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Exact solution for a one-dimensional multichannel model of correlated electrons with an Anderson-like impurity

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Abstract. We study a one-dimensional n-channel highly correlated electron model (based on the supersymmetric $t-J$ model) with a magnetic impurity of arbitrary spin S that can hybridize with up to one itinerant electron per channel. The model extends the multichannel Kondo problem to correlations in the host and to the mixed valence regime. The Bethe ansatz equations are derived and solved for the ground state and for low temperatures. We conclude that the critical non-Fermi-liquid (overscreened) behaviour cannot be reached for this interacting electron system. Possible applications of the model are discussed.

The Mn–O bond length is believed to play a fundamental role in the colossal magnetoresistance [1] recently discovered in $La_{1-x}Ca_xMnO_3$ films close to the metal–insulator and para-/ferro-magnetic transitions. The Mn ions exist in a mixed tri-/tetra-valent state in which the three t_{2g} orbitals are simply occupied with their spins forming a total spin $S = 3/2$. In Mn^{3+} there is, in addition, an electron populating one of the two e_g orbitals with its spin ferromagnetically correlated with the t_{2g} spin quartet. The mixed valent character of the Mn ions then arises from the e_g electron, which may be localized at the Mn ion or become a correlated itinerant electron via hybridization. The Mn–O bond lengths are changed when the degeneracy of the two e_g orbitals is lifted.

We consider here an integrable impurity model with some of the key ingredients of the Mn ions in the manganates, namely, a localized spin S (representing the t_{2g} states) hybridizing with itinerant electrons to form the (Mn^{3+}) configuration of total spin $S + \frac{1}{2}$. The model has n orbitals to take into account the degeneracy of the e_g levels. The one-dimensional (1D) conduction states have infinite local repulsion within each channel (only one spin state is occupied) and interactions with electrons on the neighbouring sites. Our model can also be considered the extension of the multichannel Kondo problem [2–4] to include correlations in the host and a hybridization of two magnetic impurity configurations with the itinerant electrons.

We construct the Bethe ansatz equations for our model using the quantum inverse scattering method [5] from the electron–electron scattering matrix of the host and the electron–impurity scattering matrix by imposing periodic boundary conditions. (Note that this approach is different from studying an open chain with the boundary potential playing the role of the impurity [6].) Our problem is then similar to other magnetic impurities (e.g. Kondo and Anderson) embedded into a free electron gas solved with the coordinate Bethe

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ansatz [4, 7], except that the starting point is the scattering matrices. The Hamiltonian can be constructed as the logarithmic derivative of the transfer matrix.

An impurity introduced into an exactly solvable correlated host usually destroys the integrability. There are only a few exceptions, namely, (i) the SU(2) Heisenberg chain of spin S' with an impurity of spin S embedded into the chain [8] and (ii) some magnetic impurities (Kondo and Anderson-like) in a single channel correlated electron host [9]. Whereas in case (i) all three forms of spin-compensation (under-/over-screening and exact spin-compensation) can take place, the one-electron channel impurity models in case (ii) only reveal underscreened and exact spin-compensated regimes, but no critical behaviour. Our present model can also be considered as the extension of (ii) to include the situation where the number of channels is larger than $2S$.

The host is the multichannel extension of the 1D supersymmetric $t-J$ model [10] with the two-electron scattering matrix given by

$$\hat{X}(p) = (p\hat{I}_s + \mathrm{i}\hat{P}_s)(p\hat{I}_o - \mathrm{i}\hat{P}_o)(p^2+1)^{-1} \tag{1}$$

where $\hat{I}_s$, $\hat{P}_s$, $\hat{I}_o$ and $\hat{P}_o$ are the identity and permutation operators for the spin and channels (orbits), respectively. In (1) the spin and orbital parts factorize and each separately satisfy the triangular Yang–Baxter relation, so that $\hat{X}$ also obeys the triangular relation. Here $p = \frac{1}{2}\cot\frac{1}{2}k$ are the charge rapidities and k is the wavenumber in the coordinate representation. To preserve the integrability the electron–impurity scattering matrix, $\hat{S}$ has to satisfy the triangular Yang–Baxter equation with $\hat{X}$ [7]

