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Spin–electron pairing in a magnetic field in the one-dimensional Kondo lattice: exact results

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Abstract. An exact solution of the Kondo problem has been obtained with allowance for the pairing of band electrons with the spins localized at impurity sites. The dependence of the gap in the conduction electron state density on the value of the magnetic field has been calculated.

The application of the Bethe *ansatz* for calculating the properties of the one-dimensional Kondo model, in which the singlet pairing of conduction electrons with spins localized at impurity sites is taken into account, permitted us to derive a number of exact results [1]. A peculiarity of these solutions is the presence of a gap in the band electron state density near the Fermi energy ε_F. Since the solutions obtained are stable, it is possible to regard the proposed electron pairing mechanism in [1] as one of the mechanisms explaining the high-temperature superconduction phenomenon.

The pairs consisting of electrons and localized magnetic moments are localized; therefore the Josephson effect is not realized. Taking into account this mechanism of pairing the Josephson effect should be considered in the framework of the Anderson model, but not in the Kondo model. It is known that the Anderson model with half-filled conduction bands for $V/U \ll 1$ (V and U are the parameters of the mixing interaction and Coulomb repulsion, respectively) is reduced to the s–d exchange model.

In the present paper the behaviour of the system in a magnetic field H in the weak-field limit $H \ll \varepsilon_F$ is considered. The electronic states in a magnetic field are believed to consist of two phases: some of the electrons are paired and the remaining electrons form states, which are characteristic of the Kondo problem [2, 3]. When this treatment is used, the magnetic state of the system is described, in the case of weak bonding, by the solutions of the Kondo problem [2, 3]. This makes it possible to use the solutions obtained in this paper to calculate the dependence of the value of the gap in the conduction electron state density on the magnetic field amplitude. As in [1], the impurity concentration n_i is considered to be arbitrary and is not limited by $n_i = 1$, which describes the Kondo lattice.

We write the Hamiltonian of the exchange s–d model as

$$\mathcal{H} = -\mathrm{i}\sum_{\sigma}\int \mathrm{d}x\, c_{\sigma}^{+}(x)\frac{\mathrm{d}}{\mathrm{d}x}[c_{\sigma}(x)] + \frac{J}{2}\sum_{n,\sigma,\sigma'}\int \mathrm{d}x\,\delta(x - x_n)c_{\sigma}^{+}(x)\sigma_{\sigma\sigma}^{\alpha'}c_{\sigma'}(x)S_n^{\alpha} \qquad (1)$$

where interactions exist only between right- or left-going wavenumbers. $c_{\sigma}^{+}(x)$, $c_{\sigma}(x)$ are the operators of the conduction electrons, J is the exchange integral, $J > 0$ (antiferromagnetic case); $\sigma^{\alpha}_{\sigma'\sigma}$ are the Pauli matrices; S_n is the spin operator, localized at the lattice site x_n (we shall consider the case $S = \frac{1}{2}$).

Let us introduce anomalous averages which describe the contact singlet pairing of spinons and band electrons:

$$\Delta_{\sigma\sigma'} = \langle X_n^{0\sigma'} c_{-\sigma}(X_n)\rangle.$$

($X_n^{0\sigma}$ is the projection operator, which translates the state with the magnetic quantum number σ to the empty shell.) In a magnetic field the matrix $\Delta_{\sigma\sigma'}$ is degenerate in the spin components, which renders the problem unintegrable in the general case. Let us consider the solution of the problem by regarding the matrix $\Delta_{\sigma\sigma'}$ as isotropic, i.e. $\Delta_{\sigma\sigma'} = \Delta_{\sigma-\sigma}$.

Separating the anomalous averages in (1) we have one more term in the Hamiltonian $\mathcal{H}$:

$$\mathcal{H}_\Delta = \frac{3J\Delta}{4}\sum_n \int \mathrm{d}x\, \delta(x - x_n)[c_\sigma^+(x)X_n^{-\sigma 0} - c_{-\sigma}^+(x)X_n^{\sigma 0}] + \text{hc.} \qquad (2)$$

Now we consider the scattering of electrons on localized spins. The wavefunction is determined in the following form:

$$|\Psi_k\rangle_\sigma^s = \int \mathrm{d}x\, [f_{k\sigma}^s(x, x_n)c_\sigma^+(x)X_n^{s0} + \delta(x - x_n)\bar{f}_{k\sigma}^s(x_n)]|0\rangle \qquad (3)$$

where $|0\rangle$ is the function of the vacuum $c_\sigma(x)|0\rangle = 0$; $S_n^\alpha\ |0\rangle = 0$; k is the electron wavevector.

