Ground State Properties of an Anderson Impurity in a Gapless Host

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Using the Bethe ansatz method, we study ground state properties of a $U \to \infty$ Anderson impurity in a "gapless" host, where a density of band states vanishes at the Fermi level ϵ_F as $|\epsilon - \epsilon_F|$. As in metals, the impurity spin is proven to be screened at arbitrary parameters of the system. However, the impurity occupancy as a function of the bare impurity energy is shown to acquire novel qualitative features which demonstrate a nonuniversal behavior of the system. The latter explains why the Kondo screening is absent (or exists only at quite a large electron-impurity coupling) in earlier studies based on scaling arguments. [S0031-9007(98)08269-6]

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The physics of "gapless" dilute magnetic alloys, where an effective density of band electron states varies near the Fermi level as $|\epsilon - \epsilon_F|^r$, $r > 0$, has been attracting a significant theoretical interest. Using "poor-man's" scaling for the spin-$\frac{1}{2}$ Kondo model, Withoff and Fradkin [1] have predicted that the Kondo effect in gapless systems takes place only if an effective electron-impurity coupling exceeds some critical value; otherwise, the impurity decouples from the electron band. Numerical renormalization group (RG) calculations, large-N studies, and quantum Monte Carlo simulations [2–7] have confirmed this prediction and revealed a number of additional intriguing features of the physics of magnetic impurities in unconventional Fermi systems.

In a conventional metallic system with (i) a linear dispersion of electrons near the Fermi level, $\epsilon(k) = v_F(k - k_F)$, and (ii) an energy independent band electron-impurity hybridization, basic "impurity" models are exactly solved by the Bethe ansatz (BA) [8–11]. It has recently been shown [12] also that integrability of the degenerate and $U \to \infty$ nondegenerate Anderson models is not destroyed by a nonlinear dispersion of particles and an energy dependent hybridization, but it becomes only hidden [13]. The approach developed has allowed us to study [14] the thermodynamic and ground state properties of an Anderson impurity embedded in a BCS superconductor, and can be used to obtain an exact solution of the Kondo problem in other unconventional systems.

In this Letter, we report an exact BA solution of a model describing a $U \to \infty$ Anderson impurity embedded in a gapless host. The model is diagonalized by BA at the arbitrary density of band states $\rho(\epsilon)$ and hybridization $t(\epsilon)$. In the RG approach, the physics of the system is assumed to be governed only by an effective electron-impurity coupling $\Gamma(\epsilon) = \rho(\epsilon)t^2(\epsilon)$ rather than by separate forms of $\rho(\epsilon)$ and $t(\epsilon)$. However, to derive thermodynamic BA equations, one has to specify separate forms of an effective electron-impurity coupling and an inverse dispersion of band states $k(\epsilon)$. While an effective coupling determines the electron-impurity and effective electron-electron scattering amplitudes, an inverse dispersion accounts for the spatial behavior of electron wave functions, and naturally enters BA equations via periodic boundary conditions imposed on eigenfunctions of the system. The physics of the system is thus governed by both an effective electron-impurity coupling $\Gamma(\epsilon)$ and an inverse dispersion of band electrons $k(\epsilon)$ [15].

Here, we treat the case of an energy independent hybridization, $t(\epsilon) = t = \text{const}$, so that an energy dependence of an effective coupling $\Gamma(\epsilon) = 2\Gamma\rho(\epsilon)$, where $2\Gamma = t^2$, is determined only by a nonlinear band dispersion. We assume also a simple form for the density of states of a gapless host,

$$\rho(\epsilon) = \frac{|\epsilon|^r}{|\epsilon|^r + \beta^r}, \qquad (1)$$

where the energy ϵ is taken relative to the Fermi value ϵ_F. The parameter β characterizes the size of the region with an unconventional behavior of $\rho(\epsilon)$. At $\beta = 0$, the model reduces to the metallic Anderson model. If β exceeds essentially a band half-width D, $\beta \gg D$, one obtains the density of states $\rho(\epsilon) \sim |\epsilon|^r$. To derive thermodynamic BA equations one has to fix the power r in Eq. (1). The magnitude of r is one of the key factors in determining the spectrum of the system in terms of Bethe excitations. In this Letter, we focus on the simplest case $r = 1$, which is, however, of particular physical interest [3–7].

