Exact solution of *s-d* exchange model at $T = 0$

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It is shown that the *s-d* exchange model is completely integrable. The magnetic susceptibility of a magnetic impurity in a nonmagnetic metal at $T = 0$ is determined.

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1. The interaction of the conduction electrons of a nonmagnetic metal with a magnetic impurity is usually studied by using the so-called *s-d* model as an example:

$$\mathcal{H}_{sd} = \sum_{k,\sigma=\uparrow,\downarrow} \epsilon_k C^+_{k\sigma} C_{k\sigma} + J \sum_{k,k'} C^+_{k\sigma} \bar{\sigma}_{\sigma\sigma'} C_{k'\sigma'} \bar{S}; \quad S = 1/2; \quad J > 0. \tag{1}$$

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It is well known that for $T<T_c$ [$T_c=\epsilon_F\exp(-1/J\rho)$ is the Kondo temperature], even for $J\ll 1$ the effective interaction of electrons with the impurity is considerable and perturbation theory cannot explain the properties of the system.[1] At present, there is apparently no correct approximation scheme that allows the Kondo problem to be solved. On the other hand, the problem is solved exactly if the following simplifications are made. Let us assume that only the s wave interacts with the impurity. Since the kinetic energy of electrons is diagonal with respect to the partial waves, the particles with different momentum directions are scattered independently by the impurity, and, in essence, we are dealing with a one-dimensional problem. In addition, we assume that the coupling constant is so small, $J\ln J\ll 1$, that at low temperatures and weak magnetic fields we can ignore electron states lying far from the Fermi surface. Therefore, it is sufficient to consider only the linear portion of the spectrum $\epsilon_k-\epsilon_F\approx v_F k$. Under these assumptions the problem is completely integrable.

2. The Schrödinger equation for a system of N particles has the form

$$\left(-E-i\sum_{j=1}^{N}\frac{\partial}{\partial x_j}\right)\psi^{a}_{a_1\ldots a_N}(x_1\ldots x_N)+J\sum_{j=1}^{N}\bar{\sigma}_{a_j a_j'}\bar{S}_{aa'}\delta(x_j)$$

$$\times\ \psi^{a}_{a_1'\ldots a_j'\ldots a_N'}(x_1\ldots x_N)=0. \tag{2}$$

$\{\alpha_j\}$ are the spins of the particles whose $\{x_j\}$ coordinates are concentrated on an arbitrarily chosen straight line passing through the impurity. Before writing the solution of Eq. (2) for arbitrary N, we shall make the following comment. Let us assume that $N=2$. In the region $x_1,x_2<0$ the particles are free and the ψ function can be chosen in the form of a plane wave

$$\psi^{a}_{a_1a_2}(x_1,x_2)=A^{a}_{a_1a_2}e^{ik_1x_1+ik_2x_2}-A^{a}_{a_2a_1}e^{ik_1x_2+ik_2x_1}, \tag{3}$$

where $A^{a}_{\alpha_1\alpha_2}$ is an arbitrary constant matrix. Let us also try to find a ψ function in the other regions in the form of a plane wave, but with another matrix A. The Schrödinger equation determines the discontinuities in the A coefficients at $x_j=0$. For example,

$$A^{a}_{a_1a_2}(x_1>0)=R^{a_1'a}_{a_1a}A^{a}_{a_1'a_2}(x_1<0), \tag{4}$$

where

$$R_{10}\equiv R^{a_1'a}_{a_1a}=a+bP_{10};\qquad R^{+}_{10}\equiv R_{01}.$$

The quantities b and a are, respectively, the amplitudes of the electron scattering by the impurity with and without spin reversal

$$a = -e^{-iJ}\cos 2J; \qquad b = ie^{-iJ}\sin 2J, \tag{5}$$

and $P_{10} = 2(\frac{1}{2}\times\frac{1}{2} + \bar{\sigma}\bar{S})$ is the permutaion operator of the particle and impurity spin. However, the condition (4), determining the discontinuities in $A^{\alpha}_{\alpha_1\alpha_2}$, are contradictory. In fact, let us assume that two electrons, one with spin ↑ and the other with spin ↓, are scattered by the impurity whose spin is ↑. If the first electron is scattered first, and then the second electron, the impurity spin is inverted. If, however, the scattering occurs in the opposite sequence, then the impurity spin remains the same as it was before. It is clear that the scattering sequence should not matter, since the particles are identical. In other words, the matrices R_{10} and R_{20} do not commute. This means that the electrons cannot be examined independently, i.e., it is a multiparticle problem.