$$\hat{X}^{12}(p_1-p_2)\hat{S}^{1M}(p_1-p_0)\hat{S}^{2M'}(p_2-p_0) = \hat{S}^{2M}(p_2-p_0)\hat{S}^{1M'}(p_1-p_0)\hat{X}^{12}(p_1-p_2) \tag{2}$$

where $|M| \leqslant S$ is the z-projection of the impurity spin S. The Yang–Baxter equations are the necessary and sufficient conditions for the integrability.

An impurity scattering matrix satisfying relation (2) is

$$\hat{S}^{\sigma\sigma'}_{MM'}(x) = \hat{I}_o\left[\delta_{\sigma\sigma'}\delta_{MM'} + (M\sigma|M+\sigma)\times(M'\sigma'|M'+\sigma')\frac{\mathrm{i}(2S+1)}{x-\mathrm{i}(2S+1)/2}P^{\sigma\sigma'}_{MM'}\right] \tag{3}$$

where $P^{\sigma\sigma'}_{MM'} = \delta_{\sigma\sigma'}\delta_{MM'} + \delta_{-\sigma\sigma'}\delta_{M'M+2\sigma}$. The impurity scattering is diagonal in the orbital (channel) sector. The Clebsch–Gordan coefficient $(M\sigma|M+\sigma)$, which is a shorthand notation for $(SM;\frac{1}{2}\sigma|S\frac{1}{2}(S+\frac{1}{2})M+\sigma)$, selects the coupling of the impurity spin and the spin of the itinerant electron to form an effective spin $(S+\frac{1}{2})$ within each orbital channel. Hence, the impurity exists in two different spin configurations, namely, one of spin S (only the t_{2g} orbitals are singly occupied) and the other of spin $(S+\frac{1}{2})$ (there is an additional electron in an e_g orbital ferromagnetically coupled to S). The impurity scattering matrix is similar to that of an Anderson impurity with two magnetic configurations embedded in a free electron gas considered previously [11]. Since the hybridization matrix element of the impurity is fixed by the condition of integrability, the only parameter determining the properties of the impurity is thus p_0 (except for the magnitude of the spin S). It will be seen that $|p_0|$ plays the role of the Kondo exchange coupling constant. Note, however, that $\hat{S}$ is not unique, in the sense that there are other electron–impurity scattering matrices satisfying (2) that can be constructed [9].

The (non-trivial) impurity-host part of the lattice Hamiltonian can be written as (suppose the impurity is situated at site 0)

$$\begin{aligned}\mathcal{H}_{\mathrm{imp}} = J(\mathcal{H}_{L,0} + \mathcal{H}_{0,1} + \{\mathcal{H}_{L,0},\mathcal{H}_{0,1}\} + (J^{-1} - 3S(S+1) - \tfrac{1}{4})\mathcal{H}_{L,1} \\ +2p_0[(\mathcal{H}_{L,0}+\mathcal{H}_{0,1},\mathcal{H}_{L,1}])\end{aligned} \tag{4}$$

