Integrable model describing the behavior of magnetic impurities in metals

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We present an integrable impurity model describing the exchange and the correlated hybridized interactions between localized electronic states of an impurity and conduction electrons of a metal. The impurity magnetization, the Kondo limit, and the Fermi-liquid behavior at low temperatures are treated analytically on the basis of the Bethe ansatz solution.

I. INTRODUCTION

The continuous single-impurity models such as the Kondo-problem and the Anderson model are solved by means of the Bethe ansatz, by invoking the onedimensional nature of the impurity problem.¹⁻³ It should be noted that the approximation of electrons in metals to the fermion gas, used in these and subsequent papers (see Refs. 4 and 5 and references therein) allows us to obtain exact solutions of these models. On this assumption, most of the integrable single-impurity models have been constructed. Solutions were formulated to the orbitally degenerate extensions of these models, namely the Coqblin-Schrieffer^{5,6} and infinite-U Anderson models.⁷

The nondegenerate and orbital-degenerate Anderson models describe qualitatively the principal feature of rare-earth compounds which are characterized by two items: first, the almost localized electrons from the inner shells forming the localized spin; second, the heavyfermion behavior of 4f electronic states. It is well known that rare-earth systems are a possible better realization of local moments, because the 4f shells of atoms are well localized. In the compounds and alloys the f shell of ions hybridizes with conduction electron states. The valence instability and large spin fluctuations are realized as a result of the interaction of conduction electrons with 4fconfigurations of rare-earth atoms.

Aligia, Balseiro, and Proetto⁸ obtained the solution of the model which includes two configurations of the impurity shell with arbitrary angular momentum J_0 and J_1 (where $J_1 = J_0 \pm \frac{1}{2}$) hybridized through the promotion of conduction electrons. In the Tm systems so-called intermediate-valence systems and the valence of rareearth ions fluctuates between electronic configurations $4f^{12}$ and $4f^{13}$. The model is intended to describe some of the properties of Tm, Sm, Eu, Yb, and Ce compounds and alloys.

II. THE MODEL AND THE BETHE ANSATZ EQUATIONS

The electrons of the 4f shell exchange their spin component with that of conduction electrons without an actual charge transfer from the f shell to the conduction band, therefore the s-f direct exchange interaction takes place. In this paper we consider an isotropic impurity model involving both hybridization between localized and conduction electrons and exchange contact interaction between their spin components. The model offered is a more realistic one due to the model Hamiltonian describing both the exchange interaction and the correlated hybridization of localized and conduction electronic states. This model extends the class of integrable impuri-ty models.⁸⁻¹⁰ The model consists of the conduction states of the metal and levels of impurities, which can be singly occupied with either an up- or down-spin electron or a doubly occupied one. The Hamiltonian of the model considered has the following form:

$$\mathcal{H} = -i \sum_{\sigma} \int dx \ c_{\sigma}^{\dagger}(x) \frac{\partial}{\partial x} c_{\sigma}(x) + \varepsilon_{d} \sum_{\sigma} \sum_{i=1}^{N_{i}} n_{i\sigma} + U \sum_{i=1}^{N_{i}} n_{i_{1}} n_{i_{1}} + \sum_{\sigma} \sum_{i=1}^{N_{i}} \int dx \ \delta(x - X_{i}) [W n_{i-\sigma} c_{\sigma}^{\dagger}(x) d_{i\sigma} + \mathrm{H.c.}]$$

$$+ J \sum_{\sigma, \sigma', s, s'} \sum_{i=1}^{N_{i}} \int dx \ \delta(x - X_{i}) c_{\sigma}^{\dagger}(x) \sigma_{\sigma\sigma'} c_{\sigma'}(x) d_{is}^{\dagger} \mathbf{S}_{ss'} d_{is'}, \qquad (1)$$

where $c_{\sigma}^{\dagger}(x)$ and $c_{\sigma}(x)$ are the operators of the conduction electrons; $d_{i\sigma}^{\dagger}$ and $d_{i\sigma}$ are the operators of the electrons localized at an impurity with coordinate the $x = X_i$; $n_{i\sigma} = d_{i\sigma}^{\dagger} d_{i\sigma}$ is the number of spin- σ electrons localized at the impurity ($\sigma = \uparrow, \downarrow$); ε_d is the energy of the oneelectron impurity level; U is the on-site Coulomb repul-

sion; W is the constant of the correlated hybridized interaction; J is the constant of the exchange interaction of the band electrons with electrons localized at impurities; $\sigma = \{\sigma^x, \sigma^y, \sigma^z\}$ are the usual Pauli matrices; $S = \{S^x, S^y, S^z\}$ are the Pauli matrices of spin- $\frac{1}{2}$ impurity; and N_i is the number of impurity atoms. First of all, we consider the mathematical problem of the diagonalization of the model Hamiltonian. In order to describe the integrable of the model, let us define the expression for the T_j matrix. Let us first consider a scattering of one conduction electron on an impurity. In this case, a general state vector of the Hamiltonian (1) can be written as

$$|\Psi\rangle_{k\sigma}^{s} = \int dx \left[\psi_{k\sigma}^{s}(x)c_{\sigma}^{\dagger}(x)d_{0s}^{\dagger} + \delta(x)\delta_{\sigma-s}\varphi_{k}d_{0}^{\dagger}d_{0}^{\dagger}\right]|0\rangle , \qquad (2)$$

where $|0\rangle$ is the Fock vacuum, $c_{\sigma}(x)|0\rangle = 0$, $d_{is}|0\rangle = 0$; and k is the electron wave vector. It is considered that the impurity occupies the origin.

