Theory of the Kondo effect at low temperatures

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(Submitted February 5, 1973)
Zh. Eksp. Teor. Fiz. **65**, 307–318 (July 1973)

A model is proposed for describing scattering of conduction electrons of a nonmagnetic metal by magnetic impurities at temperatures considerably below the Kondo temperature T_K. Since at $T \to 0$ the impurity spin vanishes as a result of screening by the conductivity electrons it is suggested that at $T \ll T_K$ the picture is equivalent to inelastic scattering of electrons by nonmagnetic impurities with a localized level near the Fermi energy. The impurity part of the specific heat and magnetic susceptibility, conductivity, thermal conductivity and differential thermo-emf are found for such a model. Dependences of the superconducting transition temperature and energy gap at $T = 0$ on impurity concentration are derived. Interference between inelastic and potential scattering is taken into account in all cases.

1. THE MODEL

The effect of magnetic impurities on the properties of metals has been the subject of many investigations in recent years (see the review [4]). The unique character of the scattering of conduction electrons by such impurities is attributed to the so-called Kondo effect,[1-4] wherein the temperature dependence of the resistance of a nontransition metal with a slight admixture of a transition metal exhibits a minimum. This resistance minimum exists only in the case of antiferromagnetic interaction of the electron with the impurity (when the exchange integral I in the interaction energy $-(1/2)I\mathbf{s}\cdot\sigma$ is negative; $\mathbf{s}$ is the impurity spin and $\sigma/2$ is the spin of the conduction electron). At this sign of the interaction, however, the expression for the scattering amplitude has a pole at the Kondo temperature $T_K \sim \epsilon_F \exp(-2\epsilon_F/3Iz)$[2,3] ($\epsilon_F$ is the Fermi energy and z is the number of conduction electrons per atom of the host metal). Strictly speaking, therefore, the expression is valid only at temperatures above T_K. There is no rigorous theory for $T < T_K$.

In the cited papers, the impurity spin was assumed given. This model is obviously reasonable so long as the exchange interaction of the conduction electrons with the impurity is weak. When the Kondo temperature is approached, however, the scattering increases and this means that the interaction of the electron with the impurity spin becomes strong. Since exchange does take place in fact between the conduction electrons and the electrons of the inner shells of the impurity atom, the very concept of a fixed impurity spin at low temperatures raises many doubts. The known experimental data (see, e.g., [5,6]) and practically all the theories (even though they cannot be regarded as rigorous) indicate that the impurity spin vanishes at low temperatures (it is sometimes said to be "screened"). It is therefore more reasonable to use a model camable of describing the very formation of the impurity spin in the metal. The simplest model of this type was proposed by Anderson.[7] The corresponding Hamiltonian is

$$\hat{\mathcal{H}} - \hat{N}\mu = \sum_{p\alpha} \xi_p \hat{n}_{p\alpha} + \sum_{a\alpha} \varepsilon_d' \hat{n}_{a\alpha} + \frac{U}{2} \sum_{a\alpha} \hat{n}_{a\alpha}\hat{n}_{a-\alpha} + \frac{V'}{\sqrt{N_0}} \sum_{a\alpha} (\hat{\psi}_\alpha^+(\mathbf{r}_a)\hat{d}_{a\alpha} + \hat{d}_{a\alpha}^+ \hat{\psi}_\alpha(\mathbf{r}_a)), \tag{1}$$

where $\mathbf{p}$ is the electron quasimomentum, α is the spin, $\hat{n}_{p\alpha}$ is the number of electrons with momentum $\mathbf{p}$, $\xi_p = p^2/2m - \epsilon_F$; m is the electron mass; $\hat{n}_{a\alpha} = \hat{d}_{a\alpha} + \hat{d}_{a\alpha}$; $d_{a\alpha}$ is the operator for electron annihilation at a localized level on the a-th impurity atom; $\hat{\psi}_\alpha(\mathbf{r})$ is the annihilation operator of the conduction electron at the point $\mathbf{r}$; $\mathbf{r}_a$ is the coordinate of the a-th impurity atom; N_0 is the density of the atoms of the host metal. Each impurity atom corresponds to a localized level with energy $\epsilon_d' < 0$ (reckoned from the Fermi level). The term with U ensures satisfaction of Hund's rule ($U + \epsilon_d' > 0$). The last term describes the exchange interaction that leads to a possible transition of a conduction electron to a localized level and back.

