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

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The valence and magnetic susceptibility of an impurity atom for $H \ll$ min $[\sqrt{U\Gamma}, \Gamma(U/U+2\epsilon_d)]$ and for an arbitrary position of the impurity level are determined on the basis of an exact solution of the Anderson model.

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1. The physical properties of alloys of normal metals with a small amount of transition-element impurity atoms or rare-earth impurity atoms differ markedly from the properties of pure metals. Whether the states with a localized magnetic moment and the Kondo effect or the states with an intermediate valence are observed depends on the location of the impurity level $d(f)$ of an electron relative to the Fermi surface of the metal, (ϵ_d), and on the width of this level, (Γ). Both these effects are described by the Anderson model[1]:

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

where U is the Coulomb repulsion of electrons at the impurity orbital, and V is the hybridization amplitude $[\Gamma = \pi\rho(\epsilon_F)V^2]$.

2. It was shown in Ref. 2 that the Anderson Hamiltonian (1) is fully integrable and is diagonalized exactly. In a previous paper[3] the magnetic susceptibility of the impurity in an arbitrary magnetic field H was calculated for the symmetric case $2\epsilon_d + U = 0$. In this letter we present the results for an arbitrary location of the ϵ_d level and an intermediate magnetic field $H \ll min(\sqrt{U\Gamma}, \Gamma U/U+2\epsilon_d)$. We shall consider mainly the region of the variable valence $|\epsilon_d| \sim \Gamma \ln U/\Gamma \ll U$.

3. It was shown in Ref. 2 that the energy levels of the Hamiltonian (1), which are relatively close to the Fermi level, can be determined by solving $N(N/2 - S^z)$ algebraic equations for the surge of the charge $\{k_j\}$ and spin $\{\Lambda_a\}$ waves. (N is the total number of particles, and S^z is the spin of the system.) These equations are found in Ref. 3. Kawakami and Okiji[4] have shown that in the thermodynamic limit (N, $L \to \infty$, $\pi N/L = \epsilon_F$) the system of algebraic equations transforms to two linear integral equations for the distribution functions $\rho(k)$ and $\sigma(\Lambda)$. They have analyzed these equations numerically.

We have determined the $\rho(k)$ and $\sigma(\Lambda)$ functions within the intervals $(-\infty, B)$ and $(Q, +\infty)$, respectively. We assume that they are equal to zero outside these intervals. We shall determine, however, the distribution functions of the "holes," $\rho(k)$ and $\sigma(\Lambda)$, which are nonzero in the intervals (B, ∞) and $(-\infty, Q)$. Thus we can write the integral equations as follows[4]:

$$\tilde{\rho}(k) + \rho(k) = 1/2\pi + \frac{1}{L}\delta(k) + g'(k)\int_{-\infty}^{\infty} a_1(g(k) - \Lambda)\sigma(\Lambda)\, d\Lambda, \tag{2}$$

$$\tilde{\sigma}(\Lambda) + \sigma(\Lambda) + \int_{-\infty}^{\infty} a_2(\Lambda - \Lambda')\sigma(\Lambda')\, d\Lambda' + \int_{-\infty}^{\infty} a_1(\Lambda - g(k))\rho(k)dk$$
$$= \int_{-\infty}^{\infty} a_1(\Lambda - g(k))(1/2\pi + 1/L\,\delta(k))dk; \tag{3}$$

where $g(k) = (k - \epsilon_d - U/2)^2$, and $\delta(k) = \Gamma((k - \epsilon_d)^2 + \Gamma^2)^{-1}$.

The ground-state energy, the total number of particles and the projection of the total spin are given by

$$E/L = 2\mathrm{Re}\int_{Q}^{\epsilon_F^2} [(\Lambda + iU\Gamma)^{1/2} + \epsilon_d + U/2]\,\delta(\Lambda)d\Lambda + \int_{-\infty}^{B} k\rho(k)\, dk, \tag{4}$$

$$N/L \equiv \epsilon_F/\pi = 2\int_{Q}^{\epsilon_F^2} \sigma(\Lambda)d\Lambda + \int_{-\infty}^{B} \rho(k)\, dk, \tag{5}$$

$$S^z/L = \frac{1}{2} \times \int_{-\infty}^{B} \rho(k)\, dk. \tag{6}$$

[The symbols in Eqs. (2)-(6) have the same meaning as in Ref. 3.]

Integrating Eq. (3) and using condition (5), we obtain a convenient formula which, together with Eqs. (2) and (3), determines the limit of Q:

$$\int_{-\infty}^{Q} \tilde{\sigma}(\Lambda)d\Lambda = \epsilon_d + U/2. \tag{7}$$

In the symmetric case, we have $Q = -\infty$ and $\sigma = 0$ and at $S^z = 0$ we have the limits $B = -\infty$ and $\rho = 0$.

