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The open spin chain with impurity: an exact solution

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Abstract. Using a model of an open spin chain that is exactly soluble by means of a Bethe *ansatz*, we study the effects of a boundary magnetic field and an impurity spin coupled to the chain. An impurity spin only scatters forward, while the boundary is purely a back-scatterer. Two parameters for the impurity and one for the boundary permit us to mimic the effect of real magnetic impurity, with both forward and backward scattering.

Studies of impurities in one-dimensional correlated quantum systems have a long history: field theoretical methods such as those of bosonization and boundary conformal field theory have been applied to describe the effect of local potentials and to study the transport properties in the presence of these—see, e.g. [1–7]. On the other hand, exactly soluble models of one-dimensional quantum systems have provided results essential to the understanding of a number of physical problems involving impurities: examples are the Kondo effect [8, 9], point contact spectroscopy of quantum wires [10] and x-ray absorption singularities [11, 12]. The impurities studied within this approach are either static ones, i.e. boundary potentials in open systems, or dynamical ones such as those in the Kondo problem. In this paper we wish to compare the behaviour of these in a simple integrable model, namely an open spin-$\frac{1}{2}$ antiferromagnetic Heisenberg chain, coupled to an integrable spin-S' impurity, subject to boundary magnetic fields at its ends. Within the framework of the quantum inverse scattering method [13], such an impurity can be described by a two-parameter family of operators $\mathcal{L}_{S'}(\lambda+\lambda_0)$, which can be expressed in terms of spin-S' operators:

$$\mathcal{L}_{S'}(\lambda) = \frac{1}{\lambda + \mathrm{i}/2 + \mathrm{i}S'} \begin{pmatrix} \lambda + \mathrm{i}/2 + \mathrm{i}S'^z & \mathrm{i}S'^- \\ \mathrm{i}S'^+ & \lambda + \mathrm{i}/2 - \mathrm{i}S'^z \end{pmatrix} \qquad \langle \boldsymbol{S}'^2 \rangle = S'(S'+1). \tag{1}$$

Here λ is a spectral parameter. In reference [14] impurities of this type with $\lambda_0 = 0$ in a periodic chain have been studied (see also references [15, 16] for impurities of this type in a spin-$S > \frac{1}{2}$ chain). The $\mathcal{L}_{S'}$-operators satisfy the Yang–Baxter equation with the vertex of the host (equation (1) with spin $S' = \frac{1}{2}$); thus the associated transfer matrices with different spectral parameters commute. This commutativity is the necessary and sufficient condition for exact integrability: one can construct an infinite number of local conservation laws for the system (e.g. the Hamiltonian is the logarithmic derivative with respect to the spectral

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parameter of the transfer matrix). At the impurity vertex, which defines the integrable spin chain, the additional shift $\lambda \to \lambda + \lambda_0$ (see also [17]) of the spectral parameter in (1) leads to a two-parameter family (S', λ_0) characterizing the impurity [18]. In addition to the impurity, a (boundary) magnetic field acting on the two boundary sites can be incorporated using the reflection equation formalism [19, 20]. This leads to the Hamiltonian

$$\mathcal{H} = \sum_{j=1}^{L-1} \boldsymbol{S}_j \cdot \boldsymbol{S}_{j+1} + \mathcal{H}_{imp} + \mathcal{H}_{bound}. \qquad (2)$$

As a peculiarity of the quantum inverse scattering method, the eigenvalues of the system do not depend on the position of the impurity spin in the chain. The reason for this is that all vertices, including the impurity one, are forward scatterers by construction. Hence they produce the phase shifts, but have no amplitude for reflection. A boundary, on the other hand, is a perfect back-scatterer with vanishing transmission. The combination of an impurity vertex and a boundary field thus mimics a real impurity, which should have both reflection and transmission properties.