According to Anderson's estimates $U \sim 10$ eV and $V' \sim 2$ eV, so that the Hund term is not small and it is difficult to solve the problem with the Hamiltonian (1). To describe the system at very low temperatures, however, we can propose another model based on the fact that as $T \to 0$ the impurity spin vanishes completely and can appear only in the form of a fluctuation. In this model the magnetic impurity atoms are represented as nonmagnetic impurities with localized levels near the Fermi energy. The conduction electrons can be inelastically scattered by these atoms. The Hamiltonian in this model is

$$\hat{\mathcal{H}} - \hat{N}\mu = \sum_{p\alpha} \xi_p \hat{n}_{p\alpha} + \sum_{a\alpha} \tilde{\varepsilon}_d \hat{n}_{a\alpha} + \frac{V}{\sqrt{N_0}} \sum_{a\alpha} (\hat{\psi}_\alpha^+(\mathbf{r}_a)\hat{d}_{a\alpha} + \hat{d}_{a\alpha}^+ \hat{\psi}_\alpha(\mathbf{r}_a)) + \sum_{a\alpha} \int \hat{\psi}_\alpha^+(\mathbf{r}) U(\mathbf{r} - \mathbf{r}_a) \hat{\psi}_\alpha(\mathbf{r})\, d^3\mathbf{r}. \tag{2}$$

It differs outwardly from (1) only in the absence of the Hund term (the last term accounts for the usual potential scattering). However, the quantities V and $\tilde{\epsilon}_d$ in (2) do not coincide with the analogous coefficients of Anderson's Hamiltonian. It is proposed that at low temperatures the Anderson model is equivalent to the Hamiltonian (2) and the new coefficients are expressed in terms of the coefficients in (1).

We assume V, $|\tilde{\epsilon}_d| \ll \epsilon_F$ and $c_i = N_i/N_0 \ll 1$ (N_i is the concentration of the impurity atoms) and that the temperature is low enough (an exact criterion will be established later). The potential scattering is assumed for simplicity to be isotropic, i.e., $U(\mathbf{r}) = U_0\delta(\mathbf{r})$. Under these assumptions we calculate the main characteristics of the metal in the normal state, namely the specific heat, the magnetic susceptibility, the electric conductivity and the thermal conductivity. The results agree well with the experimental facts; this justifies the use of so simple a model.

In the conclusion, we use the described model to analyze the influence of a transition-metal impurity on superconductivity at $T \ll T_K$.

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2. THE GREEN FUNCTIONS

We use for the complete temperature Green functions the notation[1)]

$$\mathcal{G}(x,x') \equiv -\langle T\tilde{\psi}(x)\tilde{\bar{\psi}}(x')\rangle \equiv \overset{x}{\Longrightarrow}\overset{x'}{}$$

$$\mathfrak{D}_{a,b}(\tau,\tau') \equiv -\langle T\tilde{d}_a(\tau)\tilde{\bar{d}}_b(\tau')\rangle \equiv \overset{a,\tau}{=\!=\!\gg}\overset{b,\tau'}{=\!=\!=}$$

where $x=(\mathbf{r},\tau)$ and τ is the imaginary time. The zeroth Green functions

$$\mathcal{G}^{(0)} \equiv \longrightarrow\,, \quad \mathfrak{D}^{(0)} \equiv - - \!\rightarrow\! - -$$

are respectively equal in the Fourier representation $(\omega_n, \mathbf{p})$, to

$$\mathcal{G}^{(0)}(\omega_n,\mathbf{p}) = (i\omega - \xi_p)^{-1}, \quad \mathfrak{D}^{(0)}_{ab}(\omega_n) = \delta_{ab}(i\omega_n - \tilde{\varepsilon}_d)^{-1},$$

where $\omega_n = (2n+1)\pi T$.

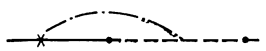
The matrix element of the potential interaction is

$$\overset{\omega,\mathbf{p}}{\rightarrow}\overset{\omega,\mathbf{p}'}{\rightarrow} \;(a) = U_0 e^{-i(\mathbf{p}-\mathbf{p}')\mathbf{r}_a}$$

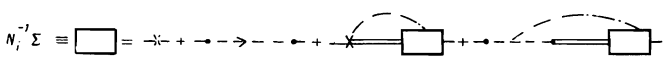
and that of the exchange interaction is

$$\overset{\omega}{\rightarrow}\overset{\omega,\mathbf{p}}{\rightarrow} \;(a) = V/\sqrt{N_0}\, e^{i\mathbf{p}\mathbf{r}_a}$$

After averaging over the impurity positions, the mass operator contains diagrams with several crosses and (or) dashed lines due to one impurity atom. We shall join such crosses and dashed lines by dash-dot lines, e.g.,



As usual (see Sec. 39 of [8]), diagrams with intersecting dash-dot lines can be neglected; then each diagram for the mass operator of the conduction electron $\Sigma(\omega, \mathbf{p})$ begins and ends with a cross or a dashed line pertaining to one impurity atom. Consequently



The solution of this equation is

$$\Sigma(\omega,\mathbf{p}) = \frac{N_i}{\pi\nu}\frac{1}{1+b^2}\left\{b - ib^2\operatorname{sign}\omega + \frac{\Gamma(1-ib\operatorname{sign}\omega)^2}{i\omega - \varepsilon_d + i\Gamma\operatorname{sign}\omega}\right\},$$

where

$$\nu = p_0 m/2\pi^2, \quad b = \pi\nu U_0, \quad \varepsilon_d = \tilde{\varepsilon}_d - b\Gamma, \quad \Gamma = \tilde{\Gamma}/(1+b^2),$$

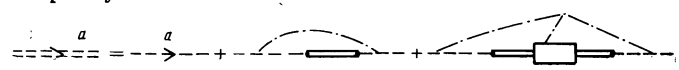
$$\tilde{\Gamma} = \pi\nu V^2/N_0 = 3\pi z V^2/4\varepsilon_F \ll V \ll \varepsilon_F,$$

p_0 is the Fermi momentum.