The presence of the function $\bar{f}_{k\sigma}^s(x_n)$ in (3) takes into account the pairing of a band electron with a spin localized at the lattice site x_n.

The amplitudes $f_{k\sigma}^s(x, x_n)$ and $\bar{f}_{k\sigma}^s(x_n)$ are determined from the Schrödinger equation. Using the solution for $f_{k\sigma}^s(x, x_n)$ we obtain the following expression for the scattering matrix of electrons on localized spins:

$$R_{\sigma\sigma'}^{ss'}(k) = \{[g(k) + 1 + \mathrm{i}cP_{\sigma\sigma}^{ss'}]/[g(k) + 1 + \mathrm{i}c]\}\exp(\mathrm{i}\vartheta) \qquad (4)$$

where

$$g(k) = \Delta_0^2(1 + cJ/8)/[E(k) - \Delta_0^2] \qquad \vartheta = -2\tan^{-1}(J/8) \qquad c = J/2(1 - 3J^2/64).$$

$E(k)$ is the electron energy which is measured from the Fermi energy; $P_{\sigma\sigma'}^{ss'}$ is the permutation operator: $\Delta_0^2 = (9/8)J|\Delta|^2$.

Following (4) the scattering matrix of electrons pairing with localized spins depend on the electron wavevector. When the unpaired electrons are considered, it is necessary to put $\Delta = 0$ and the matrix **R** does not depend on the electron wavevector, as in the case of the Kondo problem [2, 3]. Let us consider the two-electron function $\varphi_{k_1\sigma_1k_2\sigma_2}^s(x_1, x_2)$ (x_1 and x_2 are the coordinates of electrons). From equation (3) for the one-electron wavefunctions we write $\varphi_{k_1\sigma_1k_2\sigma_2}^s(x_1, x_2)$ as

$$\begin{aligned}\varphi_{k_1\sigma_1k_2\sigma_2}^s(x_1, x_2)|0\rangle &= \Psi_{k_1\sigma_1k_2\sigma_2}^s(x_1, x_2)c_{\sigma_1}^+(x_1)c_{\sigma_2}^+(x_2)X_0^{s0}|0\rangle \\ &\quad + \exp(\mathrm{i}k_1x_1)\bar{f}_{k_2\sigma_2}^s(o)c_{\sigma_1}^+(x_1)|0\rangle + \exp(\mathrm{i}k_2x_2)\bar{f}_{k_1\sigma_1}^s(0)c_{\sigma_2}^+(x_2)|0\rangle \qquad (5)\end{aligned}$$

where the last two terms describe the one-electron state without impurity spin. The wavefunction $\varphi_{k_1\sigma_1k_2\sigma_2}^s(x_1, x_2)$ satisfies the Schrödinger equation. The last two terms do not depend on the electron distance; therefore the electron scattering matrix is determined by the amplitude $\Psi^s_{k_1\sigma_1k_2\sigma_2}(x_1,x_2)$. The expression for $\Psi^s_{k_1\sigma_1k_2\sigma_2}(x_1,x_2)$ is obtained from the solution of the Schrödinger equation:

$$\begin{aligned}\Psi^s_{k_1\sigma_1k_2\sigma_2}(x_1,x_2) &= [\exp(\mathrm{i}k_1x_1+\mathrm{i}k_2x_2)-\exp(\mathrm{i}k_2x_1+\mathrm{i}k_1x_2)]A^s_{k_1\sigma_1k_2\sigma_2} && x_1>x_2\\ &= [\exp(\mathrm{i}k_1x_1+\mathrm{i}k_2x_2)-\exp(\mathrm{i}k_2x_1+\mathrm{i}k_1x_2)]s^{\sigma_1\sigma_1'}_{\sigma_2\sigma_2'}A^s_{k_1\sigma_1'k_2\sigma_2'} && x_1<x_2\end{aligned} \tag{6}$$

where $A^s_{k_1\sigma_1k_2\sigma_2}$ is an arbitrary constant tensor and $s^{\sigma_1\sigma_1'}_{\sigma_2\sigma_2'}(k_1,k_2)$ is the two-particle scattering matrix of electrons:

$$s^{\sigma_1\sigma_1'}_{\sigma_2\sigma_2'}(k_1,k_2)=[g(k_1)-g(k_2)-\mathrm{i}cP^{\sigma_1\sigma_1'}_{\sigma_2\sigma_2'}]/[g(k_1)-g(k_2)-\mathrm{i}c]. \tag{7}$$