where $J = \sqrt{2S+1}[p_0^2 + (S+\frac{1}{2})^2]^{-1}(M\sigma|M+\sigma)$ is the effective coupling constant (note that exchange is antiferromagnetic), an electron situated at site 0 has spin S, and the interaction in the channel sector is just 1. One can see that by enlarging $|p_0|$ one reduces the absolute value of the local exchange coupling J, so that the most important resonance situation corresponds to small values of J. The model is exactly diagonalized using the standard Bethe ansatz approach [7]. Each eigenstate is characterized by $(n+2)$ sets of quantum numbers, namely, one set of charge rapidities $\{p_j\}$, $j = 1, \ldots, N$ (N is the total number of electrons), one set of spin rapidities $\{\lambda_\alpha\}$, $\alpha = 1, \ldots, M^*$ (M^* is the number of down-spin electrons), and n sets of channel rapidities $\{\mu_\beta\}$, $\beta = 1, \ldots, m^{(i)}$, $i = 1, \ldots, n$ (with $m^{(i)} = \sum_{k=i+1}^{n} n^{(k)}$ and $n^{(k)}$ being the number of electrons in channel k). Each state corresponds to a particular solution of the nested Bethe ansatz

$$\prod_{\tau=\pm1}\prod_{\beta=1}^{m^{(k+\tau)}} e_1(\mu_\alpha^{(k)} - \mu_\beta^{(k+\tau)}) = \prod_{\gamma=1}^{m^{(k)}} e_2(\mu_\alpha^{(k)} - \mu_\gamma^{(k)})$$

$$e_{2S}(\lambda_\alpha - p_0)\prod_{j=1}^{N} e_1(\lambda_\alpha - p_j) = \prod_{\beta=1}^{M^*} e_2(\lambda_\alpha - \lambda_\beta)$$

$$e_{2S+1}(p_j - p_0)e_1^L(p_j) = \prod_{\alpha=1}^{M^*} e_1(p_j - \lambda_\alpha)\prod_{\beta=1}^{m^{(1)}} e_1(\mu_\beta^{(1)} - p_j) \tag{5}$$

where $e_n(x) = (2x + \mathrm{i}n)/(2x - \mathrm{i}n)$, $\mu_j^{(0)} = p_j$, $m^{(0)} = N$, $m^{(n+1)} = 0$, and L is the length of the chain. The energy and the magnetization are given by $E = \sum_j^N (p_j^2 + \frac{1}{4})^{-1}$, and $S^z = (N/2) - M^* + S$, respectively. The impurity contributions to equation (5) are the first factors in the second and third equations.

There are several differences between the present model and the multichannel Kondo problem in the free electron host worth pointing out. First, due to the correlations in the host the charges contribute in a non-trivial way as can be seen in the second equation of (5). Second, the present model involves forward and backward moving electrons in contrast to the s-wave-only formulation of the multichannel Kondo impurity embedded in a free electron gas [2, 3]. Third, the hybridization couples the impurity spin to itinerant electrons on both neighbouring sites, breaking parity and time-reversal symmetries separately, but conserving their product (TP).

It is instructive to discuss the long-wave limit of the model by linearizing the kinetic energy about the Fermi level. The Fermi points $\pm k_\mathrm{F}$ are related to Fermi charge rapidities $\pm p_\mathrm{F}$ by $2p_\mathrm{F} = \cot\frac{1}{2}k_\mathrm{F}$ and the Fermi velocity is $v_\mathrm{F} = [2\sin(\frac{1}{2}k_F)]^{-2}$. Dividing the charge rapidities by v_F and also rescaling the spin and channel rapidities, we obtain the generalization of Wiegmann–Tsvelik's Bethe ansatz [2] for the non-interacting multichannel electron gas (interaction just renormalizes the Fermi velocity as usual for the 1D Luttinger liquid approach) with an Anderson-like impurity (their case corresponds to $S = 0$). The continuum Hamiltonian can be written as

$$\mathcal{H} = -v_\mathrm{F}\int \mathrm{d}x c_{\sigma,f}^\dagger(x)\left(\frac{\partial}{\partial x}\right)c_{\sigma,f}(x) + v_\mathrm{F}\epsilon\sum_{M',f}|S', M', f\rangle\langle S', M', f|$$
$$+v_\mathrm{F}^{1/2}\sum_{M,M',\sigma,f}(M', \sigma|M'+\sigma)\int \mathrm{d}x\delta(x)[c_{\sigma,f}^\dagger(x)|S', M', f\rangle\langle S, M, f| + \mathrm{HC}] \tag{6}$$

