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Coqblin–Schrieffer impurity in a one-dimensional correlated electron lattice

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Abstract. We consider electrons of effective spin S on a chain with nearest-neighbour hopping t constrained by the excluded multiple occupancy of the lattice sites, and spin exchange J between neighbouring sites. The spin space of the model is SU$(2S+1)$ invariant, and at the supersymmetric point, $J=t$, the charge and the spin play identical roles forming an integrable SU$(2S+2)$ superalgebra. Without compromising the integrability we introduce a Coqblin–Schrieffer-like impurity of spin S, which interacts with the correlated conduction states of the host. The discrete Bethe *ansatz* equations diagonalizing the host with impurity are derived and the ground-state properties of the impurity are studied as a function of the Kondo exchange coupling. An undercompensated impurity of spin S embedded into a chain of interacting spin-$\frac{1}{2}$ electrons is also discussed.

1. Introduction

Impurities play an important role in strongly correlated electron systems, especially in one dimension (1D), where even a small quantity of defects may change the properties drastically. Interactions in the host are particularly important in 1D, where the system changes from a normal Fermi liquid to a Luttinger liquid [1]. The effects of the interactions on the properties of an impurity have been investigated by means of bosonization, renormalization groups, 'poor man's' scaling, boundary conformal field theory [2], and the Bethe *ansatz* [3–7].

An impurity introduced into an integrable host usually destroys the integrability. The interaction between the host and impurity has to have a special form in order to preserve the integrability. Andrei and Johannesson [8] (see also references [9, 10]) incorporated a magnetic impurity of arbitrary spin into the isotropic spin-$\frac{1}{2}$ Heisenberg chain without spoiling the integrability. It has been argued [11] that this model, however, corresponds to a non-generic fixed point.

In recent papers we succeeded in constructing 1D integrable correlated electron lattice models with a magnetic impurity via the quantum inverse scattering method [4–7]. Several combinations of hosts, e.g. two supersymmetric variants of the t–J model (a brief discussion of these host models is given in the appendix) and the Hubbard model, and impurities, e.g. exchange and intermediate-valence impurities, have been considered. The scattering matrix of the electrons in the host and the scattering matrix of electrons with the impurity have to satisfy the triangular Yang–Baxter relation. This is the necessary and sufficient condition for the integrability, which imposes restrictions on the impurity. The overall picture emerging from this study is as follows.

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(i) Correlations in the host strongly couple to the charge sector of the impurity without affecting the spin sector. The screening of the impurity spin is then unchanged with respect to free electrons.

(ii) The correlations drive the impurity away from integer-valence into the mixed-valence region with a concomitant increase of the Kondo temperature. A fraction of an itinerant electron (hole) is localized at the impurity site.

(iii) The impurity is placed on a link of the chain and interacts with both neighbouring lattice sites. Hence, the impurity interacts with both partial waves, i.e. with states of even and odd parity with respect to the impurity site, in contrast with the situation in a non-interacting host, where the coupling is only with even-parity (s-wave) conduction states.

(iv) The coupling parameter of the impurity and host is the impurity rapidity, p_0, which on the one hand determines the Kondo temperature and on the other hand introduces a chirality (right–left asymmetry) into the chain.

(v) The impurity is a forward scatterer only, and hence does not give rise to bound states in the system.

None of the cases studied so far involve orbital degeneracy. In this paper we extend this investigation to an impurity with orbital degrees of freedom. The simplest generalization is the degenerate Kondo exchange problem or Coqblin–Schrieffer model. In section 2 we introduce the scattering matrices, obtain the discrete Bethe *ansatz* equations diagonalizing the interacting lattice gas with impurity, and discuss the ground-state properties of the impurity. In section 3 we address the situation of an impurity of spin S embedded into an interacting lattice gas of electrons with spin $\frac{1}{2}$. Concluding remarks follow in section 4.

2. An interacting host with Coqblin–Schrieffer impurity

2.1. The host

The host consists of electrons on a chain with nearest-neighbour hopping and excluded multiple occupancy of the sites. The electrons can have $N = 2S + 1$ spin components and interact with each other via a nearest-neighbour exchange interaction. The Hamiltonian is given by [12, 13]

$$H_0 = -t \sum_{i\sigma} P(c^\dagger_{i\sigma} c_{i+1\sigma} + c^\dagger_{i+1\sigma} c_{i\sigma}) P + J \sum_{i\sigma\sigma'} c^\dagger_{i+1\sigma} c^\dagger_{i\sigma'} c_{i\sigma} c_{i+1\sigma'} + J \sum_i n_i n_{i+1} \tag{1}$$

where $c^\dagger_{i\sigma}$ creates an electron of spin component σ at site i, $\sigma = -S, \ldots, S$, P is a projector that excludes the multiple occupancy of each site, $n_i = \sum_\sigma c^\dagger_{i\sigma} c_{i\sigma}$ is the number operator for site i, and J is the antiferromagnetic exchange coupling. The hopping t can be equated to 1.

The spin space of model (1) is SU($2S+1$) invariant by construction for all values of J/t. In particular, for $J = t$ the charges play an identical role to the spin degrees of freedom. This leads to an SU($2S + 2$)-invariant superalgebra (all degrees of freedom are boson-like) and to the integrability of the model. Due to this supersymmetry the sets of wavenumbers of the incoming and outgoing particles are identical [12, 13], and there is a scattering phase shift if two electrons are in a spin-triplet state, but to no phase shift if they are in a singlet state. This situation is then reversed with respect to the degenerate supersymmetric t–J model (corresponding to a graded permutation algebra of $2S + 1$ fermions and one boson), where two electrons in a spin-singlet state scatter, while they do not scatter in the triplet state. A more detailed discussion can be found in the appendix and in references [12, 13].

