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# INFLUENCE OF MAGNETIC FIELD ON THE KONDO EFFECT ANDERSON MODEL

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The effect of an external magnetic field on the scattering of conduction electrons by magnetic impurity is investigated. The method of Green's functions is applied to the Anderson model and an integral equations for scattering matrices are solved in the strongly correlated limit. The temperature dependence of the critical magnetic field and magnetoresistivity of dilute magnetic alloy are calculated.

## 1. *Introduction*

The interaction of the localized magnetic moment with conduction electrons has been the object of studies in a great number of works. Most of them are concerned with the $s-d$ exchange model (for reference see [1]). Recently, more attention has been focused on the investigation of the Anderson model. Theumann [2] and Mamada and Takano [3] using the equation of motion approach derive an integral equation which in the limit of infinite intra atomic Coulomb energy can be treated in analogy to Nagaoka's equation in the $s-d$ exchange model.

The effect of a magnetic field on the properties of metal with paramagnetic impurities has been investigated in various approximations in the framework of $s-d$ exchange model only [1], [4].

The purpose of the present work is to obtain some information about the system of electrons interacting with a paramagnetic impurity in the presence of arbitrary magnetic field at finite temperatures. In Section 2 the necessary Green's functions are introduced and their equations of motion are set up. These equations can be reduced to the system of two integral equations for the scattering matrices, which are solved in Section 3 in the strongly correlated limit. In Section 4 an equation for critical magnetic field, at which perturbation theory diverges, as the function of temperature is determined. Also the magnetoresistivity in some approximation is calculated.

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## 2. *Equations of motion*

As stated above we consider a system consisting of conduction electrons interacting with one impurity located at the origin of the coordinate system. We assume a non degenerate $d$-level of impurity and energy independent interaction. Then the Anderson Hamiltonian of the system in the presence of a magnetic field $H$ is given by

$$\mathscr{H} = \sum_{ks} \varepsilon_{ks} c_{ks}^{+} c_{ks} + \sum_{s} E_s n_s + \tfrac{1}{2} U \sum_{s} n_s n_{-s} + \sum_{ks} (V c_{ks}^{+} d_s + V^* d_s^{+} c_{ks}) \tag{2.1}$$

where

$$\varepsilon_{ks} = \varepsilon_k - \tfrac{1}{2} s \frac{g_e}{g} h, \quad E_s = E - \tfrac{1}{2} sh,$$

$$h = g\mu_B H, \quad s = \pm 1.$$

$g_e(g)$ are the Lande $g$-factors of the conduction (impurity $d$-level) electrons and other symbols have their usual meaning.

The properties of our system are most conveniently expressed by the Green's functions

$$\langle\langle c_{k's}(\tau) | c_{ks}^{+} \rangle\rangle = -\langle T c_{k's}(\tau), c_{ks}^{+}(0) \rangle, \tag{2.2}$$

$$\langle\langle d_s(\tau) | d_s^{+} \rangle\rangle = -\langle d_s(\tau), d_s^{+}(0) \rangle. \tag{2.3}$$

The Fourier transform of function (2.2) given by

$$\langle\langle c_{k's} | c_{ks}^{+} \rangle\rangle = \int_0^{\beta} e^{z\tau} \langle\langle c_{k's}(\tau) | c_{ks}^{+} \rangle\rangle d\tau$$

with

$$z = i\omega_n = i \frac{\pi}{\beta} (2n+1)$$

satisfies the equation of motion

$$(z - \varepsilon_{k's}) \langle\langle c_{k's} | c_{ks}^{+} \rangle\rangle = \delta_{kk'} + V \langle\langle d_s | c_{ks}^{+} \rangle\rangle. \tag{2.4}$$

For the new Green function in the right hand side of Eq. (2.4) we obtain the equation:

$$(z - E_s) \langle\langle d_s | c_{ks}^{+} \rangle\rangle = U \langle\langle n_{-s} d_s | c_{ks}^{+} \rangle\rangle + V^* \sum_{l} \langle\langle c_{ls} | c_{ks}^{+} \rangle\rangle. \tag{2.5}$$

