Solution of the Kondo problem for an orbital singlet

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An exact solution is derived for the behavior of an alloy of a normal metal with a small admixture d of a magnetic impurity in an orbital singlet state. The solution is generalized to an arbitrary impurity spin S. Under the condition $2S > 2l + 1$, where l is the orbital angular momentum of the unfilled shell of the impurity ion, the Gell-Mann–Low function vanishes at some finite point. A nontrivial scaling, first observed in a one-dimensional quantum many-body system, is analyzed on the basis of the exact solution.

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1. The Mn^{+3} ion in a metal is an orbital singlet ($L = 0$) and has a spin $S = 5/2$. Its term is ($3d^5\,{}^6S_{5/2}$). Accordingly, when this impurity scatters conduction electrons of the metal, the projection of the orbital angular momentum of the electrons is conserved. The exchange spin interaction is customarily described by the Hamiltonian[1]

$$\mathcal{H} = \sum_{k,m,\sigma} \epsilon_k C^+_{km\sigma} C_{km\sigma} + J \sum_{\substack{m=1\\ k,k',\sigma,\sigma'}}^{n} C^+_{km\sigma} \vec{\sigma}_{\sigma\sigma'} \mathbf{S}\, C_{k'm\sigma'} . \quad (1)$$

Here the operator $C_{km\sigma}$ represents the conduction electron with momentum modulus k, spin $\sigma = \pm 1/2$, and orbital-angular-momentum projection m; $l = (n-1)/2$; and $\mathbf{S}$ is the spin operator of the impurity ion (only the d partial wave of the conduction electrons interacts with the impurity). Hamiltonian (1) also describes alloys with Co

($n = 2S = 3$) and V ($n = 2S = 2$) in a strong cubic crystal field.[2] For arbitrary n and $2S$, Hamiltonian (1), called the "n-channel Kondo problem" in the English-language literature, is a model Hamiltonian.[1)]

2. It has recently been shown that the exchange models which are customarily studied in the theory of magnetic alloys are completely integrable, and most have been solved exactly by the Bethe method.[3,4] An exceptional case is the Kondo problem for an orbital singlet, (1); a naive application of the Bethe Ansatz to this problem has resulted in physically meaningless results (see Ref. 5, for example). We recall that some of the basic conditions for the integrability of exchange Hamiltonians are (a) that the impurity can be treated as a point impurity and (b) it is sufficient to consider only the linear part of the spectrum of the conduction band near the Fermi surface.[6] It turns out that under these assumptions it is not possible to correctly take into account the quantum axial anomaly in the divergence of the density of particles with a given projection of the orbital angular momentum (this difficulty does not arise in the other exchange models which can be solved). Approximations (a) and (b) lead to a situation in which the "bare" S matrix of the interaction of the particle with the impurity does not depend on the energy of the particle. In our case, $S = \exp(iJ\vec{\sigma}\cdot\mathbf{S})_{\sigma\sigma'}\delta_{mm}$ is the tensor product $SU(2) \otimes GL(n)$ of the spin and orbital scattering processes. The formal application of the Bethe method[5] leads to the result that the physical S matrix, although now dependent on the energy, leaves the spin and orbital channels independent. The absurdity of this result can be seen even in second-order perturbation theory. In the present letter we drop the assumption that the interaction is a point interaction.

3. For this purpose we consider an integrable Anderson model, which describes the orbitally degenerate shell of the impurity ion, of such a nature that, with the appropriate choice of parameters, this model is equivalent to the exchange Hamiltonian (1):

$$\mathcal{H} = \sum_{k,m,\sigma} v_F(k - k_F)\, C^+_{km\sigma} C_{km\sigma} + V \sum_{k,m,\sigma} (C^+_{km\sigma} d_{m\sigma} + h.c.) + \mathcal{H}_{at}, \tag{2}$$

where

$$\mathcal{H}_{at} = \epsilon_d \sum_{m,\sigma} d^+_{m\sigma} d_{m\sigma} - \frac{U}{2} \sum_{m,m',\sigma,\sigma'} d^+_{m\sigma} d^+_{m'\sigma'} d_{m'\sigma} d_{m\sigma'}, \tag{3}$$

and the operator $d_{m\sigma}$ represents an electron in the impurity shell. Under the condition $0 < [U(n-1)]/2 < \epsilon_d < [U(n+2)]/2$, the ground state of the shell is the orbital singlet ($n_d = n$, $S = n/2$, $L = 0$). Models (1) and (2) are equivalent if the hybridization amplitude $\Gamma = \pi\rho(\epsilon_F)V^2$ is small enough that all the excited states are virtual. Specifically, the following condition must be satisfied:

$$(U, \epsilon_d - U(n-1)/2) \gg n\Gamma. \tag{4}$$

4. It is a simple matter to construct a Bethe Ansatz for Hamiltonian (3). For simplicity, we consider only the hybridization of states with $n_d = n$ and $n_d = n - 1$, assuming $U \gg \epsilon_d - U(n-1)/2$. The two-particle S matrix of the "bare" particles in this model is the tensor product

$$S(k-p) = S_\sigma(k-p) \otimes S_m(k-p). \tag{5}$$

Here S_σ is the matrix of the Anderson model without orbital degeneracy and with repulsion in the atomic shell; S_m is the corresponding matrix for a model without spin degeneracy but with attraction,[7,8]

$$S_{\sigma(m)}(k) = (k/2\Gamma \,(\mp)\, iP)/(k/2\Gamma \,(\mp)\, i),$$

where P is the permutation operator which acts in the spin (orbital) space.

A spectral equation for the quantized momenta of the particles is found by "gluing together" the spin and orbital parts:

$$\exp(ik_j L)(k_j - \epsilon_d - i\Gamma)/(k_j - \epsilon_d + i\Gamma) = t^\sigma(k_j)\, t^m(k_j), \tag{6}$$

where t^a are the eigenvalues of the operators

$$T^a(k_j) = \prod_{\substack{p=1 \\ p\neq j}}^{N} S^a_{jp}(k_j - k_p) \qquad (a = \sigma, m).$$

The energy of the state, $E = \Sigma_{j=1}^N k_j$, now does not break up into independent spin and orbital parts. These parts are related by Eq. (6).

The quantities t^a are well known (see Refs. 7 and 8, for example):

$$t^\sigma(k) = \prod_{\alpha=1}^{M} e_1(k/2\Gamma - \lambda_\alpha); \qquad t^m(k) = \prod_{\alpha=1}^{m^{(1)}} e_1^{-1}(k/2\Gamma - \mu_\alpha^{(1)}), \tag{7}$$

where λ and μ satisfy

$$\prod_{j=1}^{N} e_1(\lambda_\alpha - k_j/2\Gamma) = \prod_{\beta=1}^{M} e_2(\lambda_\alpha - \lambda_\beta), \tag{8}$$

$$\prod_{\tau=\pm 1} \prod_{\beta=1}^{m(j+\tau)} e_1(\mu_\alpha^{(j)} - \mu_\beta^{(j+\tau)}) = \prod_{\beta=1}^{m(j)} e_2(\mu_\alpha^{(j)} - \mu_\beta^{(j)}); \quad (j = 1, \dots n-1),$$

Here $e_n(x) = (x - in/2)/(x + in/2)$; N is the total number of particles; $m^{(j)} = \Sigma_{k=j+1}^n n_k$; and $N/2 - S$, where S is the total spin, and n_k is the number of particles with orbital-angular-momentum projection $n/2 - k$.

5. Omitting the technical details and the calculations, we write the integral equation which describes the impurity part of the distribution of the solutions of Eqs. (6), $\rho(k)$, directly in the Kondo limit (4):

$$\rho(k) - \int_0^\infty F(k-k')\,\rho(k')\,dk' = \left(2 \operatorname{ch} \pi \left(k - \frac{1}{\pi} \ln H/T_H\right)\right)^{-1} \tag{9}$$

where H is the magnetic field,

$$F(k) = \frac{1}{2\pi}\int_{-\infty}^{+\infty} e^{-i\omega k}\left(1 - \frac{\text{th}\,\omega/2}{1 - e^{-n|\omega|}}\right)d\omega\,, \tag{10}$$

and T_H is the Kondo temperature, found from the solution of another integral equation, which we will not reproduce here. We simply note that under the condition $J \ll 1$ we have $T_H \sim J^{1/n} e^{-1/J}$, in accordance with the perturbation-theory results.[2] We are interested in the magnetization of the impurity in the external magnetic field:

$$M_{imp}(H) = \int_0^{\infty} \rho(k)\, dk. \tag{11}$$

6. We offer without proof a generalization of the results (9)—(11) to arbitrary values of n and S. We need only a single change, but an important one, in Eqs. (9)—(11): The right side of Eq. (9) becomes

$$= \frac{1}{4\pi}\int_{-\infty}^{+\infty} d\omega\, e^{-2i\omega k}\left(e^{-|n-2S||\omega|} - e^{-(n+2S)|\omega|}\right) \tag{9*}$$

$$\times\ (1 - e^{-2n|\omega|})^{-1}\,(2\,\text{ch}\,\omega)^{-1}.$$

7. Equation (9*) is solved explicitly by the Wiener-Hopf method, so that the magnetization can be written in the form

$$M_{imp}(H) = -\frac{-in}{4\pi^{3/2}}\int \frac{d\omega}{\omega - i0}\exp(2i\omega \ln H/T_H)\left(\frac{i\omega + 0}{e}\right)^{i\omega n} \tag{12}$$

$$\frac{\Gamma(1+i\omega)\Gamma(1/2 - i\omega)}{\Gamma(1+i\omega n)}\left(\exp(-\pi|n-2S||\omega|) - \exp(-\pi(n+2S)|\omega|)\right)$$

$$\times\ (1 - \exp(-2\pi n|\omega|))^{-1}.$$

This expression generalizes the result derived in Ref. 9 for $n = 1$. Let us analyze (12) for various values of the parameters H/T_H, n, and S.

