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THE EXACT SOLUTION OF THE s-d EXCHANGE
MODEL WITH ARBITRARY IMPURITY SPIN S
(KONDO PROBLEM)

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An exact solution of the s-d exchange model with arbitrary impurity spin S (Kondo problem) is proposed. On the basis of this solution, the magnetic susceptibility as a function of an arbitrary magnetic field is calculated in explicit form.

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Recently, an exact solution of the s-d exchange model with localized spin $S = \frac{1}{2}$ was proposed¹⁾. In this paper, we extend this approach to the case of arbitrary impurity spin S .

The canonical Hamiltonian which describes a magnetic atom in a non-magnetic host metal, the so-called "s-d exchange model", has the form:

$$H_{s.d.} = \sum_{k, \mu=\pm 1} \epsilon_k c_{k, \mu}^+ c_{k, \mu} + J \sum_{\substack{k, k' \\ \mu, \mu'}} c_{k, \mu}^+ \vec{\sigma}_{\mu, \mu'} c_{k', \mu'} \vec{S} \quad (1)$$

where $\vec{\sigma} = (\sigma_1, \sigma_2, \sigma_3)$ are the usual Pauli matrices, $J > 0$ and $\vec{S} = (S_1, S_2, S_3)$ are the spin operators of impurity.

The conduction bound states are to be decomposed according to their orbital angular momentum relative to the impurity, and it is supposed that only $\ell = 0$ (s wave) components can interact with a point-like impurity. The s wave electrons obey a one-dimensional wave equation in an arbitrary line intersecting the impurity position at $x = 0$. Furthermore, we suppose that $J \ll 1$, that the temperature and magnetic field are much smaller than the Fermi energy ϵ_F , and that we may consider only the linear expansion $\epsilon_k = \epsilon_F + V_F (|k| - k_F)$ for the electron spectrum.

Under these assumptions, the Hamiltonian (1) will be diagonalized exactly. The method employed goes back to H. Bethe. Its application towards the solution of the Kondo problem was exposed in Ref. 1). For this reason, only the basic points will be outlined below. On the basis of this solution, the magnetic susceptibility as a function of an arbitrary magnetic field will be calculated in an explicit form.

1) The wave function of the system consisting of N one-dimensional particles, the spins and the co-ordinates of which are $\{\mu_j\}$ and $\{x_j\}$, and of a localized magnetic moment with spin S , satisfies the Schrödinger equation:

$$\begin{aligned} & (-E - i \sum_{j=1}^N \frac{\partial}{\partial x_j}) \Psi_{\mu_1, \dots, \mu_N, S}(x_1, \dots, x_N) + \\ & + \gamma \sum_{j=1}^N \vec{\sigma}_{\mu_j, \mu'_j} \vec{S}_{SS'} \delta(x_j) \cdot \Psi_{\mu_1, \dots, \mu'_j, \dots, \mu_N, S'}(x_1, \dots, x_N) \stackrel{(2)}{=} \\ & = 0 \end{aligned}$$

The solution of this equation is given by the Bethe ansatz. Let $Q = \{q_0, \dots, q_N\}$ be a certain permutation of integers $\{0, 1, \dots, N\}$. Then in the region $X_Q = \{x_{q_0} < x_{q_1} < \dots < x_{q_N}\}$

$$\begin{aligned} & \Psi_{\mu_1, \dots, \mu_N, S}(x_1, \dots, x_N) = \\ & = \sum_P A_{\mu_1, \dots, \mu_N, S}(Q'P) (-1)^P \exp\{i \sum_{j=1}^N k_{P_j} x_j\} \quad (3) \end{aligned}$$

where $k_1, \dots, k_N$ is a set of unequal numbers, Q' is a remainder of Q with $q_1 = 0$ deleted, P is a permutation of integers $\{1, \dots, N\}$, PQ' is a product of permutations, and we put $x_0 = 0$.