3. The function (3) is not the only solution of Schrödinger equation. In fact, if ψ_0 is a solution, then $\psi_0 f(x_1 - x_2)$ is also a solution. It turns out that the ψ function in he region $x_1, x_2 < 0$ can be chosen in such a way that in the remaining regions it will have the same form as in the region $x_1, x_2 > 0$. This function reflects an "ordering" of the spins in terms of the coordinate and has the form

$$\psi^{\alpha}_{\alpha_1\alpha_2} = \{A^{\alpha}_{\alpha_1\alpha_2}\theta(x_1 - x_2) + A^{\alpha}_{\alpha_2\alpha_1}\theta(x_2 - x_1)\}(e^{ik_1x_1 + ik_2x_2} - e^{ik_1x_2 + ik_2x_1}) \tag{6}$$

In this case the A coefficients have discontinuities at $x_j = 0$, which are given by Eqs. (4) and (5). In examining the scattering of two particles, we must follow the ordering of their coordinates, regardless of whether they are separated by the impurity. As before, the $A^{\alpha}_{\alpha_1\alpha_2}$ in the regions $x_1 < x_2 < 0$ and $0 < x_2 < x_1$ can be related to each other by two different methods, but now they give identical results, since the factorization condition

$$P_{12}R_{10}R_{20} = R_{20}R_{10}P_{12} \tag{7}$$

is valid. Therefore, Eq. (6) with the conditions (4) and (5) gives the solution of the Schrödinger equation for $N = 2$. The quantities k_1 and k_2 in (6) are never equal to each other, even when the particle spins are opposite. Both the sum $k_1 + k_2$, which is the energy of the system, and each k_j remain the same as a result of scattering of the particles by the impurity.

4. For a system of N particles the *Bethe substitution* is valid: assume that $k_1 \cdots k_N$ are numbers not equal to each another. In the region $Q = \{x_{q_1} < \cdots < 0 < \cdots < x_{q_{N+1}}\}$

$$\psi^{\alpha}_{\alpha_1\ldots\alpha_N}(x_1\ldots x_N) = \sum_P (-1)^P A^{\alpha}_{\alpha_1\ldots\alpha_N}(QP)\exp\{i\sum_{j=1}^{N} x_j k_{p_j}\} \tag{8}$$

here $P = \{p_1 \cdots p_{N+1}\}$ and $Q = \{q_1 \cdots 0 \cdots q_{N+1}\}$ are the permutations of the numbers 0, 1⋯N, and QP is the product of the permutations. The coefficients $A(QP)$, which are related to each other, can be expressed in terms of $A(I)$ ($I = \{1\cdots N, 0\}$ is the unit permutation)

$$A^{a}_{a_1\dots a_N}(Q) = S^{a'_1\dots a'_N,a}_{a_1\dots a_N,a'}(QI)A^{a'}_{a'_1\dots a'_N}(I).$$

The $S(QI)$ matrix is two-particle factorized—it is the product of the matrices corresponding to permutations of the two particles. In order to construct this matrix, it is necessary to represent Q in the form of a successive product of pair permutations. Moreover, the P_{ij} matrix correlates to each factor if it performs a permutation of the particles $(x_i x_j)$, and the matrix R_{j0} if it is a permutation of a particle and the impurity. For example, the coefficients for $\exp\{i\Sigma k_j x_j\}$ in the regions I and $I_1 = \{2\cdots N,0,1\}$ are related to the matrices $P_{10}P_{1N}\cdots P_{13}P_{12}$. Of course, the decomposition into pair permutations is not unique. However, just as in the case of two particles, the fulfillment of the factorization condition (7) and of the unitarity condition

$$P_{ij}P_{ji} = 1, \quad R_{j0}R_{0j} = 1 \tag{9}$$

is necessary and sufficient for the validity of the Bethe hypothesis,[2,3] i.e., different methods of decomposition into successive pair permutations produce identical results. The fact that the system in different regions Q is described by the same set $\{k_j\}$ means that there is an infinite series of conservation laws.