Because of a separation of charge and spin quantum numbers, the spectrum of the metallic $U \to \infty$ Anderson model is described in terms of unpaired charge excitations, charge complexes, and spin excitations including bound spin complexes [8–11]. Since the ground state of the system is composed only of charge complexes (a charge complex contains one spin wave and two charge excitations) carrying no spin, the Kondo effect takes place: The impurity spin vanishes at zero temperature.

In the gapless model described above, the structure of the spectrum is shown to preserve basic characteristic features of the metallic version. In particular, the ground state of the system is still composed only of charge complexes carrying no spin. Therefore, as in metals, the Kondo screening of the impurity spin takes place at arbitrary parameters of the system, which contradicts dramatically to results of earlier studies [1–7].

However, the behavior of the impurity occupancy n_d as a function of the bare impurity level energy ϵ_d is drastically changed compared to a metal host. At positive values of ϵ_d, the impurity occupancy is still given by the standard formulas [8], where the renormalized impurity level energy $\epsilon_d^* = \epsilon_d + \frac{\Gamma}{\pi}\ln\frac{D}{\Gamma} + \beta$ contains now the parameter β. The mixed-valence regime shrinks: the impurity occupancy quickly grows from $n_d \approx 0$ at $\epsilon_d = 0$ to $n_d = 1$ (precisely) at $\epsilon_d \leq -\Gamma^2/4\beta$. In the Kondo (local-moment) regime, $n_d = 1$, and it does not depend on ϵ_d. Only in the empty-level regime ($\epsilon_d > 0$) the impurity occupancy is a universal function of the renormalized impurity energy e_d^* rather than a function of the bare parameters of the model.

The behavior of the impurity occupancy in the mixed-valence and Kondo regimes is not universal that manifests nonuniversal properties of a gapless system in contrast to a metallic one. This explains why the Kondo screening is absent (or exists only at quite a large electron-impurity coupling) in earlier studies based on scaling arguments.

We start with the Hamiltonian of the nondegenerate Anderson model rewritten in terms of the Fermi operators $c_\sigma^\dagger(\epsilon)$ $[c_\sigma(\epsilon)]$ which create [annihilate] an electron with spin $\sigma = \uparrow, \downarrow$ in an s-wave state of energy ϵ,

$$H = H_c + H_d + H_h\,. \tag{2a}$$

Here

$$H_c = \sum_\sigma \int_{-D}^{D} \frac{d\epsilon}{2\pi}\, \epsilon c_\sigma^\dagger(\epsilon) c_\sigma(\epsilon)\,, \tag{2b}$$

$$H_d = \epsilon_d \sum_\sigma d_\sigma^\dagger d_\sigma + U d_\uparrow^\dagger d_\uparrow d_\downarrow^\dagger d_\downarrow\,, \tag{2c}$$

$$H_h = \sum_\sigma \int_{-D}^{D} d\epsilon \sqrt{\Gamma(\epsilon)}\,[c_\sigma^\dagger(\epsilon) d_\sigma + d_\sigma^\dagger c_\sigma(\epsilon)]\,, \tag{2d}$$

are the conduction band, impurity, and hybridization terms, respectively. All notation in Eqs. (2) are standard. An electron localized in an impurity orbital with the energy ϵ_d is described by the Fermi operators d_σ. The electron energies and momenta are taken relative to the Fermi values, which are set to be equal to zero. The integration over the energy variable ϵ is restricted by the band half-width D. In what follows, we assume that D is the largest parameter on the energy scale, $D \to \infty$. In the energy representation, the effective particle-impurity coupling $\Gamma(\epsilon) = \rho(\epsilon) t^2(\epsilon)$ combines the density of band states, $\rho(\epsilon) = dk/d\epsilon(k)$, and the energy dependent hybridization $t(\epsilon)$.