In view of the supersymmetry with SU($2S+2$) invariance, the Hamiltonian (1) can also be written in terms of spin-($S+\frac{1}{2}$) operators as a Heisenberg chain [12]:

$$H_S = \sum_i (\mathcal{P}_{i,i+1} + 1) \tag{2}$$

where $\mathcal{P}_{i,i+1}$ permutes the $2S+2$ spin components of the sites i and $i+1$.

The scattering matrix for two electrons with wavenumbers k_1 and k_2 is [13]

$$\hat{X}(k_1, k_2) = -\frac{(p_1 - p_2)\hat{I} + \mathrm{i}\hat{P}}{p_1 - p_2 - \mathrm{i}} \tag{3}$$

where $p = \frac{1}{2}\tan(k/2)$, and $\hat{I}$ and $\hat{P}$ are the identity and permutation operators, respectively. This scattering matrix satisfies the triangular Yang–Baxter relation, which is the necessary and sufficient condition for the integrability of equation (1).

2.2. The impurity

We introduce the impurity via its scattering matrix, $\hat{S}$, describing its interaction with the itinerant electrons. If the integrability of the SU($2S+2$)-invariant t–J model is to be preserved, $\hat{S}$ has to satisfy the triangular Yang–Baxter relation with $\hat{X}$ [14, 15], which is the case for

$$\hat{S}(p - p_0) = \frac{(p - p_0)\hat{I} + \mathrm{i}\hat{P}}{p - p_0 + \mathrm{i}} \tag{4}$$

where $\hat{I}$ and $\hat{P}$ are the identity and permutation operators (permuting the spin components of the impurity and the itinerant electron), respectively. Here p_0 is the rapidity of the impurity, which is related to the Kondo exchange coupling.

The impurity when embedded into the lattice of N_a sites interacts only with the two nearest-neighbour sites. Without loss of generality we may assume that the impurity is on the link joining the sites N_a and 1. The general form of the Hamiltonian describing the interaction between the impurity and the itinerant electrons is [4–7]

$$\begin{aligned} H_{imp} = {} & g_1(p_0)(\mathcal{P}_{N_a,imp} + \mathcal{P}_{imp,1} + \{\mathcal{P}_{N_a,imp}, \mathcal{P}_{imp,1}\}) \\ & + g_2(p_0)\mathcal{P}_{N_a,1} + \mathrm{i}g_3(p_0)[(\mathcal{P}_{N_a,imp} + \mathcal{P}_{imp,1}), \mathcal{P}_{N_a,1}] \end{aligned} \tag{5}$$

where $g_1(p_0)$ and $g_2(p_0)$ are even functions of p_0, while $g_3(p_0)$ is odd and the square (curly) brackets denote a commutator (an anti-commutator). Here $\mathcal{P}_{N_a,1}$, $\mathcal{P}_{N_a,imp}$, and $\mathcal{P}_{imp,1}$ are $(2S+2)$-component permutators as defined in equation (2). The parity and time-reversal symmetries are separately broken by the impurity, but the PT symmetry is preserved.

The impurity Hamiltonian is more transparent in the continuum limit. As the lattice constant tends to zero the lattice Hamiltonian reduces to a standard Luttinger liquid. We 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 $p_{FS} = \frac{1}{2}\tan(k_{FS}/2)$, then the group velocity of the electrons is $v = [2\cos(k_{FS}/2)]^{-2}$. Identifying $|p_0|/v$ with the inverse of the Kondo exchange coupling $\mathcal{J}$ we essentially obtain the scattering matrix for the Coqblin–Schrieffer model [14, 16–18]:

$$H_{imp} = \mathcal{J} \sum_{\sigma,\sigma'} d^\dagger_\sigma d_{\sigma'} \int \mathrm{d}x\ \delta(x) c^\dagger_{\sigma'}(x) c_\sigma(x) \tag{6}$$

where the interaction is with even-parity states with respect to the impurity. Odd-parity states only affect the impurity indirectly via the Luttinger liquid host. The Luttinger liquid properties of the interacting host are the main difference from the Coqblin–Schrieffer impurity in a free-electron gas.

2.3. Bethe ansatz equations

Consider now N_e itinerant electrons and the impurity in a box of N_a sites with periodic boundary conditions. Following standard procedures this problem is solved by means of $(2S+1)$ nested Bethe *ansätze*. Each Bethe *ansatz* gives rise to a set of rapidities, i.e. $\{p_j\}$, $j = 1, \ldots, N_e$, for the charges, and $\{\Lambda_\alpha^{(l)}\}$, $\alpha = 1, \ldots, m_l$, $l = 1, \ldots, 2S$ for the spin degrees of freedom. If N_k, $k = 1, \ldots, 2S+1$, are the numbers of particles with spin component $k - S - 1$, $N_1 \geqslant N_2 \geqslant \cdots \geqslant N_{2S+1}$, then the m_l are defined as $m_l = \sum_{k=l+1}^{2S+1} N_k$. The rapidities satisfy the following discrete Bethe *ansatz* equations:

$$\left[\frac{p_j + \mathrm{i}/2}{p_j - \mathrm{i}/2}\right]^{N_a} = (-1)^{N_e} \prod_{l=1}^{N_e} \frac{p_j - p_l + \mathrm{i}}{p_j - p_l - \mathrm{i}} \prod_{\beta=1}^{m_1} \frac{p_j - \Lambda_\beta^{(1)} - \mathrm{i}/2}{p_j - \Lambda_\beta^{(1)} + \mathrm{i}/2} \qquad j = 1, \ldots, N_e \tag{7}$$

$$\prod_{\tau=\pm 1} \prod_{\beta=1}^{m_{l+\tau}} \frac{\Lambda_\alpha^{(l)} - \Lambda_\beta^{(l+\tau)} + \mathrm{i}/2}{\Lambda_\alpha^{(l)} - \Lambda_\beta^{(l+\tau)} - \mathrm{i}/2} = -\prod_{\beta=1}^{m_l} \frac{\Lambda_\alpha^{(l)} - \Lambda_\beta^{(l)} + \mathrm{i}}{\Lambda_\alpha^{(l)} - \Lambda_\beta^{(l)} - \mathrm{i}} \qquad \alpha = 1, \ldots, m_l \qquad l = 1, \ldots, 2S-1 \tag{8}$$

$$\frac{\Lambda_\alpha^{(2S)} - p_0 + \mathrm{i}/2}{\Lambda_\alpha^{(2S)} - p_0 - \mathrm{i}/2} \prod_{\beta=1}^{m_{2S-1}} \frac{\Lambda_\alpha^{(2S)} - \Lambda_\beta^{(2S-1)} + \mathrm{i}/2}{\Lambda_\alpha^{(2S)} - \Lambda_\beta^{(2S-1)} - \mathrm{i}/2} = -\prod_{\beta=1}^{m_{2S}} \frac{\Lambda_\alpha^{(2S)} - \Lambda_\beta^{(2S)} + \mathrm{i}}{\Lambda_\alpha^{(2S)} - \Lambda_\beta^{(2S)} - \mathrm{i}} \qquad \alpha = 1, \ldots, m_{2S}. \tag{9}$$

Here $m_0 = N_e$ and the set $\{\Lambda_\alpha^{(0)}\}$ is identical to the set $\{p_j\}$. The first factor on the left-hand side of equation (9) arises from the impurity. The remaining factors correspond to the supersymmetric SU$(2S+2)$-invariant t–J model without impurity. The impurity acts like a distinguishable particle, i.e. a particle in a fictitious $N+1$ spin component, whose rapidity is not selfconsistently determined and does not explicitly appear in the expression for the energy. The energy and the magnetization of the system are given by [13]

$$\begin{aligned} E &= 2N_e - 2\sum_{j=1}^{N_e} \frac{1/2}{p_j^2 + 1/4} \\ S_z &= \sum_{l=0}^{2S} (S-l)(m_l - m_{l+1}) + S \end{aligned} \tag{10}$$

with $m_{2S+1} \equiv 0$. If we suppress the charge fluctuations in equations (7) and (8), i.e. equating $p_j = 0$ for all j on the right-hand side of (7) and on the left-hand side of (8), and setting $|p_0| = v/\hat{J}$ ($\hat{J}$ being the Kondo coupling), then we essentially (except that there are two partial waves) recover the Bethe *ansatz* equations of the degenerate Kondo problem.

For the ground state all rapidities are real and densely distributed. The distribution functions for the charge and spinon rapidities, $\rho(p)$ and $\sigma^{(l)}(\Lambda)$, for $l = 1, \ldots, 2S$, and their 'holes', $\rho_h(p)$ and $\sigma_h^{(l)}(\Lambda)$, are introduced in the standard way. The density functions satisfy the following linear integral equations:

$$\rho_h(p) + \rho(p) + \int_{-Q}^{Q} \mathrm{d}p'\ a_2(p-p')\rho(p') = \int_{-B_1}^{B_1} \mathrm{d}\Lambda\ a_1(p-\Lambda)\sigma^{(1)}(\Lambda) + a_1(p) \tag{11}$$

$$\sigma_h^{(l)}(\Lambda) + \sigma^{(l)}(\Lambda) + \int_{-B_l}^{B_l} \mathrm{d}\Lambda'\ a_2(\Lambda - \Lambda')\sigma^{(l)}(\Lambda')$$

$$= \sum_{\tau=\pm 1} \int_{-B_{l+\tau}}^{B_{l+\tau}} \mathrm{d}\Lambda'\ a_1(\Lambda-\Lambda')\sigma^{(l+\tau)}(\Lambda') \qquad l = 1, \ldots, 2S-1 \tag{12}$$

$$\sigma_h^{(2S)}(\Lambda) + \sigma^{(2S)}(\Lambda) + \int_{-B_{2S}}^{B_{2S}} \mathrm{d}\Lambda'\ a_2(\Lambda-\Lambda')\sigma^{(2S)}(\Lambda')$$
$$= \int_{-B_{2S-1}}^{B_{2S-1}} \mathrm{d}\Lambda'\ a_1(\Lambda-\Lambda')\sigma^{(2S-1)}(\Lambda') + \frac{1}{N_a}a_1(\Lambda - p_0) \tag{13}$$

where $a_n(x) = (n/2\pi)/(x^2 + (n/2)^2)$. In zero magnetic field we have $B_l = \infty$, and all of the spinon bands are full. With increasing magnetic field the B_l decrease monotonically. In zero field the number of electrons (charges) in the system is an increasing function of Q. The energy, and the number of electrons with each spin component are given by

$$\begin{aligned} E/N_a &= 2\int_{-Q}^{Q} \mathrm{d}p\ \rho(p)[1 - \pi a_1(p)] \\ N_e/N_a &= n = \int_{-Q}^{Q} \mathrm{d}p\ \rho(p) \\ m_l/N_a &= \int_{-B_l}^{B_l} \mathrm{d}\Lambda\ \sigma^{(l)}(\Lambda) \end{aligned} \tag{14}$$

and $m_l = \sum_{k=l+1}^{2S+1} N_k$. In other words, the N_k determine the integration limits Q and B_l. Equations (11)−(13) 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. The distribution densities for the host are even functions of the rapidities, while those for the impurity are asymmetric due to the chiral character of the impurity.

