Multichannel Anderson impurity behavior in a pure hybridization impurity model

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A single multichannel quantum impurity model with pure hybridizations between the localized and orbital degenerate conducting electrons is shown to exhibit several interesting impurity properties resembling that of the multichannel Anderson model. Particularly for two special kinds of hybridization parameters the model can be solved exactly by the Bethe ansatz method. In these integrable cases, the competition between the direct and exchange correlated hybridizations can produces either a Fermi-liquid or non-Fermi-liquid behavior at low temperatures.

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I. INTRODUCTION

A prototype model of quantum hybridization impurity problem is the well-known Anderson model (AM), which describes the formation of the local magnetic moment in nonmagnetic host metals. The model exhibits the quantum nature of an impurity embedded in a Fermi liquid (FL), such as mixed-valance behavior and the Kondo effect, and provides some interesting interpretations of the deviations from the FL which have been widely observed in the normal-state properties of cuprates and in some Ce- and U-based heavy-fermion compounds.[1] The deviations are in some cases also ascribed to the existence of a quantum critical point (QCP) associated with degenerate impurity states at zero temperature, such as the quadrupolar Kondo effect and electron-assisted tunneling of an atom in a double-well potential.[2] Thus, in order to make a closer connection between theory and experiment, it is interesting to investigate the different types of impurity correlations in a single-impurity model and to clarify if it is responsible for the non-Fermi liquid (NFL) behavior.

The simplest single-impurity model Hamiltonian exhibiting NFL behavior is the multichannel Kondo model[3](MKM) in the overscreened case, which has been studied extensively by the Bethe ansatz (BA) method,[4–7] conformal field theory,[8] and bosonization technique.[9] Unlike other NFL scenarios, the overscreened Kondo effect manifests itself as the ground-state degeneracy due to the residue degrees of freedom at the impurity site, resulting in divergent susceptibility at low temperatures.[6] Many efforts have been made to clarify if this unusual impurity behavior is limited only to the Kondo regime. One may consider a generalized AM with additional screening channels. As long as the normalized local level is pinned at the Fermi surface the valence fluctuation may give rise to a NFL.[10] Another remarkable approach is to consider the response of channel anisotropy to NFL behavior in the MKM by use of a BA solution. In this case, a new energy scale is generated characterizing the neighbors of the fixed points, reflecting the structure of symmetry breaking in the channel sector.[11] Depending on the anisotropy parameter, the BA solution provides a unified description for the crossover from FL to NFL behavior. It is then interesting to seek a similar BA solution for the Anderson-like model where a similar crossover would take place. For this purpose, Karnaukhove and Yu suggested to consider a single-impurity model describing the exchange interaction and correlated hybridization in a degenerate AM.[12] More recently, by using the BA method, Bolech and Andrei have studied the two-channel AM with the single-occupancy constraint on the localized level,[13] and Zvyagin has investigated a generalized AM with both in-shell Hubbard-like interaction and Hunds exchange.[14]

In this paper, we propose to study a class of hybridization impurity models without direct Coulomb in-shell coupling between localized electrons. Recall that in the AM, the hybridization is a one-particle process; the only two-particle interaction is the direct d-d correlation parametrized by repulsion U on an impurity shell. In our model, the latter is absent. Instead, two competing correlated hybridizations [H_{W_1} and H_{W_2} in Eq. (1)] corresponding to off-diagonal Coulomb processes are introduced. We will show that the model Hamiltonian shares some features similar to those of the multichannel AM and is exactly solvable in some specified parameter regions. Though the conventional U term is absent, the electrons on the impurity shell experience Pauli exclusion due to correlated two-body impurity-metal hybridizations and the exclusion of three- or more-particle occupancy at the impurity site. The latter requirement is necessary for the validity of the BA solutions in a number of multichannel models involving three (or more) hybridizing impurity valences (conveniently chosen as empty, singly, or doubly occupied impurity states).[15] As the model parameters vary, the system exhibits both the traditional Kondo effect and NFL behavior due to the different degenerate ground states similar to the multichannel Anderson model.

