1\rangle\langle SM| + |SM\rangle\langle S_1 M_1|c_\sigma(x)] \tag{B13}$$

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

$$\sum_{M_1} |S_1 M_1\rangle\langle S_1 M_1| + \sum_{M} |SM\rangle\langle SM| = 1. \tag{B14}$$

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