The eigenvalues of the Hamiltonian are

$$E = \sum_{j=1}^N k_j \quad (4)$$

2) Not all the coefficients $A(Q)$ in (3) are independent. The Schrödinger equation determines the discontinuities of A on the boundary of the region X_Q . If X_Q and $X_{\tilde{Q}}$ only differ by permutation of the particle x_j and the impurity $x_0 = 0$,

then:

$$A_{\mu_1, \dots, \mu_n, s}(Q) = (R_{j0})_{s s'}^{\mu_j \mu_j'} A_{\mu_1, \dots, \mu_j', \dots, \mu_n, s'}(\tilde{Q}) \quad (5)$$

where $R_{j0} = \exp(-iJ\vec{\sigma} \vec{S})$.

If two regions differ by permutation of the particles x_i and x_j , then the coefficients A are connected by the permutation operator:

$$\begin{aligned} (P_{ij})_{\mu_j \mu_j'}^{\mu_i \mu_i'} &= \frac{1}{2} \delta_{\mu_i'}^{\mu_i} \delta_{\mu_j}^{\mu_j'} + \frac{1}{2} \vec{\delta}_{\mu_i \mu_i'} \vec{\delta}_{\mu_j \mu_j'} = \\ &= \delta_{\mu_j'}^{\mu_i} \delta_{\mu_i'}^{\mu_j} \end{aligned} \quad (6)$$

These rules enable one to express an arbitrary $A(Q)$ in terms of, say,

$$A(1, \dots, n, 0) = \Phi_{\mu_1, \dots, \mu_n, s}$$

As was pointed out by C.N. Yang²⁾, for the Bethe hypothesis (3) to hold, the necessary and sufficient conditions are the unitarity and factorization relations, which in our case have a form:

$$\begin{aligned} R_{j0} R_{0j} &= \mathbb{I} \quad ; \quad P_{ij} P_{ji} = \mathbb{I} \\ R_{j0} R_{i0} P_{ij} &= P_{ij} R_{i0} R_{j0} \end{aligned} \quad (7)$$

3) In order to find the spectrum of the Hamiltonian (1), we put the system into the sphere of radius $L/2$ around the impurity and impose the periodic boundary conditions. This leads in the standard way to an eigenvalue problem:

$$\exp(ik_j L) \phi_{\mu_1, \dots, \mu_N, s} = T_{\mu_1, \dots, \mu_N, s}^{\mu'_1, \dots, \mu'_N, s'} \phi_{\mu'_1, \dots, \mu'_N, s'} \quad (8)$$

where

$$T = P_{12} \cdot P_{12} \cdots P_{1N} \cdot R_{10} \quad (9)$$

To diagonalize the operator T we construct, following Baxter³⁾, a parametric family of self-commuting operators $T(u)$. Namely, the operator T belongs to:

$$T(u) = \sum_{\alpha_1 = \alpha_{N+1} = \pm 1} L^{\alpha_1 \alpha_{N+1}}(u) \quad (10)$$

where the 2×2 operator-valued matrix $L^{\alpha_1 \alpha_{N+1}}(u)$ is represented in the form:

$$\begin{aligned} L(u; v_1, \dots, v_{N+1}) &\equiv \begin{pmatrix} A & B \\ C & D \end{pmatrix} = \\ &= \sum_{\alpha_1, \alpha_2, \dots, \alpha_N = \pm 1} \prod_{j=1}^N \tau_{\mu_j \mu'_j}^{\alpha_j \alpha_{j+1}}(u - v_j) \cdot R_{s s'}^{\alpha_N \alpha_{N+1}}(u - v_{N+1}) \quad (11) \end{aligned}$$

Here r and R are the operator matrices of special form:

$$-r_{\mu\mu'}^{\alpha\alpha'} = \frac{[a(u)+b(u)]}{2} \delta_{\alpha'}^{\alpha} \delta_{\mu'}^{\mu} + \frac{[a(u)-b(u)]}{2} \vec{\delta}_{\alpha\alpha'} \vec{\delta}_{\mu\mu'} \quad (12)$$

$$R_{ss'}^{\alpha\alpha'} = \frac{[a(u)+b(u)]}{2} \delta_{\alpha'}^{\alpha} \delta_{s'}^s + \frac{[a(u)-b(u)]}{2} \vec{\delta}_{\alpha\alpha'} (2 \vec{S}_{ss'}) \quad (13)$$

and

$$a(u) = \frac{u-i\gamma}{u+i\gamma} \quad ; \quad b(u) = \frac{u}{u+i\gamma} \quad (14)$$

At $v_j = -\delta_{N+1,j}$ and $u = 0$, operators (11) and (9) coincide.

