Integrable multiparametric impurity model

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We present a one-dimensional model describing the interaction of spin-$\frac{1}{2}$ impurities with band electrons of a paramagnetic host metal. The model naturally describes the creation and annihilation of electron pairs localized at impurities, and the interaction between localized and band electrons. Using the Bethe-ansatz solution the thermodynamic properties of the system are calculated.

The Kondo problem and the Anderson model that describe the behavior of a localized magnetic moment in paramagnetic host metals are of great physical interest. The models of dilute systems of magnetic impurities are calculated using various methods such as Wilson's renormalized group,[1,2] and the Bethe ansatz.[3-5] The last method of attack is preferred since we are dealing with exact results. The exact solutions of the Kondo problem and the Anderson model obtained by Andrei[6] and Wiegmann[7,8] are relevant for any dimension of a system. These models are special because of their integrability. The single impurity models are integrable for the linearized dispersion of band electrons. This is due to the spherical symmetry of kinetic energy of band electrons and contact interaction, and the localized nature of the impurity. The eigenvalue problem for the above models has been solved exactly directly in a momentum space by Kebukawa.[9]

In this paper, based on Andrei and Wiegmann's idea of a calculation of the Kondo problem, we present an exact solution of the multiparametric one-dimensional single impurity model. We propose a model that is again solvable in one dimension, and combines and extends some of the interesting features of the Kondo problem and the Anderson model. The model considered takes into account different interactions between conduction electrons and electrons localized at impurities.

Before we present the Hamiltonian of the new impurity model, we briefly discuss some physical aspects of the model. It has been found that electrons in the materials that exhibit high-T_c superconductivity form spin-singlet pairs of Cooper type, which are much smaller than in traditional superconductors. We shall consider a creation and annihilation of electron pairs localized at impurities and suggest the integrable model, which keeps the main idea of approach to superconductivity, namely the existence of singlet pairs of electrons in narrow energy-band-electron systems. The model describes two types of electrons with spin $\frac{1}{2}$ on a chain; the conduction electrons from the partially filled atomic shells and almost localized electrons from the inner shells of impurities. The conduction electrons exchange interact with the localized spins of impurities and are hybridized with electron states of impurity shells, which can be singly or doubly occupied by electrons. The model Hamiltonian, which takes into account these interactions has been discussed in Ref. 10. In contrast to Ref. 10 we also consider terms describing a creation and annihilation of electron pairs localized at impurities.[11] The model proposed presents a logical generalization of the ones recently considered. In terms of the Hubbard operators $X_i^{ab}=|ai\rangle\langle ib|$ $(a,b=0,\uparrow,\downarrow,2)$ which define the states of impurity shell, the model Hamiltonian is chosen in the form

$$\mathcal{H}=\mathcal{H}_0+\mathcal{H}_{\rm int}\ , \tag{1}$$

$$\mathcal{H}_0=\sum_\sigma \int dx\, c_\sigma^\dagger(x)\left[-i\frac{\partial}{\partial x}\right]c_\sigma(x) +\varepsilon_d\sum_\sigma\sum_{i=1}^{N_i}X_i^{\sigma\sigma}+(2\varepsilon_d+U)\sum_{i=1}^{N_i}X_i^{22}\ , \tag{2}$$

$$\mathcal{H}_{\rm int}=\sum_{i=1}^{N_i}\int dx\,\delta(x-x_i)[Wc_\uparrow^\dagger(x)X_i^{\downarrow 2}-Wc_\downarrow^\dagger(x)X_i^{\uparrow 2}+\text{H.c.}]$$

$$+J\sum_{\sigma,\sigma'}\sum_{i=1}^{N_i}\int dx\,\delta(x-x_i)c_\sigma^\dagger(x)\vec{\sigma}_{\sigma\sigma'}c_{\sigma'}(x)\vec{S}_i+I\sum_{\sigma,\sigma'}\sum_{i=1}^{N_i}\int dx\,\delta(x-x_i)c_{\sigma'}^\dagger(x)c_{\sigma'}(x)X_i^{\sigma\sigma}$$

$$+\sum_{i=1}^{N_i}\int dx\,\delta(x-x_i)[\Delta_1c_\uparrow^\dagger(x)X_i^{\downarrow 0}-\Delta_1c_\downarrow^\dagger(x)X_i^{\uparrow 0}+\text{H.c.}]+\sum_{i=1}^{N_i}(\Delta_2X_i^{20}+\text{H.c.})\ , \tag{3}$$

