Solution of the symmetric Anderson model at $T=0$

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The impurity part of the magnetic susceptibility is calculated as a function of the magnetic field in the symmetric case. An exact solution of the Anderson model, which describes the formation of localized magnetic moments in a metal, is used in the calculation.

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1. The formation of a localized moment in a metal is customarily studied using the Anderson model **I**:

$$\mathcal{H}_A = \sum_{k,\sigma=\uparrow\downarrow} \epsilon_k c^+_{k\sigma} c_{k\sigma} + V \sum_{k,\sigma} (c^+_{k\sigma} d_\sigma + d^+_\sigma c_{k\sigma}) + \sum_\sigma \epsilon_d d^+_\sigma d_\sigma + U d^+_\uparrow d_\uparrow d^+_\downarrow d_\downarrow , \tag{1}$$

where ϵ_d is the location of the impurity level with respect to the Fermi level, U is the Coulomb repulsion of electrons which are localized at the impurity center, and the amplitude V describes the tunneling of impurity electrons into the conduction band. We know that in the limit $\Gamma \equiv \pi p(\epsilon_F) V^2 \ll \min(\epsilon_d, \epsilon_d + U)$ the impurity has a magnetic moment and is described by the Kondo Hamiltonian.[2]

It was shown in Refs. 3 and 4 that the Anderson and Kondo Hamiltonians are fully integrable and are diagonalized exactly. In this letter we are reporting the results of magnetic susceptibility in an arbitrary magnetic field for the symmetric case $\epsilon_d + U/2 = 0$. The precise ground-state energy was calculated in Ref. 5.

2. The energy levels of the Anderson Hamiltonian, which are in relatively close proximity to the Fermi level, can be determined from the following transcendental equations:

$$\exp(ik_j L) = \prod_{\alpha=1}^{M} \frac{g(k_j) - \Lambda_\alpha + iU\Gamma}{g(k_j) - \Lambda_\alpha - iU\Gamma} \, \frac{k_j - \epsilon_d + i\Gamma}{k_j - \epsilon_d - i\Gamma} , \tag{2}$$

$$-\prod_{j=1}^{N} \frac{g(k_j) - \Lambda_\alpha - iU\Gamma}{g(k_j) - \Lambda_\alpha + iU\Gamma} = \prod_{\beta=1}^{M} \frac{\Lambda_\alpha - \Lambda_\beta + 2iU\Gamma}{\Lambda_\alpha - \Lambda_\beta - 2iU\Gamma} , \tag{3}$$

where

$$g(k) = (k - \frac{U}{2} - \epsilon_d)^2 .$$

Here N is the total number of particles, L is the size of the system, and the number $M = N/2 - S^z$ is related to the total-spin projection. The energy of the system is

$$E = \sum_{j=1}^{N} k_j .$$

3. Kawakami and Okiji[5] have shown that at $U>0$ a part of the charge excitations k_j in the ground state forms "bound" states with spin excitations

$$g(k_a) = \Lambda_a \pm iU\Gamma. \tag{4}$$

In the thermodynamic limit in which $N, L, M \to \infty$, $N/L = \epsilon_F/\pi$ and M/L remain finite numbers of Λ_α, and the "unbound" numbers k_j $(j = M+1, \ldots N)$ are distributed continuously over the intervals $(-Q, \epsilon_F^2)$, $(-\epsilon_F, B)$ with the densities $\sigma(\Lambda)$ and $\rho(k)$, respectively. Thus equations (2) and (3) yield linear integral equations for the $\sigma(\Lambda)$ and $\rho(k)$ distributions:

$$\rho(k) = \frac{1}{2\pi} + \frac{1}{L}\delta(k) + 2k\int_{-Q}^{+\infty} a_1(k^2 - \Lambda)\sigma(\Lambda)d\Lambda\,; \tag{5}$$

$$\sigma(\Lambda) + \int_{-Q}^{+\infty} a_2(\Lambda - \Lambda')\,\sigma(\Lambda')\,d\Lambda' + \int_{-\infty}^{B} a_1(\Lambda - k^2)\rho(k)dk = \int_{-\infty}^{-\infty} a_1^B(\Lambda - k^2)\left(\frac{1}{2\pi} + \frac{1}{L}\delta(k)\right)dk, \tag{6}$$

where

$$a_n(x) = \frac{1}{4\pi}\,\frac{n}{x^2 + n^2(U\Gamma)^2}, \qquad \delta(k) = \frac{1}{4\pi}\,\frac{\Gamma}{(k - \epsilon_d)^2 + \Gamma^2},$$

but B and Q are defined by the conditions

$$S^z/L = \frac{1}{2}\int_{-\epsilon_F}^{B} \rho(k)\,dk; \qquad N/L = 2\int_{-Q}^{\epsilon_F^2} \sigma(\Lambda)d\Lambda + \int_{-\epsilon_F}^{B} \rho(k)dk. \tag{7}$$