The amplitudes $\psi_{k\sigma}^{s}(x)$ and φ_{k} satisfy the Schrödinger equation $\mathcal{H}|\Psi\rangle_{k\sigma}^{s} = E(k)|\Psi\rangle_{k\sigma}^{s}$, which can be rewritten in the following form:

$$-i\frac{\partial}{\partial x}\psi_{k\sigma}^{s}(x) - k\psi_{k\sigma}^{s}(x) + W\varphi_{k}\delta(x)(\delta_{s_{\downarrow}}\delta_{\sigma_{\uparrow}} - \delta_{s_{\uparrow}}\delta_{\sigma_{\downarrow}}) + J\sigma_{\sigma\sigma'}\mathbf{S}_{ss'}\psi_{k\sigma'}^{s'}(0)\delta(x) = 0, \quad (3)$$

$$(\varepsilon - k)\varphi_k + W^*[\psi_{k_{\uparrow}}^{\downarrow}(0) - \psi_{k_{\downarrow}}^{\uparrow}(0)] = 0 , \qquad (4)$$

where $\varepsilon = \varepsilon_d + U$, and E(k) is the eigenvalue of the Hamiltonian (1).

The solution $\psi_{k\sigma}^{s}(x)$ determines the scattering matrix of conduction electrons on impurity which will now be denoted as the *R* matrix

$$\psi^{s}_{k\sigma}(x) = A^{s}_{k\sigma} \exp(ikx) ,$$

$$A^{s}_{k\sigma}(x>0) = R^{\sigma\sigma'}_{ss'}(k) A^{s'}_{k\sigma'}(x<0) ,$$
(5)

where $A_{k\sigma}^s$ is an arbitrary tensor. According to Eqs. (3) and (4) the components of the tensor $A_{k\sigma}^s$ are independent of spin indexes at x = 0.

Substituting expression (5) into Eqs. (3) and (4) we determine the expression for the scattering matrix of electrons on impurity,

$$R_{i0} = \frac{g(k_i) - iP_{i0}}{g(k_i) - i} \exp(i\Phi) , \qquad (6)$$

$$g(k) = \frac{k - \varepsilon + c |W|^2 / 4}{c [k - \varepsilon - |W|^2 / (2J)]} , \qquad (7)$$

where P_{i0} is the spin permutation operator $P_{i0} = \frac{1}{2}(1 + \sigma_i \mathbf{S}_0)$, c is the effective coupling constant determined by the value of the exchange interaction $c = 2J/(1 - 3/4J)^2$; and $\Phi = -2 \tan^{-1}(J/2)$.

The integrability of a single-impurity system such as (1), such as the Kondo problem and the Anderson model, requires two particles interacting only on the same site and their scattering matrices satisfying the Yang-Baxter equations. Let us consider the factorization conditions which take place for the model (1). To do the scattering of two electrons on impurity should be born in mind. In accordance with (2) the general state vector of the Hamiltonian (1) has the following form:

$$|\Psi\rangle_{k_{1}\sigma_{1}k_{2}\sigma_{2}}^{s} = \int dx_{1}dx_{2}[f_{k_{1}\sigma_{1}k_{2}\sigma_{2}}^{s}(x_{1},x_{2})c_{\sigma_{1}}^{\dagger}(x_{1})c_{\sigma_{2}}^{\dagger}(x_{2})d_{0s^{\dagger}} + g_{k_{1}\sigma_{1}k_{2}}(x_{1},0)\delta_{\sigma_{2}-s}\delta(x_{2})c_{\sigma_{1}}^{\dagger}(x_{1})d_{0_{1}}^{\dagger}d_{0_{1}}^{\dagger} + g_{k_{1}k_{2}\sigma_{2}}(0,x_{2})\delta_{\sigma_{1}-s}\delta(x_{1})c_{\sigma_{2}}^{\dagger}(x_{2})d_{0_{1}}^{\dagger}d_{0_{1}}^{\dagger}]|0\rangle .$$
(8)