II. MODEL HAMILTONIAN

The free part of the model includes the electron energies in the conducting band and the local impurity level, given by

$$H_0 = -i\sum_{m\sigma}\int dx c^{\dagger}_{m\sigma}(x)\frac{\partial}{\partial x}c_{m\sigma}(x) + \epsilon_d\sum_{m\sigma} d^{\dagger}_{m\sigma}d_{m\sigma},$$

where $c^{\dagger}_{m\sigma}(x)$ ($d^{\dagger}_{m\sigma}$) creates a conducting band (local orbital) electron with spin index $\sigma=\uparrow,\downarrow$ and orbital channel (flavor) index $m=1,\ldots,f$. The one-particle hybridization between localized and band electrons is described by

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$$H_V = -\sum_{m\sigma} \int dx\,\delta(x)[Vc^\dagger_{m\sigma}(x)d_{m\sigma} + V^* d^\dagger_{m\sigma}c_{m\sigma}(x)].$$

Among two-particle impurity-metal correlations, we consider two kinds of correlated hybridizations, represented by W_1 and W_2, respectively, as

$$H_{W_1} = \sum \int dx\,\delta(x)[W_1 d^\dagger_{m\sigma}c^\dagger_{m'\sigma'}(x)d_{m'\sigma'}d_{m\sigma} + \text{H . c . }],$$

$$H_{W_2} = \sum \int dx\,\delta(x)[W_2 d^\dagger_{m\sigma}c^\dagger_{m'\sigma'}(x)d_{m'\sigma}d_{m\sigma'} + \text{H . c . }].$$

Obviously, these two terms are truncated from the off-diagonal Coulomb processes preserving the spin and orbital rotational invariance. Our total model Hamiltonian is given by

$$H = H_0 + H_V + H_{W_1} + H_{W_2}. \tag{1}$$

The pure hybridization Hamiltonian, Eq. (1), shares in some aspects the features of degenerate asymmetric AM's. For simplicity, we fix $V>0$, $W_1>0$ and consider W_2 as a running parameter. Let us first consider $W_2=0$—i.e., the spin-orbital degenerate case. Usually, both the one-particle hybridization H_V and the correlated hybridization H_{W_1} will induce the antiferromagnetic exchange between the local and conducting electrons. But due to the absence of direct on-site repulsion U, the effective s-d exchange J_V induced by V via valence fluctuations, $d^1+e^- \rightleftharpoons d^2, d^1 \rightleftharpoons d^0+e^-$, is vanishing, while the one induced by W_1 via $d^1+e^- \rightleftharpoons d^2$ is $J_{W_1} \sim -VW_1/\epsilon_d$. We always assume that the local level ϵ_d is below the Fermi surface. The case with $f=1$ (i.e., the single-channel model without the W_2 term) was first discussed by Karnaukhov.[16] The Kondo regime closes to $W_1=V$, where double occupation at the impurity site is forbidden. This is because $H_V+H_{W_1}$ is given by

$$V \int dx\,\delta(x)\left[1 - \frac{W_1}{V}n_d\right]c^\dagger_\sigma(x)d_\sigma,$$

indicating the limit $W_1 \to V$ being the same as that of the $U \to \infty$ degenerate Anderson model.[6,16] In fact, as we will see in the following, the two-electron scattering S matrix turns out to be the same as that of the infinite-U degenerate Anderson model[6] and the model is exactly solvable for arbitrary f. As the spin and orbital channels are degenerate [preserving SU($2f$) symmetry], there is a characteristic energy scale T_K (the Kondo temperature) below which both the spin and orbital degrees of freedoms of the impurity are exactly compensated by the conducting electrons.