2.4. Results

In the absence of external magnetic field all of the spin-rapidity bands are completely filled, i.e. $\sigma_h^{(l)}(\Lambda) \equiv 0$, so the spinon density functions can be eliminated from equations (11)−(13) via Fourier transformation. The problem is then reduced to the solution of one integral equation of the Fredholm type for $\rho(p)$:

$$\rho_h(p) + \rho(p) + \int_{-Q}^{Q} \mathrm{d}p'\ K_{2S+2}(p-p')\rho(p') = a_1(p) + \frac{1}{N_a}K_1(p-p_0) \tag{15}$$

$$K_l(p) = \int \frac{\mathrm{d}\omega}{2\pi}\ \exp(\mathrm{i}p\omega - l|\omega|/2)\sinh(\omega/2) \Big/ \sinh(N\omega/2) \tag{16}$$

where again $N = 2S + 1$.

Equation (15) can be solved analytically in the limits $Q \to 0$ and $Q \to \infty$. Q grows monotonically with the number of electrons in the system, so

$$0 \leqslant \frac{N_e}{N_a} \leqslant \frac{N}{N+1} \qquad 0 \leqslant n_{imp} \leqslant \frac{1}{N+1}. \tag{17}$$

For intermediate values of Q, the integral equation (15) has to be solved numerically by discretizing the integral. For the calculation displayed in figure 1 we fixed Q so $N_e/N_a = 0.5$ for each N. The impurity localizes a fraction of a conduction electrons, n_{imp}, which is a decreasing function of p_0 and N, but an increasing function of Q (the number of electrons in the host). The localization of this charge is driven by the interactions in the conduction band and the Kondo exchange coupling. The impurity has then to some

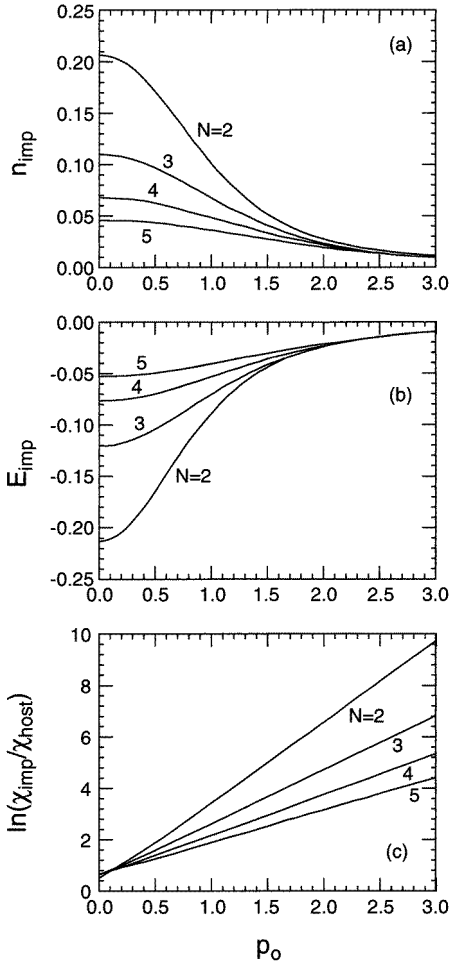

Figure 1. (a) The number of itinerant charges localized at the impurity site, (b) the ground-state energy of the impurity, and (c) the logarithm of the spin susceptibility as a function of $|p_0|$ for four spin values $S = \frac{1}{2}, 1, \frac{3}{2}$, and 2. $|p_0|$ corresponds to $1/(\mathcal{J}\rho_F)$, where $\mathcal{J}$ is the Kondo exchange coupling and ρ_F the density of states. The host has 0.5 electrons per site, corresponding to $Q = 0.594$, 0.541, 0.523, and 0.515 for $N = 2, 3, 4$, and 5, respectively.

degree mixed-valence character, the admixed configuration having one electron more than the original impurity state of spin S. The valence admixture and the formation of the Kondo singlet yields an energy gain E_{imp}. E_{imp} tracks the p_0-, N-, and Q-dependences of n_{imp}. As $S \to \infty$ (the classical spin limit), n_{imp} also tends to zero (no valence fluctuations).