The ground-state energy with a given S^z is given by

$$E/L = \int_{-\epsilon_F}^{B} k\rho(k)dk + 2\int_{-Q}^{\epsilon_F^2} \mathrm{Re}\sqrt{\Lambda + iU\Gamma}\,\sigma(\Lambda)\,d\Lambda. \tag{8}$$

In the diagonalization of Hamiltonian (1) we took into account only the states near the Fermi level and only the linear part of the conduction-electron spectrum, which is justifiable for $U, \Gamma \ll \epsilon_F$. This leads to the fact that $\sigma(\Lambda) \approx \Lambda^{-1/2}$ and $\rho(k) \approx 1/2\pi$ in the momentum region far from the Fermi surface, i.e., in the limit $\Lambda \to +\infty$, $k \to -\infty$, and the integrals in Eqs. (7) and (8) diverge. These integrals must therefore be cut off for the momenta of the order of ϵ_F, but all the integrals in Eqs. (5) and (6) converge, and incorporation of the finite band width gives small corrections on the order of $\sqrt{U\Gamma}/\epsilon_F \ll 1$.

In the symmetric case $2\epsilon_d + U = 0$ we have the limit $Q = \infty$, and if $S^z = 0$ we have the limit $B = \infty$.

The ground-state energy and charge susceptibility of the impurity were calculated in Ref. 5 for the symmetric case. Equations (5) and (6) were also solved numerically in Ref. 5.

4. The impurity part of the magnetic susceptibility can be easily determined by using the following procedure. Since the equations (5) and (6) describe the free electron gas in the leading order in $1/L$, $S^z = H/4\epsilon_F$ (we assume that $g_L \mu_B = 1$). This condition correlates the parameter B with the magnetic field H. The impurity moment is now determined by the densities ρ and σ, i.e., by the solution of Eqs. (5) and (6) whose right-hand sides have terms with the coefficient $1/L$.

Equations (5) and (6) with arbitrary sign of B are solved by the Wiener-Hopf method. After dropping $\sigma(\Lambda)$ in Eq. (5), we have

$$\rho(k) + 2k \int_{-\infty}^{B} R(k^2 - p^2)\rho(p)\, dp = \frac{1}{2\pi} + \frac{1}{L}\delta(k) + 2k \int_{-\infty}^{+\infty} R(k^2 - p^2)\left(\frac{1}{2\pi} + \frac{1}{L}\delta(p)\right) dp\,, \tag{9}$$

where

$$R(x) = \frac{1}{\pi}\int_0^\infty \cos(\omega x)/(1 + e^{\omega})^{-1} d\omega.$$

For $B \leqslant 0$ ($H \leqslant H_C = \text{const}\sqrt{U\Gamma}$),

$$\frac{H}{\sqrt{U\Gamma}} = \sum_{n=0}^{\infty} e^{-\pi b^2 (2n+1)} \frac{G^-(-i\pi(2n+1))}{\pi(2n+1)^{3/2}}, \tag{10}$$

where $G^-(2\pi\omega) = (i\omega/e)^{i\omega}\sqrt{2\pi}/\Gamma(\tfrac{1}{2} + i\omega)$ is the analytic function in the lower half-plane, and $b \equiv B/\sqrt{2U\Gamma}$. Note that b depends solely on $H/\sqrt{U\Gamma}$ and is independent of ϵ_F. Equation (10) is valid for $H \leqslant H_C$, where H_C is determined by the same equation for $B = 0$.

The magnetic moment of the impurity is given by

$$M^{\text{imp}} = M^{\text{Kondo}} + \frac{1}{\sqrt{2\pi}} \sum_{n=0}^{\infty} \frac{G^-(-i\pi(2n+1))}{2n+1} e^{-\pi b^2(2n+1)} \int_{-\infty}^{+\infty} dt\, e^{-\frac{\pi t^2(2n+1)}{2U\Gamma}} \delta(it), \tag{11}$$

where

$$M^{\text{Kondo}} = -\frac{i}{2\sqrt{2\pi}} \int_{-\infty}^{+\infty} \frac{d\omega}{\omega - i0} G^-(\omega) e^{-i\omega(b^2 - (U^2 - 4\Gamma^2)/8U\Gamma)} \frac{1}{2\text{ch}\,\omega/2}. \tag{12}$$

Equations (10)-(12) completely determine the dependence of the impurity part of the magnetic moment for $H < H_C$ and of the arbitrary U and Γ. It follows from these equations that the impurity paramagnetism vanishes as $H \to 0$, irrespective of the relationship between U and Γ. The ground state of the impurity is a singlet state. The magnetic susceptibility, which is finite at $H = 0$, has the form

$$\chi(0) = \frac{1}{2\sqrt{2U\Gamma}}\left(\exp\left(\frac{U^2 - 4\Gamma^2}{8U\Gamma}\pi\right) + \int_{-\infty}^{+\infty} e^{\frac{-\pi t^2}{2U\Gamma}} \delta(it) dt\right). \tag{13}$$

At $U \gg 2\Gamma$ the magnetic susceptibility is exponentially large:

$$\chi(0) = \frac{1}{2\pi T_K}, \qquad T_K = \frac{1}{\pi}\sqrt{2U\Gamma}\, e^{-U/8\Gamma}$$ – is the Kondo temperature (Ref. 6).