In order to take into account the correlation between conduction and $d$-electrons we must consider higher order Green's functions. The equations for them are

$$\begin{aligned}(z - E_s - U) \langle\langle n_{-s} d_s | c_{ks}^{+} \rangle\rangle &= V^* \sum_{l} \langle\langle n_{-s} c_{ls} | c_{ks}^{+} \rangle\rangle + \\ &+ V^* \sum_{l} \langle\langle d_{-s}^{+} c_{l-s} d_s | c_{ks}^{+} \rangle\rangle - V \sum_{l} \langle\langle c_{l-s}^{+} d_{-s} d_s | c_{ks}^{+} \rangle\rangle,\end{aligned} \tag{2.6}$$

$$\begin{aligned}(z - \varepsilon_{k's}) \langle\langle n_{-s} c_{k's} | c_{ks}^{+} \rangle\rangle &= \langle n_{-s} \rangle \delta_{kk'} + V \langle\langle n_{-s} d_s | c_{ks}^{+} \rangle\rangle - \\ &- V \sum_{l} \langle\langle c_{l-s}^{+} d_{-s} c_{k's} | c_{ks}^{+} \rangle\rangle + V^* \sum_{l} \langle\langle d_{-s}^{+} c_{l-s} c_{k's} | c_{ks}^{+} \rangle\rangle,\end{aligned} \tag{2.7}$$

$$(z-\varepsilon_{k'-s}+sh)\langle\langle d^+_{-s}c_{k'-s}d_s|c^+_{ks}\rangle\rangle = V\langle\langle n_{-s}d_s|c^+_{ks}\rangle\rangle-$$

$$-V\sum_l \langle\langle c^+_{l-s}c_{k'-s}d_s|c^+_{ks}\rangle\rangle+V^*\sum_l \langle\langle d^+_{-s}c_{k'-s}c_{ls}|c^+_{ks}\rangle\rangle, \tag{2.8}$$

$$(z+\varepsilon_{k'-s}-2E-U)\langle\langle c^+_{k'-s}d_{-s}d_s|c^+_{ks}\rangle\rangle = -V^*\langle\langle n_{-s}d_s|c^+_{ks}\rangle\rangle+$$

$$+V^*\sum_l \langle\langle c^+_{k'-s}d_{-s}c_{ls}|c^+_{ks}\rangle\rangle+V^*\sum_l \langle\langle c^+_{k'-s}c_{l-s}d_s|c^+_{ks}\rangle\rangle. \tag{2.9}$$

If analogous equations of motion starting with the function (2.3) are set up and an appropriate decoupling procedure

$$\langle\langle c^+_{l-s}d_{-s}c_{k's}|c^+_{ks}\rangle\rangle = \langle c^+_{l-s}d_{-s}\rangle\langle\langle c_{k's}|c^+_{ks}\rangle\rangle \quad etc.$$

and

$$\langle\langle d^+_{-s}c_{k-s}d_s|d^+_s\rangle\rangle = \langle d^+_{-s}c_{k-s}\rangle\langle\langle d_s|d^+_s\rangle\rangle \quad etc.$$

is applied, the closed system of equations of motion can be obtained. It is possible to solve this system, by means of simple but lengthy procedure, with respect to functions (2.2)

$$\langle\langle c_{k's}|c^+_{ks}\rangle\rangle = \frac{\delta_{kk'}}{z-\varepsilon_{k's}}+|V|^2\frac{t_s(z)}{(z-\varepsilon_{ks})(z-\varepsilon_{k's})} \tag{2.10}$$

and (2.3)

$$\langle\langle d_s|d^+_s\rangle\rangle = t_s(z). \tag{2.11}$$

Another two Green's functions that we will need in following may also be expressed in terms of $t$-matrices as

$$\langle\langle d_s|c^+_{ks}\rangle\rangle = V^*\frac{t_s(z)}{z-\varepsilon_{ks}} \tag{2.12}$$

and

$$\langle\langle c^+_{ks}|d^+_s\rangle\rangle = V\frac{t_s(z)}{z-\varepsilon_{ks}}. \tag{2.13}$$