The magnetization of the impurity is obtained from the integral equations obeyed by the spinon densities $\sigma^{(l)}$:

$$\sigma^{(l)}(\Lambda) + \sum_{k=1}^{2S} \int_{|\Lambda'|>B_k} \mathrm{d}\Lambda' \; G_{k,l}(\Lambda - \Lambda')\sigma_h^{(k)}(\Lambda') = \int_{-Q}^{Q} \mathrm{d}p \; F_{N-l}(\Lambda - p)\rho(p) + \frac{1}{N_a} F_l(\Lambda - p_0) \tag{18}$$

where $G_{k,l}(\Lambda)$ and $F_l(\Lambda)$ are the Fourier transforms of

$$\hat{G}_{k,l}(\omega) = \exp(|\omega|/2)\frac{\sinh[(N-\max(k,l))\omega/2]\sinh[\min(k,l)\omega/2]}{\sinh(N\omega/2)\sinh(\omega/2)}$$
$$\hat{F}_l(\omega) = \sinh(l\omega/2)\big/\sinh(N\omega/2). \tag{19}$$

In a small magnetic field, $B_k \gg Q$ for all k, so the feedback of the magnetic field to the charge distributions is of order H^2, and can be neglected. As $H \to 0$ we obtain

$$m_l = N_a\frac{N-l}{N}\int_{-Q}^{Q} \mathrm{d}p\ \rho(p) + \frac{l}{N} \tag{20}$$

which leads to a vanishing magnetization, i.e. a singlet state for both impurity and host. In a small but finite magnetic field, equations (18) can be reduced to a sequence of Wiener–Hopf integral equations (the spinon Fermi points at B_k and $-B_k$ are very far apart, and do not interfere), and all of the driving terms are proportional to $\exp(-2\pi|\Lambda|/N)$. The latter is the consequence of the (marginal) Fermi liquid properties of the system. The proportionality constants are the magnetic susceptibility. The ratio of the susceptibility of the impurity and the host is then [14, 15]

$$\frac{\chi_{imp}}{\chi_{host}} = \left(\mathrm{e}^{2\pi|p_0|/N} + \int_{-Q}^{Q}\mathrm{d}p\ \mathrm{e}^{2\pi p/N}\rho_{imp}(p)\right)\Big/\left(\int_{-Q}^{Q}\mathrm{d}p\ \mathrm{e}^{2\pi p/N}\rho_{host}(p)\right). \tag{21}$$

The first term in the numerator is the expected Kondo exponential, which is usually much larger than the susceptibility induced by the valence fluctuations (the term involving the integral over ρ_{imp}). The logarithm of the susceptibility is shown in figure 1(c) as a function of $|p_0|$. The small deviations from the straight line at small p_0 are then due to the valence admixture.

3. Undercompensated Kondo impurity

3.1. Bethe ansatz equations

We now consider an undercompensated Kondo impurity embedded into the correlated host introduced in section 2 with $N = 2$. The spin space is SU(2) invariant, and at the supersymmetric point the combined spin and charge space for the host is generated by a SU(3)-invariant superalgebra. The impurity is defined by the scattering matrix of the itinerant electrons with the impurity [19]:

$$S^{\sigma\sigma'}_{MM'}(p-p_0) = a(p-p_0)\frac{(p-p_0+\mathrm{i}/2)\delta_{MM'}\delta_{\sigma\sigma'} + \mathrm{i}\boldsymbol{S}_{MM'}\cdot\boldsymbol{\sigma}_{\sigma\sigma'}}{p-p_0+\mathrm{i}}$$
$$a(p-p_0) = \left[\frac{p^2+1}{p^2+(S+1/2)^2}\right]^{1/2} \tag{22}$$

where $\boldsymbol{\sigma}$ is the vector of Pauli matrices for the host and the $\boldsymbol{S}$ are the spin matrices of the impurity of spin S and spin components M (M'). The scattering matrix is unitary and satisfies the triangular Yang–Baxter relation with the scattering matrix of the host. The interaction Hamiltonian is essentially the spin exchange between an impurity of spin S and itinerant electrons with spin $\frac{1}{2}$, and is a generalization of the impurity model considered in section 2.

The model is diagonalized by means of two nested Bethe *ansätze*, each giving rise to one set of rapidities. Using the same notation as in the previous section we obtain the

following discrete Bethe *ansatz* equations:

$$\exp(-\mathrm{i}\phi)\left[\frac{p_j+\mathrm{i}/2}{p_j-\mathrm{i}/2}\right]^{N_a}=(-1)^{N_e}\prod_{l=1}^{N_e}\frac{p_j-p_l+\mathrm{i}}{p_j-p_l-\mathrm{i}}\prod_{\beta=1}^{M^*}\frac{p_j-\Lambda_\beta-\mathrm{i}/2}{p_j-\Lambda_\beta+\mathrm{i}/2} \tag{23}$$

where

$$\phi=\arctan\left(\frac{2(p_j-p_0)}{2S+1}\right)-\arctan(p_j-p_0)\qquad j=1,\ldots,N_e$$

and

$$\frac{\Lambda_\alpha-p_0+\mathrm{i}S}{\Lambda_\alpha-p_0-\mathrm{i}S}\prod_{j=1}^{N_e}\frac{\Lambda_\alpha-p_j+\mathrm{i}/2}{\Lambda_\alpha-p_j-\mathrm{i}/2}=-\prod_{\beta=1}^{M^*}\frac{\Lambda_\alpha-\Lambda_\beta+\mathrm{i}}{\Lambda_\alpha-\Lambda_\beta-\mathrm{i}}\qquad \alpha=1,\ldots,M^*. \tag{24}$$

Here M^* is the number of reversed spins. The first factors on the left-hand sides of equations (23) and (24) arise from the impurity. The energy is still given by equation (10), and the magnetization is $S_z=\frac{1}{2}N_e-M^*+S$. Suppressing the charge fluctuations, i.e. equating $p_j=0$ for all j on the right-hand side of (23) and on the left-hand side of (24), we recover (except that there are two partial waves) the Bethe *ansatz* equations of the traditional Kondo problem.