When $W_2 \neq 0$, the above picture will be modified in each spin-orbital channel, resulting in an orbital singlet or spin singlet, respectively, depending on the effective coupling. This is because while W_1 is spin-orbital SU($2f$) invariant, W_2 breaks it into $\text{SU}_{\text{spin}}(2) \otimes \text{SU}_{\text{orbital}}(f)$. The meaning of H_{W_2} is clear: when there is an electron in the d orbital, it leads to another d electron attracting (repelling) a c electron if they are in the same (different) channels with different (the same) spins. Therefore the correlated hybridizations for a spin singlet and orbital triplet (ss,ot) is W_1-W_2, while for an orbital singlet and spin triplet (os,st) is W_1+W_2. The situation resembles that of the multichannel AM with both direct and exchange correlations among d electrons.[5,6,17,14] Generally, these asymmetric spin or orbital singlet ground states will lead to non-Fermi-liquid behavior at low temperatures.

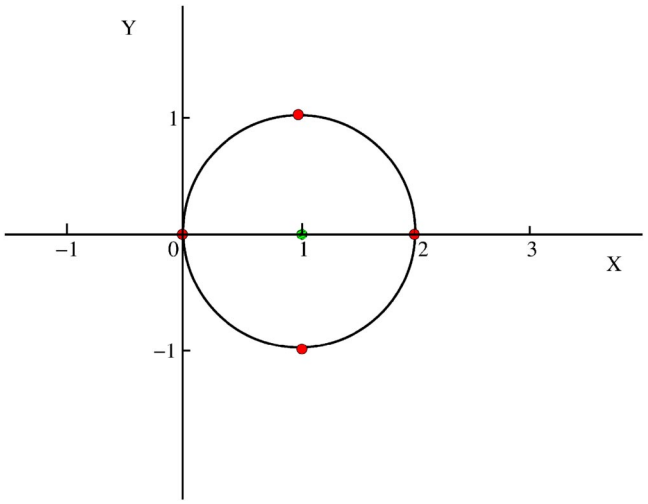

FIG. 1. The integrable cases parametrized by $X=W_1/V$ and $Y=W_2/V$. Case (i) (spin-orbital degenerate) is along the X axis; case (ii) (spin-orbital nondegenerate) is a circle centered at (1,0) with radius 1. The two integrable lines insect at (0, 0) and (2, 0). The effective coupling (c) along the X axis is negative (positive) in between (or outside) the two points. Along the circle the effective coupling changes sign alternatively at the four free spin points (0, 0), (1, 1), (2, 0), and $(1,-1)$.

At first glance, the model seems to be integrable for generic W_2, as the two-electron scattering matrices in both (ot,ss) and (os,st) sectors satisfy the Yang-Baxter relation (YBR). However, the explicit two-electron scattering matrix in a general spin-orbital configuration cannot be expressed in terms of the product of those obtained in each (ot,ss) and (os,st) sector, owing to the hybridizing dynamics.[15] So the model is not integrable for generic W_2. Fortunately, we will find that there is a nontrivial circle $W_2 = \pm\sqrt{W_1(2V-W_1)}$, along which the exact solution of Hamiltonian (1) is again available. In the phase diagram parametrized by $W_1/V, W_2/V$ (see Fig. 1), the center of the circle is located at (1, 0)—i.e., the Kondo regime in the degenerate case. There are four special points at the circle—i.e., (0, 0), (1, 1), (2, 0), and $(1,-1)$—corresponding to the exact free spin regimes.

III. INTEGRABLE CASES

The integrability of the model in two special cases, especially the spin-orbital nondegenerate case, is nontrivial. This is explored by *explicitly solving the two-particle scattering matrix (TPSM) $S_{12}(k_1,k_2)$ of two conduction electrons* in the following.[15] Here, we need to solve the three valence states with $n_d=0$, 1, 2 by use of Bethe wave functions. These states, however, are mixed into each other due to the one-particle and correlated hybridizations. A generic state of the two-particle system, parametrized by two different quasimomenta $|k_1,k_2\rangle$, is defined by