For the time being the $t$-matrices depend on thermal averages that follow from the decoupling procedure. However using Eqs (2.10) to (2.13) with relations of the form

$$\langle c^+_{ks}d_s\rangle = \frac{1}{\beta}\sum_{\omega_n} e^{i\omega_n}\langle\langle d_s|c^+_{ks}\rangle\rangle \equiv \mathscr{F}\{\langle\langle d_s|c^+_{ks}\rangle\rangle\}, \tag{2.14}$$

the $t$-matrices can be expressed in terms of integrals of themselves yielding a system of two singular integral equations for $t_s(z)$.

For arbitrary $U$ these integral equations are very complicated and we will not write them down. As it was mentioned above, we are mainly interested in the strongly correlated limit (high $U$) which seems to correspond to the $s-d$ exchange model and describes the

Kondo effect. Thus we can expand our equations in the power series of $U^{-1}$ and take into account the leading terms only. It follows after a simple transformation

$$t_s(z) = \frac{1-\langle n_{-s}\rangle - \mathscr{F}\left\{\frac{F(i\omega)-F(z)}{z-i\omega}\, t(-s;\, i\omega)\right\}}{z-E-\frac{3}{2}F(z)-R(s;z)-\mathscr{F}_s\left\{\frac{[F(i\omega)-F(z)]^2}{z-i\omega}\, t(-s;\, i\omega)\right\}} \tag{2.15}$$

$$t(s;z) = t_s(z-\tfrac{1}{2}sh),\; F(z) = \sum_k \frac{|V|^2}{z-\varepsilon_k}, \tag{2.16}$$

where

$$R(s;z) = \mathscr{F}_s\left\{\frac{F(i\omega)-F(z)}{z-i\omega}\right\} - \tfrac{1}{2}F(z) \tag{2.17}$$

and $\mathscr{F}_s$ means the "shifted" frequency sum of form (2.14) which, when converted into integral bent over to the real axis, can be written as

$$\mathscr{F}_s\{f(i\omega)\} \equiv \mathscr{F}\{f(i\omega-\tfrac{1}{2}sh)\}.$$

$$= \frac{1}{4\pi i}\int_{-\infty}^{\infty} \mathrm{th}\,\frac{\beta(\omega+\frac{1}{2}sh)}{2}\,[f_r(\omega)-f_a(\omega)]d\omega. \tag{2.18}$$

A certain approximation was also made in (2.15), namely we omit the quantity $(g-g_e)\mu_B H/2$ in the arguments of functions $F$. This causes a negligibly small errors of the order $(g-g_e)\mu_B H/2D$, where $2D$ is the conduction electrons band width.

### 3. *Solution of integral equations*

In order to solve Eq. (2.15) we follow the method most frequently exploited in the Kondo problem. However, since we have the system of two equations, some generalization in needed. In the following we assume the Lorentzian form for the density of states

$$N(\omega) = N(0)\varrho(\omega) = N(0)\frac{D^2}{\omega^3+D^2} \tag{3.1}$$

which is sufficiently regular function in complex plane. One then finds for $F(z)$

$$F_{r,a}(z) = \frac{\Delta D}{z\pm iD}, \qquad \Delta = \pi N(0)|V|^2. \tag{3.2}$$