As U is reduced, the term M^{Kondo} becomes exponentially small and a smooth transition to the region, in which the perturbation theory of U/Γ is valid, occurs. In this case we have $\chi(0) = (1/2\pi\Gamma)x\,[1 + 0(\Gamma/U)]$. Four known terms of the series in

U[7] can be determined from Eq. (13).

5. At $H \ll H_C$ we can limit ourselves solely to the first term of the series in (10), so that $b^2 = (1/\pi) \ln [(U\Gamma/\pi e^{1/2}/H]$. If $U \gg \Gamma$, then the main contribution in Eq. (11) comes from the M^{Kondo} term which coincides with the magnetic moment of the impurity. This magnetic moment was calculated using the Kondo exchange Hamiltonian.[3] Note that the models are equivalent only when $U \gg \Gamma$ and $H \ll \sqrt{U\Gamma}$.

For arbitrary values of U and Γ in the entire region $H \ll T_K, H_C$ (see Fig. 1) the impurity magnetization is expanded in a series in integral powers of H and the localized magnetic moment is missing. For $T_K \ll H \ll H_C$ Eqs. (10)-(12) give logarithmic asymptotic forms which are well-known in the perturbation theory of Γ/U.[8] For

$$H = H_C \qquad \chi(H_C) = \frac{1}{2\pi}\,\frac{\Gamma}{\Gamma^2 + U^2/4}. \tag{14}$$

6. If $H \geqslant H_C (B \geqslant 0)$, we derive from Eq. (9) the expression

$$\frac{H}{\sqrt{U\Gamma}} = \frac{i}{\pi}\int_{-\infty}^{+\infty}\frac{d\omega}{\omega + i0}\, e^{-i\omega b^2}\, G^-(\omega)\int_0^{\infty} e^{i\omega k^2}\, dk \tag{15}$$

and

$$M^{\text{imp}} = \frac{i}{2\sqrt{2\pi}}\int_{-\infty}^{+\infty}\frac{d\omega}{\omega + i0}\, e^{-i\omega B^2}\, G^-(\omega)\int_0^{\infty} e^{\frac{i\omega k_2^2}{2U\Gamma}}\, \delta(k)\, dk\,. \tag{16}$$

At $H \gg H_C$ the magnetic moment of the impurity is expanded in powers of max $(\Gamma/U)/H$. In the regions $U \gg \Gamma$ and $\Gamma \gg U$ (the hatched regions in Fig. 1) the electron in the impurity atom is nearly free. In these regions we can ignore in the Hamiltonian (1) either the hybridization term for $\Gamma \ll H \ll H$ or the Coulomb repulsion for $U \ll H \ll \Gamma$, or both of them if $H \gg U, \Gamma$.

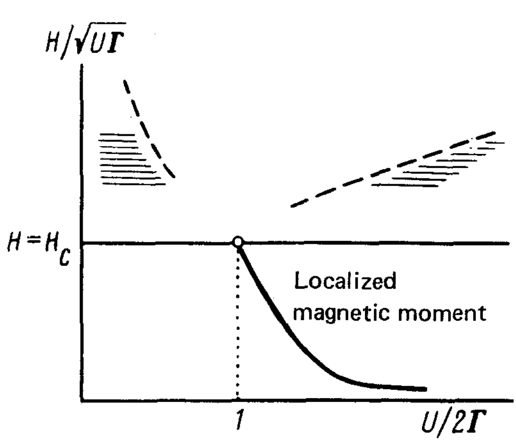

FIG. 1.

7. We shall consider the impurity part of the specific heat $T \to 0$ without deriving it:

$$\frac{C}{T} = \frac{\pi^2}{3} \frac{1}{\sqrt{2U\Gamma}} \left(e^{\pi \frac{U^2 - 4\Gamma^2}{8U\Gamma}} + \int_{-\infty}^{+\infty} (\delta(it) + \delta(t))\, e^{-\frac{\pi t^2}{2U\Gamma}} dt \right). \tag{17}$$

Equations (13) and (17) define the function $R(U/\Gamma) \equiv 4/3\pi^2 \; T\chi/C$, which, as we know, varies (see, for example, Refs. 6, 7, and 9) in the range of 1 to 2 as U/Γ varies in the range of 0 to ∞.

8. The solution of the asymmetric Anderson model and the low-temperature thermodynamics for arbitrary values of ϵ_d will be published in the next issue of JETP Letters.

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