In constructing the Hamiltonian, we have to distinguish two different situations, which are described by the same Bethe *ansatz* equations: if the impurity spin is added in the bulk—say, situated between sites $m > 1$ and $m + 1 < L$ of the system (2)—we find (here $\{\ ,\ \}$ denotes an anticommutator)

$$\begin{aligned} \mathcal{H}_{imp} &= J_0\big((\boldsymbol{S}_m + \boldsymbol{S}_{m+1}) \cdot \boldsymbol{S}' + \{\boldsymbol{S}_m \cdot \boldsymbol{S}', \boldsymbol{S}_{m+1} \cdot \boldsymbol{S}'\} \\ &\qquad + 2\lambda_0 \boldsymbol{S}_m \cdot (\boldsymbol{S}' \times \boldsymbol{S}_{m+1}) + (\lambda_0^2 - 2S'(S'+1))\boldsymbol{S}_m \cdot \boldsymbol{S}_{m+1}\big) \\ \mathcal{H}_{bound} &= h_1 S_1^z + h_L S_L^z \qquad J_0 = J_0(S', \lambda_0) = \left(\left(S' + \frac{1}{2}\right)^2 + \lambda_0^2\right)^{-1}. \end{aligned} \qquad (3)$$

Note that the impurity contribution to the Hamiltonian for $\lambda_0 = 0$ coincides with the one studied in reference [14]. The second possibility is to put the spin-S' impurity vertex at one end of the chain. The corresponding Hamiltonian can be obtained from (3) by making the replacement $\boldsymbol{S}_m \to h_1 \hat{\boldsymbol{z}}$ (this property holds for any SU(2)-symmetric Bethe-*ansatz*-integrable system). The combined contribution from boundary fields and impurity spin (at site '0') is given by

$$\begin{aligned} \mathcal{H}_{imp} + \mathcal{H}_{bound} = J_0\Bigg(&\boldsymbol{S}' \cdot \boldsymbol{S}_1 + h_1\Big[S'^z + 2\lambda_0(S_1^x S'^y - S_1^y S'^x) + \{S'^z, \boldsymbol{S}' \cdot \boldsymbol{S}_1\} \\ &+ \left(\lambda_0^2 - S'(S'+1) + \frac{1}{4}\right)S_1^z\Big]\Bigg) + h_L S_L^z \end{aligned} \qquad (4)$$

(see also reference [21]). Upon tuning of the system parameters, $\mathcal{H}_{imp}$ simplifies in a number of limits:

(i) $S' = \frac{1}{2}$, $\lambda_0 = 0, \infty$: the model reduces to the well known open spin-$\frac{1}{2}$ Heisenberg chain with $L + 1$ and L sites respectively;

(ii) $h_1 = 0$: in this case the impurity spin (at the edge) is coupled by an exchange term to $\boldsymbol{S}_1$; the sign and magnitude of the coupling constant J_0 depend on λ_0, which can be chosen either purely real or purely imaginary in this case, and on the impurity spin value S'.

Note that the edge impurity Hamiltonian (4) for $h_1 = 0$ has a 'natural' physical form: there are no three-spin interactions and no changes of coupling between the host spins (so the impurity–host link differs from other links, and the spin value of the impurity is different from the ones of the host).

The model defined above can be solved using the algebraic Bethe *ansatz*. The eigenvalues and eigenfunctions of $\mathcal{H}$ are determined by solution of the Bethe *ansatz* equations (BAE):

$$\left(e_1(\lambda_j)\right)^{2L} e_{2S'}(\lambda_j+\lambda_0)e_{2S'}(\lambda_j-\lambda_0)e_{\xi_1}(\lambda_j)e_{\xi_L}(\lambda_j) = \prod_{k=1,k\neq j}^{M} e_2(\lambda_j-\lambda_k)e_2(\lambda_j+\lambda_k) \tag{5}$$

where $e_n(x) = (x + (\mathrm{i}/2)n)/(x - (\mathrm{i}/2)n)$, L is the number of sites, M is the number of down spins (the total spin is $S^z = L/2 + S' - M$), $\{\lambda_j\}_{j=1}^{M}$ is the set of rapidities, parametrizing the eigenfunctions and eigenvalues, and the boundary magnetic field enters through $\xi_{1,L} = -1 + 1/h_{1,L}$. Later, to take the thermodynamic limit in a controlled way, we will consider two situations: (a) lattices with an even number of sites (including the impurity one) and vanishing boundary fields $h_{1,L} = 0$ (i.e. without the phases $e_{\xi_{1,L}}$ in (5)); and (b) lattices with an odd number of sites and both $h_{1,L}$ finite. Each solution of equations (5) corresponds to an eigenstate of the Hamiltonian (2) with the energy