The imaginary part of the denominator of the retarded time-dependent Green function is

$$\frac{1}{2\tau(\omega)} \equiv -\operatorname{Im}\Sigma_R = \frac{N_i}{\pi\nu}\frac{1}{1+b^2}\left\{b^2 + \frac{\Gamma^2(1-b^2)+2b\Gamma(\omega-\varepsilon_d)}{\Gamma^2+(\omega-\varepsilon_d)^2}\right\}. \quad (3)$$

Analogously, the Green function of the electron at the impurity level is



i.e.,

$$\mathfrak{D}_{aa}(\omega) = (i\omega - \varepsilon_d + i\Gamma\operatorname{sign}\omega)^{-1}. \quad (4)$$

3. SPECIFIC HEAT

To calculate the specific heat it is convenient to use the fact that

$$\frac{\partial\Omega}{\partial\tilde{\varepsilon}_d} = N_i\langle d_{a\alpha}^{+}d_{a\alpha}\rangle = 2N_iT\sum_{\omega}\mathfrak{D}_{a,a}(\omega)e^{-i\omega\tau}_{\tau\to+0} = 2N_i\left\{2T\sum_{\omega>0}\operatorname{Re}\mathfrak{D}(\omega)+\frac{1}{2}\right\},$$

in addition,

$$S = -\frac{\partial\Omega}{\partial T}, \quad c_v = T\frac{\partial S}{\partial T},$$

where Ω, S, and c_V are the specific thermodynamic potential, the specific entropy, and the specific heat.

Thus, according to (4),

$$\frac{\partial S}{\partial\varepsilon_d} \equiv 4N_i\frac{\partial}{\partial T}T\sum_{\omega>0}\frac{\varepsilon_d}{(i\omega+i\Gamma)^2-\varepsilon_d^2} = -\frac{N_i}{\pi i}\frac{\partial}{\partial T}\int_{-\infty}^{\infty}d\omega\,\operatorname{th}\frac{\omega}{2T}$$
$$\times\frac{\varepsilon_d}{(\omega+i\Gamma)^2-\varepsilon_d^2} = \frac{N_i}{2\pi i}\frac{\partial}{\partial T}\int\frac{d\omega}{2T}\operatorname{ch}^{-2}\frac{\omega}{2T}\ln\frac{i\Gamma-\varepsilon_d+\omega}{i\Gamma+\varepsilon_d+\omega}.$$

In the case under consideration, when $T \ll \max\{\epsilon_d, \Gamma\}$, we can expand the logarithms in powers of ω and obtain in first order in T

$$\frac{\partial S}{\partial\varepsilon_d} = -\frac{4\pi}{3}N_iT\frac{\varepsilon_d\Gamma}{(\varepsilon_d^2+\Gamma^2)^2}.$$

The correction to the specific heat is therefore

$$\Delta c_v = \Delta S = \frac{2\pi}{3}N_iT\frac{\Gamma}{\varepsilon_d^2+\Gamma^2}. \quad (5)$$

It follows from the results given below for the conductivity and the magnetic susceptibility that in the considered model $\max\{\epsilon_d, \Gamma\}$ plays the role of the Kondo temperature T_K. Therefore the specific heat per impurity atom is of the order of T/T_K, i.e., the impurity atoms are much more "effective" for the specific heat than the conduction electrons (the specific heat per conduction electron is of the order of T/ϵ_F).

4. MAGNETIC SUSCEPTIBILITY

To find the static impurity susceptibility χ_i we can calculate the magnetic moment $\mathbf{M}_a$ of one impurity atom in a weak homogeneous magnetic field $\mathbf{H}$ directed along the z axis. In such a field, the Green function of the d-electron is

$$\mathfrak{D}_\sigma = (i\omega - \varepsilon_d + \sigma g\mu H + i\Gamma\operatorname{sign}\omega)^{-1},$$

where $\sigma = \pm 1$ is the sign of the spin projection on the z axis, $g \sim 1$ is the d-electron g factor, and μ is the Bohr magneton

$$\mathbf{M}_a \equiv g\mu\langle\boldsymbol{\sigma}\rangle,$$
$$M_{az} = g\mu\langle\tilde{\bar{d}}_+\tilde{d}_+ - \tilde{\bar{d}}_-\tilde{d}_-\rangle = g\mu T\sum_{\omega}[\mathfrak{D}_+(\omega)-\mathfrak{D}_-(\omega)]_{\tau\to+0}e^{-i\omega\tau} =$$
$$= -2g^2\mu^2HT\sum_{\omega}(i\omega-\varepsilon_d+i\Gamma\operatorname{sign}\omega)^{-2}.$$