Baxter³⁾ has shown the self-commutativity $[T(u), T(u')] = 0$ to be equivalent to the factorization relation and to hold at all values of the spectral parameter u :

$$\begin{aligned} \tau_{ij}(u) R_{io}(u+u') R_{jo}(u') &= \\ &= R_{jo}(u') R_{io}(u+u') \tau_{ij}(u) \end{aligned} \quad (15)$$

This relation generalizes Eqs. (7). The requirement that conditions (15) are valid determines the functional form of $a(u)$ and $b(u)$. Note that these functions do not depend on the spin S^* .

4) It is convenient to diagonalize $T(u)$, following the quantum inverse scattering method developed in Ref. 5). Equation (15) defines commutation properties of the elements $L^{\alpha_1 \alpha_2} N+1(u)$, which also do not depend on spin S . For example, the commutation relation which we will use to diagonalize $T(u) \equiv A(u) + D(u)$ have the form:

$$\begin{aligned} A(v) B(u) &= \frac{a(u-v)}{b(u-v)} B(u) A(v) - \\ &\quad - \frac{a(u-v) - b(u-v)}{a(u-v)} B(v) A(u) \\ D(v) B(u) &= \frac{a(v-u)}{b(v-u)} B(u) D(v) - \\ &\quad - \frac{a(v-u) - b(v-u)}{b(v-u)} B(v) D(u) \\ [B(v), B(u)] &= 0 \end{aligned} \tag{16}$$

Consider now the state ϕ_0 with maximal value of the total spin projection $S^Z = N/2 + S$.

$$\phi_0 = \phi_{1, \dots, 1, S} \tag{17}$$

It is an eigenstate of the operators $A(u)$, $D(u)$ and $C(u)$ with eigenvalues

*) The operators $T(u)$ (10 - 14) belong to the more general family of self-commuting operators constructed in Ref. 4).

$$\begin{aligned}\Lambda_A^0 &= [a(u-v_{N+1})(S+\frac{1}{2}) - b(u-v_{N+1})(S-\frac{1}{2})] \cdot \prod_{j=1}^N a(u-v_j) \\ \Lambda_D^0 &= [-a(u-v_{N+1})(S-\frac{1}{2}) + b(u-v_{N+1})(S+\frac{1}{2})] \cdot \prod_{j=1}^N b(u-v_j)\end{aligned}\quad (18)$$

and $\Lambda_C^0 = 0$ respectively.

Other eigenstates can be constructed by the successive applications on Φ_0 of the "annihilation" operator $B(u_\alpha)$ which decreases the total spin projection by one:

$$\Phi_M(u; u_1, \dots, u_N) = \prod_{\alpha=1}^M B(u_\alpha) \Phi_0 \quad (19)$$

Using (16) and (18) it is easy to see that the vector Φ_M is the eigenvector of $T(u)$ only provided that "wrong" terms coming from the second terms on the right-hand side of Eqs. (16) vanish. This condition leads to the equations on the values of u_α :

$$\begin{aligned}& \prod_{j=1}^N \frac{a(u_\alpha - v_j)}{b(u_\alpha - v_j)} \cdot \frac{[a(u_\alpha - v_{N+1})(S+\frac{1}{2}) - b(u_\alpha - v_{N+1})(S-\frac{1}{2})]}{[-a(u_\alpha - v_{N+1})(S-\frac{1}{2}) + b(u_\alpha - v_{N+1})(S+\frac{1}{2})]} = \\ &= \prod_{\beta=1}^M \frac{a(u_\alpha - u_\beta)}{a(u_\beta - u_\alpha)} \frac{b(u_\beta - u_\alpha)}{b(u_\alpha - u_\beta)}\end{aligned}\quad (20)$$

If these equations hold, the eigenvalue $t(u)$ of the operator $T(u)$ is:

$$t(u) = \Lambda_A^0(u) \prod_{\beta=1}^M \frac{a(u_\beta - u)}{b(u_\beta - u)} + \\ + \Lambda_B^0(u) \prod \frac{a(u - u_\beta)}{b(u - u_\beta)} \quad (21)$$

where $\Lambda_A^0(u)$ and $\Lambda_B^0(u)$ are given by (18).

