Bethe-*Ansatz* Solution of the Anderson Model of a Magnetic Impurity with Orbital Degeneracy

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A model for Ce impurities is considered, consisting of the $4f^0$ singlet and a multiplet of total angular momentum j of the $4f^1$ configuration hybridized with conduction states of the metal ($U\to\infty$ limit of Anderson's model). The model is solved by a Bethe *Ansatz* and exact expressions for ground-state properties, e.g., valence, spin and charge susceptibilities, and resistivity, are given.

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Several models for magnetic impurities in metals, e.g., the Kondo problem and the Anderson model, have recently been exactly diagonalized[1-6] by means of Bethe's *Ansatz*.[7] In particular for the nondegenerate Anderson impurity, Tsvelick and Wiegmann[6] have shown that the model is completely integrable and Kawakami and Okiji[8] determined the structure of the ground state. Wiegmann and co-workers[9-12] obtained the low-temperature thermodynamics of the nondegenerate (symmetric and asymmetric) Anderson impurity.

The purpose of this Letter is to present exact ground-state properties of a model for Ce impurities (mixed- or integer-valent) which includes the *orbital degeneracy* of the $4f$ levels. The model[13] consists of highly correlated f states of the impurity and conduction states of the metal. From the f states only the $4f^0$ configuration and the Hund's-rule ground multiplet of the $4f^1$ configuration of total angular momentum $j=\frac{5}{2}$ are considered. All other states, e.g., the $4f^n$ configurations for $n>1$, are excluded because of the large Coulomb repulsion and a large spin-orbit coupling. The conduction electron states are expanded in partial waves around the impurity. Only the conduction states with total angular momentum j hybridize with the impurity $4f$ states. If we assume a contact hybridization, $V\delta(r)$, only "s waves" are scattered by the impurity. The problem can then be regarded as half-dimensional and only forward-moving particles need to be considered.[1-6] The Hamiltonian is given by

$$H=\sum_m\int dx\, c_m^\dagger(x)(-i\,\partial/\partial x)c_m(x)+\epsilon\sum_m|jm\rangle\langle jm|+V\sum_m\int dx\,\delta(x)[c_m^\dagger(x)|0\rangle\langle jm|+|jm\rangle\langle 0|c_m(x)], \quad (1)$$

where ϵ is the f-level energy and the bras and kets denote the impurity states, i.e., $|0\rangle$ the $4f^0$ singlet and $|jm\rangle$ the $4f^1$ multiplet ($|m|\leq j$). The dispersion of the conduction electrons has been linearized in the momentum around the Fermi energy. Note that depending on $\epsilon-\epsilon_F$, ϵ_F being the Fermi energy, the impurity has a magnetic moment, has a mixed valence, or is nonmagnetic.

Bethe's *Ansatz*[7] for the N-electron wave function of the model (1) can be constructed in analogy to Ref. 3. It is the superposition of two terms[14]: (a) The N-particle Fermi sea with no f electron and (b) the $(N-1)$-electron Fermi sea with the impurity in a state $|jm\rangle$. The term (a) completely specifies the latter term. The form of part (a) is the standard one,[15]

$$\psi_Q=\sum_P[Q,P]\exp[ik_{P1}x_{Q1}+\dots+ik_{PN}x_{QN}], \quad (2a)$$

where Q and P are permutations of the coordinates and charge rapidities k_j, respectively. The columns ξ_P of the $N!\times N!$ matrix $[Q,P]$ satisfy the relations

$$\xi_P=Y_{ij}{}^{ab}\xi_{P'},\quad Y_{jk}{}^{ab}Y_{ik}{}^{bc}Y_{ij}{}^{ab}=Y_{ij}{}^{bc}Y_{ik}{}^{ab}Y_{jk}{}^{bc},$$

$$Y_{ij}{}^{ab}=-\frac{-iV^2}{k_i-k_j-iV^2}+\frac{k_i-k_j}{k_i-k_j-iV^2}\hat{P}_{ab}, \quad (2b)$$

where $\hat{P}_{ab}$ permutes the coordinates a and b. The energy of the system is given by

$$E=\sum_{j=1}^{N}k_j. \quad (2c)$$

For $j=\frac{1}{2}$ the above equations reduce to the $U\to\infty$ limit of Wiegmann's solution.[3]

Periodic boundary conditions reduce the problem to a set of eigenvalue equations. These eigenvalue equations are the same as those derived by Yang [see Eqs. (4)–(11) in Ref. 15] for the fermion gas with δ-function interaction, if we identify the interaction strength c with $-V^2$. Model (1) then corresponds to a one-dimensional electron gas with *attractive* contact interaction, but with the energy given by (2c).