Similar to the two-particle state (2), the amplitudes $f_{k_1\sigma_1k_2\sigma_2}^s(x_1,x_2)$, $g_{k_1\sigma_1k_2}(x,0)$, and $g_{k_1k_2\sigma_2}(0,x)$ satisfy the Schrödinger equation, which in our case has the form

$$-i\frac{\partial}{\partial x_{1}}f_{k_{1}\sigma_{1}k_{2}\sigma_{2}}(x_{1},x_{2})+J\sigma_{\sigma_{1}\sigma_{1}}S_{ss}f_{k_{1}\sigma_{1}k_{2}\sigma_{2}}^{s'}(0,x_{2})\delta(x_{1}) +Wg_{k_{1}k_{2}\sigma_{2}}(0,x_{2})(\delta_{s_{1}}\delta_{\sigma_{1}}-\delta_{s_{1}}\delta_{\sigma_{1}})\delta(x_{1})-i\frac{\partial}{\partial x_{2}}f_{k_{1}\sigma_{1}k_{2}\sigma_{2}}^{s}(x_{1},x_{2}) +J\sigma_{\sigma_{2}\sigma_{2}'}S_{ss'}f_{k_{1}\sigma_{1}k_{2}\sigma_{2}'}^{s'}(x_{1},0)\delta(x_{2})+Wg_{k_{1}\sigma_{1}k_{2}}(x_{1},0)(\delta_{s_{1}}\delta_{\sigma_{2}}-\delta_{s_{1}}\delta_{\sigma_{2}})\delta(x_{2})=(k_{1}+k_{2})f_{k_{1}\sigma_{1}k_{2}\sigma_{2}}^{s}(x_{1},x_{2}), \quad (9)$$

$$-i\frac{\partial}{\partial x}g_{k_{1}\sigma_{1}k_{2}}(x,0) + (\varepsilon - k_{1} - k_{2})g_{k_{1}\sigma_{1}k_{2}}(x,0) + W^{*}[f_{k_{1}\sigma_{1}k_{2}}^{\downarrow}(x,0) - f_{k_{1}\sigma_{1}k_{2}}^{\dagger}(x,0)] = 0, \qquad (10)$$

$$-i\frac{\partial}{\partial x}g_{k_1k_2\sigma_2}(0,x) + (\varepsilon - k_1 - k_2)g_{k_1k_2\sigma_2}(0,x) + W^*[f_{k_1,k_2\sigma_2}^{\dagger}(0,x) - f_{k_1,k_2\sigma_2}^{\downarrow}(0,x)] = 0.$$
(11)

As we know, e.g., from Wiegmann's paper,¹ the new basis of eigenfunctions must contain an arbitrary function denoted as Z(x) which depends on the difference in position between scattered electrons. So, we split the function into its even and odd parts and define one in the form¹

$$Z(x) = 1/2(1 + \text{sgn}x)$$
 (12)

Then, the corresponding solutions for the amplitudes $f_{k_1\sigma_1k_2\sigma_2}^s(x_1,x_2)$, $g_{k_1\sigma_1k_2}(x,0)$, and $g_{k_1k_2\sigma_2}(0,x)$ of the threeparticle wave function (8) has the following solutions:

$$f_{k_{1}\sigma_{1}k_{2}\sigma_{2}}^{s}(x_{1},x_{2}) = \{\exp(ik_{1}x_{1}+ik_{2}x_{2})[Z(x_{1}-x_{2})\delta_{\sigma_{1}\sigma_{1}'}\delta_{\sigma_{2}\sigma_{2}'}+S_{\sigma_{2}\sigma_{2}'}^{\sigma_{1}\sigma_{1}'}(k_{1},k_{2})Z(x_{2}-x_{1})] - \exp(ik_{1}x_{2}+ik_{2}x_{1})[Z(x_{2}-x_{1})\delta_{\sigma_{2}\sigma_{1}'}\delta_{\sigma_{1}\sigma_{2}'}+S_{\sigma_{1}\sigma_{2}'}^{\sigma_{2}\sigma_{1}'}(k_{1},k_{2})Z(x_{1}-x_{2})]\}A_{k_{1}\sigma_{1}'k_{2}\sigma_{2}'}^{s},$$
(13)

$$g_{k_{1}\sigma_{1}k_{2}}(x,0) = W^{*} \sum_{s,\sigma_{2}} (\delta_{s_{1}}\delta_{\sigma_{2^{\dagger}}} - \delta_{s_{1}}\delta_{\sigma_{2^{\dagger}}}) \left\{ \frac{1}{k_{2}-\varepsilon} \exp(ik_{1}x) [Z(x)\delta_{\sigma_{1}\sigma_{1}'}\delta_{\sigma_{2}\sigma_{2}'} + S_{\sigma_{2}\sigma_{2}'}^{\sigma_{1}\sigma_{1}'}(k_{1},k_{2})Z(-x)] - \frac{1}{k_{1}-\varepsilon} \exp(ik_{2}x) [Z(-x)\delta_{\sigma_{2}\sigma_{1}'}\delta_{\sigma_{1}\sigma_{2}'} + S_{\sigma_{1}\sigma_{2}'}^{\sigma_{2}\sigma_{1}'}(k_{1},k_{2})Z(x)] \right\} A_{k_{1}\sigma_{1}'k_{2}\sigma_{2}'}^{s}, \quad (14)$$