$$E(\{\lambda_j\}) = E_{FM} - H\left(\frac{L}{2} + S'\right) - \frac{1}{2}\sum_{j=1}^{M}\left(\frac{1}{\lambda_j^2 + \frac{1}{4}} - 2H\right) \tag{6}$$

where $E_{FM} = \frac{1}{4}(L-1) + J_0 C + \frac{1}{2}(h_1 + h_L)$ is the energy of the ferromagnetic state ($C = (\lambda_0^2 + 2S')/4$ for the bulk impurity, $C = S'/2$ for the impurity at the edge) and H is the bulk magnetic field. To solve the BAE (5) for the open chain we follow the procedure of references [22, 23]: extending the set of rapidities to $\{\lambda_j\}_{j=-M}^{M}$ with $\lambda_j = -\lambda_{-j}$ for $j = -1, \ldots, -M$ and $\lambda_0 = 0$, equations (5) can be rewritten as

$$\left(e_1(\lambda_j)\right)^{2L+1} e_2(\lambda_j)e_{2S'}(\lambda_j+\lambda_0)e_{2S'}(\lambda_j-\lambda_0)e_{\xi_1}(\lambda_j)e_{\xi_L}(\lambda_j) = \prod_{k=-M}^{M} e_2(\lambda_j-\lambda_k). \tag{7}$$

In this form the BAE for the open chain considered here are similar to the ones for the periodic system [14], with the obvious replacements $L \to 2L+1$ and $M \to 2M+1$ (reflection), and several 'impurity-like' terms in the lhs: two (because of reflection) of them correspond to the impurity vertex, and one is connected with each boundary. The remaining ones are due to the extended set of rapidities introduced above. We note here that in (7) the boundary fields mimic impurities with effective 'spin' $S_{eff} = \xi_{1,L}/2$ which is a function of the boundary magnetic field: for $h_{1,L} = 0$ it is infinite (leading to an effective twist of π at the free boundary). At $h_{1,L} = 1$ the effective spin changes its sign leading to the appearance of a complex root of the BAE in the ground-state configuration in this regime. Finally, for $h_{1,L} \to \infty$ we have $S_{eff} = -\frac{1}{2}$, effectively removing one site from the system.

In addition to real λ_0 which corresponds to weak antiferromagnetic coupling of the impurity spin to the host, we can choose λ_0 to be purely imaginary in the system with open boundaries. Small imaginary λ_0 leads to increasing antiferromagnetic coupling of the impurity; at $\lambda_0 = \pm\mathrm{i}(S' + \frac{1}{2})$ the coupling between the impurity and the host changes to ferromagnetic coupling, leading to an effective impurity spin $S' + \frac{1}{2}$. We will show that for the low-temperature low-magnetic-field case it corresponds to the effective asymptotically free spin S'. Hence, at least for the impurity spin situated at the edge, one covers any possible *physical* situations of the edge impurity spin S' coupled via one link of any possible exchange coupling to the host (at zero boundary field). Once again we want to emphasize that while the BAE do not depend on the impurity position, i.e. describe both the bulk and edge impurity, the systems are clearly described by different Hamiltonians. The difference is present in the set of eigenfunctions. In the following we shall consider real λ_0 mostly.

This is the most interesting case of moderate *anti*ferromagnetic coupling between impurity and host.