where bra and ket denote impurity states ($\sum_M |S, M, f\rangle\langle S, M, f| + \sum_{M'} |S', M', f\rangle\langle S', M', f| = 1$), and σ and f denote the spin projection and the channel of itinerant

electron. Two-electron states at each place are excluded, as in the Hund-rule situation. In the continuum limit (with 'contact' impurity–host coupling) only the odd parity about the impurity waves interact with the impurity, even ones were disregarded. (Note that in [2] only the spin-compensated case was studied rigorously and for other cases a special conjecture had to be used.) The impurity rapidity p_0 is related to the impurity level energy ϵ of the linearized model via $v_F\epsilon = |p_0|$.

The thermodynamics of the model is analysed in terms of the usual string hypothesis. In the thermodynamic limit, in which $L, N, M, m^{(j)} \to \infty$ with their ratios kept fixed, the Bethe ansatz equations have the following solutions: (i) unbound electrons with charge rapidities p_j, (ii) spin–charge singlet pairs $p_j = \lambda_j \pm i/2$, (iii) spin strings (bound states of any number of down-spins), and (iv) channel strings of arbitrary length for each channel. In fact our n-channel $t-J$ model has an infinite on-site repulsion to exclude the double occupation within each channel, so that the structure of bound states is analogous to the asymmetric limit studied in [2, 12]. For simplicity we only consider the channel-singlet situation and neglect all channel symmetry breaking fields [13], for instance crystalline fields. The orbital singlet condition leads to spin-composites for the itinerant electrons in the ground state, which spin-compensate the impurity.

We first study the ground-state properties of the impurity as a function of the band filling and the external magnetic field. In complete analogy to the standard multichannel Kondo problem in the ground state only unbound charges (class (i)), spin–charge singlet pairs (class (ii)) and channel strings of length 1 and 2 for each channel (class (iv)) can be occupied. The latter correspond to unbound channel states and pairs of them. The occupation of these states determines the Dirac seas of the model. For the orbital singlet condition the rapidities of the channel strings fill the entire band without leaving holes. Introducing distribution density functions for particles and holes for each class of states, the channel strings can then be eliminated from the problem via Fourier transformation. Denoting with $\rho(p)$ ($\rho_h(p)$) and $\sigma(\lambda)$ ($\sigma_h(\lambda)$) the densities for unbound charges and spin–charge pairs and their holes, respectively, we find that they satisfy the following integral equations

$$a_1(p) + \frac{1}{L}a_{2S+1}(p-p_0) = \rho_h(p) + (1 - a_1 \star s_1) \star (\rho(p) + a_1 \star \sigma(\lambda))$$
$$a_2(\lambda) + \frac{1}{L}a_{2S+2}(\lambda - p_0) = \sigma_h(\lambda) + (1 + a_2) \star (1 - a_1 \star s_1) \star (\sigma(\lambda) + s \star \rho(p)) \tag{7}$$

where $\star$ denotes convolution, and the p and λ integrations are over the intervals $|p| > B$ and $|\lambda| > Q$, respectively. Here the integration limits $\pm B$ and $\pm Q$ play the role of Fermi points for unbound electrons and singlet spin–charge pairs. The kernels a_n, s and s_1 are the Fourier transforms of

$$\exp(-n|\omega|/2) \qquad [2\cosh(\omega/2)]^{-1} \qquad \sinh[(n-1)|\omega|/2]/\sinh[n|\omega|/2] \tag{8}$$

respectively. The driving terms proportional to L^{-1} are due to the impurity, while the extensive ones describe the interacting electron gas. Equations (7) are linear in densities, and can be separated into a bulk and an impurity contribution. The host determines the integration limits, e.g. $B = \infty$ corresponds to a zero magnetic field (no unbound charges), while the limit $Q \to \infty$ refers to the low singlet-pair density, and $Q \to 0$ to a band-filling n (one electron per channel and site).