The set of eigenvalue equations has been solved by Sutherland[16] for arbitrary Young tableau for the δ-function gas. Specializing this result for $(2j+1)$ spin components we obtain $(2j+1)$ sets of nonlinearly coupled rapidities $\xi_\alpha^{(l)}$, where $l=0, \ldots, 2j$ labels the sets and α is the running index within each set. The equations determining the rapidities $\xi_\alpha^{(l)}$ are to be solved in the thermodynamic limit.

Attractive forces between fermions tend to *bind* the electrons in *complexes*, which are characterized by complex rapidities.[8-10,17-19] Since only electrons of different spin components interact, we may build complexes of up to $2j+1$ electrons. A complex of n electrons ($n \leq 2j+1$) is characterized by one real $\xi^{(n-1)}$ value and in general complex $\xi^{(l)}$ values, $l<n-1$, which are related by

$$\xi_p^{(l)} = \xi^{(n-1)} + ipV^2, \quad l \leq n-1, \quad p = -\tfrac{1}{2}(n-l-1), -\tfrac{1}{2}(n-l-3), \ldots, \tfrac{1}{2}(n-l-1). \tag{3}$$

Hence a complex of n electrons is completely determined by one *real* $\xi^{(n-1)}$ rapidity.

For the ground state the number of $(2j+1)$-particle complexes, M, is maximum in the absence of an external magnetic field. Taking the thermodynamic limit such that M/L remains constant, where L is the length of the box, we obtain a Wiener-Hopf integral equation for the density distribution function σ of the $\xi_\alpha^{(2j)}$ rapidities:

$$\sigma(\xi) + \frac{1}{\pi}\sum_{p=1}^{2j}\int_{-\infty}^{Q} d\xi' \frac{pV^2\sigma(\xi')}{(\xi-\xi')^2+(pV^2)^2} = \frac{2j+1}{2\pi}\varphi(\xi) + \frac{1}{\pi L}\frac{[\frac{1}{2}(2j+1)]V^2}{(\xi-\epsilon)^2+\{[\frac{1}{2}(2j+1)]V^2\}^2}. \tag{4}$$

Here Q is the Fermi level determined by

$$M/L = \int_{-\infty}^{Q} d\xi\, \sigma(\xi), \tag{5}$$

and φ is a cutoff function for large ξ, which is 1 around the Fermi level and bounds the energy spectrum from below. The last term in Eq. (4) is the impurity contribution.

The solution of the Wiener-Hopf equation can be constructed in analogy to other impurity models.[1,2,5,6,10] The density σ is split into $\sigma_{\rm host}$ and $\sigma_{\rm imp}$; the former determines Q and the latter yields the f-level occupation

$$n_f = \frac{1}{2} + \frac{i}{2\pi}\int_{-\infty}^{\infty}\frac{dx}{x}\,\frac{\Gamma(1-\frac{1}{2}i(2j+1)x)}{\Gamma(1-\frac{1}{2}ix)}[-ix+0]^{ijx}\exp[i\tilde{\epsilon}x - \tfrac{1}{2}(2j+1)\pi|x|], \tag{6}$$

where $\tilde{\epsilon}$ is a dimensionless invariant coupling related to the f-level position. The valence varies smoothly from the localized moment ($n_f=1$) to the nonmagnetic ($n_f \simeq 0$) region as illustrated in Fig. 1(a). The charge susceptibility $\chi_{\rm ch} = -\partial n_f/\partial\tilde{\epsilon}$ shows a peak in the mixed-valence regime [Fig. 1(b)].