Let us first study the case of non-negative $\xi_{1,L}$ (i.e. $h_{1,L} \leqslant 1$). The solution of the BAE (7) is straightforward, along the lines of references [14, 24, 25]. The energy can be written as a series in L^{-1}: $E = LE_\infty + E_i + L^{-1}E_{mes} + \cdots$. The energy density of the bulk E_∞ is the same for the periodic system and for the open one, and does not depend on characteristics of the impurity. The mesoscopic corrections E_{mes} determine the asymptotics of the correlation functions, and will be considered later. Now we will concentrate on the boundary and impurity effects of order L^0, namely E_i. Taking the thermodynamic limit $L, M \to \infty$ with their ratio fixed, the solutions of the BAE can be classified in terms of so-called 'strings' $\lambda_j = \lambda_{j,k} + \mathrm{i}k/2$, where $k = -(n-1), -(n-3), \ldots, (n-1)$. The integer n denotes the length of the string. Introducing densities of n-strings, $\rho_n(\lambda)$, and the corresponding 'hole' densities, $\rho_n^{(h)}(\lambda)$, the BAE can be written as an infinite set of coupled integral equations:

$$\rho_n^{(h)}(\lambda) + \sum_{k=1}^{\infty} \int \mathrm{d}\lambda' \; A_{nk}(\lambda - \lambda')\rho_k(\lambda') = a_n(\lambda) + \frac{1}{2L}(a_n(\lambda) + a_{n+1}(\lambda) + \delta_{n>1}a_{n-1}(\lambda) + \Xi_{n,S'}(\lambda) + \Xi_{n,\xi}(\lambda)) \qquad (8)$$

where the kernels are

$$A_{n,k}(x) = a_{n+k}(x) + 2\sum_{l=1}^{\min(n,k)-1} a_{n+k-2l}(x) + a_{|n-k|}(x)$$

with $a_n(x) = 2n/\pi(4x^2 + n^2)$, $a_0(x) = \delta(x)$ and

$$\begin{aligned} \Xi_{n,S'}(\lambda) &= \sum_{l=1}^{\min(n,2S')} (a_{n+2S'+1-2l}(\lambda + \lambda_0) + a_{n+2S'+1-2l}(\lambda - \lambda_0)) \\ \Xi_{n,\xi}(\lambda) &= \sum_{l=1}^{n} (a_{n+\xi_1+1-2l}(\lambda) + a_{n+\xi_L+1-2l}(\lambda)). \end{aligned} \qquad (9)$$

Note that $2M + 1 = \sum_n n\ell_n$, where $\ell_n = 2L\int \mathrm{d}\lambda \; \rho_n(\lambda)$ is the number of n-strings. The equilibrium state at temperature T is obtained by minimization of the free energy $F = E - T\mathcal{S}$ ($\mathcal{S}$ is the combinatoric entropy). This procedure leads to an additional set of non-linear integral equations for the dressed energies $\varepsilon_n(\lambda) = T\ln(\rho_n^{(h)}(\lambda)/\rho_n(\lambda))$:

$$T\ln[1 + \exp(\varepsilon_n/T)] = nH - \pi a_n(\lambda) + T\sum_{k=1}^{\infty} \int \mathrm{d}\lambda' \; A_{nk}(\lambda - \lambda')\ln[1 + \exp(-\varepsilon_k/T)]. \qquad (10)$$

Note that only the bulk field H enters these equations, while the impurity and the boundary field h only affect the string densities according to (8). The ground-state configuration at $T = 0$ is determined by the host alone through equation (10): all states with negative dressed energy $\varepsilon_n(\lambda) < 0$ have to be filled. Using equations (8) and (10), the free energy can be written as

$$F(H,T) = LF_\infty(H,T) + 1 - \left(S' + \frac{1}{2}\right)H - \frac{1}{2}T\sum_{n=1}^{\infty} \int \mathrm{d}\lambda \; \ln(1 + \exp(-\varepsilon_n/T)) \times \{a_n(\lambda) + a_{n+1}(\lambda) + \delta_{n>1}a_{n-1}(\lambda) + \Xi_{n,S'}(\lambda) + \Xi_{n,\xi}(\lambda)\}. \qquad (11)$$

We now study the $T = 0$ ground state. From equations (10) one finds that only ε_1 may be negative. Hence, the ground state is constructed by filling the Dirac sea of 1-string states with negative energy. The $T \to 0$ limit of (10) for $n = 1$ can be written as

$$\varepsilon_1(\lambda) = \frac{1}{2}H - \frac{\pi}{2\cosh(\pi\lambda)} + \left(\int_{-\infty}^{-\Lambda} + \int_{\Lambda}^{\infty}\right) \mathrm{d}\mu\ J(\lambda-\mu)\varepsilon_1(\mu). \tag{12}$$