Accurate to second order in T we have:

$$\chi_i = N_ig^2\mu^2\frac{2\Gamma}{\pi(\Gamma^2+\varepsilon_d^2)}\left[1-\frac{\pi^2}{3}\frac{\Gamma^2-3\varepsilon_d^2}{(\Gamma^2+\varepsilon_d^2)^2}T^2\right]. \quad (6)$$

for $\epsilon_d \ll \Gamma$ we have

$$\chi_i = N_ig^2\mu^2\frac{2}{\pi\Gamma}\left[1-\frac{\pi^2}{3}\frac{T^2}{\Gamma^2}\right],$$

and for $\epsilon_d \gg \Gamma$,

$$\chi_i = N_ig^2\mu^2\frac{2\Gamma}{\pi\varepsilon_d^2}\left[1+\pi^2\frac{T^2}{\varepsilon_d^2}\right].$$

Thus, as $T\to 0$ the quantity χ_i tends to a constant equal to $N_ig^2\mu^2/\Theta$, where $\Theta \sim \max\{\Gamma, \epsilon_d^2/\Gamma\}$, and the low-temperature criterion is

$$T \ll \max\{|\varepsilon_d|, \Gamma\}.$$

At high temperatures, as is well known, the impurities produce the usual paramagnetic susceptibility $\chi_i = N_i g^2 \mu^2 / 3T$. The existing experimental data correspond to a monotonic approach of χ_i to a constant limit with decreasing temperature. It follows from (6) that another case is also possible, namely $\chi_i(T)$ should have a maximum at $\Gamma^2 < 3\epsilon_d^2$.

5. THE KINETIC COEFFICIENTS

An expression for the thermal conductivity κ in terms of the complete Green functions of the conduction electrons was derived by Zittartz.[9] For our case, it takes the form

$$\varkappa = \frac{1}{T}\lim_{\omega\to 0}\omega^{-1}\operatorname{Im} P(\omega+i\delta),$$

$$P(i\nu) = -\frac{1}{6}\lim_{\gamma\to 0}\frac{\partial^2}{\partial\gamma^2}\int\frac{d^3\mathbf{p}}{(2\pi)^3}T\sum_{\omega}\frac{\mathbf{p}}{m^2}\Pi(\mathbf{p},\omega;\mathbf{p},\omega-\nu)e^{i\gamma(2\omega-\nu)},$$

$$\nu = 2\pi n T,$$

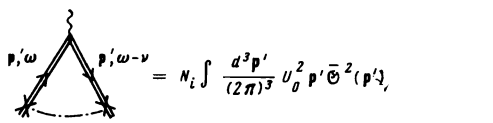
where $\Pi(p_1, p_2)$ are the Fourier components (p_1 and p_2 are 4-momenta) of

$$\Pi(x-y, y-x') = -\frac{i}{2}(\nabla_y - \nabla_{y'})_{y'\to y}\overline{\mathcal{G}(x,y')\mathcal{G}(y,x')}$$

$$= \frac{T^2}{(2\pi)^6}\sum_{\omega_1,\omega_2}\int d^3\mathbf{p}_1\, d^3\mathbf{p}_2 \exp[ip_1(x-y)+ip_2(y-x')]\Pi(p_1,p_2)$$

(the bar denotes averaging over the impurity positions).

Since the scattering is isotropic, the mean value of the product of two Green functions can be replaced in $\Pi(\mathbf{p}, \omega; \mathbf{p}, \omega-\nu)$ by the product of the mean values. Indeed, taking as an example the correction corresponding to the diagram



$$= N_i\int\frac{d^3\mathbf{p}'}{(2\pi)^3}U_0^2\,\mathcal{G}(\mathbf{p}',\omega)\,\bar{\mathcal{G}}^2(\mathbf{p}',\omega-\nu)$$

we see that the integral with respect to the momenta causes this correction to vanish. Consequently

$$P(i\nu) = -\frac{1}{6}\lim_{\gamma\to 0}\frac{\partial^2}{\partial\gamma^2}\int\frac{d^3\mathbf{p}}{(2\pi)^3}\frac{p^2}{m^2}T\sum_{\omega}\mathcal{G}(\mathbf{p},\omega)\mathcal{G}(\mathbf{p},\omega-\nu)e^{i\gamma(2\omega-\nu)}$$

(the averaging bar will henceforth be omitted).

To calculate this expression, analogous expressions must be added to and subtracted from the Green functions $\mathcal{G}_0$ of the pure metal, which can be summed directly. Its imaginary part is equal to zero. The integral containing the difference $\mathcal{G}\mathcal{G} - \mathcal{G}_0\mathcal{G}_0$ (we designate it $P'(i\nu)$) converges quite rapidly and the order of summation and integration can be reversed in it by replacing p^2/m^2 under the integral sign by p_0^2/m^2. As a result we get

$$\operatorname{Im} P(\nu+i\delta) = \operatorname{Im} P'(\nu+i\delta),$$

where

$$P'(i\nu) = \frac{\pi N}{m}T\sum_{0<\omega<\nu}(2\omega-\nu)^2[2\nu+\tau^{-1}(i\omega)+\tau^{-1}(i\omega-i\nu)]^{-1},$$