The resistivity due to the impurity is determined from the scattering phase shift, δ, given by Friedel's sum rule,[20] $\delta = \pi n_f/(2j+1)$. The resistivity normalized to its value for the localized moment is shown in Fig. 1(d). Andrei, Furuya, and Lowenstein[5] have obtained the phase shift for the spin-$\frac{1}{2}$ Kondo problem through the "hole" excitation spectrum for the magnetic rapidities. Analogously, the δ obtained from the "hole" excitations of Eq. (4) agrees with Friedel's sum rule.

In an external magnetic field the ground state has a finite fraction of complexes of fewer than $2j+1$ electrons. Let us recall that a complex of n electrons is characterized by one real $\xi^{(n-1)}$ rapidity. When the thermodynamic limit is taken we introduce $2j+1$ density functions for the real rapidities $\xi^{(l)}$, $\sigma^{(l)}(\xi)$, $l=0,\ldots,2j$. Here $\sigma^{(2j)}$ reduces to the density σ in Eq. (4) for vanishing field. A system of $2j+1$ linearly coupled Wiener-Hopf integral equations for the densities is then obtained. If we assume that the Zeeman energy is much smaller than the bandwidth, $\sigma^{(2j)}$ can be eliminated from the system of equations. We obtain for $l=0,\ldots,2j-1$

$$\sigma^{(l)}(\xi) + \sum_{q=0}^{2j-1}\int_{-\infty}^{B_q} d\xi'\,\sigma^{(q)}(\xi')\int_{-\infty}^{\infty}\frac{dx}{2\pi}e^{-i(\xi-\xi')x}K_{lq}(x)$$

$$= \frac{1}{2\pi L}\int_{-\infty}^{\infty}dx\, e^{-i(\xi-\epsilon)x}\frac{\sinh[(j-\frac{1}{2}l)V^2x]}{\sinh[(j+\frac{1}{2})V^2x]} + a_l\exp\left[\frac{\pi\xi}{(j+\frac{1}{2})V^2}\right], \tag{7}$$

where

$$K_{lq}(x)=\{\exp[(p_{l,q}{}^*-l-q)(V^2/2)|x|]\sinh[\tfrac{1}{2}(p_{l,q}{}^*+1)V^2x]$$
$$-\exp(-jV^2|x|)\sinh[\tfrac{1}{2}(l+1)V^2x]\sinh[\tfrac{1}{2}(q+1)V^2x]/\sinh[(j+\tfrac{1}{2})V^2x]\}[\sinh(\tfrac{1}{2}V^2x)]^{-1}, \quad (8)$$

$$a_l=\frac{\sin\{\pi[(l+1)/(2j+1)]\}}{(j+\frac{1}{2})V^2}\int_Q^\infty d\xi'\,\tilde{\sigma}^{(2j)}(\xi')\exp\left[-\frac{\pi\xi'}{(j+\frac{1}{2})V^2}\right], \quad (9)$$

and $p_{l,q}{}^*=\min(l,q)$ if $l\neq q$ and $p_{l,l}{}^*=l-1$. The integration limits B_q are determined from the Zeeman-split f-level occupation numbers. The B_q are in general not all equal. The first term of the right-hand side of Eq. (7) is the Kondo part and the second term is the mixed-valent contribution induced by charge fluctuations. The mixed-valent contribution has been linearized in the field since the Zeeman energy is much smaller than V^2.

For small fields the magnetization can be extracted by inspection[10] from Eqs. (7)–(9) and we obtain for the zero-field magnetic susceptibility

$$\chi_s\Gamma=\frac{j(j+1)}{6}\left\{\frac{2\pi}{(2j+1)}\,\frac{1}{\Gamma[1+1/(2j+1)]}\,e^{-\tilde{\epsilon}/(j+1/2)}\right.$$
$$\left.-\frac{i}{(2j+1)}\int_{-\infty}^{\infty}dx\,\frac{\Gamma(1-i(j+\frac{1}{2})x)}{\Gamma(1-ix/2)}\,\frac{[-ix+0]^{ijx}}{x-i/(j+\frac{1}{2})}\exp[i\tilde{\epsilon}x-\tfrac{1}{2}(2j+1)\pi|x|]\right\}. \quad (10)$$