The distribution functions for the charge and spinon rapidities for the ground state satisfy

$$\rho_h(p)+\rho(p)+\int_{-Q}^{Q}\mathrm{d}p'\ a_2(p-p')\rho(p')$$
$$=\int_{-B}^{B}\mathrm{d}\Lambda\ a_1(p-\Lambda)\sigma(\Lambda)+a_1(p)+\ \frac{1}{2N_a}[a_2(p-p_0)-a_{2S+1}(p-p_0)] \tag{25}$$

$$\sigma_h(\Lambda)+\sigma(\Lambda)+\int_{-B}^{B}\mathrm{d}\Lambda'\ a_2(\Lambda-\Lambda')\sigma(\Lambda')$$
$$=\int_{-Q}^{Q}\mathrm{d}p\ a_1(\Lambda-p)\rho(p)+\frac{1}{N_a}a_1(\Lambda-p_0). \tag{26}$$

In zero magnetic field, $B=\infty$, and B decreases monotonically with increasing magnetic field. The energy and the total number of electrons are still given by equation (15), while the impurity magnetization is

$$S_z^{imp}=\frac{1}{2}\int_{-Q}^{Q}\mathrm{d}p\ \rho_{imp}(p)-\int_{-B}^{B}\mathrm{d}\Lambda\ \sigma_{imp}(\Lambda)+S=S-\frac{1}{2}+\frac{1}{2}\int_{|\Lambda|>B}\mathrm{d}\Lambda\ \sigma_{imp,h}(\Lambda). \tag{27}$$

Hence, the zero-field ground-state magnetization is $S-\frac{1}{2}$.

3.2. Results

For the zero-field ground state the band of spin rapidities is completely filled, so $\sigma_h(\Lambda)\equiv 0$, and $\sigma(\Lambda)$ can be eliminated from equations (25) and (26) via Fourier transformation. The resulting Fredholm equation satisfied by $\rho(p)$ is

$$\rho_h(p)+\rho(p)+\int_{-Q}^{Q}\mathrm{d}p'\ G_3(p-p')\rho(p')$$
$$=a_1(p)+\frac{1}{N_a}G_{2S}(p-p_0)+\frac{1}{2N_a}[a_2(p-p_0)-a_{2S+1}(p-p_0)] \tag{28}$$

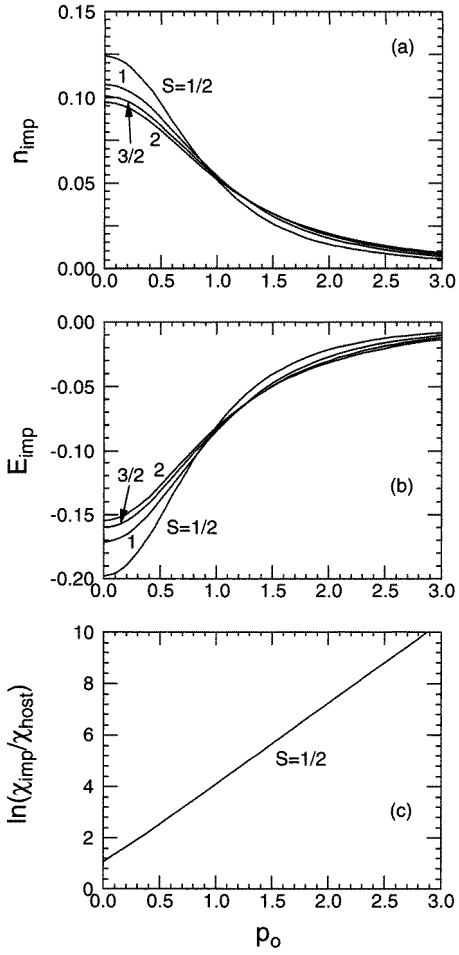

Figure 2. (a) The number of itinerant charges localized at the impurity site, and (b) the ground-state energy of the impurity as a function of $|p_0|$ for four impurity spin values $S = \frac{1}{2}, 1, \frac{3}{2}$ and 2. (c) The logarithm of the spin susceptibility for $S = \frac{1}{2}$ as a function of $|p_0|$. For all other spin values the impurity ground state is not a singlet. $|p_0|$ is inversely proportional to the Kondo exchange coupling. The host has 1/3 of an electron per site, corresponding to $Q = 0.310$.

$$G_l(p) = \int \frac{\mathrm{d}\omega}{2\pi}\ \exp(\mathrm{i}p\omega - l|\omega|/2) \ \Big/\ [2\cosh(\omega/2)]. \tag{29}$$

The density functions can be separated into a host and an impurity part. The host contribution is identical to the one discussed in section 2 for the Coqblin–Schrieffer model, if N is set equal to 2. The impurity driving terms are, however, different, because this impurity has an undercompensated spin. By numerically solving the integral equation it is straightforward to obtain the fraction of an electron localized at the impurity site, and the impurity ground-state energy. The fraction of a localized electron, n_{imp}, and the energy are displayed in figures 2(a) and 2(b) as functions of $|p_0|$ for $N_e/N_a = 1/3$ and several impurity spin values. n_{imp} decreases monotonically with $|p_0|$, i.e. it is a maximum when the impurity rapidity is on resonance with the conduction states, and gradually decreases as the p_0 gets off resonance. Here $|p_0|$ is inversely proportional to the Kondo exchange.

