Hidden Kondo Effect in a Correlated Electron Chain

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We develop a general *Bethe ansatz* formalism for diagonalizing an integrable model of a magnetic impurity of arbitrary spin coupled ferro- or antiferromagnetically to a chain of interacting electrons. The method is applied to an open chain, with the exact solution revealing the existence of a "hidden" Kondo effect driven by forward electron scattering off the impurity. We argue that the so-called "operator reflection matrices" proposed in recent *Bethe ansatz* studies of related models emulate only forward electron-impurity scattering, which may explain the absence of complete Kondo screening for certain values of the impurity-electron coupling in these models. [S0031-9007(98)07209-3]

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The study of magnetic impurities in one-dimensional (1D) strongly correlated electron or spin systems has attracted great interest in the last few years. The availability of nonperturbative methods in one dimension has allowed for a detailed picture of the relevant physics, revealing some rather unexpected features, such as the complete screening of an impurity spin for a *ferromagnetic* Kondo exchange [1]. Future possible experiments on magnetic impurities implanted in quantum wires or carbon nanotubes, as well as analogies with related phenomena (x-ray boundary effects, metal point-contact spectroscopies, etc.), provide additional impetus for studying this problem.

The *Bethe ansatz* (BA) has played a particularly important role in the study of magnetic impurities. As is well known, the method has successfully been employed for the exact treatment of a Kondo impurity in a free electron host as well as for mixed-valence impurities (with hybridized impurity and host wave functions) [2]. The method has also been used to study magnetic impurities in spin chains [3], and more recently in *correlated* electron hosts [4]. In most of this work *periodic* boundary conditions (PC) were imposed on the electron (or spin) host. However, there exists an alternative approach, also exact, where *open* boundary conditions (OC) are implemented within a BA framework [5]: A boundary potential at the edge of the system here plays the role of impurity scatterer. In a recent series of very interesting papers, Wang and collaborators [6] proposed several new BA solutions for magnetic impurities in correlated hosts with OC. In their approach the magnetic impurity is attached to the edge of the chain together with an auxiliary boundary potential that preserves integrability. The effect of the resulting composite edge on the electrons is coded in a "reflection matrix," interpreted in [6] as simulating backscattering (BS) of electrons off an ordinary (nonintegrable) Kondo impurity in a correlated electron system. However, the absence of complete Kondo screening—as predicted by Furusaki and Nagaosa [1]—for certain values of the ferromagnetic exchange coupling in [6] raises some concern about this interpretation.

In this Letter, we revisit the problem via an alternative route, exploiting the quantum inverse scattering method (QISM) [7] to study the algebraic structure of this class of models. This allows us to explicitly exhibit the form of the reflection matrix used in [6] and show that it contains only forward electron scattering (FS) off the magnetic impurity, with the backscattering against the (infinite wall) free edge potential playing no essential role for the physics of the impurity. This is different from a nonintegrable Kondo impurity in a correlated host, where the *dynamic* backscattering against the impurity crucially influences the properties of the system [1,8]. By a more general construction, valid for an integrable impurity spin of *arbitrary* magnitude coupled ferro- *or* antiferromagnetically to an electron host, we show that a Kondo effect is still operative also when the impurity appears to be unscreened: The associated hidden Kondo screening becomes manifest only in the presence of an external magnetic field or at nonzero temperatures. Most importantly, our analysis shows that forward electron-impurity scattering, without the assistance of backward scattering off a free edge potential, can drive Kondo screening in a correlated electron host. For transparency, we focus on the supersymmetric t-J model of 1D correlated electrons with a spin-S impurity. However, the principal results of our analysis hold for *any* integrable electron model with gapless low-lying excitations, and do not depend on the specific form of the host Hamiltonian.

The key object in the QISM [7] is the two-particle scattering matrix, $X_{a,m}(u)$, where u is a spectral parameter, a labels a subspace V_a of an auxiliary particle, and m labels the Hilbert space V_m of a particle at a site m on a 1D lattice [7]. The necessary and sufficient condition for integrability is that the scattering matrix satisfies the Yang-Baxter equation (YBE) $X_{ab}(u - v)X_{am}(u)X_{bm}(v) = X_{bm}(v) \times X_{am}(u)X_{ab}(u - v)$, implying that only *forward* scattering (FS) is allowed. To maintain integrability in the presence of an impurity, located at a site n say, the impurity-host scattering matrix $R_{an}(u)$ also must satisfy a YBE: $X_{ab}(u - v)R_{an}(u)R_{bn}(v) = R_{bn}(v)R_{an}(u)X_{ab}(u - v)$.