$$g_{k_{1}k_{2}\sigma_{2}}(0,x) = W^{*} \sum_{s,\sigma_{1}} (\delta_{s_{1}}\delta_{\sigma_{1}^{1}} - \delta_{s_{1}}\delta_{\sigma_{1}^{1}}) \left\{ \frac{1}{k_{1}-\varepsilon} \exp(ik_{2}x) [Z(-x)\delta_{\sigma_{1}\sigma_{1}'}\delta_{\sigma_{2}\sigma_{2}'} + S_{\sigma_{2}\sigma_{2}'}^{\sigma_{1}\sigma_{1}'}(k_{1},k_{2})Z(x)] \right\}$$

$$\frac{1}{k_2 - \varepsilon} \exp(ik_1 x) [Z(x) \delta_{\sigma_2 \sigma_1'} \delta_{\sigma_1 \sigma_2'} + S_{\sigma_1 \sigma_2'}^{\sigma_2 \sigma_1'} (k_1, k_2) Z(-x)] \bigg] A_{k_1 \sigma_1' k_2 \sigma_2'}^s , \quad (15)$$

where $S_{12} = S_{\sigma_2 \sigma'_2}^{\sigma_1 \sigma'_1}(k_1, k_2)$ is the matrix of mutual scattering of conduction electrons and $A_{k_1 \sigma_1 k_2 \sigma_2}^s$ is an arbitrary tensor. At $x_1 = x_2 = 0$, components of the tensor $A_{k_1 \sigma_1 k_2 \sigma_2}^s$ are independent of spin indexes and are determined from the norm calculation of the wave function (8).

It should be noted that the form of solutions (13)-(15)is similar to that for the Kondo problem¹ and the Anderson model.³ By definition, S_{ij} is a linear operator which depends on the difference between two parameters, $g(k_i)$ and $g(k_i)$, and satisfies the Yang-Baxter equations

$$R_{i0}R_{j0}S_{ij} = S_{ij}R_{j0}R_{i0} , \quad S_{ij}S_{il}S_{jl} = S_{jl}S_{il}S_{ij} .$$
(16)

These relations follow from solutions (13)-(15) and were obtained by Wiegmann¹ and Andrei² for the Kondo problem. The S matrix is the solution of Eqs. (16), in our case it has the well-known form

$$S_{ij} = \frac{g(k_i) - g(k_j) - iP_{ij}}{g(k_i) - g(k_j) - i} , \qquad (17)$$

where P_{ij} is the permutation operator of scattered electrons $P_{ij} = \frac{1}{2}(1 + \sigma_i \sigma_j)$.

To calculate the eigenvector of the Hamiltonian (1), we find the amplitudes of the wave function corresponding to the state with N_i impurities with coordinates $0 < X_1 < X_2 < \cdots < X_{N_i}$ and with N_e conduction electrons with coordinates $X_{N_i} < x_{Q1} < x_{Q2} < \cdots < x_{QN_e} < L$ and M_e spins directed upward (\uparrow) (L is the chain length). The amplitude of the N_e wave function is determined in the form of the Bethe ansatz for the present configuration of electrons Q

$$f(X_{1},s_{1};\ldots;X_{N_{i}}s_{N_{i}};x_{Q1},\sigma_{1};\ldots;x_{QN_{e}},\sigma_{N_{e}}) = \sum_{P} (-1)^{P} A_{k_{1}\sigma_{1}}^{s_{1}s_{2}\cdots s_{N_{i}}} (Q/P) \exp\left[i\sum_{j=1}^{N_{e}} k_{Pj}x_{Qj}\right],$$
(18)

where $\{k_j\}$ is the set of unequal numbers; the sums are over all permutations $P = [P_1, \ldots, P_{N_n}]$.

The wave function which was constructed with the use of coefficients (18) is the eigenfunction of the model Hamiltonian (1) if these coefficients satisfy the following conditions:

$$A(\ldots x_i > x_j, \ldots) = S_{ij} A(\ldots x_j > x_i, \ldots) , \qquad (19)$$

$$\mathbf{A}(\ldots,\mathbf{x}_i > \mathbf{X}_j,\ldots) = \mathbf{R}_{ij} \mathbf{A}(\ldots,\mathbf{x}_i < \mathbf{X}_j,\ldots) .$$
 (20)

The energy and the magnetization appropriate to this wave function are

$$E = \sum_{j=1}^{N_e} k_j + N_i \varepsilon_d - HM_z , \qquad (21)$$

$$M_z = N/2 - M$$
, (22)

where H is the external magnetic field, N is the number of particles, and M is the number of down-spin particles.