The dependence of n_{imp} on the impurity spin is not monotonic, as a consequence of the last two terms (arising from the normalization of the impurity scattering matrix, equation (22)) on the right-hand side of equation (28). In contrast to the case for the Coqblin–Schrieffer model, n_{imp} does not tend to zero as $S \to \infty$ (the classical limit for the impurity, but the host still has fluctuations). The binding energy for the spin compensation follows a similar trend to n_{imp}.

Since $n_{imp} \neq 0$, the impurity is in a mixed-valence state of two magnetic configurations, of spin S and $S - \frac{1}{2}$, respectively. On the lattice the impurity Hamiltonian has the general form (5). In the continuum limit the Hamiltonian for the impurity placed at the origin can be written as [20, 21]

$$H_{imp} = \epsilon \sum_{M_1} |S_1 M_1\rangle\langle S_1 M_1| + V \sum_{\sigma M M_1} (M\sigma|M_1) \int \mathrm{d}x\ \delta(x) \times [c_\sigma^\dagger(x)|SM\rangle\langle S_1 M_1| + |S_1 M_1\rangle\langle SM|c_\sigma(x)] \tag{30}$$

where the bra and ket denote the impurity states, $S_1 = S - \frac{1}{2}$, ϵ is a function of $|p_0|/v$ (v is the Fermi velocity) and is the energy difference between the two configurations relative to the Fermi level, and

$$(M\sigma|M+\sigma) = (SM; \tfrac{1}{2}\sigma|S\ \tfrac{1}{2}\ (S-\tfrac{1}{2})\ M+\sigma) \tag{31}$$

is a Clebsch–Gordan coefficient. The completeness condition for the impurity requires

$$\sum_{M_1} |S_1 M_1\rangle\langle S_1 M_1| + \sum_M |SM\rangle\langle SM| = 1. \tag{32}$$

The impurity in the non-interacting host has two free parameters, namely ϵ and the hybridization V, so charge and spin fluctuations can occur on different energy scales. In contrast, the integrability in the presence of interactions in the host restricts V to $V^2 = (2S+1)/v$, so the impurity (besides the value of S) has only one free parameter, namely p_0. In the non-interacting host, n_{imp} varies with ϵ between 0 and 1, while in the interacting host the maximum n_{imp} is 1/3. This difference arises from the normalization term $a(p - p_0)$ in the impurity scattering matrix.

The ground-state magnetization is obtained from equation (26), which is a Fredholm integral equation for σ with two driving terms, namely, an independent term depending on p_0 and a term involving ρ. The magnetization is then the sum of the magnetization due to the internal degrees of freedom of the impurity and the one arising from the valence admixture. For $S = \frac{1}{2}$ the ground state is a singlet, and hence the zero-field susceptibility is finite, and given by

$$\frac{\chi_{imp}}{\chi_{host}} = \left(\mathrm{e}^{\pi|p_0|} + \int_{-Q}^{Q} \mathrm{d}p\ \mathrm{e}^{\pi p} \rho_{imp}(p)\right) \Big/ \left(\int_{-Q}^{Q} \mathrm{d}p\ \mathrm{e}^{\pi p} \rho_{host}(p)\right) \qquad S = \tfrac{1}{2}. \tag{33}$$

The Kondo exponential in the numerator is the dominating feature, as shown in the plot of $\ln(\chi_{imp}/\chi_{host})$ as a function of $|p_0|$ (see figure 2(c)).

For $S > \frac{1}{2}$ the ground state is magnetic, so the susceptibility diverges as $H \to 0$. We can then neglect the contribution of the valence fluctuations to the magnetization (for magnetic fields much smaller than the bandwidth), and the Fredholm equation can be reduced to a hierarchical sequence of Wiener–Hopf integral equations, of which the leading contribution is given by ($y(\Lambda) = \sigma_{imp}(\Lambda - B)$)

$$y(\Lambda) + y_h(\Lambda) - \int_{-\infty}^{0} \mathrm{d}\Lambda'\ G_1(\Lambda - \Lambda') y_h(\Lambda') = G_{2S-1}(\Lambda - B + |p_0|). \tag{34}$$

Adopting the parametrization $|p_0| - B = (1/\pi)\ln(H/T_K)$, where T_K is the Kondo temperature, the leading contribution to the magnetization is a universal function of H/T_K, and is identical to that of the ordinary Kondo problem without interactions in the host. The next-order contribution in the hierarchical sequence is smaller by a factor $1/B$ and also depends on $|p_0| + B$, i.e. the bandwidth explicitly enters as a third energy scale (in addition to T_K and H). This non-universal dependence arises from the interference of the two Fermi points of the spinon band (backward scattering). In the limit of very large $|p_0|$, i.e. $T_K/D \ll 1$ and $H/D \ll 1$, the non-leading contributions in the Wiener–Hopf sequence become small and can be neglected.

The universal dependence of the magnetization is given by [14, 15, 17]

$$M_{imp} = (S - \tfrac{1}{2})[1 + \tfrac{1}{2}\mathcal{L}^{-1} - \tfrac{1}{4}\ln(\mathcal{L})/\mathcal{L}^2 + \cdots] \qquad H \ll T_K, S > \tfrac{1}{2} \tag{35}$$

$$M_{imp} = S[1 - \tfrac{1}{2}\mathcal{L}^{-1} - \tfrac{1}{4}\ln(\mathcal{L})/\mathcal{L}^2 + \cdots] \qquad H \gg T_K \tag{36}$$

where $\mathcal{L} = |\ln(H/T_K)|$. Hence, in a small field the impurity has an asymptotically free spin $S - \frac{1}{2}$, while in strong magnetic fields the effective spin is S, weakly coupled (logarithms characterize asymptotic freedom) to the itinerant electrons. For intermediate fields the magnetization smoothly interpolates between these two limits.