Taking the log of (20) and (21) and putting $u_\alpha = J(-\lambda_\alpha + i/2)$ and $V_j = -\delta_{j, N+1}$ we have

$$k_j L = 2\pi I_j + \sum_{\alpha=1}^M \theta(\lambda_\alpha) - \mathcal{I} \cdot S \\ j = 1, \dots, N; \quad (22)$$

$$N\theta_{\frac{1}{2}}(\lambda_\alpha) + \theta_S(\lambda_\alpha - \frac{1}{2}\mathcal{I}) = 2\pi \mathcal{I}_\alpha + \sum_{\beta=1}^M \theta_2(\lambda_\alpha - \lambda_\beta) \quad (23) \\ \alpha = 1, \dots, M.$$

where $\theta_\sigma(x) = 2\arctg x/\sigma$, and the integers $2I_\alpha$ and $2J_\alpha$ are the quantum numbers of the system. The energy and the total spin projection are:

$$E = \sum_{j=1}^N k_j \\ S_z = \frac{N}{2} - M + S \quad (24)$$

5) The further analysis of Eqs. (22) - (24) in the limit of $N, L \rightarrow \infty$ ($\pi N/L = \epsilon_F$) is rather similar to Ref. 1).

In the ground state with the fixed spin projection S_Z the quantum numbers $J_\alpha = -N/2, -N/2+1, \dots, N/2+2S-2S_Z$. Then in the thermodynamic limit, in the main order in $1/N$, Eqs. (23) take the form:

$$\rho(\lambda) = \frac{4}{1+4\lambda^2} - \int_{-\infty}^b \frac{2}{1+(\lambda-\lambda')^2} \rho(\lambda') d\lambda' \quad (25)$$

The impurity contributions of the energy and the total spin projection are:

$$\Delta E = - \int_{-\infty}^b \theta_s(\lambda - \frac{1}{4}) \rho(\lambda) d\lambda \quad (26)$$

$$S_Z/N = \frac{1}{2} - \int_{-\infty}^b \rho(\lambda) d\lambda \quad (27)$$

where $\rho(\lambda) = \lim_{N \rightarrow \infty} 1/N(\lambda_\alpha - \lambda_{\alpha+1})$ is the λ distribution density, and Eq. (27) determines b as a function of S_Z/N .

At leading order in $1/N$, the total spin of the system is determined by the magnetism of the conductive band. Therefore $S_Z/N = 4H/\epsilon_F$, where H is a magnetic field.

Equation (25) is of the Wiener-Hopf type and can be solved analytically. Then, using (26) and (27), we can obtain the explicit expression for the impurity part of the energy as a function of the ratio of the arbitrary magnetic field and the Kondo temperature $T_k = \epsilon_F \exp(-2\pi/J)$. [For details, see Ref. 1)].

The explicit formula for the impurity magnetic moment for the arbitrary spin S seems similar to the $S = \frac{1}{2}$ case. Nevertheless, the infra-red properties ($H \ll T_k$) are quite different in these cases.

$$M(H) = S + \frac{i}{4\pi^{3/2}} \int_{-\infty}^{\infty} \Gamma(\frac{1}{2} + i\omega) f_+^{2s}(\omega) \cdot f_-^{2s-1}(\omega) \times \\ \times \exp\{-2i\omega \ln \frac{H}{T_k}\} \cdot \frac{d\omega}{\omega - i0} \quad (28)$$

where $f_{\pm}(\omega) = (e^{\pm i\pi/2} \omega/e)^{\pm i\omega}$ are analytic in the upper and lower half-planes respectively and factorize the function

$$\exp(-\pi/|\omega|) = f_+(\omega) f_-(\omega) \quad (29)$$

and

$$T_k = \epsilon_F \exp(-2\pi/g)$$

In the lower (upper) half-plane $f_{\pm}(\omega)$ has a cut which we draw along the lower (upper) half imaginary axis. The discontinuities on these axes are

$$\text{disc } f_{\pm}^n(\omega) = \pm 2i e^{-n/|\omega| \log |\omega/e|} \sin \pi n/|\omega| \quad (30)$$