where $c_\sigma^\dagger(x)$ and $c_\sigma(x)$ are the operators of the conduction electrons; ε_d is the one-electron energy of impurity level, U is the on-site Coulomb repulsion, W is the constant of the correlated hybridized interaction, J is the constant of the exchange interaction of the band electrons with impurity spin, $\vec{\sigma}=\{\sigma^x,\sigma^y,\sigma^z\}$ are the Pauli matrices, and $\vec{S}_i$ is the spin operator of the spin-$\frac{1}{2}$ impurity. The last terms, which are proportional to complex constants of prime interactions Δ_1 and Δ_2, describe a creation and annihilation of singlet electron pairs on an impurity: band electron-localized electron and pair of localized electrons. Additionally, we include a potential scattering term with interaction constant I.

We construct the exact solution of the one-dimensional model (1)–(3) for N_e conduction electrons interacting with N_i impurities in the chain length L. The total number of particles is not conserved since the operator $\hat{N}=\hat{N}_e+\hat{N}_i[\hat{N}_e=\sum_\sigma\int dx\, c_\sigma^\dagger(x)c_\sigma(x)$, $\hat{N}_i=\sum_{j=1}^{N_i}(\sum_\sigma X_j^{\sigma\sigma}+2X_j^{22})]$ does not commute with $\mathcal{H}$ (the last terms in (3), which are proportional to Δ_1 and Δ_2, nonconserve the total number of electrons). As the number operator $\hat{N}_-=\hat{N}_e-\sum_{j=1}^{N_i}\sum_\sigma X_j^{\sigma\sigma}$ commutes with $\mathcal{H}$ (Ref. 12) we can add a term $-\varepsilon_F\hat{N}_-$ to the Hamiltonian without changing the set of eigenvalues. That allows us to introduce the Fermi energy ε_F for the system in which the total number of particles are not conserved. The Hamiltonian $\mathcal{H}_0$ can be rewritten as

$$\mathcal{H}_0=\sum_\sigma\int dx\left[c_\sigma^\dagger(x)\left[-i\frac{\partial}{\partial x}\right]c_\sigma(x)-\varepsilon_F c_\sigma^\dagger(x)c_\sigma(x)\right]+(\varepsilon_d+\varepsilon_F)\sum_\sigma\sum_{i=1}^{N_i}X_i^{\sigma\sigma}+(2\varepsilon_d+U)\sum_{i=1}^{N_i}X_i^{22}\,. \tag{4}$$

The multiparametric model (1), (3), and (4) generalizes the integrable impurity models, which have been recently proposed by the author: In the limit $\Delta_1\to 0$, $\Delta_2\to 0$, and $I\to 0$, the Hamiltonian coincides with the one in Ref. 10 and, for $I=0$ and $U\to\infty$, it coincides with the one in Ref. 11.

Let us consider a scattering of electrons on a magnetic impurity localized at the origin. The two-particle wave function can be written as

$$|\Psi\rangle_{k\sigma}^s=\int dx[\psi_{k\sigma}^s(x)c_\sigma^\dagger(x)X_0^{s0}+\delta(x)(\delta_{\sigma\uparrow}\delta_{s\downarrow}-\delta_{\sigma\downarrow}\delta_{s\downarrow})(\varphi_k X_0^{2_0}+f_k)]|0\rangle\,, \tag{5}$$

where k is the electron wave vector, $\delta_{\sigma\sigma'}$ is Kronecker's symbol, and the unknown amplitudes are solutions of Schrödinger's equation,

$$-i\frac{\partial}{\partial x}\psi_{k\sigma}^s(x)-k\psi_{k\sigma}^s(x)+(W\varphi_k+\Delta_1 f_k)\delta(x)(\delta_{s\downarrow}\delta_{\sigma\uparrow}-\delta_{s\uparrow}\delta_{\sigma\downarrow})+I\delta(x)\psi_{k\sigma}^s(x)+J\delta(x)\vec{\sigma}_{\sigma\sigma'}\vec{S}_{ss'}\psi_{k\sigma'}^{s'}(x)=0\,, \tag{6}$$

$$[\varepsilon-\varepsilon(k)]\varphi_k+W^*[\psi_{k_\uparrow}^\downarrow(0)-\psi_{k_\downarrow}^\uparrow(0)]+\Delta_2 f_k=0\,, \tag{7}$$

$$-\varepsilon_0(k)f_k+\Delta_1^*[\psi_{k_\uparrow}^\downarrow(0)-\psi_{k_\downarrow}^\uparrow(0)]+\Delta_2^*\varphi_k=0\,, \tag{8}$$

where $\varepsilon(k)=k-\varepsilon_F$, $\varepsilon=\varepsilon_d+U-\varepsilon_F$, and $\varepsilon_0(k)=\varepsilon(k)+\varepsilon_d+\varepsilon_F$. Let us seek the solution for the amplitude $\psi_{k\sigma}^s(x)$ in standard form

$$\psi_{k\sigma}^s(x)=A_{k\sigma}^s\exp(ikx)\,, \tag{9}$$

where $A_{k\sigma}^s$ is an arbitrary tensor.