As usual, the periodic boundary condition can be expressed in terms of the T_i matrix of the considered model

$$T_i A(I) = \exp(ik_i L) A(I)$$
,

where I denotes the identity in the permutation group and the T_i matrix is defined as

$$T_{j} = S_{jj+1}S_{jj+2}\cdots S_{jN_{e}}R_{j1}R_{j2}\cdots R_{jN_{i}}S_{j1}S_{j2}\cdots S_{jj-1}.$$
(23)

The diagonalization of the T_j matrix is achieved by a purely algebraic procedure based on the algebra of monodromy matrices. The eigenvalue problem reduces to solving a set of N_e coupled algebraic equations for the N_e quasimomenta k_j ,

$$\exp(ik_jL + iN_i\Phi) = \prod_{\alpha=1}^{M} \frac{g(k_j) - \lambda_{\alpha} - i/2}{g(k_j) - \lambda_{\alpha} + i/2}$$

for $j = 1, 2, \dots N_e$. (24)

The λ 's in Eq. (24) are the set of real numbers related to the k's through

$$\prod_{i=1}^{N_e} \frac{\lambda_{\alpha} - g(k_j) - i/2}{\lambda_{\alpha} - g(k_j) + i/2} \left[\frac{\lambda_{\alpha} - i/2}{\lambda_{\alpha} + i/2} \right]^{N_i}$$
$$= -\prod_{\beta=1}^{M} \frac{\lambda_{\alpha} \lambda_{\beta} - 1}{\lambda_{\alpha} - \lambda_{\beta} + i} \text{ for } \alpha = 1, 2, \dots M . \quad (25)$$

f

In the next section we consider the solution of our model in the thermodynamic limit.

III. THE GROUND STATE OF THE MODEL

In the thermodynamic limit $(L \rightarrow \infty)$, with $n_e = N_e / L$, M/L, $n_i = N_i/L$ are fixed) the structure of solutions of the Bethe equations (24) and (25) for the ground-state system includes real momenta and rapidities. Since the function g(k) must be real the complex charge rapidities are not realized. The ground state of the model is the Fermi sea, characterized by two distribution functions: $\rho(k)$ is the distribution function of charge rapidities with momentum k, and $\sigma(\lambda)$ describes the distribution of down spins with respect to the spin-wave rapidity λ . The "Fermi surfaces" are determined by the k_F and B values, the ground-state configuration corresponds to filling of all states with $0 < k < k_F$ and $-B < \lambda < \infty$. The momenta k vary from 0 to k_1 , i.e., $0 < k < k_1$ (where k_1 determines the conduction band width) and rapidities λ range in the infinite limits $-\infty < \lambda < \infty$. According to (24) and (25) the functions $\rho(k)$ and $\sigma(\lambda)$ satisfy the following integral equations:

$$\rho(k) = \frac{1}{2\pi} - g'(k) \int_{-B}^{\infty} d\lambda a_1 [\lambda - g(k)] \sigma(\lambda) , \qquad (26)$$

$$\sigma(\lambda) + \int_{-B}^{\infty} d\lambda' a_2(\lambda - \lambda')\sigma(\lambda')$$

=
$$\int_{0}^{k_F} dk \ a_1[\lambda - g(k)]\rho(k) + n_i a_1(\lambda) , \quad (27)$$

where n_i is the concentration of impurity.

The kernels a_1 and a_2 of these integral equations are given by

$$a_n(\lambda) = \frac{n}{2\pi} \frac{1}{\lambda^2 + (n/2)^2} .$$
 (28)

The values of k_F and B are fixed by the following equations:

$$\int_{0}^{k_{F}} \rho_{e}(k) dk = n_{e} , \qquad (29)$$

$$\int_{-B}^{\infty} \sigma_e(\lambda) d\lambda = n_e / 2 - \mathcal{M}_e .$$
(30)

In Eqs. (29) and (30) n_e is the density of conduction electrons, $\mathcal{M}_e = (N_e^{\dagger} - N_e^{\downarrow})/2L$ is the density of the magnetization of conduction electrons, and the distribution functions can be divided into a host and impurity part, $\rho(k) = \rho_e(k) + n_i \rho_i(k)$ and $\sigma(\lambda) = \sigma_e(\lambda) + n_i \sigma_i(\lambda)$. The density of the ground-state energy of the Hamiltonian (1) is

$$\mathcal{E} = \int_{0}^{k_{F}} k \rho(k) dk - H \mathcal{M} + n_{i} \varepsilon_{d} , \qquad (31)$$

where $\mathcal{M} = (N^{\uparrow} - N^{\downarrow})/2L$ is the total density of the magnetization.