In the limit of a large Coulomb repulsion in an impurity orbital, $U \gg D$, eigenvalues of the model (2) with the arbitrary inverse dispersion $k(\epsilon)$ and effective coupling $\Gamma(\epsilon)$ are found from the following BA equations [12]:

$$e^{ik_jL}\,\frac{h_j - \epsilon_d/2\Gamma - i/2}{h_j - \epsilon_d/2\Gamma + i/2} = \prod_{\alpha=1}^{M} \frac{h_j - \lambda_\alpha - i/2}{h_j - \lambda_\alpha + i/2}\,, \tag{3a}$$

$$\prod_{j=1}^{N} \frac{\lambda_\alpha - h_j - i/2}{\lambda_\alpha - h_j + i/2} = -\prod_{\beta=1}^{M} \frac{\lambda_\alpha - \lambda_\beta - i}{\lambda_\alpha - \lambda_\beta + i}\,, \tag{3b}$$

where N is the total number of electrons in an interval of size L and M is the number of electrons with spin "down." The eigenenergy E and the z component of total spin of the system are found to be

$$E = 2\Gamma \sum_{j=1}^{N} \omega_j\,, \qquad S^z = \frac{N}{2} - M\,. \tag{3c}$$

In Eqs. (3), $\omega = \epsilon/2\Gamma$ is a dimensionless energy, and $k_j = k(\omega_j)$ are charge excitation momenta. From Eq. (1), one easily obtains

$$\frac{k}{2\Gamma} = \begin{cases} \omega + \delta \ln(1 - \frac{\omega}{\delta}), & \omega < 0\,, \\ \omega - \delta \ln(1 + \frac{\omega}{\delta}), & \omega > 0\,, \end{cases} \tag{4a}$$

where $\delta = \beta/2\Gamma$. The BA equations (3) are quite similar to those in the conventional Anderson model [8–11]. The only, but very essential, difference is a nonlinear energy dependence of momenta and charge "rapidities" $h_j = h(\omega_j)$. At arbitrary $\rho(\epsilon)$ and $t(\epsilon)$, the rapidity $h(\epsilon) = (\epsilon - \epsilon_d)/\Gamma(\epsilon)$. In our model of a gapless host, where $t^2(\epsilon) = 2\Gamma$ and $\rho(\epsilon)$ is defined as in Eq. (1) with $r = 1$,

$$h(\omega) = \left(\omega - \frac{\epsilon_d}{2\Gamma}\right) \frac{|\omega| + \delta}{|\omega|} + \frac{\epsilon_d}{2\Gamma}\,. \tag{4b}$$

As in the metallic Anderson model, in the thermodynamic limit spin rapidities λ_α, $\alpha = 1, \ldots, M$ are grouped into bound spin complexes of size n,

$$\lambda_\alpha^{(n,j)} = \lambda_\alpha + \frac{i}{2}(n + 1 - 2j)\,, \qquad j = 1, \ldots, n\,. \tag{5}$$

Apart from unpaired charge excitations with real rapidities h_j, the system spectrum contains also charge complexes, in which two charge excitations with complex rapidities bound to a spin wave with a real rapidity λ_α,

$$h_\alpha^{(\pm)}(\omega) = \lambda_\alpha \pm \frac{i}{2}\,. \tag{6}$$

Without an impurity term [the second term in the left-hand side of Eq. (3a)], BA equations of impurity models describe a free host in terms of interacting Bethe particles with an arbitrary rapidity $h(\omega)$. Introducing an impurity fixes $h(\omega)$, and fixes thus the spectrum of Bethe excitations of a host. For instance, the finite-U and $U \to \infty$ Anderson impurities require different descriptions of the same host with the different spectra of Bethe excitations [8]. In a gapless system, the impurity energy ϵ_d is involved both in the impurity term and in the expression for $h(\omega)$. The magnitude of ϵ_d thus both determines a particle-impurity scattering phase and dictates an appropriate choice of the Bethe spectrum of a host.