$$|k_1,k_2\rangle = \sum_{m_i\sigma_i}\int dx_1dx_2 g^{\sigma_1\sigma_2}_{m_1m_2}(x_1,x_2)c^\dagger_{m_1\sigma_1}(x_1)c^\dagger_{m_2\sigma_2}(x_2)|0\rangle + \sum_{m_i\sigma_i}\int dx e^{\sigma_1|\sigma_2}_{m_1|m_2}(x)c^\dagger_{m_1\sigma_1}(x)d^\dagger_{m_2\sigma_2}|0\rangle + \sum_{m_i\sigma_i} f^{\sigma_1\sigma_2}_{m_1m_2}d^\dagger_{m_1\sigma_1}d^\dagger_{m_2\sigma_2}|0\rangle,$$

where $g(x_1,x_2)$, $e(x)$, and f are the wave functions satisfying the following Schrödinger equations:

$$(-i\partial_{x_1}-i\partial_{x_2}-E)g(x_1,x_2) = \frac{V}{2}[\delta(x_1)Pe(x_2)-\delta(x_2)e(x_1)], \tag{2}$$

$$(-i\partial_x+\epsilon_d-E)e(x)+2V^*g(x,0)+2[(V+W_1)f+W_2P_\sigma f]\delta(x) = 0, \tag{3}$$

$$(2\epsilon_d-E)f+\frac{1}{2}(V^*+W_1^*)(1-P)e(0)+\frac{1}{2}W_2^*(P_\sigma-P_m)e(0) = 0. \tag{4}$$

In the above, P_σ, P_m, and $P\equiv P_\sigma\otimes P_m$ are permutation operators defined in the spin, orbital, and total spaces, respectively.

According to Wiegmann and Tsvelick,[5] we assume the following Bethe wave functions:

$$2!\, g(x_1,x_2) = [Ag_{k_1}(x_1)g_{k_2}(x_2)-PBg_{k_2}(x_1)g_{k_1}(x_2)]\theta(x_1-x_2) + [Bg_{k_1}(x_1)g_{k_2}(x_2)-PAg_{k_2}(x_1)g_{k_1}(x_2)]\times\theta(x_2-x_1),$$

where $g_k(x)$ is the one-electron wave function satisfying $(-i\partial_x-k)g_k(x)+Ve_k\delta(x)=0$ and $e_k=[V^*/(k-\epsilon_d)]g_k(0)$. It is solved by $g_k(x)=\exp\{i[kx+\phi\,\mathrm{sgn}(x)]\}$, with $\phi=2\tan^{-1}[-V^2/2(k-\epsilon_d)]$. Once the Bethe function for $g_{k_1k_2}(x_1,x_2)$ is adopted, $e_{k_1k_2}(x)$ and f_{k_1,k_2} can be derived directly from Eqs. (2) and (4), respectively:

$$e_{k_1k_2}(x) = [Ae_{k_2}g_{k_1}(x)-PBe_{k_1}g_{k_2}(x)]\theta(x)+[Be_{k_2}g_{k_1}(x)-PAe_{k_1}g_{k_2}(x)]\theta(-x), \tag{5}$$

$$f_{k_1k_2} = e_{k_1}e_{k_2}\frac{V^*+W_1^*+W_2^*P_s}{4V^*}(1-P)(A+B). \tag{6}$$

By substituting the above expressions into Eq. (3), we obtain the following constraint on the amplitudes A and B:

$$\Delta_1+\Delta_2+\Delta_3 = 0, \tag{7}$$

where $\Delta_1=-(V/2)(1-P)(A+B)$, $\Delta_2=(i/V^*)[(k_1-\epsilon_d)+(k_2-\epsilon_d)P](B-A)$, and $\Delta_3=[(|V+W_1+W_2P_s|^2)/2V^*](1-P)(A+B)$. It is straightforward to derive from Eq. (7) the two-particle scattering matrix defined by $B=S(k_1,k_2)A$. The expression for $S(k_1,k_2)$ is rather complicated, and it does not satisfy the following YBR for generic W_2:

$$S_{12}S_{13}S_{23} = S_{23}S_{13}S_{12}. \tag{8}$$

However, we find two special cases where the S matrices do satisfy Eq. (8).