4. Conclusions

We considered (i) a Coqblin–Schrieffer impurity of spin S and (ii) an undercompensated Kondo impurity of spin S embedded into a one-dimensional lattice with strongly interacting electrons. The integrable model providing the background of itinerant electrons for (i) is the SU($2S + 2$)-invariant and for (ii) the SU(3)-invariant supersymmetric t–J model. The translational invariance is broken by introducing the additional spin S, but the integrability is preserved by construction. The impurity is introduced via the scattering matrix, equations (4) and (22) for (i) and (ii) respectively, which obeys the triangular Yang–Baxter relation with the scattering matrix of the host. This is the necessary and sufficient condition for the integrability of the model with impurity. The interaction of the itinerant electrons with the impurity is via spin exchange with the two neighbouring sites of the impurity. The exchange is proportional to the inverse of the absolute value of the impurity rapidity. This rapidity introduces a chirality into the system, so the impurity interacts with both partial waves (even- and odd-parity states with respect to the impurity site).

We derived the Bethe *ansatz* equations diagonalizing the host with impurity, and studied the ground-state properties of the impurity. The properties of the host influence the impurity, so some impurity properties are then different from those of an impurity in an uncorrelated host. The impurity localizes a fraction of an itinerant electron and acquires mixed-valence character. For the Coqblin–Schrieffer model this fraction is constrained to the interval $0 \leqslant n_{imp} \leqslant 1/(2S + 2)$, while for the undercompensated spin (case (ii)) we obtain $0 \leqslant n_{imp} \leqslant 1/3$. In both cases n_{imp} monotonically decreases with $|p_0|$, and for $|p_0| \to \infty$, i.e. when the Kondo exchange coupling tends to zero, $n_{imp} \to 0$. Hence, in this limit the impurity has integer valence and we recover the traditional Kondo problem.

There are two contributions to the magnetic properties, namely the Kondo magnetization and the magnetization arising from the valence admixture. The latter is always smaller than the Kondo effect and can be neglected for most purposes. The integral equations governing the spin-rapidity distributions are of the Fredholm type. Each rapidity band has two Fermi points, which however in the Kondo limit (large $|p_0|$) do not interfere. In this limit the Fredholm equations can be reduced to a Wiener–Hopf integral equation, and the traditional Coqblin–Schrieffer and Kondo problems are recovered.

The two models studied in this paper confirm the general results derived previously for other combinations of interacting host and magnetic impurity [4–7]. The trends are the same, namely (a) the interactions in the host drive the impurity into a mixed-valence state, (b) the Kondo exchange coupling is parametrized by the impurity rapidity, (c) the impurity is on a link of the chain and interacts with both neighbouring sites (i.e. with even- and odd-parity states), and (d) the impurity is a forward scatterer only and does not produce a bound state split off from the continuum. The latter property is clearly a non-universal feature of our model. All of the other properties are believed to be general and generic.

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Appendix: The host Hamiltonian

The t–J–V model is defined as

$$H_{tJV} = -t \sum \mathrm{i}\sigma P(c^{\dagger}_{i\sigma} c_{i+1\sigma} + c^{\dagger}_{i+1\sigma} c_{i\sigma}) P + J \sum_{i\sigma\sigma'} c^{\dagger}_{i+1\sigma} \boldsymbol{S}_{\sigma\sigma'} c_{i+1\sigma'} \cdot c^{\dagger}_{i\sigma'} \boldsymbol{S}_{\sigma'\sigma} c_{i\sigma} + V \sum_{i} n_i n_{i+1} \tag{A1}$$

where $c^{\dagger}_{i\sigma}$ creates an electron of spin component $\sigma = \pm\frac{1}{2}$ at the site i, P is a projector excluding the multiple occupancy of each site, $\boldsymbol{S}$ is the vector of spin-$\frac{1}{2}$ operators, and n_i is the number operator at site i. As a consequence of supersymmetries, the model is integrable for $2t = \pm J$ at (i) $V = -\frac{1}{4}J$ and (ii) $V = \frac{3}{4}J$ [12, 13]. Point (i) corresponds to a phase shift if two scattering electrons form a spin singlet and to no phase shift if they are in a triplet state. On the other hand, case (ii) represents the situation where there is no scattering in the singlet state and there is a scattering phase shift if the electrons are in a triplet state.

In equation (A1) the model is formulated in terms of electron fermion operators. Alternatively, we may consider the three allowed states at each site, namely an up- or down-spin electron and the holon (empty site). For case (ii) these three states correspond to hard-core bosons, i.e. the spinons are identical to the holons. This can be represented in terms of Hubbard projection operators as a BBB (three bosons) superalgebra, which has SU(3) symmetry. On the other hand, for case (i) the spin states act as fermions, while the holon is still a boson, but are otherwise identical [22, 23]. This is known as a graded FFB superalgebra and denoted as SU(2, 1).

The model used in this paper, equation (1), is the extension of case (ii) to N spin degrees of freedom. There are now $N+1$ states per site, all being hard-core bosons, so the symmetry is SU($N+1$). The supersymmetric point now corresponds to $J = \pm t = \pm V$. On the other hand, the Hamiltonian corresponding to the extension of case (i) to N spin degrees of freedom ($\mathrm{F}^N\mathrm{B}$) is again Hamiltonian (1), but with a changed sign for the last term.

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