To set the stage, let us first look at the simplest case of an impurity in a spin-$\frac{1}{2}$ chain [3]. The host as well as the impurity scattering matrices here belong to the SU(2)-symmetric rational solutions of the YBE: $X_{am}(u) = A(u)[u\hat{I} + ic\hat{P}_{am}]$ $(m = 1, 2, \ldots, N)$ and $R_{an}(u) = A(u - i\alpha)[(u - i\alpha)\hat{I} + ic\hat{P}_{an}]$, respectively. Here c is a coupling constant (fixed by the YBE to be the same for host and impurity exchange), $|\alpha|$ measures the shift of the impurity level from the Kondo resonance [4], $A(v)$ with $v = u, u - i\alpha$ are normalization constants, and P_{aj} is a permutation operator on the corresponding spaces, with V_j carrying a spin$-\frac{1}{2}$ (spin-S) representation of SU(2) for $j{=}m{\neq}n$ $(j{=}n)$. Given $X_{am}(u)$ and $R_{an}(u)$ and imposing PC, QISM constructs the Hamiltonian of the system as a logarithmic derivative (with respect to the spectral parameter) of the *transfer matrix* $\tau_{PC}(u)$ of the associated 2D statistical mechanics problem: $\tau_{PC}(u) \equiv Tr_a \prod_m^L X_{am}(u)R_{an}(u - i\alpha)$. It is important to note that the position of the impurity matrix in this product has no influence on the dynamics: The auxiliary particle simply scatters off all spins on the chain consecutively, including the impurity. For the OC case, one introduces additional *reflection* matrices, $K_a(u)$ [9] which describe the backscattering off the open boundary. In contrast to the host or impurity scattering matrices, these are c-number matrices. They satisfy the reflection equation (RE) $X_{ab}(u - v)K_a(u)X_{ab}(u + v)K_b(v) = K_b(v)X_{ab}(u + v)K_a(u) \times X_{ab}(u - v)$, as required by integrability. Given the reflection matrices, the analog of the transfer matrix for the OC, $\tau_{OC}(u)$, is defined by $\tau_{OC}(u) = Tr_a K_a(u)T_a(u) \times K_a(u)T_a^{-1}(-u)$, where $T_a(u) = \prod_m^L X_{am}(u)R_{an}(u - i\alpha)$ is the PC monodromy matrix. The recently proposed operator reflection matrix for the spin model in [6] has the simple structure $R(u)K(u)R^{-1}(-u)$ with $K(u) = \hat{I}$, i.e., it is just the ordinary c-number reflection matrix $K(u)$ of a free boundary sandwiched between two FS impurity matrices [6,10]. The auxiliary particle here scatters off the impurity, reflects at the free edge, and then scatters off the impurity once more, but moving in the opposite direction.

The QISM for correlated PC [11] or OC [12] electron chains with an impurity works similar to the scheme above, with one essential difference: electrons carry spin *and* charge, and, hence, two *nested* transfer matrices have to be introduced. The first-level transfer matrix describes the charge sector, while the second-level transfer matrix describes the spin sector. Because of the nesting, a magnetic impurity inserted into a correlated electron chain has to carry both spin *and* charge degrees of freedom in order to preserve integrability. Its spin part drives the Kondo effect while the charge part provides the mixed-valence behavior of an impurity [13].

Specializing to the supersymmetric t-J model [14] with a magnetic impurity, its Hamiltonian can be decomposed as $\mathcal{H} = \mathcal{H}_{\rm bulk} + \mathcal{H}_{\rm imp} + \mathcal{H}_{\rm bound}$. Here $\mathcal{H}_{\rm bulk} = K_{\alpha\beta}\sum_{n=1}^{L-1}(J_n^\alpha J_{n+1}^\beta + \text{H.c.})$ defines the bulk Hamiltonian for a chain of length L, with J_n^α the generators in the defining representation of the supersymmetric algebra $sl(1|2)$, and $K_{\alpha\beta} \equiv TrJ^\alpha J^\beta$ [11]. The impurity Hamiltonian $\mathcal{H}_{\rm imp}$ (with the impurity coupled to sites n and $n + 1$) has the form

$$\begin{aligned}\mathcal{H}_{\rm imp} = \ & c_0(H_{n,S} + H_{S,n+1} - (\alpha^2 + 2S(S + 1))H_{n,n+1} \\ & - 2i\alpha[H_{S,n} + H_{S,n+1}, H_{n,n+1}] \\ & + \{H_{n,S}, H_{S,n+1}\}) \,. \qquad (1)\end{aligned}$$