5. To determine the spectrum of the system, we must satisfy the boundary conditions, which, for convenience, can be periodic, by placing the system in a sphere with a radius $L/2$. The conditions imposed on the $A(Q)$ coefficients in this case do not depend on Q. We shall write them, for example, for $A(I) = \Phi^{\alpha}_{\alpha_1\cdots\alpha_N}$

$$T(J)^{a'_1\dots a'_N,a}_{a_1\dots a_N,a'}\Phi^{a'}_{a'_1\dots a'_N} \equiv P_{jj+1}\cdots P_{jN}R_{j0}P_{j1}\cdots P_{jj-1}\Phi = e^{ik_jL}\Phi. \tag{10}$$

It is easy to prove that all the $T(J)$ operators are equal to each another. The eigenvalues of the T determine k_j, and hence the spectrum of the system.

6. The eigenvalue problem was first solved by Yang and Gaudin[2,4] and, from more general positions, by Baxter.[3] The solution is given by the system of equations (11) and (12). Let us assume that the spin of the system is $S^z = N/2 - M$. Thus,

$$Lk_j = 2\pi I_j + \sum_{\alpha=1}^{M}\theta(2\lambda_\alpha); \quad j = 1\dots N. \tag{11}$$

$$N\theta(2\lambda_\alpha) + \theta(2\lambda_\alpha + {}^{2}/_{g}) = 2\pi J_\alpha + \sum_{\alpha'=1}^{M}\theta(\lambda_\alpha - \lambda_{\alpha'}); \quad \alpha = 1\dots M$$

$$E = \Sigma k_j, \tag{12}$$

where $g = \tan 2J$ and $\theta(x) = 2\arctan x$.

The quantities I_j and J_α are integers, not equal to each another, the quantum numbers of the system.

7. Let us add Eqs. (11) and (12):

$$LE = 2\pi(\Sigma I_j + \Sigma J_\alpha) - \sum_\alpha \theta(2\lambda_\alpha + {}^2/_g) = E + \epsilon. \tag{13}$$

The first term in Eq. (13), which determines the equidistant part of the energy levels, describes the spectrum of a free electron gas. The second term, which produces a relative change in the energy by an amount of the order of N^{-1}, is the energy associated with the impurity. Within this accuracy the second term in Eq. (12) can be dropped.

The sequential allotment of number sfrom $N/4 - S^z$ to $N/4$ corresponds to the ground state of the system with a given spin. In this case we can turn to the thermodynamic limit in Eqs. (11)–(13): $N,M,L \to \infty$, by introducing the "spin momentum" density

$$\rho(\lambda) = \frac{4}{1+4\lambda^2} - \frac{1}{2\pi}\int_{-b}^{\infty} \frac{2\rho(\lambda')d\lambda'}{1+(\lambda-\lambda')^2}, \tag{14}$$

$$\epsilon = -\frac{N}{L}\int_{-b}^{\infty} \rho(\lambda)\,\theta\left(2\lambda + \frac{2}{g}\right)\frac{d\lambda}{2\pi}; \quad \frac{S^z}{N} = \frac{1}{2} - \int_{-b}^{\infty} \rho(\lambda)\frac{d\lambda}{2\pi}, \tag{15}$$

and $b = \infty$ if $S^z = 0$. At $b = \infty$ Eq. (14) is identical to an analogous equation that describes the one-dimensional Heisenberg antiferromagnetic model (see, for example, Ref. 5).

8. Let us calculate the susceptibility of the magnetic impurity in a nonmagnetic metal at $T = 0$ and as a function of the magnetic field $H \ll \epsilon_F$. To do this, it is convenient here, like in Ref. 5, to switch to the $r(-\lambda - b)$ function which is defined for all λ and which coincides with $\rho(\lambda)$ for $-b < \lambda < \infty$. This function satisfies the Wiener–Hopf equation

$$r(\lambda) = \frac{\pi}{\cosh \pi(\lambda + b)} - \int_0^{\infty} R(\lambda - \lambda')\, r(\lambda')\, d\lambda', \tag{16}$$

where $R(\lambda)$ is the resolvent of Eq. (14) for $b = \infty$. In this case the energy and spin are

$$\epsilon(H) - \epsilon(0) = \frac{N}{2L}\int_0^{\infty} r(\lambda)\,\text{arc tan sinh}\,\pi\left(-\lambda - b + \frac{1}{g}\right)d\lambda; \quad S^z = N\int_0^{\infty} r(\lambda)\frac{d\lambda}{4\pi}. \tag{17}$$