Here the boundaries Λ of integration are to be determined from the condition $\varepsilon(\pm\Lambda) = 0$ as a function of the bulk magnetic field H. The kernel is given in terms of its Fourier transform as $(1 + \exp(|u|))^{-1}$. For vanishing bulk field H one finds $\Lambda = \infty$; the ground state is obtained by filling the sea of 1-strings completely. In this case the ground state has spin $S - \frac{1}{2}$ for the case of $L + 1$ even and $h_{1,L} = 0$, and has $S^z = -\frac{1}{2}$ for $L + 1$ odd and non-zero boundary fields. Its energy is (ψ is the digamma function)

$$\begin{aligned} E_0 - E_{FM} = &-\left(L + \frac{1}{2}\right)\ln 2 + \frac{\pi}{4} - \frac{1}{4}\sum_{x=\pm\lambda_0}\left(\psi\left(\frac{2S'+3}{4} + \mathrm{i}x\right) - \psi\left(\frac{2S'+1}{4} + \mathrm{i}x\right)\right) \\ &- \frac{1}{4}\sum_{j=1,L}\left(\psi\left(\frac{\xi_j+3}{4}\right) - \psi\left(\frac{\xi_j+1}{4}\right)\right). \end{aligned} \tag{13}$$

Since the spectral properties of the system do not depend on the location of the impurity, equation (13) applies also to the case where the spin S' is situated at the edge and $h_{1,L} = 0$. In particular, this allows one to compute the local correlation function $\langle \boldsymbol{S}' \cdot \boldsymbol{S}_1 \rangle$ for the system (4) by taking the derivative of the ground-state energy w.r.t. J_0. In the region of antiferromagnetic coupling this quantity varies between 0 and $-(S'+1)/2$ as a function of the parameter λ_0. As an example, we find the enhancement of the antiferromagnetic correlations at the edge for $J_0 = 1$ and $S' = \frac{1}{2}$ to be (see also reference [26] for a recent numerical study of this quantity)

$$-\langle \boldsymbol{S}_0 \cdot \boldsymbol{S}_1 \rangle = \frac{1}{4}(1 - 3\zeta(3)) \approx 0.6515\ldots\ . \tag{14}$$

In the following we consider the ground-state properties of the impurity and the boundaries in a magnetic field H separately. Fourier transforming the L^0-terms in (11) for vanishing boundary fields (i.e. putting $\Xi_{n\xi} \equiv 0$), we obtain ($f^{(\pm)}(x) = \theta(\pm x) f(x)$, θ being the step function)

$$E_i = E_i(H=0) - H\left(S' - \frac{1}{2}\right) + \int \frac{\mathrm{d}u}{8\pi}\ \frac{\varepsilon_1^{(+)}(u)}{\cosh(u/2)}\left(1 + \mathrm{e}^{-|u|/2} + 2\cos(u\lambda_0)\mathrm{e}^{-(S'-1/2)|u|}\right). \tag{15}$$

In the integrand, the last term is due to the impurity, while the second one is a consequence of the open-chain boundary conditions.

For small values of the bulk magnetic field $H \ll 1$, i.e. Zeeman splitting small compared to the bandwidth, the Fredholm equation (12) can be transformed into a sequence of Wiener–Hopf equations. The latter can be solved perturbatively [27], giving $\Lambda = -(1/\pi)\ln(H/H_0)$ with $H_0 = \sqrt{\pi^3/e}$. The same procedure applied to the equation for the density of 1-strings (equation (8)) gives the leading asymptotics for the magnetization:

$$\begin{aligned} M^z &= M^z_{edge} + M^z_{imp} \\ M^z_{edge} &= \frac{1}{2}\left(\frac{1}{2|\ln H/H_0|} - \frac{\ln\frac{1}{2}|\ln H/H_0|}{4(\ln H/H_0)^2}\right) + \cdots \\ M^z_{imp} &= \mu\left(1 + \sum_{\sigma=\pm}\left(\pm\frac{1}{2|\ln H/H_\sigma|} - \frac{\ln\frac{1}{2}|\ln H/H_\sigma|}{4(\ln H/H_\sigma)^2}\right)\right) + \cdots. \end{aligned} \tag{16}$$