The N-particle wavefunction is determined according to the Bethe *ansatz*. The matrix **R** (4) and the matrix **S** (7) satisfy the Yang–Baxter equations and therefore the problem is integrable.

For definiteness it is considered that $N_e \geqslant N_i$ (N_e is the number of conduction electrons; N_i is the number of impurity atoms). In the case $H=0$, $N_i^{\uparrow}=N_i^{\downarrow}$ and $N_e^{\uparrow}=N_e^{\downarrow}$ ($N_i^{\downarrow}$ *and* $N_i^{\uparrow}$ *are the numbers of spin-up and spin-down magnetic moments;* $N_e^{\downarrow}$ and $N_e^{\uparrow}$ are the numbers of spin-up and spin-down electrons).

If $H \neq 0$ we have $N_i^{\uparrow} \neq N_i^{\downarrow}$ and $N_e^{\uparrow} \neq N_e^{\downarrow}$. We obtain the solution of the problem with a magnetic field as in the case $H=0$, assuming that $N_e^s = 2N_e^{\downarrow}$ are the number of electrons paired with localized spins and the rest of the electrons, $N_e - N_e^s$ in number, form electronic states as in the case of the Kondo problem. The two-particle wavefunction of the unpaired electron is determined from (3) with $\bar{f}^s_{k\sigma}(x_n)=0$. For N_e^s paired and $N_e - N_e^s$ unpaired electrons the wavefunction is defined by the two-particle wavefunctions (3) with $\bar{f}^s_{k\sigma}(x_n)\neq 0$ and $\bar{f}^s_{k\sigma}(x_n)=0$, respectively; therefore the matrix **S** is determined from (7) with $\Delta \neq 0$ and $\Delta = 0$, respectively. In this approach the matrix $\Delta_{\sigma\sigma'}$ is still isotropic, as in the case $H=0$, and the value of Δ depends on H. To determine the eigenvalues of the Hamiltonian (1) and (2) we must impose periodic boundary conditions on the N-particle wavefunction. The problem is reduced to the problem of eigenvalues of the T_j matrix:

$$T_j = S_{jj+1}(k_j,k_{j+1})\ldots S_{jN_e}(k_j,k_{N_e})R_{j1}(k_j,k_s)\ldots R_{jN_i}(k_j,k_s)\ldots S_{jj-1}(k_j,k_{j-1}).$$

We shall write the Bethe equations for the Kondo model using the Bethe *ansatz* formalism, and taking into account the spinon–electron pairing:

$$\begin{aligned}&\exp(\mathrm{i}k_iL)=\prod_{\alpha=1}^{M}\frac{g(k_i)-\lambda_\alpha-\mathrm{i}c/2}{g(k_i)-\lambda_\alpha+\mathrm{i}c/2}\exp(-\mathrm{i}N_i\vartheta)\\ &\prod_{j=1}^{N_e}\frac{\lambda_\alpha-g(k_j)-\mathrm{i}c/2}{\lambda_\alpha-g(k_j)+\mathrm{i}c}\left(\frac{\lambda_\alpha+1-\mathrm{i}c/2}{\lambda_\alpha+1+\mathrm{i}c/2}\right)^{N_i}=-\prod_{\beta=1}^{m}\frac{\lambda_\alpha-\lambda_\beta-\mathrm{i}c}{\lambda_\alpha-\lambda_\beta+\mathrm{i}c}.\end{aligned} \tag{8}$$

Here

$$g(k_i)=\begin{cases}\Delta_0^2(1+cJ/8)/[E(k_i)-\Delta_0^2] & i\leqslant N_e^s\\ 0 & N_e^s<i\leqslant N_e.\end{cases}$$

L is the chain length; M is the number of spin-down particles. The energy of the ground state is defined in a particular way:

$$E_0 = \sum_{i=1}^{N_e} k_i$$

where the values of k_i are obtained from equations (8).