a) Strong magnetic fields, $H/T_H \gg 1$. This region is controlled by perturbation theory. We find the invariant charge z of the Gell-Mann-Low equation from the final result of the two-loop approximation[2]:

$$\frac{1}{z} - \frac{n}{2}\ln|z| = \ln H/T_H. \tag{13}$$

The general requirement of renormalizability would mean that all the physical quantities are expanded in a series in integer powers of $|z| \ll 1$. From (12) we have

$$M_{imp}(H) = S\left(1 - z + \sum_{k=2}^{\infty} a_k(n,S)\, z^k\right);\ H \gg T_H. \tag{14}$$

In the limit $n \to \infty$ we find $a_k \sim n^{k-2}$. Accordingly, perturbation-theory series (14) holds for $nz \ll 1$, i.e., for $H \gg e^n T_H$.

b) Weak magnetic fields, $H \ll T_H$. Here we expect to find the behavior very different for different values of n and S.

(1) At $n < 2S$, the ground state of the magnetic impurities is $(2S + 1 - n)$-fold degenerate, and $M_{\rm imp}(0) = S - n/2$, corresponding to the strong-coupling limit. This result means that the fixed point of Hamiltonian (1) is $J^* = \infty$. At $H \ll T_H$ the exchange interactions are ferromagnetic in nature. Near the ferromagnetic stable fixed point $J^* = \infty$ (i.e., in the limit $H \to 0$), as near the antiferromagnetic unstable fixed point $J^* = 0$ (i.e., in the limit $H \to \infty$), the physical quantities are logarithmic in nature. From (12) we see the "duality" of the high-and low-energy expansions:

$$M_{imp}(H) = (S - {}^n/_2)\left(1 - z + \sum_{k=2}^{\infty} a_k(n, S - {}^n/_2)\, z^k\right); \quad H \ll T_H . \tag{15}$$

(2) At $n = 2S$, the ground state is a singlet. The fixed point is also the strong-coupling limit, but the physical quantities behave completely differently:

$$M_{imp}(H) = \sum_{k=1}^{\infty} b_k(n)(H/T_H)^{2k-1} . \tag{16}$$

Between the regions $H \ll T_H$ and $H \gg e^n T_H$, in which Eqs. (14) and (16) apply, there is a peculiar intermediate regime $T_H \ll H \ll e^n T_H$ in the limit $n \to \infty$:

$$M_{imp}(H) = \frac{1}{\pi}\left(n \ln {}^H/_{T_H}\right)^{1/2}\left(1 + \frac{\pi \ln 2}{2 \ln {}^H/_{T_H}} + \ldots\right). \tag{17}$$

(3) The most interesting case is $n > 2S$. This situation was discussed qualitatively by Nozieres and Blandin.[2] They mention that in this case a fixed point cannot be a strong-coupling limit, since at $n > 2S$ this limit is antiferromagnetic and thus unstable. Nozieres and Blandin argued on this basis that a fixed point of Hamiltonian (1) with $n > 2S$ corresponds to a finite value of the effective interaction, $J^* < \infty$. This result would mean that at low energies the physical quantities have a *power-law scaling*.[2)] The magnetic moment in the limit $H \to 0$, for example, would be

$$M_{imp}(H) \sim (H/T_H)^{\alpha}, \tag{18}$$

where $0 < \alpha < 1$ is a number which may depend on n or S. It follows from (12) that this is in fact the case, and we have $\alpha = 2/n$ at $n \neq 2$. With $n = 2$, $S = 1/2$, and $H < T_H$, we have

$$M_{imp}(H) = \sum_{k=0}^{\infty} (H/T_H)^{2k+1} A_k \ln {}^H/_{b_k T_H} . \tag{19}$$

Hamiltonian (1) is apparently the first example of a one-dimensional quantum many-body system of this type.

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[1)]With $n \neq 2S$, Hamiltonian (1) may hold for alloys with certain isotopes of manganese whose hyperfine splitting is comparable to the Kondo temperature.

[2)]The formal possibility of scaling has been discussed previously,[10,9] but the discussions dealt with the case $n=1$, in which there is no scaling.

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