According to (9), the relation among the components of the tensor $A_{k\sigma}^s$ for $x<0$ and $x>0$ determines the scattering matrix of conduction electrons on an impurity, which is denoted below as the R matrix. This leads to the following result for the R matrix:

$$R_{i0}=\frac{g(k_i)}{g(k_i)}\frac{-iP_{i0}}{-i}\exp(i\phi)\,, \tag{10}$$

$$g(k)=\frac{1}{c_1}-\frac{c'\nu(k)}{1+\nu(k)/(2J)}\,, \tag{11}$$

$$\nu(k)=-\frac{|\Delta_1|^2}{\varepsilon_0(k)}+|W+\Delta_1\Delta_2^*/\varepsilon_0(k)|^2\frac{1}{\varepsilon-\varepsilon(k)+|\Delta_2|^2/\varepsilon_0(k)}\,, \tag{12}$$

where P_{i0} is the spin permutation operator $P_{i0}=\frac{1}{2}(1+\vec{\sigma}_i\vec{S}_0)$ and c' is the effective coupling constant

$$c'=\frac{1}{2c_1}[1/J+(c_1+c_2)/2]\,. \tag{13}$$

c_1 and c_2 are equal to

$$c_1=\frac{2J}{1+I^2/4-IJ/2-3J^2/4}\,,\qquad c_2=\frac{2I}{1+I^2/4-IJ/2-3J^2/4}\,, \tag{14}$$

and, finally, $\phi=-2\tan^{-1}[(J+I)/2]$. The three-particle wave function satisfies Schrödinger's equation and is determined by the two-particle scattering matrix of electrons S on the basis of solutions containing a step function.[7,13] The S matrix is the solution of the Yang-Baxter equations and has a well-known form

$$S_{ij}=\frac{g(k_i)}{g(k_i)}\frac{-g(k_j)}{-g(k_j)}\frac{-iP_{ij}}{-i}\,, \tag{15}$$

where P_{ij} is the spin permutation operator of scattered electrons.

The Bethe-ansatz wave function explicitly depends on the relative ordering of the conduction electrons. We present this dependence by a permutation Q of the N_e

elements ordered coordinates of electrons

$$\psi(x_{Q1},\sigma_1,\ldots,x_{QN_e},\sigma_{N_e}) = \sum_P (-1)^P A(Q/P)\exp\left[i\sum_{j=1}^{N_e} k_{Pj}x_{Qj}\right], \quad (16)$$

where $\{k_j\}$ is the set of unequal wave numbers; the sums are over all permutations $P=[P_1,..,P_{N_e}]$. The amplitudes $A(Q/P)$ depend on spins of band electrons and impurities and on Q through the coordinates of conduction electrons.

Imposing periodic boundary conditions on the Bethe function (16) leads to the following equations for the electron momenta k_j and rapidities λ_α derived in Ref. 11,

$$\exp(ik_jL+iN_i\phi)=\prod_{\alpha=1}^{M}\frac{g(k_j)-\lambda_\alpha-i/2}{g(k_j)-\lambda_\alpha+i/2}, \quad (17)$$

$$\prod_{j=1}^{N_e}\frac{\lambda_\alpha-g(k_j)-i/2}{\lambda_\alpha-g(k_j)+i/2}\left[\frac{\lambda_\alpha(-i/2}{\lambda_\alpha+i/2}\right] = -\prod_{\beta=1}^{M}\frac{\lambda_\alpha-\lambda_\beta-i}{\lambda_\alpha-\lambda_\beta+i}. \quad (18)$$

The energy and the magnetization of the system in the state corresponding to a solution of (17) and (18) are equal to

$$E=\sum_{j=1}^{N_e}\varepsilon(k_j)+(\varepsilon_d+\varepsilon_F)N_i-HM_z;\quad M_z=N/2-M, \quad (19)$$

where H is an external magnetic field and N is the total number of particles.