In the thermodynamic limit, equations (8) are written for the electron momentum distribution density $\rho(k)$ and for the rapidity distribution density $\sigma(\lambda)$:

$$\rho(k) = \frac{1}{2\pi} - \frac{c}{2\pi} g'(k) \int_{-B}^{\infty} \mathrm{d}\lambda\, \sigma(\lambda) \frac{1}{[\lambda - g(k)]^2 + c^2/4}$$

$$\sigma(\lambda) + \frac{c}{\pi} \int_{-B}^{\infty} \mathrm{d}\lambda'\, \sigma(\lambda') \frac{1}{(\lambda - \lambda')^2 + c^2} = \frac{c}{2\pi} \int_{-k_0}^{k_0} \mathrm{d}k\, \rho(k) \frac{1}{[\lambda - g(k)]^2 + c^2/4} + \frac{c}{2\pi} n_i \frac{1}{(\lambda + 1)^2 + c^2/4}. \tag{9}$$

The set of equations (9) must be completed by conditions which determine the magnetization density m, i.e.

$$m = \frac{(n_i + n_e)}{2} - \int_{-B}^{\infty} \mathrm{d}\lambda\, \sigma(\lambda) \tag{10}$$

and the band electron density n_e, *i.e.*

$$n_e = \int_{-k_0}^{k_0} \mathrm{d}k\, \rho(k). \tag{11}$$

Let us consider the solution of the set of equations (9) in a magnetic field. The value of B is determined by equation (10) as a function of the magnetic field. The case of strong interaction ($J \sim 1$) is not considered. The dependence of $\rho(k)$ on H is weak in the case of weak interaction ($J \ll 1$), as follows from equations (9) and (10), and is proportional to H/π. The value of Δ in the magnetic field depends on H as a function of the density of impurity spins paired with conduction electrons. We denote this density by n_i^s. Taking into account only the dependence of Δ on H, we obtain an integral equation for $p^s(z)$ with the symmetrical kernel $\mathscr{L}(z)$:

$$p^s(z) - \int_{-Z_2}^{-Z_1} \mathrm{d}z'\, \mathscr{L}(z - z') p^s(z') - \int_{Z_1}^{Z_2} \mathrm{d}z'\, \mathscr{L}(z - z') p^s(z') = -\frac{\Delta_0^2(1 + cJ/8)}{2\pi z^2} - n_i^s \mathscr{L}(z + 1) \tag{12}$$

$$\mathscr{L}(z) = \frac{1}{2\pi} \int_{-\infty}^{\infty} \mathrm{d}\omega \exp(\mathrm{i}\omega z) \frac{1}{1 + \exp(|\omega| c)}$$

where

$$p^s(z) = \rho(k)/g'(k) \Big|_{k = (k_F + \Delta_0^2)\,\mathrm{sgn}\, k + \Delta_0^2(1 + cJ/8)/z}$$

describes only paired conduction electrons, whose density is n_e^s.

The limits of integration with respect to z are determined according to [1]:

$$Z_1 = \Delta_0^2(1 + cJ/8)/(k_F + \Delta_0^2) \qquad Z_2 = \Delta_0^2(1 + cJ/8)/(k_F - k_0 + \Delta_0^2).$$

At an arbitrary exchange integral value, equation (12) can be solved by expanding the functions into a Fourier series. Taking into consideration the condition (11), the solution for $p^s(z)$ in the case of weak interaction is [1]

$$p^s(z) = -n_e^s\mathscr{L}(z) - \Delta_0^2(1 + cJ/8)/2\pi z^2 - n_i^s\mathscr{L}(z + 1) + O(\Delta^3). \tag{13}$$

From equation (11) we obtain the value of k_0:

$$k_0 = k_F - \Delta_0\sqrt{2(1/c + J/8)}\,[n_e^s \ln 2 + \pi c n_i^s \mathscr{L}(1)]^{1/2}. \tag{14}$$