Below we shall consider the case where H=0. In the absence of magnetic field the number of electrons is the same for each spin component. According to (30) $B = \infty$ and the function $\rho(k)$ may be calculated as the solution of the following equation:

$$p(k) + g'(k) \int_{0}^{\kappa_{F}} dk' R[g(k) - g(k')]\rho(k')$$

$$= \frac{1}{2\pi} - n_{i}g'(k)R[g(k)] . \quad (32)$$

The kernel R(x) of this equation is given by

$$R(x) = \frac{1}{2\pi} \int_{-\infty}^{\infty} d\omega \exp(i\omega x) \frac{1}{1 + \exp(|\omega|)} .$$
 (33)

According to (7) g(k) is the discontinuous function of k; it is equal to $+\infty$ at $k = k_0 \pm v [k_0 = \varepsilon + |W|^2/(2J)$, $v \rightarrow 0$]. We have two branches of values of g(k). Let us consider the solution of Eq. (32) in the weak interaction limit for the constant W, namely, $|W|^2/|J\varepsilon| \ll 1$ and $|W|^2/|J(k_1-\varepsilon)| \ll 1$. In this approximation the value of g(k) is the same at k=0 and $k=k_1$ $g(0)=g(k_1)=1/c$, the error is $0(|W|^2/|J\varepsilon|)$ or $0[|W|^2/|J(k_1-\varepsilon)|]$ and it is of no interest here. We shall consider the solution for $\rho(k)$ assuming that it is the periodic function with period k_1 (the value of k_1 is determined by lattice spicing). Since the g(k) is the continuous function of k in the interval from k_0 to $k_0 + k_1$, Eq. (32) can be exactly solved for the case $k_0 = k_F [\varepsilon - k_F = -|W|^2/(2J)]$ using standard Wiener-Hopf techniques. The value of g(k) varies in the $1/c \leq g(k) < -\infty$ limits at $0 \leq k < k_F$ and $\infty < g(k) \le 1/c$ for $k_F < k \le k_1$. Let us determine the kernel of the integral equation (33) as a product of the functions which are analytic in the upper and lower complex ω plane

$$1 + \exp(-|\omega|) = G_+(\omega)G_-(\omega)$$

where the functions $G_{+}(\omega)$ and $G_{-}(\omega)$ are the well known

$$G_{-}(\omega) = G_{+}(-\omega) = \sqrt{2\pi} \left(\frac{i\omega}{2\pi e}\right)^{i\omega/2\pi} \frac{1}{\Gamma(1/2 + i\omega/2\pi)} ,$$
(34)

where $\Gamma(x)$ is the gamma function.

Using this factorization in Eq. (32) and taking into account Eq. (29) we calculate the value of the density of conduction electrons as the k_F function,

$$n_{e} = k_{F} / \pi - \frac{1}{\sqrt{2}\pi^{2}} \int_{0}^{\infty} \frac{d\omega}{\omega} \sin(\omega) G_{+}^{-1}(i\omega) \\ \times \int_{0}^{k_{F}} dk \exp\{\omega[g(k) - 1/c]\} .$$
(35)

Similarly, the valence of impurity is obtained from Eq. (32) at c > 0,

$$\bar{n}_i = 2 - \frac{\sqrt{2}}{\pi} \int_0^\infty \frac{d\omega}{\omega} \sin(\omega) G_+^{-1}(i\omega) \exp(-\omega/c) , \qquad (36)$$

and at c < 0

$$\bar{n}_i = 1 + \frac{1}{\sqrt{2\pi}} \int_0^\infty \frac{d\omega}{\omega} tg(\omega/2) G_+(i\omega) \exp(\omega/c) .$$
 (37)

Equations (36) and (37) yield a smooth monotonic decrease in the valence of impurity from 2 in the nonmag-

netic state $(0 < c \ll 1)$ to $1 (0 < -c \ll 1)$ [according to (1) the valence of impurity changes from 1 to 2]. The intermediate-valence state is realized for small values of $\varepsilon - k_F$, namely, according to (36) and (37) $J \cong 1$ in the weak interaction limit.

Let us consider the magnetic states of the system in a small magnetic field. The magnetic field enters the problem through the limit of integration B, which is determined from magnetization calculation in the absence of impurities (30). Equating the magnetic response of the conduction electrons to the Pauli magnetization and making the physically reasonable assumption that the magnetic-field energies are slightly comparable to the Fermi energy give sufficient conditions for determining the value of B. We have used the fact that in the small magnetic field the corrections to $\rho(k)$ are of the order of H^2 , therefore we can use Eqs. (28) and (29) to compare the magnetization as a function of the magnetic field assuming that the distribution function of momenta $\rho_0(k)$ is independent of H.