4. It is unlikely that Eqs. (2) and (3) can be solved analytically for arbitrary values of B and Q. For $H \ll H_0 \equiv \Gamma\, U/(U + 2\epsilon_d)$, however, an iteration scheme, which allows the coefficients of the powers of H/H_0 to be determined, can be easily constructed. Under this condition $B^2 \gg Q$, $B < 0$ and all the quantities are expanded in a series in $\exp[-\pi(B^2 - Q)]$. In this scheme the integral with $\rho(k)$ in Eq. (3) for $\Lambda < Q$ is the perturbation.

Eliminating $\sigma(\Lambda)$ from Eqs. (2) and (3) for $k < B$ and $\Lambda < Q$, we find

$$\rho(k) + g'(k)\int_{-\infty}^{B} R(g(k) - g(p))\,\rho(p)\, dp = 1/2\pi + \frac{\delta(k)}{L}$$
$$+ g'(k)\int_{-\infty}^{\infty} R(g(k) - g(p))$$
$$\times\left(\frac{1}{2\pi} + \frac{1}{L}\delta(p)\right)dp + \sum_{n=0}^{\infty} (-1)^n \exp[-\pi(2n+1)(g(k)/2U\Gamma - q)$$
$$\times\,\sigma^{(-)}(-i\pi(2n+1))], \tag{8}$$

$$\tilde{\sigma}(\Lambda) - \int_{-\infty}^{Q} R(\Lambda - \Lambda')\tilde{\sigma}(\Lambda')d\Lambda' = \int_{-\infty}^{\infty} \operatorname{sech}[\pi(\Lambda - g(k))/2U\Gamma]\frac{1}{4\pi}$$

$$+ \frac{\delta(k)}{2L}\, dk - \sum_{n=0}^{\infty} (-1)^n \rho^{(+)}(i\pi(2n+1))\exp[-\pi b(2n+1)], \tag{9}$$

where

$$R(x) = \int_0^{\infty} \cos(\omega x/2U\Gamma)(1+e^{\omega})^{-1} d\omega/2\pi U\Gamma$$

and

$$\sigma^{(-)}(\omega) = \int_{-\infty}^{0} \tilde{\sigma}(\Lambda + Q)\exp(i\omega/2U\Gamma)\, d\Lambda/2U\Gamma;\ \rho^{(+)}(\omega)$$

$$= \int_{-\infty}^{B} e^{i\omega[g(k)/2U\Gamma - b]}\rho(k)\, kdk/U\Gamma$$

are the analytic functions in the lower and upper half-planes, respectively, $aq = Q/2U\Gamma$, and $b = g(B)/2U\Gamma$.

5. As in Ref. 3, the limits of b and q can be determined in the leading order in $1/L$; i.e., they can be determined by eliminating the extra terms with the coefficient $1/L$ on the right sides of Eqs. (8) and (9) and by assuming that $S^z/N = H/4\epsilon_F$.

In the leading order in $\exp(-\pi b)$, we have

$$H/\sqrt{2U\Gamma} = \sqrt{\frac{2}{\pi e}}\, e^{-\pi b}\left(1 + \sigma^{(-)}(-i\pi)e^{\pi q}\right);\ \epsilon_d + U/2 = \sqrt{2U\Gamma}\,\sigma^{(-)}(0), \tag{10}$$

where

$$\sigma^{(-)}(\omega) = \frac{-i}{2\sqrt{\pi}} G^{(-)}(\omega) \int_{-\infty}^{\infty} \frac{d\omega'}{\omega - \omega' - i0} \frac{\exp\left(-\frac{|\omega'|}{2} - i\omega' q\right)}{G^{(-)}(\omega')(-i\omega' + 0)^{1/2}}.$$

$G^{(-)}(\omega) = \sqrt{2\pi}(i\omega + 0/2\pi e)^{i\omega/2\pi}/\Gamma(1/2 + i\omega/2\pi)$ is the solution of Eq. (9) for $b = \infty$.

In a nearly symmetric case, we have $-q \gg 1$; therefore, $\epsilon_d + U/2 \cong \sqrt{2U\Gamma}\, e^{-\pi q}$, and the correction in Eq. (10) for $\sigma^{(-)}(-i\pi)$ is small in $(\epsilon_d + U/2)/\sqrt{U\Gamma}$.

In the asymmetric case, we have $q \gg 1$. In this region the $\sigma^{(-)}(\omega)$ function is expanded in a series in q^{-1}, where $q = q_* + 1/2\pi \ln(2\pi e q_*)$.

$$(U/2 + \epsilon_d)/\sqrt{2U\Gamma} = q_*^{1/2} + O(q_*^{-3/2}). \tag{11}$$

Thus the term with $\sigma^{(-)}(-i\pi)$ in Eq. (10) is exponentially large and

$$H/\sqrt{2U\Gamma} \cong (\pi e \sqrt{q_*})^{-1} e^{-\pi(b-q)}. \tag{12}$$

6. The valence and magnetic susceptibility of the impurity ion are determined by the $1/N$ corrections for Eqs. (5) and (6). These corrections are obtained by solving Eqs. (8) and (9), the right sides of which contain only the extra terms with the coefficient $1/L$.