$N = zN_0$ is the concentration of the conduction electrons. By changing in standard fashion from summation to integration along a contour in the complex ω plane we obtain

$$\varkappa = \frac{2NT}{m}\int_{-\infty}^{\infty}\frac{\omega^2\,d\omega}{(2T)^3}\frac{\tau(\omega)}{\operatorname{ch}^2(\omega/2T)}. \tag{7}$$

Expression (7) coincides with the one obtained from the kinetic equation. The same can be stated also concerning the formula for the determination of the static conductivity σ (see, e.g., [3]):

$$\sigma = \frac{Ne^2}{2m}\int_{-\infty}^{\infty}\frac{d\omega}{2T}\frac{\tau(\omega)}{\operatorname{ch}^2(\omega/2T)}. \tag{8}$$

On the same basis we can use the relation obtained from the kinetic equation for the differential thermoelectric power α:

$$\sigma\alpha = \frac{Ne}{m}\int_{-\infty}^{\infty}\frac{\omega\,d\omega}{(2\pi)^2}\frac{\tau(\omega)}{\operatorname{ch}^2(\omega/2T)}. \tag{9}$$

After substituting the values of τ from (3) in (7)–(9) we obtain

$$\rho \equiv \sigma^{-1} = c_i\frac{2m}{\pi v z e^2}\frac{1}{1+b^2}\frac{(\Gamma-b\varepsilon_d)^2}{\Gamma^2+\varepsilon_d^2}\left[1-\frac{\pi^2}{3}\left(\frac{T}{T_1}\right)^2\right], \tag{10}$$

where

$$T_1^2 = \frac{(\Gamma-b\varepsilon_d)^2(\Gamma^2+\varepsilon_d^2)}{\Gamma[\Gamma(1+3b^2)+2b\varepsilon_d]}, \tag{11}$$

$$\varkappa^{-1} = c_i\frac{3}{\pi^2}\frac{2m}{\pi v z T}\frac{1}{1+b^2}\frac{(\Gamma-b\varepsilon_d)^2}{\Gamma^2+\varepsilon_d^2}\left[1-\frac{7\pi^2}{20}\left(\frac{T}{T_1}\right)^2\right];$$

$$\alpha = -\frac{2\pi^2}{3}\frac{T}{e}(1+b^2)\frac{\Gamma(\varepsilon_d+b\Gamma)}{(\Gamma^2+\varepsilon_d^2)(\Gamma-b\varepsilon_d)} = -\frac{2\pi^2}{3}\frac{T}{e}\frac{\tilde{\Gamma}\tilde{\varepsilon}_d}{(\tilde{\Gamma}-b\tilde{\varepsilon}_d)[(\tilde{\Gamma}-b\tilde{\varepsilon}_d)^2+\tilde{\varepsilon}_d^2]}(1+b^2). \tag{12}$$

The Lorentz number $L \equiv \kappa/\sigma T$ depends on the temperature:

$$L(T) = \frac{\pi^2}{3e^2}\left[1+\frac{\pi^2}{60}\left(\frac{T}{T_1}\right)^2\right]. \tag{13}$$

Formulas (10)–(13) are accurate to the first terms of the expansion with respect to T, which is assumed to be small in the sense of

$$T \ll T_1,\ \max\{|\varepsilon_d|, \Gamma\}.$$

A curious case is $\tilde{\epsilon}_d = 0$, in which the "localized level" in the Hamiltonian (2) lies exactly on the Fermi surface. Then

$$\alpha = 0,\quad \rho = c_i\frac{2m}{\pi v z e^2}\left[1-\frac{\pi^2}{3}\left(\frac{T}{\tilde{\Gamma}}\right)^2\right]$$

$$\chi_i = \frac{2N_i g^2\mu^2}{\pi\tilde{\Gamma}}\left[1-\frac{\pi^2}{3}\left(\frac{T}{\tilde{\Gamma}}\right)^2(1-3b^2)\right],$$

$$\Delta c_v = \frac{2\pi}{3}N_i\frac{T}{\tilde{\Gamma}}.$$

In this case there exists for all the phenomena a single temperature scale $\tilde{\Gamma}$, which plays the role of the "Kondo temperature." But then $\alpha = 0$, which does not agree with experiment. In the general case when $\tilde{\epsilon}_d \neq 0$ it is impossible to introduce a single scale. Formulas (12), (5), and (6) are quite similar to the results of Nagaoka[10]

$$\rho = c_i\frac{2m}{\pi v z e^2}\left[1-\frac{\pi^2}{3}\left(\frac{T}{\Delta}\right)^2\right],\quad c_v = \frac{2\pi}{3}\frac{T}{\Delta} \tag{14}$$

and Klein[11]

$$\chi_i = \frac{5{,}4}{\pi}\frac{N_i\mu^2}{T_K}\left[1-2{,}4\left(\frac{T}{T_K}\right)^2\right].$$