(i) *Spin-orbital degenerate case with* SU(2f) *symmetry:* $W_2=0$, $c=2W_1(W_1-2V)$*:*

$$S(k_1,k_2) = \frac{k_1-k_2-icP}{k_1-k_2-ic}. \tag{9}$$

(ii) *Spin-orbital nondegenerate case with* SU(2)$\otimes$SU(f) *symmetry:* $W_2^2-2VW_1+W_1^2=0, c=2W_2(W_1-V)$*:*

$$S(k_1,k_2) = S_\sigma(k_1,k_2)\otimes S_m(k_1,k_2), \tag{10}$$

where

$$S_\sigma(k_1,k_2) = \frac{k_1-k_2-icP_\sigma}{k_1-k_2-ic}, \tag{11}$$

$$S_m(k_1,k_2) = \frac{k_1-k_2+icP_m}{k_1-k_2+ic}. \tag{12}$$

We notice that the same TPSM of the conducting electrons keeping SU(2)$\otimes$SU(f) symmetry in the spin-orbital nondegenerate case was first obtained in the MKM by the fusion rule[4] and equivalently in the degenerate AM (but is valid only in the Kondo regime).[5] In that case, the electron-impurity TPSM is determined by the electron-impurity exchange correlation, but the electron-electron TPSM is basically arbitrary, as there are no true interactions between two conduction electrons with linear dispersion. The integrability is then guaranteed by choosing a proper electron-electron TPSM satisfying the YBR associated with that of electron-impurity ones. The ambiguity in choosing the electron-electron TPSM appears also in the hybridization impurity model if only two valence states such as $n_d=1,2$ or $n_d=0,1$ are considered.[12] However, once the mixing of three impurity valences ($n_d=0,1,2$) in the hybridization models is concerned, such an ambiguity no longer exists. Moreover, as we can see from Eq. (7), $S=I$ when $W_1=W_2=0$. So *the electron-electron TPSM is unambiguously fixed by* H_V *even in the absence of interactions*. This is a striking dynamical constraint on the wave functions of the hybridization impurity models involving three impurity valences, in contrast to that of the conventional impurity models.

IV. BETHE ANSATZ EQUATIONS AND THE SOLUTIONS

In the SU(2f) case, the solution[6,19,20] is identical to that of the single-channel Anderson model provided the number of spin components is simply replaced by $2f$. So we turn to the more interesting SU(2)$\otimes$SU(f) case where the TPSM is expressed as a product of individual ones defined in spin and orbital spaces, respectively. This characteristic is crucial for the formation of orbital (spin) singlet ground states, which in turn leads to the NFL behavior. In this case, the eigenstates are parametrized by three sets of rapidities: the charge rapidities $\{k_j\}_{j=1}^N$, the spin rapidities $\{\lambda_\alpha\}_{\alpha=1}^M$, and the orbital rapidities $\{\mu_q^{(r)}\}_{q=1}^{M_r}$, where N, M, and M_r are the numbers of conduction electrons, of down spins, and of electrons in the rth orbital. Each eigenstate corresponds to a solution of the following BA equations (BAE's) (obtained on a periodic interval of length L):

$$\exp[ik_jL + 2i\phi(k_j)] = \prod_{\alpha=1}^{M} e_1[k_j - \lambda_\alpha] \prod_{q=1}^{M_1} e_1^{-1}[k_j - \mu_q^{(1)}],$$

$$\prod_{j=1}^{N} e_1[\lambda_\alpha - k_j] = -\prod_{\beta=1}^{M} e_2[\lambda_\alpha - \lambda_\beta],$$