The commutator-anticommutator structure in (1) is generic and applies to *any* impurity model [with SU(2) or $sl(n|m)$ symmetry] constructed by QISM. It is here realized by taking $H_{n,S} = K_{\alpha\beta}(J_n^\alpha J_S^\beta + \text{h.c.})$, where J_S^α are the generators for the spin-S impurity, with $c_0 = f[(S + \frac{1}{2})^2 - \alpha^2]^{-1}$ being an effective impurity-host coupling constant [$f = 1$ for an exchange impurity, while $f = (M\sigma|M + \sigma)\sqrt{2S + 1}$ for a hybridization impurity, with $(M\sigma|M + \sigma)$ the Clebsch-Gordan coefficients [4]]. The boundary Hamiltonian $\mathcal{H}_{\rm bound}$ has a trivial structure for PC: $\mathcal{H}_{\rm bound} = K_{\alpha\beta}J_1^\alpha J_L^\beta + \text{H.c.}$ The OC boundary Hamiltonian, on the other hand, is obtained by making the replacement $(J^\alpha)_{1,L} \rightarrow h_{1,L}$, where $h_{1,L}$ define the *boundary fields* at the edges at $m = 1$ and $m = L$ [15]. This procedure is directly applicable when the impurity is located in the bulk. However, a similar construction can be used also for an impurity *at the edge:* We now put $n = L$, and replace the operator at the "phantom site" with index $n + 1$ in Eq. (1) by the boundary field h_L. Note that by this procedure the three-particle commutator and anticommutator terms in (1) collapse to two-particle terms.

Inspection of Eq. (1) shows that the parameter α determines the coupling between impurity and host. For imaginary α, and for real α with $|\alpha| < S + \frac{1}{2}$, we have an antiferromagnetic (AFM) coupling, while for real α with $|\alpha| > S + \frac{1}{2}$ we get a ferromagnetic (FM) coupling. A real α, however, corresponds to a non-Hermitian impurity Hamiltonian, making the ferromagnetic case unphysical unless one places the impurity at the edge with a *zero boundary field* [4,10]. For this special choice, $h_L = 0$, only the first term survives in Eq. (1): $\mathcal{H}_{\rm imp} = c_0 H_{L,S}$. Thus, the FS impurity is here connected to the host by a single link with coupling constant c_0, providing a simple and natural impurity Hamiltonian. Analogous to the spin-chain case, the reflection matrix including the impurity is obtained by sandwiching the ordinary *free edge* reflection matrix $K(u) = \hat{I}$ between two FS impurity matrices: $R_{aL}(u)\hat{I}R_{aL}(-u)$ with $R_{aL}(u)$ from [4]. This structure is general and holds also for the models considered in [6] as is evident from inspection of the resulting BA equations.

Its form implies that the backscattering from the free edge, which is present in any open chain, decouples from the scattering governed by the FS impurity matrices. As a consequence, the position of the impurity on the chain is immaterial to the physics when the interaction is AFM with imaginary α. On the other hand, as we have just seen, for real α (including FM interaction) a real energy spectrum requires the impurity to be attached to the edge *with zero boundary potential*.

Eigenfunctions and eigenvalues of the model are parametrized by sets of quantum numbers, partitioned into *charge rapidities* $\{u_j\}_{j=1}^{N}$ (with N the number of electrons) and *spin rapidities*, $\{v_q\}_{q=1}^{M}$ (with M the number of "down spins"). The rapidities are the solutions of the BA equations, which for the OC zero-boundary case take the form

$$\prod_{\pm} e_{2S\pm\alpha}(v_p)\prod_{j=1}^{N} e_1(v_p \pm u_j) = \prod_{\pm}\prod_{q=1}^{M} e_2(v_p \pm v_q)$$

$$e_1^{2L}(u_j) = \prod_{\pm} Y_{\pm}(u_j)\prod_{p=1}^{M} e_1(u_j \pm v_p), \qquad (2)$$

with $e_n(x) = (2x + in)/(2x - in)$. The functions containing α describe spin and charge degrees of freedom of the impurity [$Y_{\pm}(x) = e_{2S+1\pm\alpha}(x)$ for a hybridization impurity and $Y_{\pm}(x) = \sqrt{e_{2S+1\pm\alpha}(x)/e_{2\pm\alpha}(x)}$ for an exchange impurity [4]]. These BA equations can be transformed into a form similar to the PC case by a change of variables: $u_j \to -u_j$, $j = -N, \ldots, -1, 0$; $v_p \to -v_p$, $p = -M, \ldots, -1, 0$ which gives the OC energies $E = \sum_{j=1}^{2N+1}(u_j^2 + \frac{1}{4})^{-1}$. We also remove the roots corresponding to $u_j = v_p = 0$ (which label unphysical null states). It is important to stress that the states which are present for OC but not PC determine the BS singularities *independent* of the FS *impurity* terms.