Nagaoka derived (14) by using the Zubarev method in superconductivity to describe the binding of free electrons with magnetic impurities. Klein used the model of Takano and Ogawa, which is analogous to Gor'kov's method in superconductivity. The method by which Nagaoka obtained his results is not quite correct, but

his formulas agree well with experiment. Star[12] modified Nagaoka's formulas (and obtained better agreement with experiment) by introducing the empirical reciprocal lifetime of the conduction electrons

$$\tau^{-1}=\frac{2N_i}{\pi\nu}\left[A-\mathrm{Re}\left(e^{2i\delta}\frac{\omega-i\Delta}{\omega+i\Delta}\right)\right], \tag{15}$$

where δ is the phase shift of the potential scattering and Δ is an energy parameter of the order of the Kondo temperature. In (5) there are three fitting parameters (A, δ, and Δ). Star obtained from (15)

$$\alpha=\frac{2\pi^2}{3}\frac{1}{e}\frac{T}{\Delta}\frac{\sin 2\delta}{A+\cos 2\delta},$$

$$\rho=c_i\frac{2m}{\pi\nu e^2}(A+\cos 2\delta)\left[1-\frac{\pi^2}{3}\left(\frac{T}{\Delta}\right)^2\frac{2\cos 2\delta}{A+\cos 2\delta}\right],$$

which is quite similar to formulas (12) and (10), in which there are likewise three free parameters (Γ, ϵ_d, and b). In Star's formula α vanishes if there is no potential scattering, and expression (12) vanishes only if $\tilde{\epsilon}_d=0$.

The fundamental difference from our formulas is that ours are derived rigorously from the model (2), whereas the assumption concerning the scattering amplitude, on which the formulas of Nagaoka, Klein, and Star are based, does not follow from any macroscopic model.

We see thus that the model proposed for the description of the magnetic impurities at low temperatures, in spite of its simplicity, gives good agreement with experiment.

6. SUPERCONDUCTING STATE

As is well known,[8] the superconducting transition temperature T_c is determined from the singularities of a vertex part of the type

with zero entering 4-momentum. Accurate to first-order in ω_D/ϵ_F, this temperature is

$$\lambda(1+\lambda F)^{-1},$$

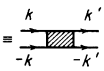
where $\lambda<0$ is the electron coupling constant, ω_D is the Debye frequency,

$$F=T\sum_{|\omega|<\omega_D}\int\frac{d^3\mathbf{k}}{(2\pi)^3}\mathfrak{G}(k)\mathfrak{G}(-k), \tag{16}$$

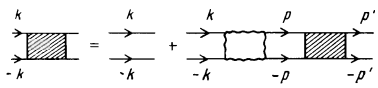
and $\mathfrak{G}$ is the Green's function of the electrons of the normal metal.

In the presence of impurities it is necessary to average (16) over their positions, and we obtain for the quantity

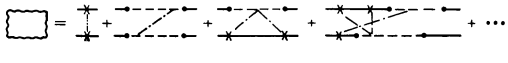
$$\frac{1}{V}\overline{\sum_{k'}\mathfrak{G}(k,k')\mathfrak{G}(-k,-k')}\equiv\Pi(k)\equiv$$



(V_K is the volume of the metal) the equation



where



In analogy with the procedure used by Abrikosov and Gor'kov,[13] we can neglect here diagrams with intersections, and then the equation for $\Pi(k)$ takes the form

$$\Pi(k)=\bar{\mathfrak{G}}(k)\bar{\mathfrak{G}}(-k)\left[1+N_i^{-1}|\Sigma(\omega)|^2\int\frac{d^3\mathbf{p}}{(2\pi)^3}\Pi(p)\right],\quad p=(\mathbf{p},\omega).$$

Solving this equation by integrating with respect to $d^3k/(2\pi)^3$, we obtain

$$F=T\sum_{|\omega_l|<\omega_D}\Lambda(\omega),\quad \Lambda(\omega)=\frac{\pi\nu}{|\omega|}\left[1+\frac{c_i\zeta\epsilon_F\Gamma}{\epsilon_d^2+(\Gamma+|\omega|)^2}\right]^{-1}, \tag{17}$$

where $\zeta^{-1}=3\pi z/4$. It is seen from (17) that the influence of the potential scattering reduces only to a renormalization of ϵ_d and Γ.

From the equation

$$1+\lambda F=0$$

it follows under the assumptions

$$T_c\ll\max\{\Gamma,\epsilon_d\},\quad \omega_D^2\gg\max\{\Gamma^2,\epsilon_d^2,c_i\zeta\epsilon_F\Gamma\}$$

that

$$\ln\frac{T_c}{T_{c0}}=-\frac{c_i\zeta\epsilon_F\Gamma}{\Gamma^2+\epsilon_d^2}\left\{\ln\frac{2\gamma}{\pi T_{c0}}\sqrt{\Gamma^2+\epsilon_d^2+c_i\zeta\epsilon_F\Gamma}-\frac{\Gamma}{\sqrt{\epsilon_d^2+c_i\zeta\epsilon_F\Gamma}}\operatorname{arctg}\frac{\sqrt{\epsilon_d^2+c_i\zeta\epsilon_F\Gamma}}{\Gamma}\right\},$$

where $T_{c0}=(\gamma/\pi)2\omega_D e^{1/\nu\lambda}$ is the superconducting transition temperature of the pure metal, $\gamma=e^C\approx1.78$, and c is Euler's constant.