Here $\Gamma=V^2/2$ on the left-hand side is the resonance width of the impurity level. The first term is the Kondo susceptibility and the second one is the mixed-valent contribution. Both contributions are shown in Fig. 1(c) as a function of the invariant coupling $\tilde{\epsilon}$. For large $|\tilde{\epsilon}|$ the invariant coupling can be related by perturbation theory to the bare f-level energy ϵ. Note that for $n_f=\frac{1}{2}$ and $j=\frac{5}{2}$ the Kondo part of χ_s is already larger than the mixed-valent contribution.

The Kondo contribution of Eqs. (7)–(9) (set $a_l\equiv 0$) is just the Coqblin-Schrieffer model. Identifying $\tilde{\sigma}_{CS}{}^{(l+1)}\equiv\sigma^{(l)}$ and inverting the matrix $\hat{1}+\hat{K}$ we obtain the Bethe-*Ansatz* equations of the Coqblin-Schrieffer Hamiltonian.[6]

The magnetic field dependence of the Kondo contribution can be obtained by solving Eqs. (7)–(9). This is in general not possible by the Wiener-Hopf method, since the B_q are not all equal for $j>1$. I succeeded in constructing an approximate solution for $j>1$ (to be published elsewhere) and obtained in this way the magnetization, the f-occupation numbers, and the magnetoresistance. The magnetization is linear in H for small fields, while for very large fields we obtain

$$M=j\left\{1-\frac{1}{(2j+1)}\,\frac{1}{\ln(H/T_H)}-\frac{\ln\ln(H/T_H)}{(2j+1)^2\ln^2(H/T_H)}\right\} \quad (11)$$

and the resistivity decreases as $O(\ln^2(H/T_H))$, T_H being the Kondo energy.

From the exact low- and high-field magnetization we obtain the Wilson numbers,[21,22] $W(j)$, for

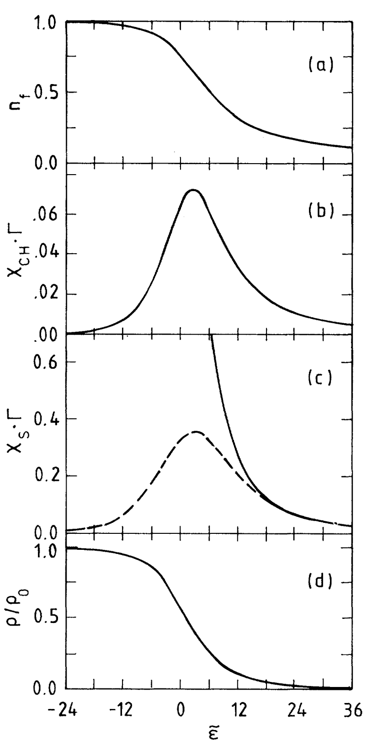

FIG. 1. (a) Valence, (b) charge susceptibility, (c) spin susceptibility, and (d) resistivity as a function of the invariant coupling $\tilde{\epsilon}$. The resistivity is normalized to its value for a localized moment. The dashed line in (c) is the mixed-valent susceptibility, the full line is the total χ_S, and the difference between the full and dashed lines is the Kondo susceptibility. The Kondo part depends exponentially on $\tilde{\epsilon}$.

the SU($2j+1$) Kondo model; in particular for Ce we have $W(\frac{5}{2})/W(\frac{1}{2}) = 1.0434$.

In summary, I have given exact expressions for several measurable quantities, χ_s, ρ, n_f, and χ_{ch}, for a Ce ion in a metal at low temperatures in terms of two parameters: the energy scale Γ and the dimensionless invariant coupling $\tilde{\epsilon}$. Hence, the measurement of two independent quantities, e.g., the valence and the spin susceptibility,[23] completely determines these two parameters and hence all other quantities. A direct comparison with experiment is, however, difficult since the model (1) neglects crystal fields.

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