Let us replace $F(z)$ with $F_{r,a}(z)$ in Eq. (2.15) we then obtain equations for $t_r(s;z)$ and $t_a(s;z)$ that can be rewritten as

$$1+[F_r(z)-F_a(z)]t_r(s;z) = \frac{X_r(s;z)}{\Phi_r(s;z)}, \tag{3.3a}$$

$$1-[F_r(z)]-F_a(z)t_a(s;z) = \frac{X_a(s;z)}{\Phi_a(s;z)} \tag{3.3b}$$

where the nominators

$$X_{r,a}(s;z)=z-E-\tfrac{1}{2}F_r(z)-F_a(z)-\langle n_{-s}\rangle[F_r(z)-F_a(z)]-R(s;z)+\chi(s;z), \tag{3.4}$$

with

$$\chi(s;z)=-\mathscr{F}_s\left\{[F(i\omega)-F_r(z)]\,[F(i\omega)-F_a(z)]\,\frac{t(-s;i\omega)}{z-i\omega}\right\}, \tag{3.5}$$

contain besides known functions, only the regular function $\chi(s;z)$. However, the function $\chi(s;z)$ is of the order $\Delta^2/E^2D$ and can be neglected in the cases when no differentiation of $\chi(s;z)$ with respect to temperature is involved. We write the denominators as

$$\Phi_{r,a}(s;z)=z-E-\tfrac{3}{2}F_{r,a}(z)-R(s;z)-F_r(z)F_a(z)L_0(s;z)t+$$
$$+[F_r(z)+F_a(z)]L_1(s;z)-L_2(s;z) \tag{3.6}$$

where

$$L_n(s;z)=\mathscr{F}_s\left\{\frac{F^n(i\omega)}{z-i\omega}\,t(-s;i\omega)\right\}. \tag{3.7}$$

The functions $R(s;z)$ and $L_n(s;z)$ are represented by Cauchy integrals which for $\operatorname{Im} z \gtrless 0$ define the functions $R^{\pm}(s;z)$ and $L_n^{\pm}(s;z)$ holomorphic on the whole complex plane excluding the real axis. For the discontinuity across the real axis, Eqs (2.17) and (3.7) yield

$$\Delta R(s;\omega)\equiv R^{+}(s;\omega)-R^{-}(s;\omega)=-\tfrac{1}{2}[F_r(\omega)-F_a(\omega)]\,\mathrm{th}\,\frac{\beta(\omega+\frac{1}{2}sh)}{2}, \tag{3.8}$$

$$\Delta L_n(s;\omega)=-\tfrac{1}{2}[F_r^n(\omega)t_r(-s;\omega)-F_a^n(\omega)t_a(-s;\omega)]\,\mathrm{th}\,\frac{\beta(\omega+\frac{1}{2}sh)}{2}. \tag{3.9}$$

Then from Eqs (3.4) and (3.6) with help of Eq. (3.3) one finds the sprung relations for $\Phi_r(s;\omega)$ and $\Phi_a(s;\omega)$

$$\Delta\Phi_r(s;\omega)=\Delta X_r(s;\omega)\,\frac{X_a^{-}(-s;\omega)}{\Phi_a^{-}(-s;\omega)}, \tag{3.10}$$

$$\Delta\Phi_a(s;\omega)=\Delta X_a(s;\omega)\,\frac{X_r^{+}(-s;\omega)}{\Phi_a^{+}(-s;\omega)}. \tag{3.11}$$

Combining these relations we can see that the function

$$w(s;z)=\Phi_r(s;z)\Phi_a(-s;z)-X_r(s;z)X_a(-s;z) \tag{3.12}$$

is continuous across the real axis, *i.e.*

$$w^{+}(s;\omega)=w^{-}(s;\omega). \tag{3.13}$$

By use of Eqs (3.2), (3.4), (3.6) and Liouville's theorem one finds

$$w(s;z)=\Delta^2\varrho^2(z)[4+3n-4\langle n_s\rangle\langle n_{-s}\rangle]-$$
$$-i\Delta s\varrho(z)\left[2(E-z)+5\Delta\varrho(z)\frac{z}{D}\right]m \tag{3.14}$$

where $n = \langle n_+\rangle + \langle n_-\rangle$ and $m = \langle n_+\rangle - \langle n_-\rangle$. Now by means of Eq. (3.12) we can eliminate the unphysical function $\Phi_r^-$ in Eq. (3.10) and arrive at a certain generalization of the Riemann problem

$$\frac{1}{\Delta D} F_r(\omega-E)\Phi_r^+(s;\omega)\,\frac{1}{\Delta D} F_a(\omega-E)\Phi_a^-(-s;\omega)$$