6) If $H \gg T_k$ the integration contour could be shifted to encircle the cut in the upper half-plane. Then

$$M(H) = S - \frac{1}{2\pi^{3/2}} \int_0^{\infty} \frac{\sin 2\pi\omega S}{\omega} \times$$

$$\times \Gamma\left(\frac{1}{2} + \omega\right) e^{-2\omega \ln \frac{H}{T_k}} \left(\frac{\omega}{e}\right)^{-\omega} d\omega \quad (31)$$

and the well known perturbation theory expansion

$$M(H) = S \left(1 - \frac{1}{\ln\left(\frac{H}{T_k}\right)^2} - \frac{\ln[\ln\left(\frac{H}{T_k}\right)^2]}{\ln^2\left(\frac{H}{T_k}\right)^2} + \dots \right) \quad (32)$$

is obtained.

If $H < T_k$, i.e., in the region inaccessible for the perturbation theory, the integration contour could be shifted to encircle the cut in the lower half-plane. As a result:

$$M(H) = S - \frac{1}{2} + \frac{1}{2\pi^{3/2}} \int_0^{\infty} \Gamma\left(\frac{1}{2} - \omega\right) \times$$

$$\times e^{-2\omega \ln \frac{H}{T_k}} \left(\frac{\omega}{e}\right)^{\omega} d\omega + \quad (33)$$

$$+ \sum_{n=0}^{\infty} \frac{1}{\Gamma\pi} \left(\frac{n+\frac{1}{2}}{e}\right)^{(n+\frac{1}{2})} \frac{(-1)^n}{(n+\frac{1}{2})n!} \cdot \cos[2\pi(S-\frac{1}{2})(n+\frac{1}{2})] \times$$

$$\times \left[\frac{H}{T_k}\right]^{2n+1}$$

At $H \ll T_k$ and $S \neq \frac{1}{2}$, the contribution of poles of the Γ function in (33) is exponentially small in comparison with the integral around the cut. Then

$$M(H) = (S - \frac{1}{2}) \left(1 + \frac{1}{\ln(T_k/H)^2} - \frac{\ln \ln(T_k/H)^2}{\ln^2(T_k/H)^2} \right) \quad (34)$$

However, if $S = \frac{1}{2}$, the only singularities of the integrand in the lower half-plane are the poles, leading to the power series in $(H/T_k)^{1)}$.

$$M(H) = \sum_{n=0} \frac{1}{1\pi} \left(\frac{n+\frac{1}{2}}{e} \right)^{n+\frac{1}{2}} \frac{(-1)^n}{n! (n+\frac{1}{2})} \left(H/T_k \right)^{2n+1} \quad (35)$$

7) Equations (28) - (35) imply that the ground state of magnetic impurity (at $H = 0$) is $2S-1$ -fold degenerated. The screening phenomenon takes place only at $S = \frac{1}{2}$ when the ground state is a singlet. This result confirms what was conjectured, on qualitative grounds, by Mattis⁶⁾.

The "duality" of the leading log approximations of $H \gg T_k$ and $H \ll T_k$ is, apparently, a general property. Elsewhere⁷⁾ we will show that at $T \neq 0$, the coefficients of the leading and next-to-leading logs at $T \gg T_k$ and $T \ll T_k$ coincide up to the substitution $S \rightarrow (S - \frac{1}{2})$. For example, for the magnetic susceptibility we will have

$$\chi(T) = \begin{cases} T \gg T_k & \frac{S(S+1)}{3} \\ T \ll T_k & \frac{S^2 - 1/4}{3} \end{cases} \times \left(1 - \frac{1}{\ln T/T_k} + \frac{\ln |\ln T_k|}{\ln^2 T/T_k} + \dots \right) \quad (36)$$

8) The Hamiltonian (1) has been studied quite extensively [see, for instance, reviews in Ref. 8)]. Still, it can hardly correspond to any real alloy. The exchange amplitude $J(k, k^1)$ is generally non-spherical; rather it contains $2S$

first-spherical harmonics. A more realistic 2S-fold degenerated model, in which the screening phenomenon takes place can also be solved exactly. This solution⁹⁾ will be published elsewhere .

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