In a nearly symmetric case at $H=0$, we easily see that the valence $n_d = 1 + O((U+2\epsilon_d)^2/U\Gamma)$.

In the asymmetric case, we find $\epsilon_d^* = -U/2 + (2U\Gamma q_*)^{1/2}$. Thus,

$$n_d = -\frac{i}{\pi\sqrt{2}} \int_{-\infty}^{\infty} \frac{d\omega}{\omega - i0} \frac{\exp(-|\omega| + i\omega/J_*)}{G^{(-)}(\omega)}, \tag{13}$$

where $J = -2U\Gamma/\epsilon_d^*(\epsilon_d^* + U)$ corresponds to the effective Schrieffer-Wolf constant.[5] At $|J_*| \ll 1$ the valence is expanded in powers of an invariant charge J_{**}, where $2J_{**}^{-1} - \ln|J_{**}|/e = 2J_*^{-1}$.[6,7] At $J_* < 0$ it follows from (13) that $n_d = -J_{**}/\pi + O(J_{**}^3)$ and for $J_* > 0$ we have $n_d\, 1 = -J_{**}/2\pi + O(J_{**}^3)$.[8,10]

At $|\epsilon_d| \ll U$ the quantity $\epsilon_d^* = \epsilon_d + \Gamma/2\pi\, [\ln(Ue\pi/4\Gamma)]$ can be interpreted as a renormalization of the impurity level.[6,7]

7. In contrast to the valence, the magnetic moment of the impurity for $H \ll \min(\sqrt{U\Gamma}, H_0)$ and $J_* \ll 1$ has characteristic Kondo anomalies. We have therefore one more energy scale—the Kondo temperature:

$$T_k = \pi^{-1}(2U\Gamma)^{1/2}\left(1 + e^{\pi q}\sigma^{(-)}(-i\pi)\right)\exp\left(-\pi\frac{U^2 - 4\Gamma^2}{8U\Gamma}\right).$$

We determine from Eqs. (6)-(8) and Eq. 12 the magnetic susceptibility of the impurity at $H=0$ and of the arbitrary values of ϵ_d, U, and Γ:

$$\chi^{imp}(0) = \frac{1}{2\pi T_c}\left\{1 + e^{-\pi\frac{(U^2-4\Gamma^2)}{8U\Gamma}} \int_{-\infty}^{\infty} e^{-\pi t^2/2\Gamma U}\delta(it)\frac{dt}{2\pi\sqrt{2U\Gamma}}\right.$$
$$\left. + e^{2\pi U\Gamma/\epsilon_d(\epsilon_d + U)} \int_{-\infty}^{\infty} \frac{d\omega}{\pi - i\omega} \frac{e^{-|\omega|/2}}{G^{(-)}(\omega)} \int_{-\infty}^{\infty} e^{i\omega(k^2/2U\Gamma - q)}\delta(k)\frac{dk}{2\pi\sqrt{U\Gamma}}\right\}. \tag{14}$$

The ground state of the impurity is the singlet state for any ϵ_d, U, and Γ.

In the asymmetric case the magnetic susceptibility for a magnetic field $H \ll H_0$, which is arbitrary with respect to T_c, is given by

$$\chi^{imp}(H) = \chi^{\rm Kondo}(H/T_c) + \frac{1}{4\sqrt{2\Gamma}} \int_{-\infty}^{\infty} \frac{d\omega}{\pi - i\omega} \frac{e^{-|\omega| + i\omega/J_*}}{G^{(-)}(\omega)} + O\left(\frac{H^2}{H_0^2}\right), \tag{15}$$

where $\chi^{\rm Kondo}(H/T_c)$ has been calculated in Refs. 2 and 3, and

$$T_c = \frac{4\Gamma}{\pi\sqrt{2\pi e}} e^{-\pi/J_*} = \frac{\sqrt{2U\Gamma}}{\pi} e^{2\pi\Gamma U/\epsilon_d(\epsilon_d + U)}$$

We note that the coefficients of the exponential function in T_c in the symmetric limit match almost exactly those in the asymmetric limit.[9]

At $J_* \sim 1$ the first two terms in Eq. (14) are of the same order of magnitude and the state with a localized moment vanishes. In this region the charge fluctuations are significant and the valence differs markedly from unity.

The first term of the expansion in $J_{**}(\epsilon_d = 0)$ in Eqs. (13) and (15) was calculated in Ref. 10.

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