$$=\frac{1}{\Delta^2 D^2} F_r(\omega-E)F_a(\omega-E)[X_r^+(s;\omega)X_a^-(-s;\omega)+w(s;\omega)]\equiv K(s;\omega) \qquad (3.15)$$

where $F_r(\omega-E)$ and $F_a(\omega-E)$ are introduced in order to guarantee the vanishing of $\ln K(s;\omega)$ at infinity. The equation (3.15) can be solved as, [5],

$$\Phi_r^+(s;\omega) = \frac{\Delta D\sqrt{K(s;\omega)}}{F_r(\omega-E)}\, e^{-i\eta(s;\omega)},$$

$$\Phi_a^-(s;\omega) = \frac{\Delta D\sqrt{K(-s;\omega)}}{F_a(\omega-E)}\, e^{i\eta(-s;\omega)} \qquad (3.16)$$

with

$$\eta(s;\omega) = \frac{P}{2\pi}\int\limits_{-\infty}^{\infty}\frac{\ln K(s;\omega')}{\omega'-\omega}\,d\omega'. \qquad (3.17)$$

The Eqs (3.16) and (3.17) with Eq. (3.3) form the complete solution for the $t$-matrices. The unknown function $\chi(s;\omega)$ can be neglected or calculated in an approximated way if needed, $n$ and $m$ can be in principle determined self-consistently from Eq. (2.11) but we will consider them to be adjustable parameters.

## 4. *The critical field and resistivity*

The quantities interesting to us in this Section are determined by the properties of the scattering matrices at the Fermi surface ($\omega = 0$) only. The Eq. (3.4) with (in following we assume that $h \ll D$ which is fulfilled in all real cases)

$$R^{\pm}(s;\omega) = \frac{\Delta}{\pi}\varrho(\omega)\left[\ln\frac{\beta D}{2\pi} - \psi\left(\tfrac{1}{2}\pm\frac{\beta}{2\pi i}(\omega+\tfrac{1}{2}sh)\right)\right] \qquad (4.1)$$

yields

$$X^{\pm}(s;\omega) = \omega - E - \frac{\Delta}{\pi}\varrho(\omega)\left[\pm i\frac{\pi}{2}(1-4\langle n_{-s}\rangle)+\right.$$

$$\left.+\ln\frac{\beta D}{2\pi} - \psi\left(\tfrac{1}{2}\pm\frac{\beta}{2\pi}(\omega+\tfrac{1}{2}sh)\right)\right]. \qquad (4.2)$$

The critical magnetic field $H_K(T)$ is determined by

$$\sum_s \mathrm{Re}\, X_s^+(0) = 0,$$

(where and in following $f_s(\omega)$ means $f(s;\omega+\frac{1}{2}sh)$, or according to Eq. (4.2)

$$\pi\frac{E}{\Delta}+\ln\frac{\beta D}{2\pi}+\mathrm{Re}\,\psi\left(\tfrac{1}{2}+\frac{\beta h}{2\pi i}\right)=0. \tag{4.3}$$

In the absence of magnetic field this equation determines the Kondo temperature

$$k_B T_K=\frac{2a}{\pi}D\exp\left(\frac{\pi E}{\Delta}\right) \tag{4.4}$$

where $\ln 4\alpha=-\psi(\frac{1}{2})$ and conditions $|E|\gg\Delta$ with $E<0$ must be satisfied [3].