In the main sequence in N^{-1} the total spin of the system is determined by the magnetism of the conduction electrons; therefore, $S^z = H/2\epsilon_F$. Since $H \ll \epsilon_F$, the quantity $b \gg 1$; therefore, it is sufficient to solve Eq. (16) in the principal approximation in $\exp(-\pi b)$. Thus,

$$H = \epsilon_F \sqrt{\frac{2\pi}{e}} \exp(-\pi b) + O\left(\exp(-3\pi b)\right),$$

and the energy is given by

$$\epsilon(H) - \epsilon(0) = \frac{iH}{4\pi\sqrt{2}} \int_{-i\infty}^{i\infty} \frac{G(x)}{x\left(x - \frac{1}{2}\right)\cos \pi x} e^{-2xz}\, dx, \tag{18}$$

where $z \equiv \ln H/T_c = -\pi(b - 1/g)$, and

$$G(x) = \sqrt{2\pi}\, \frac{\left(-\frac{x}{e}\right)^{-x}}{\Gamma\left(\frac{1}{2} - x\right)}\ ; \qquad G(\infty) = 1\ .$$

The function $G(x)$ is analytical in the entire complex half-plane with a cut along the positive part of the real axis. The behavior of the magnetic susceptibility qualitatively agrees with known experiments[6]:

$$\chi(H) = \frac{1}{2\pi^{3/2} iH} \int_{-i\infty}^{i\infty} \Gamma\left(x + \frac{1}{2}\right)\left(-\frac{x}{e}\right)^{-x} e^{-2xz}\, dx\ . \tag{19}$$

At $H/T_c \ll 1$

$$\chi(H) = \chi(0) \sum_{n=0}^{\infty} (H\chi(0))^{2n} \frac{(-1)^n}{n!} \frac{2(\pi(n + \frac{1}{2}))^{n+\frac{1}{2}}}{\sqrt{\pi}}\ ,$$

where

$$\chi(0) = \text{const}\ T_c^{-1}\ .$$

Thus, the susceptibility is finite at $T = 0$.[7-9]

At $H/T_c \gg 1$ the integral (19) has a different asymptotic form

$$\chi(H) = \frac{1}{2H\left(\ln \frac{H}{T_c}\right)^2}\left(1 + O\left(\frac{\ln \ln \frac{H}{T_c}}{\ln \frac{H}{T_c}}\right)\right).$$

The last formula can be obtained by summing the principal logarithms of perturbation theory.

9. The Bethe hypothesis is also valid for the Anderson model which describes the formation of a localized moment in the metal[10]

$$H_A = \sum_{k\sigma} \epsilon_k C^+_{k\sigma} C_{k\sigma} + V \sum_{k\sigma} (C^+_{k\sigma} d_\sigma + d^+_\sigma C_{k\sigma}) + \sum_{\sigma = 1,2} \epsilon_d d^+_\sigma d_\sigma + U d^+_1 d_1 d^+_2 d_2 .$$

For this model the equations, analogous to (11) and (12), have the form

$$\begin{aligned} L k_j + \theta\left(\frac{V^2}{k_j - \epsilon_d}\right) &= 2\pi I_j - \sum_{\alpha=1}^{M} \theta(2g(k_j) - 2\lambda_\alpha), \\ \sum_{\alpha'=1}^{M} \theta(\lambda_\alpha - \lambda_{\alpha'}) + 2\pi J_\alpha &= \sum_{j=1}^{N} \theta(2\lambda_\alpha - 2g(k_j)), \end{aligned} \tag{20}$$

$$g(k) = (k - U - \epsilon_d)(k - \epsilon_d)/V^2 U.$$

In the limit $U/V^2, \epsilon_d = V^2 \to \infty$ Eqs. (20) are converted to Eqs. (11) and (12); in this case $J = UV^2/\epsilon_d(U + \epsilon_d)$.

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