Here $H_\pm = H_0 e^{\pm\pi\lambda_0}$. There is a resonance at $|\ln H/H_0| = \pi|\lambda_0|$; hence $T_K = H_0 e^{-\pi|\lambda_0|}$ can be considered as the usual Kondo temperature. Since the parameter λ_0 breaks parity, we have two contributions to the impurity magnetization, unlike in the situation for the periodic system [14] or the ordinary Kondo problem with chiral states. In the limit of small fields, this difference can be neglected; for high fields, it is essential. For $H \ll T_K$ we take $\mu = S' - \frac{1}{2}$ and the upper sign in (16), which means that the impurity spin S' is (under)screened in the ground state leading to an effective spin $S' - \frac{1}{2}$ which is asymptotically free, analogously to the usual Kondo effect. For a strong bulk field, $1 \gg H \gg T_K$ the effective spin is $\mu = S'$ (the lower sign in (16)) and is also asymptotically free. The parameter λ_0 can be used to shift the resonance, so the Kondo effect is maximal for $\lambda_0 = 0$, and disappears for $|\lambda_0| \to \infty$. (Because $J_0^{-1} = \lambda_0^2 + (S' + \frac{1}{2})^2$, these limits correspond to strong or weak antiferromagnetic coupling of the impurity to the host, respectively.) For $S' = \frac{1}{2}$ a single spin is added to the chain, giving a singlet ground state with impurity magnetic susceptibility $\chi = (2/\pi^2)\cosh\pi\lambda_0 \sim T_K^{-1}$. Note, however, that due to the geometry there is the logarithmic contribution M^z_{edge} to the magnetization of the system, which for small fields is much stronger than the linear one due to an $S' = \frac{1}{2}$ impurity.

The analysis of the finite boundary magnetic field is completely analogous to that for the impurity. Considering the system without impurity, we find

$$
\begin{aligned}
M^z &= M^z_{edge} + M^z_{\xi_1} + M^z_{\xi_L} \\
M^z_\xi &= \begin{cases} \dfrac{1}{4}\left\{-1 + \dfrac{(\xi-1)}{|\ln H/H_0|} + \cdots\right\} & \text{for } \xi \ll |\ln H/H_0| \\ -\dfrac{1}{\pi^2(\xi-1)}|\ln H/H_0| & \text{for } \xi \gg |\ln H/H_0|. \end{cases}
\end{aligned}
\tag{17}
$$

As discussed above, the contribution $-1/4$ to M^z_ξ in a vanishing bulk field is due to the fact that we have to consider lattices of odd size in the presence of boundary fields. Note that equation (17) contains the *complete* contribution to the magnetization due to the addition of the boundary potential. Alternatively, the magnetization of the boundary spin alone may be extracted from the ξ-dependence of the ground-state energy (15) (see, e.g. [28]). For large boundary fields the result coincides with (17), while for small ones (ξ large) the expectation value of the boundary spin is only half of the expression given here. As was shown in reference [25], the boundary magnetization vanishes for zero h, H and T, while the edge susceptibility is finite. Unlike the situation for the spin impurity, the boundary magnetization can never exceed $\frac{1}{2}$. This implies that a boundary potential cannot mimic a Kondo impurity with higher spin.

An effective spin of the boundary $\xi_{1,L}/2 = \pm\frac{1}{2}$ corresponds to the addition (removal) of one site to (from) the chain, with finite zero-field susceptibility. The edge magnetization is known for boundary fields $h_{1,L} \leqslant 1$, i.e. effective boundary spin $\xi_{1,L} > 0$ [25]. For $-1 < \xi_{1,L} < 0$ there appear bound states parametrized by complex rapidities $\lambda = (i/2)(1 - 1/h_{1,L})$, localized at the edges. Taking these roots into account, the corresponding contribution to the $H = 0$ ground-state energy is again given by (13). Similarly, we find that the boundary magnetization is still given by (17), hence varying smoothly with $h_{1,L}$, despite the appearance of localized levels.