The solution of the integral equations for the impurity density distributions yields the valence and the magnetization of the impurity in the ground state. In zero magnetic field ($B \to \infty$) the valence monotonically varies from $n_{imp} = 0$ for low pair density (Q is large)

to $n_{\rm imp} = n$ for $Q = 0$ (half-filled bands). In general, the impurity valence depends on the relative values of Q and p_0, but also on S.

More interesting than the valence is the impurity magnetization. To study the magnetization we Fourier transform equations (7) and eliminate $\sigma(\lambda)$ from the first equation by using the second equation

$$\rho_{\rm h}(p) + F \star \rho = s \star \sigma_{\rm h} + s(p) + \frac{1}{L} s \star a_{2S}(p - p_0) \tag{9}$$

where F is the Fourier transform of $\tilde{F}(\omega) = \tanh(|\omega|/2)[1-\exp(-n|\omega|)]^{-1}$. In the absence of an external magnetic field we obtain an impurity magnetization of $S^z_{\rm imp} = S$ and the host has no magnetization. Since the total number of electrons is conserved, the magnetic field monotonically increases the number of unbound electrons and simultaneously decreases the number of singlet pairs. The first term on the right-hand side of equation (9) represents the number of holes in the singlet-pair band (the integration is now over the interval $[-Q, Q]$). Usually the Zeeman splitting is much smaller than the Fermi energy, so that for weak magnetic fields (the field is not necessarily small compared to the Kondo temperature) we may neglect the effect of the pair holes on the impurity magnetization, i.e. by setting $Q = 0$. Assuming that B is large the Fredholm integral equation (9) can be reduced to a hierarchical sequence of Wiener–Hopf integral equations. In the following we discuss the solution of the leading Wiener–Hopf equation, which is a valid approximation in the limit of small T_K (large $|p_0|$).

Depending on the value of S we have to distinguish two different situations [2–4].

(a) If $S \neq 0$ the impurity is said to be underscreened and asymptotically a free impurity spin behaviour is obtained

$$S^z_{\rm imp} = \mu\left[1 \pm \frac{n}{2}(Ln)^{-1} - \frac{n^2}{4}\ln|Ln|(Ln)^2 + \cdots\right] \tag{10}$$

where $Ln = |\ln(H/T_K)|$ and $T_K \propto \exp(-\pi|p_0|)$ takes the role of the Kondo temperature. In (10) the upper (lower) sign corresponds to low (high) fields compared to T_K. The magnetic moment μ is different at low and high fields, namely $\mu = S$ if $H \ll T_K$ and $\mu = S + (n/2)$ for $H \gg T_K$. This case is similar to the underscreened magnetic impurity in the free electron host, corresponding to $2S > n$.

(b) For $S = 0$ the small field impurity magnetization is given by $S^z_{\rm imp} = H\chi_s$, where $\chi_s \propto T_K^{-1}$ is finite. Since the zero-field susceptibility is finite, this case is analogous to the totally compensated Kondo impurity in the free electron gas ($2S = n$). The most essential point to emphasize is that the overscreened situation ($n > 2S$, where for small fields the excess of channels gives rise to critical non-Fermi-liquid behaviour for free electron gas) is never reached for our highly correlated multichannel electron model.

Hence, a hybridization multichannel impurity in a correlated electron system undergoes two processes at $T = 0$. First, an effective spin $S + \frac{1}{2}n_{\rm imp}$ is created via hybridization with the host spin-singlet pairs. Second, a non-zero magnetic field de-pairs electrons in the host, which screen the effective impurity spin. The latter process is similar to the spin-compensation in the multichannel Kondo effect for a free electron host [2, 3]. The saturation magnetization of the impurity at large fields (compared to T_K) is $S + (n/2)$.