It is instructive to start our analysis of the ground state properties of the system with the simplest case $\epsilon_d = 0$. The complex energies of charge excitations of a charge complex are then found to be

$$\omega_\pm(\lambda) = \begin{cases} \lambda + \delta \pm \frac{i}{2}, & \lambda < -\delta, \\ \lambda - \delta \pm \frac{i}{2}, & \lambda > \delta. \end{cases} \tag{7}$$

In contrast to the metallic case, the spectrum of charge complexes contains thus the gap of size 2δ. The existence of the gap should lead to essential changes in the thermodynamics of the system. However, it can be shown from the thermodynamic Bethe ansatz equations that the renormalized energies of unpaired charge excitations and spin complexes are still positive in the absence of an external magnetic field. Therefore, as in the conventional Anderson model, the ground state of the system is composed of charge complexes with negative renormalized energies only. The upper edge of filled states, Q_G, is now given by $Q_G = Q_A - \delta$, where $Q_A = -\frac{1}{2\pi}\ln\frac{D}{\Gamma}$ corresponds to the metallic Anderson model. The occupancy of the impurity level is also given by the standard BA formulas [8], where in the expression for the renormalized impurity level energy ϵ_d^* one needs only to replace Q_A by Q_G to get $\epsilon_d^* = \frac{\Gamma}{\pi}\ln\frac{D}{\Gamma} + \beta$. Thus, the impurity occupancy at $\epsilon_d = 0$ is essentially decreased compared to the metallic case.

At $\epsilon_d \neq 0$, the complex energies of charge excitations of a complex are found from the equation

$$\omega_\pm^2 - \left(\lambda + \delta \pm \frac{i}{2}\right)\omega_\pm + \delta\frac{\epsilon_d}{2\Gamma} = 0. \tag{8}$$

Since we study here only the ground state of the system, we may restrict our consideration to the solutions with the negative real part of energies, $\mathrm{Re}\,\omega < 0$. Then, a solution $\omega_\pm(\lambda) = x(\lambda) \pm iy(\lambda)$ is given by

$$x(\lambda) = \frac{1}{2}[\mu - u(\mu)]; \qquad y(\lambda) = \frac{1}{2}\left[\frac{1}{2} - v(\mu)\right], \tag{9a}$$

where

$$u = \frac{1}{\sqrt{2}}[\mu^2 - b + \sqrt{(\mu^2 - b)^2 + \mu^2}]^{1/2}, \tag{9b}$$

$$v = \frac{\operatorname{sgn}\mu}{\sqrt{2}}[-\mu^2 + b + \sqrt{(\mu^2 - b)^2 + \mu^2}]^{1/2}, \tag{9c}$$

and $\mu = \lambda + \delta$. The behavior of this solution is governed by the parameter $b = \frac{1}{4} + 4\frac{\epsilon_d}{2\Gamma}\delta$ [16].

Let us consider first the case of positive ϵ_d, and hence $b > \frac{1}{4}$. Then, as in the case $\epsilon_d = 0$, the function $x(\lambda)$ is negative only at $\lambda < -\delta$. The ground state of the system is still composed of charge complexes filling all the states from $\lambda = -D/2\Gamma$ to $\lambda = Q_G$. The impurity occupancy n_d is governed by the well known formulas with insignificant corrections related to small deviations of the function $x(\lambda)$ from the linear behavior.