Note, that due to the effective Kondo-like energy $T_K = H_0$ for the boundary, a perturbative analysis of the Fredholm equation at $H \gg T_K \sim 1$ is not possible. Because the bandwidth is now of the same order, the host's magnetization saturates at $H = H_s = 2$ before the effective T_K is reached. In this case the impurity magnetization becomes S'; the boundary one is $\frac{1}{2}$.

For low temperatures one can use the Sommerfeld approximation to calculate the contributions to the (zero-field) susceptibility and low-temperature specific heat ($c = \gamma T$) from the impurity and boundary, respectively. For the impurity we find $\gamma_{imp}/\chi_{imp} = 2\pi^2/3$ for $S' = \frac{1}{2}$, i.e. the universal Fermi liquid formula. For $S' > \frac{1}{2}$ one obtains the Curie behaviour $\chi_{imp} \propto (S'^2 - \frac{1}{4})/T$ and the remnant impurity entropy $S_{imp} = \sinh(2S'H/T)/\sinh(H/T)$. For the boundary a similar behaviour is found due to the remnant spin for non-zero $h_{1,L}$.

The high-temperature behaviour of the impurity is similar to that of a free effective spin S' in a magnetic field H with a Curie-like law for the zero-field susceptibility and a Schottky anomaly for the specific heat.

The case in which the bulk magnetic field H and the boundary one h are connected to each other, e.g. via $h = (1 - g)H$, with the effective g-factor of the boundary, deserves special treatment. At least, if H is small enough, and/or $g \sim 1$, the behaviour of the boundary magnetization is similar to the expression in (17). For larger field H, the perturbative solution as outlined above fails and the integral equations should be studied numerically.

Now we calculate finite-size corrections, using standard Euler–Maclaurin series for the Bethe *ansatz* equations [29]. The result is

$$E_{mes} = \pi v_F \left[\frac{(M - mL - \Theta)^2}{2z^2} + N^+ - \frac{1}{24} \right]. \tag{18}$$

Here m is the density of down spins, z is the dressed charge (its value varies from 1 to $1/\sqrt{2}$ as the magnetic bulk field H decreases from H_s to zero), and N^+ is the number of particle–hole excitations near the Fermi point. The parameter Θ is the phase shift at the Fermi point. It is produced by the edge, boundary and impurity, and it is related to the corresponding contributions to the magnetization via the Friedel sum rule. For vanishing magnetic fields, the Fermi shift 2Θ is an integer, so it can be removed from E_{mes} by making an appropriate choice of M. Note that because only open boundary conditions are considered in this paper, there are no states carrying a finite current (i.e. transfer of excitations between two Fermi points) in (18).

To summarize, we find that the behaviours of the impurity in an open and a periodic chain are very similar for small magnetic fields $H \lesssim T_K$, while a difference appears for large magnetic fields due to the broken parity for non-zero λ_0. Comparing the effect of the boundary potential to that of the impurity, we find two important features: (1) there is no shift of the Kondo resonance; and (2) the boundary potential cannot mimic the underscreened behaviour of the impurity with higher spin. Finally, we would like to stress that the appearance of a local level for sufficiently large boundary fields (i.e. $\xi_{1,L} < 0$) does not affect the low-energy physics.

As a by-product, we emphasize that, for vanishing boundary fields, the small-H behaviour of the impurity spin situated at the edge, and coupled antiferromagnetically through a single link to the open chain, is similar to that of the impurity situated in the bulk (for *any* boundary conditions) with coupling given by (3), i.e. exchange with two neighbouring spins in the host and additional three-spin interaction. The difference reveals itself in the mesoscopic (finite-size) corrections—namely, by the absence of current-carrying excitations. The impurity-induced Fermi phase shift is the same for the open and periodic cases, as are the Fermi velocity and dressed charge in (18). The differences may manifest themselves in mesoscopic finite-size effects, i.e. asymptotics of correlation functions, or in persistent current-like and Coulomb blockade oscillation effects [30, 31].

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