The thermodynamic Bethe ansatz equations for the orbital channel singlet can be obtained by minimizing the free energy $F = E - T\mathcal{S}$, where T is the temperature and $\mathcal{S}$ is the entropy. This yields integral equations for the thermal dressed energies for the excitations. The thermodynamic Bethe ansatz equations are driven by the host, and they are very similar to those of the free electron host multichannel Kondo problem [12], differing

only in the driving terms (energy of the $t-J$ model instead of the linearized free electron gas). In the high-temperature limit the driving terms are not relevant, so that the free energy of the impurity is similar to that of the Anderson impurity in a free electron host [9, 12], but with two magnetic configurations.

We now study the low-temperature thermodynamics in the Kondo limit, where the charge degrees of freedom are suppressed. Using an analysis similar to that of [3, 12] we cast the low-temperature thermodynamics into the universal form

$$\phi_j(\lambda) = s \star \ln[(1+\mathrm{e}^{\phi_{j-1}})(1+\mathrm{e}^{\phi_{j+1}})] - \delta_{j,n}\,\mathrm{e}^{\pi\lambda} \tag{11}$$

where ϕ_j is the thermodynamic dressed energy scaled with the temperature for a spin-string of length j and $\phi_0 = -\infty$. The magnetic field is introduced via the asymptotic condition $\lim_{j\to\infty}(\phi_j/j) = H/T$. For low temperatures the impurity free energy can be expressed as a function of ϕ_n

$$F_{\mathrm{imp}} = -T\int \frac{\mathrm{d}\lambda\, a_{2S}(\lambda)\ln(1+\mathrm{e}^{\phi_n})}{2\cosh[\pi\lambda + \ln(T/T_K)]}. \tag{12}$$

The results are similar to those of a multichannel impurity in a free host for a totally screened case [3, 12], but differ drastically for underscreened and overscreened cases. Once more, the overscreened case is absent for our model. In the underscreened case the low-temperature, zero-field magnetization possesses a Curie-like temperature dependence and there is non-zero entropy due to excess spin. In the totally screened case $S = 0$ the low-temperature susceptibility and specific heat are similar to the usual Fermi-liquid situation.

The effective Kondo exchange J_{eff} depends on the impurity rapidity p_0 relative to the Fermi level of the charges Q. The solution of the equation for the pair density σ in the limit of the almost filled band yields that J_{eff} is determined by the transcendental equation

$$J_{\mathrm{eff}}^{-1} - (n-2)\ln(J_{\mathrm{eff}}/2\pi) = Q - p_0$$

i.e. to leading order

$$T_K \propto J_{\mathrm{eff}}^{(n-2)/2}\exp(-\pi/J_{\mathrm{eff}}).$$

Thus for large $|Q-p_0|$ we have the usual exponential dependence, while for small $|Q-p_0|$ the Kondo temperature reveals a power-law dependence with J_{eff} [2].

Possible applications of the multichannel Kondo problem have been discussed previously [4]. For example: the underscreened situation $S \neq 0$ is realized by Tm and Tb impurities in a simple metallic host; the completely compensated case quantitatively explains the thermodynamics of Fe and Cr impurities in Cu and Ag. Additionally, in the mixed valent regime for $n = 2$ and $S = \frac{3}{2}$ the model could represent a dilute manganate alloy [1].

The stability of the critical non-Fermi-liquid fixed point of the overcompensated spin to perturbations is of great interest [13, 14]. The effects of several symmetry breaking fields have been investigated. On the one hand, the fixed point was found to be unstable (Fermi-liquid behaviour is recovered) to (i) an external magnetic field, (ii) channel-symmetry breaking in the exchange coupling (J_{eff} depends on the channel) and (iii) a crystalline field splitting. On the other hand, the fixed point is stable to exchange anisotropy ($J_\parallel \neq J_\perp$). As we have shown in this paper, it is also unstable to interactions among the conduction electrons.

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