The ground state of the supersymmetric *t*-*J* model in an external field is obtained by filling up two Dirac seas for singlet Cooper-like pairs and unbound electrons, respectively [16]. The structure of the singlet-paired ground state for zero magnetic field $H = 0$ conspires with the magnetic impurity to produce a nonzero *mixed* impurity valence n: For $H = 0$ there are no unbound electrons, but scattering of Cooper pairs off the exchange (hybridization) impurity makes n smoothly vary from zero for an empty band to $+1$ (-1) for a half-filled band, a process common to both FM and AFM impurity-host coupling. By an analysis of the counting functions that define the number of BA states [17] one can show that the impurity magnetization M_{imp} in the limit of *zero magnetic field* can take either the value $M_{\mathrm{imp}} = S - \frac{1}{2}$ (as in the ordinary Kondo effect) or $M_{\mathrm{imp}} = S$. In the latter case the Kondo screening is hidden, and becomes manifest only for nonzero fields or temperatures. This effect, which is generic to this class of theories, is particularly transparent in the present model.

To see how it comes about, let us first consider the case with AFM impurity-host coupling and imaginary α. Here the impurity "traps" a fraction of a Cooper pair which gets polarized by the field to produce an *effective* impurity spin $S_{\mathrm{eff}} = S + \frac{|n|}{2}$. However, the magnetic field also excites unbound electrons from the sea of Cooper pairs. For a sufficiently weak field, these unbound electrons partially screen the effective impurity spin, a process in complete analogy with the ordinary Kondo effect with the only difference being that an *effective spin* $S_{\mathrm{eff}} > S$ gets (partially) screened. As the field increases it eventually breaks up the impurity-screening cloud composite, leaving behind the effective (unscreened) spin S_{eff}. For $S > \frac{1}{2}$ there is a crossover between low- and high-energy behaviors of the magnetic impurity: For low fields one has an asymptotically free underscreened spin S, while for high fields the asymptotically free spin is $S + \frac{n}{2}$. We can also see the features of the hidden Kondo effect in the finite-temperature properties. For example, in the Kondo regime (with charge degrees of freedom suppressed) the effective spin is S for low temperatures, $T \ll T_K$, and $S + \frac{1}{2}$ for high temperatures, $T \gg T_K$, with Curie-like behavior and usual Kondo logarithmic corrections. The zero field residual entropy is given by $S = \ln 2S$ for imaginary α. The specific heat has a Shottky peak at $T \propto H$ and a Kondo resonance at $T \propto T_K$ for a weak magnetic field H, with the two peaks merging into one for large H. This behavior is typical for an "underscreened" magnetic impurity [2]. In contrast, *complete* Kondo screening is present for the case of an exchange impurity with $S = \frac{1}{2}$ or a hybridization impurity with $S = 0$. The impurity susceptibility is proportional to T_K^{-1}, with a specific heat linear in T at low energies, and one thus recovers a standard Fermi-liquid scenario generic for AFM impurity models.

We can illustrate the above, e.g., by explicitly calculating the impurity magnetization M_{imp} at half filling, using the BA equations (2). In fact, we find a universal expression for M_{imp}, *valid for the AFM as well as the FM case:*

$$M_{\mathrm{imp}} = S_{\mathrm{eff}}\left[1 \pm \frac{1}{2\ln(H/T_K)} - \frac{\ln\ln(H/T_K)}{4\ln^2(H/T_K)} + \ldots\right], \qquad (3)$$

where for imaginary α the Kondo energy scale is $T_K = H_0\exp(-\pi|\alpha|)$ with $H_0 = \sqrt{\pi^3/e}$, and where we have subtracted the contribution $M_{\mathrm{edge}} = |2\ln(H/H_0)|^{-1} - \ln\ln|\sqrt{H/H_0}|/4\ln^2(H/H_0) + \ldots$ from the free edges. For low fields, and $S > \frac{1}{2}$, $H \ll T_K$, $S_{\mathrm{eff}} = S$ with the upper sign in (3) defining M_{imp}. On the other hand, for fields which are large on the Kondo scale but still much smaller than the spin saturation field, $T_K \ll H \ll 1$, $S_{\mathrm{eff}} = S + \frac{1}{2}$ with M_{imp} defined by the lower sign in (3). For an $S = 0$ hybridization impurity or an $S = \frac{1}{2}$ exchange impurity one obtains $S_{\mathrm{eff}} \propto H/T_K$ for low magnetic fields, while $S_{\mathrm{eff}} = \frac{1}{2}$ for high fields [4].