Let us define the scale, characterizing the crossover in magnetic field as

$$T_{H} = \sqrt{2\pi/e} A(1) ,$$

$$A(z) = \int_{0}^{k_{F}} dk \,\rho_{0}(k) \exp[-\pi z g(k)] .$$
(38)

Using the definition of T_H we find the relation between B and H with the accuracy 0[A(3)]

$$B = 1/\pi \ln[T_H/H] . (39)$$

According to (27) and (39), the formula for the impurity magnetization is given by

$$M_{i} = N_{i} \frac{1}{2\sqrt{\pi}} \sum_{n=0}^{\infty} (-1)^{n} \frac{1}{n!(n+1/2)} \\ \times \left[\frac{n+1/2}{e}\right]^{n+1/2} (H/T_{H})^{2n+1} \\ \text{at } H < T_{H} , \quad (40)$$

$$M_{i} = N_{i} \left[\frac{1}{2} - \frac{1}{\pi \sqrt{2}} \int_{0}^{\infty} \frac{d\omega}{\omega} \sin(\omega/2) \times G_{+}^{-1}(i\omega) (T_{H}/H)^{\omega/\pi} \right]$$

at $H > T_{H}$. (41)

Expressions (40) and (41) are the same as those derived by Wiegmann and Andrei for the Kondo problem for $S = \frac{1}{2}$.^{4,5} According to (38), (40), and (41) the Kondo limit is realized if the following inequalities are satisfied:

$$\varepsilon - k_F > |W|^2 c/4$$
, $c + \frac{c|W|^2}{2J(\varepsilon - k_F)} > 0$. (42)

The first inequality in (42) determines the condition of the formation of the local magnetic moment of impurity, because the valence of impurity is near unity at $\varepsilon - k_F > 0$. The second one presents the constant of the antiferromagnetic exchange interaction calculated in the Schrieffer-Wolf approximation. The localized moment of impurity gradually vanishes at $\varepsilon \rightarrow k_F$ because in this case the intermediate-valence region is realized. According to (7) and (42) the singular point $k = k_0$ determines the change in a sign of the exchange constant describing the interaction of conduction electron with localized spin of impurity in model (1).

IV. THE THERMODYNAMICS OF THE MODEL

The value of g(k) depends on the electron energy, hence the classification of the excitation spectrum is the same as for the Kondo problem. In the thermodynamic limit the solutions of the Bethe equations may be arranged in the so-called strings. A string of length n is defined as

$$\lambda_{\alpha}^{nj} = \lambda_{\alpha}^{n} + i/2(n+1-2j) + 0[\exp(-\delta L)] .$$

$$j = 1, 2, \dots, n , \quad \delta > 0 . \quad (43)$$

The number λ_{α}^{n} is called string's center.

Using Yang and Yang's¹¹ method to obtain the partition function from the Bethe ansatz solution defined by Eqs. (24) and (25), we find the following expression for the density of the thermodynamic potential:

$$\Omega = \mathcal{E}_0 + T \int_0^{\kappa_l} dk \,\rho_0(k) \ln\{n[K(k)]\} + T \int_{-\infty}^{\infty} d\lambda \sigma_0(\lambda) \ln\{n[\varepsilon_1(\lambda)]\}, \qquad (44)$$

where $n(\varepsilon) = [1 + \exp(\varepsilon/T)]^{-1}$ is the Fermi distribution function, T is the temperature, $\sigma_0(\lambda)$ is the distribution function, and \mathcal{E}_0 is the density of the ground-state energy, independent of H and T. The functions K(k) and $\varepsilon_n(\lambda)$ satisfy the set of coupled integral equations,

$$K(k) = k - k_{F} + T \int_{-\infty}^{\infty} d\lambda s[g(k) - \lambda] \ln\{n[\varepsilon_{1}(\lambda)]\}$$

+
$$T \int_{0}^{k_{1}} dk'g'(k')R[g(k) - g(k')]$$

$$\times \ln\{n[-K(k')]\}, \qquad (45)$$

$$\varepsilon_{n}(\lambda) = -Ts^{*} \ln\{n[\varepsilon_{n+1}(\lambda)]n[\varepsilon_{n-1}(\lambda)]\}$$

$$+ T\delta_{n1} \int_{0}^{k_{1}} dk g'(k) s[g(k) - \lambda] \ln\{n[-K(k)]\},$$

$$n = 1, 2, \dots, \quad (46)$$

with the boundary conditions

$$\varepsilon_0(\lambda) = -\infty$$
, $\lim_{n \to \infty} \varepsilon_n(\lambda)/n = H$,

where the symbol a^*f denotes the convolution of the functions $a(\lambda)$ and $f(\lambda)$ in accordance with

$$a^*f(\lambda) = \int_{-\infty}^{\infty} d\lambda' a(\lambda - \lambda') f(\lambda')$$

and $s(\lambda)$ is given by

$$s(\lambda) = \frac{1}{2\cosh(\pi\lambda)}$$
.