$$\prod_{s=\pm1} \prod_{q=1}^{M_{r+s}} e_1[\mu_p^{(r)} - \mu_q^{(r+s)}] = -\prod_{q=1}^{M_r} e_2[\mu_p^{(r)} - \mu_q^{(r)}], \quad (13)$$

where $j=1,\ldots,N, \alpha=1,\ldots,M, p=1,\ldots,M_r, M_0=N$, $M_f=0$, and $e_n(x)=(x-inc/2)/(x+inc/2)$. The energy, the spin magnetization, and the orbital projection are given by $E=\Sigma_{j=1}^{N} k_j, S_z=\frac{1}{2}N-M$, and $L_z=[(f-1)/2]N-\Sigma_{r=1}^{f-1} m_r$, respectively. (The number of electrons in the rth orbital is $N_r=M_{r-1}-M_r$.)

In the thermodynamic limit, with $L,N,M,M_r\to\infty$ while keeping their ratios fixed, the solutions of the above BAE's are classified by the string hypothesis. The ground-state and thermodynamics properties can be analyzed by the standard method.[5–7,13,14,19,20] A peculiar feature of our model is that the effective coupling c can be either positive or negative, as hybridizations parameters vary along the integrable lines; see Fig. 1. For $c>0$ (<0), the effective coupling is attractive (repulsive) in the orbital sector and repulsive (attractive) in the spin sector. The former situation was discussed in detail by Schlottmann and Sacramento for the multichannel Kondo model.[7] The only difference is that in our case the effective coupling c and the hybridizition width $V^2/2$ are independent of each other. Thus the main results are briefly stated as follows. For $c>0$, the ground state is an orbital singlet. In the absence of a magnetic field, the spin rapidities are all real, the charge rapidities are bounded with opposite spin components into pairs via $k^{\pm}=\lambda\pm ic/2$, and the orbital rapidities are also complex, building bound pairs via $\mu^{(r)}=\Lambda^{(r)}\pm ic/2$ with some real parameters $\Lambda^{(r)}$. Inserting these rapidities into the BAE's, we obtain a set of coupled linear integral equations of Wiener-Hopf type for the distribution densities of the rapidities, where the integration limit Q of λ is determined by the total number of electrons. When the renormalized impurity level energy $\epsilon^*=(\epsilon_d-Q)\pi/V^2-(f/2)\ln(f/2)$ is far below the Fermi surface, the averaged impurity valence is given by $n_d/f=1-1/\epsilon^*+[(f-2)\ln|\epsilon^*|]/2|\epsilon^*|^2$. The characteristic logarithmic dependence of the multichannel Kondo problem is recovered by identifying $|\epsilon^*|\sim\ln(D/T_K)$. In the presence of the magnetic field, there are an additional $2M=2S_z$ number of real charge rapidities corresponding to unpaired propagating electrons and consequently $[(f-r)/f]2S_z$ number of real orbital rapidities in the ground state. The integration limit B for real charge rapidities is now determined by the total magnetization. In the integer valence limit, the magnetization can be obtained by simply suppressing the charge fluctuations ($Q\to\infty$) as $M=\exp(-\epsilon'-f/2)/\Gamma(f/2)$ for small fields and $M=(f/2)[1-f/2|\epsilon'|-(f/2|\epsilon'|)^2\ln|\epsilon'|]$ for large fields respectively, where the dimensionless parameter ϵ' is defined in the same form as ϵ^* but with B in place of Q.

Summarizing, we have shown that the impurity model with pure hybridizations, in cases (i) and (ii), is integrable. While the first case is spin-orbital degenerate and shows single-channel Kondo impurity behavior, the second one is spin-orbital nondegenerate, exhibiting typical multichannel Anderson impurity behavior. The latter provides an interesting new realization of a general critical theory for the hybridization impurity problem.[21] For generic model parameters W_1 and W_2, the system is not integrable. Whether it falls into the same universal class as that of the integrable one or exhibits new impurity physics at low temperatures needs further investigations.

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