In the thermodynamic limit, the ground state of the model consists of the Fermi seas each from which is determined by the k_F and B values. The ground-state configuration corresponds to the filling of all states with $0<k<k_F$ and $-B<\lambda<\infty$; the momenta are changed in the interval from 0 to k_1 $0<k<k_1$ (where k_1 is the conduction bandwidth) and the rapidities range in the infinite limits $-\infty<\lambda<\infty$. For a large system, we can introduce the density of wave numbers $\rho(k)$ and the distribution function of rapidities $\sigma(\lambda)$. By taking the continuum limit the Bethe Eqs. (17) and (18), corresponding to the ground state, can be transformed into a set of coupled integral equations for the functions $\rho(k)$ and $\sigma(\lambda)$

$$\rho(k)=\frac{1}{2\pi}-g'(k)\int_{-B}^{\infty}d\lambda\, a_1[\lambda-g(k)]\sigma(\lambda), \quad (20)$$

$$\sigma(\lambda)+\int_{-B}^{\infty}d\lambda' a_2(\lambda-\lambda')\sigma(\lambda') = \int_0^{k_F}dk a_1[\lambda-g(k)]\rho(k)+n_i a_1(\lambda), \quad (21)$$

where n_i is the concentration of impurity. The kernels of these integral equations are given by

$$a_n(\lambda)=\frac{n}{2\pi}\frac{1}{\lambda^2+(n/2)^2}. \quad (22)$$

The density of momenta and the distribution function of rapidities describing conduction electrons are normalized so that

$$\int_0^{k_F}\rho_e(k)dk=n_e,\quad \int_{-B}^{\infty}\sigma_e(\lambda)d\lambda=n_e/2-\mathcal{M}_e, \quad (23)$$

where n_e and $\mathcal{M}_e$ are the density and the density of the magnetization of conduction electrons.

Below we shall consider a valence of an impurity ion at $H=0$. In the absence of magnetic field it is easily seen that $B=\infty$. This allows the elimination of λ-dependent quantities from the Bethe-ansatz integral equation by Fourier transformation. From Eqs. (20) and (21), we obtain the following equation for the function $\rho(k)$ at $H=0$ denoted as $\rho_0(k)$:

$$\rho_0(k)+g'(k)\int_0^{k_F}dk'R[g(k)-g(k')]\rho_0(k') = \frac{1}{2\pi}-n_i g'(k)R[g(k)]. \quad (24)$$

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

$$R(x)=\frac{1}{\pi}\int_0^{\infty}d\omega\cos(\omega x)\frac{1}{1+\exp(\omega)}. \quad (25)$$

The value of $g(k)$ is tended to zero for the momenta of electron equal to $k_{\pm}^0$ $(k_+^0>k_-^0)$ and tended to infiniteness in the points $k_{\pm}^{\infty}$ $(k_+^{\infty}>k_-^{\infty})$. In contrast to the Anderson model, a strong dispersion of $g(k)$ has taken place. We have three branches of values of $g(k)$ because it is the discontinues function of the wave vector. Three branches of values of $g(k)$ are realized for deep electron levels, which correspond to inner electron shells of impurity atoms, namely, for $\varepsilon_d<-\varepsilon_F$. The case $\varepsilon_d=-\varepsilon_F$ in the infinite U limit has been considered at length.[11] The lowest of the k branch of $g(k)$ should not be taken into account if $k_-^{\infty}<-\varepsilon_F$. Therefore, if the energy of one-electron impurity state fall on a conduction band two branches of values of $g(k)$ for $k_-^{\infty}<\varepsilon(k)<k_1-k_F$ will be considered below.

The valence of an impurity atom depends on the value of $g(k)$ at $k=k_F$, which is denoted as z_F, the state of intermediate valence corresponds to region of values of z_F at close-range zero. Let us consider the solution of Eq. (24) for the state of impurity with a localized magnetic moment assuming that $k_+^{\infty}>0$ and ignoring some states with $k_+^{\infty}<\varepsilon(k)<k_1-k_F$. In this approximation, we consider only one branch of values of $g(k)$, namely $k_-^{\infty}<\varepsilon(k)<k_+^{\infty}$.