If $c_i\zeta\epsilon_F\Gamma\gg\epsilon_d^2$, we have

$$\frac{T_c}{T_{c0}}\approx1-\frac{c_i\zeta\epsilon_F\Gamma}{\Gamma^2+\epsilon_d^2}\left[\ln\frac{2\gamma\sqrt{\Gamma^2+\epsilon_d^2}}{\pi T_{c0}}-\frac{\Gamma}{\epsilon_d}\operatorname{arctg}\frac{\epsilon_d}{\Gamma}\right], \tag{18}$$

and if $c_i\zeta\epsilon_F\Gamma\gg\epsilon_d^2+\Gamma^2$ then

$$\frac{T_c}{T_{c0}}\approx\left[\frac{4\gamma^2}{\pi^2T_{c0}^2}c_i\zeta\epsilon_F\Gamma\right]^{-x/2}=(\mathrm{const}\,x)^{-x/2}, \tag{19}$$

where $x=c_i\zeta\epsilon_F\Gamma/(\epsilon_d^2+\Gamma^2)$.

Abrikosov and Gor'kov,[13] who did not take the Kondo effect into account, found that there exists a certain magnetic-impurity concentration at which T_c vanishes. From (19) it follows that, owing to the screening of the impurity spin, $T_c\to0$ only asymptotically as $x\to\infty$.

All the derived formulas are value only at $T\ll T_K$. Consequently, both (18) and (19) are meaningful at $T_{c0}\ll T_K$; on the other hand if $T_{c0}\gtrsim T_K$, then only (19) can be used, and furthermore only at concentrations such that $T_c\ll T_K$.

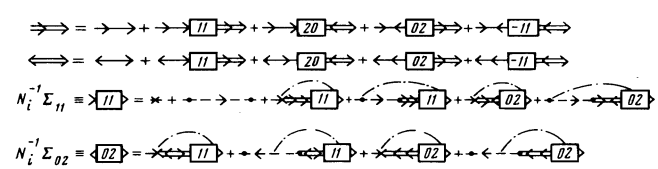
To find the energy gap it is necessary to write down the system of fundamental equations of the superconductor.

Using the notation

$\mathfrak{G}_{\alpha\beta}(x,x')\equiv-\langle T\tilde{\varphi}_\alpha(x)\tilde{\bar{\varphi}}_\beta(x')\rangle\equiv\Longrightarrow$, $\mathfrak{F}^+_{\alpha\beta}(x,x')\equiv\langle\tilde{\bar{\varphi}}_\alpha(x)\tilde{\bar{\varphi}}_\beta(x')\rangle\equiv\Longleftarrow$

$\mathfrak{G}^{(0)}\equiv\longrightarrow$, $\mathfrak{F}^{(0)}\equiv\longleftarrow$ etc.

these equations take the form



Similarly,[8]

$$\mathfrak{F}^+_{\alpha\beta}=g_{\alpha\beta}\mathfrak{F}^+,\quad \mathfrak{F}_{\alpha\beta}=-g_{\alpha\beta}\mathfrak{F},\quad \mathfrak{G}_{\alpha\beta}=\delta_{\alpha\beta}\mathfrak{G},\quad g_{\alpha\beta}=\begin{pmatrix}0&1\\-1&0\end{pmatrix}_{\alpha\beta},$$
$$(\Sigma_{20})_{\alpha\beta}=-g_{\alpha\beta}\Sigma_{20},\quad (\Sigma_{02})_{\alpha\beta}=g_{\alpha\beta}\Sigma_{02},\quad (\Sigma_{11})_{\alpha\beta}=\delta_{\alpha\beta}\Sigma_{11}.$$

In addition, if there is no external field we have in a homogeneous superconductor, after averaging over the impurity positions

$$\mathfrak{F}(p) = \mathfrak{F}^{+}(p), \quad \Sigma_{20}(p) = \Sigma_{02}(p).$$

Taking all the foregoing into account and using the explicit expressions for the Green functions of the pure superconductor,[8] we obtain from the first two equations

$$\mathfrak{G} = -\frac{i\tilde{\omega}_n + \xi'}{\tilde{\omega}_n^2 + \xi'^2 + \tilde{\Delta}_n^2}, \qquad \mathfrak{F} = \frac{\tilde{\Delta}_n}{\tilde{\omega}_n^2 + \xi'^2 + \tilde{\Delta}_n^2}, \tag{20}$$

where

$$i\tilde{\omega}_n = i\omega_n - \Sigma_{11}^{0}(\omega_n), \quad \tilde{\Delta}_n = \Delta + \Sigma_{02}(\omega_n), \quad \xi' = \xi - \Sigma_{11}^{e},$$

$$\Sigma_{11}^{0}(\omega) + \Sigma_{11}^{e}(\omega) = \Sigma_{11}(\omega), \quad \Sigma_{11}^{0}(-\omega) = -\Sigma_{11}^{0}(\omega), \quad \Sigma_{11}^{e}(-\omega) = \Sigma_{11}(\omega),$$

Δ is the electron-pair density parameter ($\Delta = |\lambda F(x, x')|_{x' \to x}$).