Significant changes in the behavior of the system occur at negative ϵ_d. At negative b ($\epsilon_d/2\Gamma < -1/16\delta$), the function $x(\lambda)$ is negative at all $\lambda \in (-\infty, \infty)$. In contrast both to the metallic model and to the gapless system with positive ϵ_d, the bare energy of charge complexes, $\xi_0(\lambda) = 4\Gamma x(\lambda)$, is now a monotonically increasing negative function at all λ. Therefore, in the ground state of the system charge complexes fill out all allowed states on the λ axis. The density of states of charge complexes $\sigma(\lambda)$ is found from the continuous limit [8–11] of Eqs. (3),

$$\frac{1}{2\pi}\frac{dq(\lambda)}{d\lambda} + \frac{1}{L}a\left(\lambda - \frac{\epsilon_d}{2\Gamma}\right) = \int_{-\infty}^{\infty} d\lambda' a(\lambda - \lambda')\sigma(\lambda') + \sigma(\lambda), \tag{10}$$

where $q(\lambda) = k_-(\lambda) + k_+(\lambda)$ is the momentum of the charge complexes, and $a(x) = [\pi(x^2 + 1)]^{-1}$. As usual, the function $\sigma(\lambda)$ is divided into the host and impurity parts, $\sigma(\lambda) = \sigma_h(\lambda) + L^{-1}\sigma_i(\lambda)$. The occupancy of the impurity level, n_d, is then given by

$$n_d = 2\int_{-\infty}^{\infty} d\lambda\,\sigma_i(\lambda), \tag{11}$$

where the impurity density of states is found from the equation

$$a\left(\lambda - \frac{\epsilon_d}{2\Gamma}\right) = \sigma_i(\lambda) + \int_{-\infty}^{\infty} d\lambda' a(\lambda - \lambda')\sigma_i(\lambda'). \tag{12}$$

Since unpaired charge excitations and spin complexes are absent in the ground state of the system, the impurity spin vanishes. Thus, as in the metallic Anderson system, the Kondo effect takes place at an arbitrary particle-impurity coupling.

Solving Eq. (12), we immediately find $n_d = 1$. Thus, at $\epsilon_d < -\Gamma^2/4\beta$ the impurity level is entirely filled out and its occupancy does not depend on a position of the impurity energy with respect to the Fermi level. Thus, the behavior of the impurity occupancy in the gapless host is not described by a universal function of the renormalized impurity energy ϵ_d^* but it depends essentially on the bare parameters of the model ϵ_d and β. Making use of the terminology of the Anderson model, we will call this regime with the entirely filled impurity level the Kondo (or local-moment) regime, despite its disappearance in the limit $\beta \to 0$, where our model reduces to the conventional Anderson model. However, for quite large δ, and even at $\delta \le 1$, the Kondo regime describes the system's behavior almost at all negative ϵ_d, except a very narrow region near the Fermi level, where $0 < b < \frac{1}{4}$.

The region $0 < b < \frac{1}{4}$ corresponds in our case to the mixed-valence regime, where the impurity occupancy is changed from $n_d \approx 0$ in the empty-level regime at $\epsilon_d \ge 0$ to $n_d = 1$ precisely in the Kondo regime at $\epsilon_d \le -\Gamma^2/4\beta$. The bare energy of charge complexes

$\xi_0(\lambda) = 4\Gamma x(\lambda)$ in this regime is negative at all λ, except the point $\lambda = -\delta$, where $x(\lambda) = 0$. The renormalized energy of charge complexes at zero temperature is found from the thermodynamic BA equation

$$\xi(\lambda) = 4\Gamma x(\lambda) - \int_{-\infty}^{Q_1} d\lambda' a(\lambda - \lambda')\xi(\lambda') - \int_{Q_2}^{\infty} d\lambda' a(\lambda - \lambda')\xi(\lambda'), \qquad (13)$$

where Q_1 and Q_2 are defined as the zeros of $\xi(\lambda)$, $\xi(Q_1) = \xi(Q_2) = 0$. This equation, as well as a corresponding equation for the density of states $\sigma(\lambda)$, is hardly solved analytically, and a numerical analysis is required.