Equation (24) is solved using the standard Wiener-Hopf technique. The key to the solution of this equation is to find a decomposition of the kernel into factors $G_{\pm}(\omega)$ that are analytic in the upper and lower complex ω plane $[1-R(\omega)]^{-1}=G_+(\omega)G_-(\omega)$,

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

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

The density of conduction electrons and the valence of impurity are equal to

$$n_e = k_F/\pi - \frac{1}{\sqrt{2}\pi^2}\int_0^\infty \frac{d\omega}{\omega}\sin(\omega)G_+^{-1}(i\omega) \times \int_0^{k_F} dk\,\exp[-\omega g(k)+\omega z_F]\,, \tag{26}$$

$$\bar{n}_i = 1+\frac{1}{\sqrt{2}\pi}\int_0^\infty \frac{d\omega}{\omega}\tan(\omega/2)G_+(i\omega)\exp(-\omega z_F)\,. \tag{27}$$

These expressions make sense for $z_F>0$ only, for $z_F\approx 0$ or $z_F<0$ we have to obtain the solution of Eq. (24) for two branches of values of $g(k)$ $[k_-^\infty<\varepsilon(k)<k_+^\infty$ and $k_+^\infty<\varepsilon(k)<k_1-k_F]$. The behavior of localized magnetic moment in a small magnetic field arbitrary with respect to the Kondo temperature T_K characterizes the magnetic scale T_H

$$T_H=\sqrt{2\pi/e}\int_0^{k_F} dk\,\rho_0(k)\exp[-\pi g(k)]\,. \tag{28}$$

In the small magnetic field, the behavior of localized magnetic moment is similar to that in the Kondo problem and the impurity magnetization is determined analogous to the Kondo problem for the spin-$\frac{1}{2}$ impurity.

The solutions for the excitations of the system are the same as for the Kondo problem, namely, M_n strings of complex spin rapidities of length n, $n=1,2,\ldots,\infty$, which corresponds to bound spin states

$$\lambda_\alpha^{nj}=\lambda_\alpha^n+ic/2(n+1-2j)+0[\exp(-\delta L)]\,, \quad j=1,2,\ldots,n,\ \delta>0\,; \tag{29}$$

where λ_α^n is a real parameter.

The density of the free energy can be written in terms of the quasienergies

$$\mathcal{F}=\mathcal{E}_0+T\int_0^{k_1} dk\,\rho_0(k)\ln\{n[K(k)]\} +T\int_{-\infty}^{\infty} d\lambda\,\sigma_0(\lambda)\ln\{n[\varepsilon_1(\lambda)]\}\,, \tag{30}$$

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 standard procedure leads from (17) and (18) to the integral nonlinear equations for the excitation energies

$$K(k)=k-\varepsilon_F+T\int_{-\infty}^{\infty} d\lambda s[g(k)-\lambda]\ln\{n[\varepsilon_1(\lambda)]\} -T\int_0^{k_1} dk' g'(k')R[g(k)-g(k')]\ln\{n[-K(k')]\} \tag{31}$$

$$\varepsilon_n(\lambda)=-Ts^*\ln\{n[\varepsilon_{n+1}(\lambda)]n(\varepsilon_{n-1}(\lambda))\} -T\delta_{n1}\int_0^{k_1} dk\,g'(k)s[g(k)-\lambda] \times\ln\{n[-K(k)]\},\quad n=1,2,\ldots, \tag{32}$$

$$\varepsilon_0(\lambda)=-\infty,\quad \lim_{n\to\infty}\varepsilon_n(\lambda)/n=H,\quad s(\lambda)=\frac{1}{2\cosh(\pi\lambda)}\,,$$

where the symbol a^*f denotes the convolution.

The Kondo limit is obtained by suppressing the charge excitation in the system: For this approximation, the impurity part of the density of the free energy is equal to

$$\mathcal{F}_{\rm imp}^{sp}=-Tn_i\int_{-\infty}^{\infty} dx\,s[x+1/\pi\ln(T_n/T_K)] \times\ln\{1+\exp[h_1(x)]\}\,, \tag{33}$$

where $T_K=\sqrt{2/\pi e}\,T_H$. The following recurrent equations are for the dimensionless functions $h_n(x)$,

$$h_n(x)=s^*\ln\{[1+\exp(h_{n-1}(x))][1+\exp(h_{n+1}(x))]\} -\delta_{n1}\exp(-\pi x),\quad \lim_{n\to\infty}h_n(x)/n=H \tag{34}$$

may be solved by iteration.

We have studied the effects of incorporating realistic features such as exchange interaction, hybridization between electron states of conduction and localized electrons, and creation and annihilation of electron pairs on the physics of the single-ion Kondo problem on the basis of the Bethe-ansatz solution. The model considered is unique because it is the only one integrable model, the Hamiltonian of which is described by six parameters of the two-particle interactions. In contrast to the Anderson model, the region of mixed valence is characterized by a strong dispersion of the components of the two-particle scattering matrices and determined by peculiar point, which corresponds to strong interaction.

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