Equations (45) and (46) and expression (44) completely determine the thermodynamic properties of the model. The solutions of Eqs. (45) and (46) may be calculated in

the low-temperature limit. The charge and spin excitations are usually coupled, but in the Kondo-limit the relevant spin excitations only involve low energies while charge fluctuations require high energies. Hence, the impurity part of Ω is obtained from (44) and (46) by neglecting the charge excitations

$$\Omega_{\rm imp}^{\rm sp} = -Tn_i \int_{-\infty}^{\infty} dx \, s[x + 1/\pi \ln(T/T_K)] \\ \times \ln\{1 + \exp[h_1(x)]\} \,. \tag{47}$$

The function $h_1(x)$ is determined by the following recurrent equations:¹²

$$h_{n}(x) = s^{*} \ln(\{1 + \exp[h_{n-1}(x)]\}\{1 + \exp[h_{n+1}(x)]\}) -\delta_{n1} \exp(-\pi x),$$

$$h_{n}(x)/n = H, \qquad (48)$$

$$n \to \infty.$$

The dimensionless functions $h_n(x)$ define the unknown functions $\varepsilon_n(\lambda)$,

$$h_n(x) = 1/T\varepsilon_n[-\lambda + 1/\pi \ln(T_K/T)], \qquad (49)$$

where T_K is the Kondo temperature $T_K = 2A(1)$.

Since the charge excitations are ignored in the above calculations, Eqs. (47)-(49) are the same as in the Kondo problem.^{4,5}

Within the low-temperature limit Ω may be determined as a sum of the terms corresponding to spin (47) and charge excitations. The charge term is determined by the solution of K(k). Let us consider the lowtemperature behavior of the system. In low-temperature limit Eq. (45) can be solved iteratively, defining $K(k) = K_0(k) + T^2 \delta K(k)$, where $K_0(k)$ is the groundstate solution. We separate the integral equation for $\delta K(k)$ in the form

$$\delta K(k) + \int_{0}^{\kappa_{F}} dk'g'(k')R[g(k) - g(k')]\delta K(k') = \frac{1}{T} \int_{-\infty}^{\infty} d\lambda s[\lambda - g(k)] \ln\{n[\varepsilon_{1}(\lambda)]\} + \frac{\pi^{2}}{6}g'(k_{F})|dK_{0}(k)/dk|_{k=k_{F}}^{-1}R[g(k) - g(k_{F})].$$
(50)

Substituting the solution for $\delta K(k)$ into (44) we obtain the low-temperature limit for the thermodynamic potential of the model. In this approach the thermodynamic potential of the model considered and the Anderson model have a similar structure:

$$\Omega_{\rm imp} = -\frac{\pi^2 T^2}{3L} (\chi_{\rm imp}^{\rm ch} + \chi_{\rm imp}^{\rm sp}) , \qquad (51)$$

where χ_{imp}^{ch} and χ_{imp}^{sp} are the charge and the magnetic susceptibility, respectively.

According to (51) the impurity part of the lowtemperature specific-heat coefficient γ is a universal function for impurity models

$$\gamma_{\rm imp} = \frac{2}{3} \pi^2 (\chi_{\rm imp}^{\rm ch} + \chi_{\rm imp}^{\rm sp}) . \qquad (52)$$

We have constructed an integrable model describing the interaction of band electrons of metal with occupied levels of impurities. The model proposed is described by three constants of interactions. The solution obtained

- ¹P. B. Wiegmann, Pis'ma Zh. Eksp. Teor. Fiz. **31**, 392 (1980) [JETP Lett. **31**, 364 (1980)].
- ²N. Andrei, Phys. Rev. Lett. 45, 379 (1980).
- ³P. B. Wiegmann, Phys. Lett. 80A, 163 (1980).
- ⁴A. M. Tsvelick and P. B. Wiegmann, Adv. Phys. **32**, 453 (1983).
 ⁵N. Andrei, K. Furuya and J. H. Lowenstein, Rev. Mod. Phys. **55**, 331 (1983).
- ⁶A. M. Tsvelick and P. B. Wiegmann, J. Phys. C 15, 1707

correlates with Wiegmann and Andrei's solution of the Kondo problem. The impurity magnetization, susceptibility, and the Kondo limit for the impurity part of the thermodynamic potential in the model considered are determined as ones in the Kondo problem for the $\frac{1}{2}$ impurity spin with the renormalized value of T_H . On the other hand, the Bethe equations are similar to ones in the Anderson model. As we conclude from the exact solution, the structure of the solutions of the Bethe equations describing the ground state of this model is completely different from the Anderson model. Another interesting feature of our model is the existence of the mixed-valence region for $\varepsilon \rightarrow k_F$. Thus, this model gives other example of the quantum integrable impurity systems.

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- ⁷P. Schlottmann, Phys. Rep. **181**, N1&2, 1 (1989).
- ⁸A. A. Aligia, C. A. Balseiro, and C. R. Proetto, Phys. Rev. B 33, 6476 (1986).
- ⁹I. N. Karnaukhov, Phys. Lett. A 160, 90 (1991); 160, 97 (1991).
- ¹⁰P. Schlottmann, Z. Phys. B 59, 321 (1985).
- ¹¹C. N. Yang and C. P. Yang, Phys. Rev. **150**, 321 (1966).
- ¹²M. Takahashi, Prog. Theor. Phys. 52, 103 (1974).

^{(1982).}