In the metallic limit, $\beta \to 0$, the lower edge of the mixed-valence regime in the gapless system is shifted to $-\infty$. Correspondingly, the mixed-valence regime of the gapless system is extended to the conventional mixed-valence ($0 < n_d < 1$) and Kondo ($n_d \approx 1$) regimes of the Anderson impurity in a metallic host.

In summary, using the BA method we have studied the ground state properties of a $U \to \infty$ Anderson impurity embedded in a gapless host with an energy independent hybridization and the density of band states given in Eq. (1) with $r = 1$. As in metals, the ground state of the system has been shown to be composed of charge complexes only. Since each complex contains two charge excitation and one spin wave, the total spin of a complex equals zero. Therefore, at zero temperature the impurity spin vanishes, and the Kondo effect takes place at arbitrary parameters of the model.

However, the appearance of an extra parameter β on the energy scale, which characterizes the size of region with an unconventional behavior of the density of band states in a gapless host, results in significant changes in the density of states of charge complexes in the ground state of the system. These changes lead to novel qualitative features in the behavior of the impurity occupancy as a function of the bare impurity level energy. The empty-level ($n_d \approx 0$) and Kondo ($n_d = 1$) regimes are extended to almost all positive and negative magnitudes of ϵ_d, respectively. While the mixed-valence regime ($0 < n_d < 1$) is squeezed to a narrow region, $-\Gamma^2/4\beta < \epsilon_d < 0$.

At $\epsilon_d < -\Gamma^2/4\beta$, $n_d = 1$ exactly and does not depend on ϵ_d. In this regime, the energy of charge complexes is negative at all λ, therefore charge complexes fill out all allowed states on the λ axis. Thus, the impurity line, represented by the driving term in Eq. (12), and domain of filled states are overlapped completely, in contrast to the metallic Anderson model, where their overlap is always partial at any finite ϵ_d, and therefore $n_d < 1$ [17].

Only in the empty-level regime the impurity occupancy is a universal function of the renormalized impurity energy $\epsilon_d^* = \epsilon_d + \frac{\Gamma}{\pi}\ln\frac{D}{\Gamma} + \beta$, which contains the parameter β. The behavior of n_d in the mixed-valence and Kondo regimes is not universal that demonstrates the nonuniversal properties of the system. The latter explains why the Kondo screening is absent—or exists only at quite a large electron-impurity coupling—in earlier studies based on scaling arguments. Nevertheless, using both poor-man's scaling and numerical RG calculations, Gonzalez-Buxton and Ingersent [6] have derived the behavior of the impurity occupancy which is qualitatively close to the above-described picture.

In the BA analysis, the power r must be fixed. The spectrum of the system is determined by the functions $k(\omega)$ and $h(\omega)$, and it is essentially different at different r. At $r \neq 1$, the spectrum of Bethe excitations is enriched that could result in qualitatively novel physical properties of the system. It seems very difficult, if not impossible, to propose any scenario of destroying the Kondo screening of an integrable Anderson impurity.

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[16] At $b > \frac{1}{4}$, the second root of Eq. (8) $x^{(+)}(\lambda) = \frac{1}{2}[\mu + u]$ also satisfies the condition $x^{(+)}(\lambda) < 0$ at $\lambda < -\delta$ that allows one to construct more complex charge complexes. However, as unpaired charge excitations and spin complexes, they do not contribute to the ground state of the system. The same scenario occurs in the finite-U metallic Anderson model [8].
[17] The reader can see here a deep analogy with a mechanism of the impurity spin screening in the $s = \frac{1}{2}$ Kondo model in terms of BA approach. In the absence of a magnetic field, spin waves fill out all states resulting in a total compensation of the impurity spin. In a magnetic field, a part of allowed states for spin waves is empty, and the compensation is only partial.