After substituting (2) in the last two equations, we obtain the following system for the determination of $\tilde{\omega}_n$ and $\tilde{\Delta}_n$:

$$\tilde{\omega}_n = \omega_n + \frac{c_i \zeta \varepsilon_F}{1 + b^2}\left\{\omega_n \tilde{\Gamma} + \frac{\tilde{\omega}_n}{\sqrt{\tilde{\omega}_n^2 + \tilde{\pi}_n^2}}[(\Gamma - b\varepsilon_d)^2 + b^2\omega_n^2]\right\}$$

$$\times\{\varepsilon_d^2 + \Gamma^2 + \omega_n^2 + 2\Gamma\omega_n\tilde{\omega}_n/\sqrt{\tilde{\omega}_n^2 + \tilde{\Delta}_n^2}\}^{-1}, \tag{21}$$

$$\tilde{\Delta}_n = \Delta + \frac{c_i \zeta \varepsilon_F}{1 + b^2}\frac{\tilde{\Delta}_n}{\sqrt{\tilde{\Delta}_n^2 + \tilde{\omega}_n^2}}\frac{(\Gamma - b\varepsilon_d)^2 + b^2\omega_n^2}{\varepsilon_d^2 + \Gamma^2 + \omega_n^2 + 2\Gamma\omega_n\tilde{\omega}_n/\sqrt{\tilde{\omega}_n^2 + \tilde{\Delta}_n^2}}.$$

Just as in [13], the gap in the energy spectrum is determined by the positive frequency ω at which an imaginary component appears for the first time in the Fourier components of the retarded time-dependent Green functions $G_R(p, \omega)$ and $iF_R(p, \omega)$ (at $T = 0$) which are obtained from $\mathfrak{G}$ and $\mathfrak{F}$ by making the transitions $i\omega_H \to \omega + i\delta$ and $T \to 0$. From (21) we can obtain (on going to the time representation by making the substitutions $i\omega_n \to \omega$, $i\tilde{\omega}_n \to \tilde{\omega}$, and $\tilde{\Delta}_n \to \tilde{\Delta}$) the relation

$$\frac{\omega}{\Delta_0} = \frac{\tilde{\omega}}{\tilde{\Delta}}\left[1 + \tilde{\Gamma}\frac{(\tilde{\Delta} - \Delta_0)\sqrt{1 - \tilde{\omega}^2/\tilde{\Delta}^2}}{(\Gamma - b\varepsilon_d)^2 - b^2\omega^2}\right]^{-1} \tag{22}$$

(Δ_0 is the value of Δ at $T = 0$). The start of the spectrum is given by the maximum real value of ω at real $\tilde{\omega}$ and $\tilde{\Delta}$. It is seen from (22) that this maximum is equal to Δ_0. Thus, the energy gap in the spectrum coincides with Δ_0, which characterizes the density of the "condensate," in contrast to the case of unscreened magnetic impurities (see [13]).

We can determine Δ_0, just as in [13], from the relation

$$\ln\frac{\Delta_0}{\Delta_{00}} = \int_0^\infty dx\left[\frac{1}{\sqrt{1 + u^2}} - \frac{1}{\sqrt{1 + x^2}}\right],$$

where

$$u = x[1 + c_i\zeta\varepsilon_F\Gamma(\varepsilon_d^2 + \Gamma^2 + \Delta_0^2x^2 + 2\Gamma\Delta_0 xu/\sqrt{1 + u^2})^{-1}]$$

Δ_{00} is the value of Δ_0 in the pure metal.

Assuming $\Delta_{00} \ll \max\{\Gamma, \epsilon_d\}$, we can calculate the integral in the limiting cases:

$c_i\zeta\varepsilon_F\Gamma \ll \Gamma^2 + \varepsilon_d^2$:

$$\ln\frac{\Delta_0}{\Delta_{00}} \approx -\frac{c_i\zeta\varepsilon_F\Gamma}{\varepsilon_d^2 + \Gamma^2}\left[\ln\frac{2\sqrt{\Gamma^2 + \varepsilon_d^2}}{e\Delta_{00}} - \frac{\Gamma}{\varepsilon_d}\operatorname{arctg}\frac{\varepsilon_d}{\Gamma}\right],$$

$c_i\zeta\varepsilon_F\Gamma \gg \Gamma^2 + \varepsilon_d^2$:

$$\ln\frac{\Delta_0}{\Delta_{00}} \approx -\frac{1}{2}\frac{c_i\zeta\varepsilon_F\Gamma}{\varepsilon_d^2 + \Gamma^2}\ln\frac{4c_i\zeta\varepsilon_F\Gamma}{\Delta_{00}}.$$

We see that the limiting functions $\Delta_0(c_i)$ are similar to the functions $T_c(c_i)$ (see (18) and (19)).

The author thanks A. A. Abrikosov for suggesting the problem and for all-out help with the work.

[1)] The spin indices can be omitted, since all the interactions are spin-conserving.

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Translated by J. G. Adashko
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