If the definition of $T_K$ is used, Eq. (4.3) can be written as

$$\mathrm{Re}\,g_+\left(\frac{\mu_B g}{2\pi k_B}\frac{H_K(T)}{T}\right)=\ln\frac{T_K}{T} \tag{4.5}$$

where

$$g_\pm(x)=\psi(\tfrac{1}{2}\mp ix)-\psi(\tfrac{1}{2}).$$

We can see with the help of asymptotic formula

$$\mathrm{Re}\,g_+(x)=\ln 4\alpha x-\frac{1}{24x^2}\quad\text{for}\quad x\gg 1$$

that

$$H_K(T)=H_K(0)\left[1+2.1\left(\frac{T}{T_K}\right)^2\right]\quad\text{near } T=0,$$

and

$$\mathrm{Re}\,g_+(x)=7\zeta(3)x^2\quad\text{for}\quad x\ll 1$$

that

$$H_K(T)=5.1H_K(0)\sqrt{1-\frac{T}{T_K}}\quad\text{near}\quad T=T_K$$

where

$$H_K(0)=\frac{\pi k_B}{2\alpha\mu_B g}T_K. \tag{4.6}$$

A more detailed calculation shows that the critical field increases with temperature increasing from 0 to about $0.3T_K$ where it reaches its maximum value $1.2H_K(0)$, while it seems, for physical reasons that $H_K(T)$ should be monotonically decreasing function for all $0<T<T_K$.

We consider now the electrical resistivity. If we restrict ourselves to the lowest order term in the Sommerfeld expansion, the resistivity is related to the retarded scattering matrices at the Fermi level in the following way

$$\varrho^{-1}=-\frac{n_0 e^2}{4m^* c|V|^2}\sum_s\frac{1}{\mathrm{Im}\,t_s^r(0)}$$

where

$$t_s^r(0) = \frac{1}{2i\Delta\varrho(\omega)}\left[1-\frac{X_s^+(\omega)}{(\omega-E+iD)\sqrt{K_s(\omega)}}\,e^{i\eta_s(\omega)}\right]_{\omega=0} \tag{4.8}$$

with $K_s(\omega)$ and $\eta_s(\omega)$ given by Eqs (3.15) and (3.17). As the $K_s(\omega)$ for $|\omega| \ll E$ is an even function of $\omega$ and the contribution to $\eta_s(0)$ from large $\omega$ is negligibly small we can neglect the phase factor in Eq. (4.7). Then

$$\varrho^{-1} = \frac{1}{2\varrho_0 c}\sum_s\left[1+\mathrm{Re}\,\frac{E+iD}{\sqrt{E^2+D^2}}\,\frac{X_s^+}{\sqrt{X_s^+X_{-s}^-+w_s}}\right]^{-1} \tag{4.7}$$

where $c$ — concentration of impurities, $\varrho_0 = \dfrac{m^x}{\pi n_0 e^2 N(0)}$,

$$X_s^\pm = \tfrac{1}{2}sh \mp \tfrac{1}{2}i\Delta(1-4\langle n_{-s}\rangle) + \frac{\Delta}{\pi}\left[\tau + g_\pm\left(\frac{sh}{2\pi k_B T}\right)\right]$$

and

$$\tau = \ln\frac{I}{T_K}.$$

The explicit form of resistivity for arbitrary $H$ is very complicated but in the case $h \ll k_B T$ can be considerably simplified. One finds by expanding Eq. (4.8) to the order $(H/k_B T)^2$

$$\varrho(H)-\varrho(0) = \varrho_0 c\left[0.22-\left(\frac{\pi^2}{4}+0.22\tau\right)\frac{\tau}{\lambda}\right]\frac{E}{\lambda\sqrt{E^2+D^2}}\left(\frac{\mu_B g H}{k_B T}\right)^2 \tag{4.9}$$

where

$$\lambda = [\tau^2+2\pi^2(2+n)]^{1/2}.$$

The resistivity in the absence of magnetic field follows from Eq. (4.7) with $H = 0$.

$$\varrho(0) = \varrho_0 c\left\{1+\left[\frac{E\tau}{\pi}+D(\tfrac{1}{2}-n)\right]\lambda^{-1}(E^2+D^2)^{-\frac{1}{2}}\right\}. \tag{4.10}$$

It is seen from Eq. (4.8) that the magnetoresistivity is negative and tends to zero for $T \gg T_K$. The solution for $t$-matrices that we have found can be used to calculate other physical quantities, in particular the magnetic susceptibility at a finite field.

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