The energy k_0 of the upper occupied state is lower than k_F; therefore, a gap whose width is $k_F - k_0$ appears near the Fermi energy in the band electron state density. According to [1] the equation for the determination of Δ can be written as

$$\frac{1}{c'} = -\frac{n_i^s}{N_e^s}\sum_{i=1}^{N_e^s}\frac{1}{E(k_i)}\left[1 + \left(\frac{c}{1 + g(k_i)}\right)^2 + n_i^s\frac{J\Delta_0^2}{2E^2(k_i)}\right]^{-1} \tag{15}$$

$$c' = 3/4J.$$

In an approximation which is linear in H, the conduction electron density in a magnetic field varies as $n_e(s) = n_e(\frac{1}{2} + Hs/\varepsilon_F)$ $(s = -\frac{1}{2}, \frac{1}{2})$; therefore $n_e^s = n_e(-\frac{1}{2})$. Analogously we determine n_i^s from equation (10) as $n_i^s = n_i(-\frac{1}{2})$. The solution of equations (9) and the value of B in the weak magnetic field approximation were obtained [2, 3]. Let us make use of the results of these studies and obtain

$$n_i^s = \frac{n_i}{4\pi\sqrt{\pi}}\int_{-\infty}^{\infty}\frac{dx}{ix + 0}\Gamma(\tfrac{1}{2} + ix)\left(-\frac{ix}{e}\right)^{-ix}\exp\left[-2ix\ln\left(\frac{H}{T_H}\right)\right] \tag{16}$$

$$T_H = (2/\pi e)^{1/2}2\varepsilon_F\exp(-\pi/c)$$

where $\Gamma(x)$ is a gamma function. The value of B does not depend on Δ to an accuracy of Δ^3. Therefore, the dependence on Δ was omitted in the expressions for T_H.

The solution of equation (15), which was obtained in [1] as a logarithmic approximation, is

$$\Delta = \tfrac{2}{3}[(J/c + J^2/8)n_e^s \ln 2]^{-1/2}k_F\exp(-\pi\nu/c') \qquad \nu = n_e^s/n_i^s. \tag{17}$$

The exponential dependence on the concentration of localized spins which form pairs with conduction electrons determines the value of Δ. The change in conduction electron concentration in a magnetic field is small as H/π, whereas the value of n_i^s depends on the field according to equation (16) with the characteristic scale T_H; the value of T_H is of the order of the Kondo temperature. At $H < T_H$, the function n_i^s can be expanded in powers of H/T_H. For $H > T_H$, equation (16) can be expanded in the powers of the invariant charge.

The dependence of the electron density n_i^s on the magnetic field is shown for comparison (figure 1(a)). Figure 1(*b*) shows the dependence of Δ on the magnetic field; it is expressed in units of T_H and was calculated from equation (16) for the Kondo lattice $n_i = n_e$. From the presented calculation, $\Delta(H)$ has a stronger non-linear dependence on the value of magnetic field than the impurity magnetization in the Kondo problem or the concentration $n_i^s(H)$ do. The stability of the superconducting phase in a magnetic

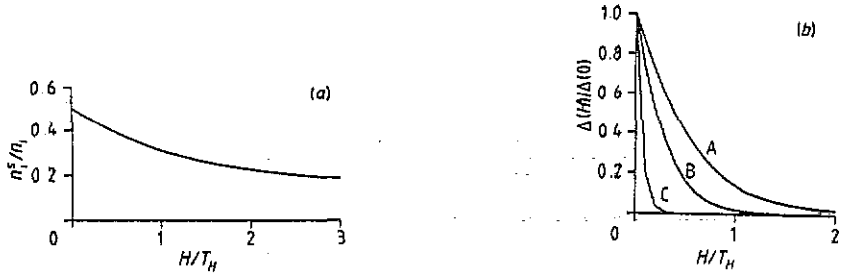

Figure 1. (*a*) Concentration of spins paired with conduction electrons n_i^s/n_i as a function of H/T_H. (*b*) $\Delta(H)/\Delta(0)$ as a function of H/T_H for different values of c': curve A, $c' = 1$; curve B, $c' = 0.5$; curve C, $c' = 0.1$.

field is defined in the same way as in [1] with the only difference that the dependence of Δ on H must be taken into account.

When superconducting pairs are subjected to breakdown in a magnetic field, the formation of Kondo states in the lattice takes place. Therefore, in a magnetic field, Kondo states exist in a superconductive phase.

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