Let us now consider the FM case, or more generally, the case of real α, with $2|\alpha| = [2|\alpha|] + \{2|\alpha|\}$, where $[x]$ $(\{x\})$ denotes the integer (fractional) part of x. Equation (3) still describes the impurity magnetization, with the fractional part determining the "Kondo temperature": $T_K = H_0/\cos(\pi\{2|\alpha|\}/2)$. This is in contrast to the case with imaginary α which exhibits a usual exponential dependence of T_K on the coupling constant. (Note that for $2|\alpha|$ an integer we have $T_K = H_0$.) Hence the crossover scale is here larger, $T_K > 1$, than the critical field that determines the transition to the spin-saturated, ferromagnetic phase of the host. It follows that for real α a *high-field region for a magnetic impurity is absent* [18]. Another feature special for real α is that incident and reflected particles effectively scatter off *different* impurity spins: $S \pm \frac{[2|\alpha|]}{2}$ and $S + \frac{1\pm[2|\alpha|]}{2}$, respectively. Thus, depending on the value of α, the impurity exhibits different characteristics. If $[2|\alpha|] < 2S - 1$, $[2|\alpha|] = \pm 2S$, or $[2|\alpha|] > 2S + 1$ (FM domain), then $S_{\mathrm{eff}} = S$ in Eq. (3): the impurity spins "seen" by incident and reflected waves are both underscreened. Thus, for the FM regime, the impurity spin is *always* underscreened, also for $S = \frac{1}{2}$. This suggests that the complete screening for FM Kondo coupling as proposed in [1] crucially depends on the presence of backscattering for this case. For the special values $[2|\alpha|] = 2S \pm 1$, $S_{\mathrm{eff}} = S \pm \frac{1}{4}(1 - \frac{H}{T_K})$ we obtain *both a remnant spin and terms linear in H*. Similar features also appear for the specific heat for these critical values: The Curie-like behavior of the remnant spin (the underscreened effective spin seen by incoming waves) is accompanied by a Fermi-liquid behavior (of the totally screened effective spin seen by reflected waves) [19]. Negative effective spins signal the appearance of local levels (bound states of host excitations). These levels, which influence the value of the remnant impurity entropy, are generated by the FS magnetic impurity, and are insensitive to the edge potential. We point out that α determines the shift of the Kondo resonance, with imaginary α (AFM coupling) corresponding to a resonance with the band excitations of the host, while for real α (FM *or* AFM coupling) local impurity levels may decouple from the bands.

To conclude, we have shown that forward electron-impurity scattering in a correlated host can drive a Kondo effect *without* the assistance of backward scattering from a free edge potential. This Kondo effect, which is present both for ferro- *and* antiferromagnetic impurity-electron coupling, is hidden for impurity spin $S > \frac{1}{2}$ (as well as for $S = \frac{1}{2}$ when the coupling is ferromagnetic) and becomes manifest only in the presence of a magnetic field or at nonzero temperatures. We have argued that the so-called operator reflection matrices proposed in recent *Bethe ansatz* studies of related models [6] emulate only forward scattering off a magnetic impurity. This may explain the observed absence of complete Kondo screening for certain values of the Kondo coupling in these models.

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[15] The boundary field couples to the $sl(1|2)$ generators and hence plays the role of a magnetic field in the spin sector. In addition, a nonzero $h_{1,L}$ acts in the charge sector to produce a nonzero phase between incoming and reflected electron waves. Here we use the case with the same boundary potentials for spin and charge sectors, [12].

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[18] As a consequence, a nonperturbative approach—as in the present Letter—is required since perturbation theory is known to break down at low energies in this class of problems [2].

[19] If one allows for *fractional* spin values (for which $T_K = H_0$) one observes a critical *overscreened* behavior of the effective spin "seen" by the reflected wave, while the other spin will be underscreened.