THE SCATTERING OF CONDUCTION ELECTRONS BY PARAMAGNETIC IMPURITIES

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Submitted December 1, 1967

Zh. Eksp. Teor. Fiz. 54, 1455-1462 (May, 1968)

Using a dispersion approach, we find an expression for the amplitude for scattering of an electron by a paramagnetic impurity. The solution found has a simple analytical structure and for integral values of the spin of the impurity it can be expressed in terms of elementary functions.

T is well known that it is impossible to solve the problem of the scattering of conduction electrons by paramagnetic impurities using perturbation theory. In the papers by Suhl and $Wong^{[1]}$ and $Maleev^{[2,3]}$ a dispersion approach was used to obtain a solution. In a paper by Maleev and the author^[41] it was shown that near the Fermi surface the results of these papers are practically the same and we shall therefore compare the results obtained in the following only with^[2,3].

In the present paper we obtain the solution of the problem in a simpler form than in^[2,3]. In particular, the scattering amplitude is for integral values of the spin of the impurity expressed in terms of elementary functions. This solution is similar in form to the solution of the equations of Chew and Low^[5-7]. The expressions obtained in the present paper for the amplitude are very convenient for a generalization to the case of superconductivity. In a paper by the present author^[8] such a kind of solution was constructed for spin one. However, a generalization of the solution obtained in^[8] to the case of larger spins leads to the appearance of energy poles in the complex plane in the scattering amplitude. In the present paper we construct a solution for arbitrary spin which is free from this difficulty and agrees well with presently available experimental data. [9]

It is well known that the scattering amplitude F has the form $F = A + BS \cdot \sigma$ where S is the impurity spin and the σ_i are Pauli matrices. For the quantities A and B there are unitarity relations (see^[3,10])

$$Im A = k\{|A|^{2} + S(S+1)|B|^{2}\},$$

Im B = k{A*B + AB* - |B|² th (\omega / 2T)}, (1)

k is the electron momentum, ω the energy reckoned from the Fermi surface, and T the temperature. Here and henceforth we assume that $\omega = \omega + i\delta$. In the following we shall use Born amplitudes which we denote by a and b.

We introduce instead of A and B amplitudes α_{\pm} and corresponding to them the S-matrix elements S_{*}:

$$a_{+} = A + BS, \quad a_{-} = A - B(S+1),$$

 $S_{\pm} = 1 + 2ika_{\pm}.$
(2)

The unitarity conditions for α_{\pm} have the form^[3]

$$\operatorname{Im} a_{+} = k \left\{ |a_{+}|^{2} + \frac{2S}{(2S+1)^{2}} |a_{+} - a_{-}|^{2}n(\omega) \right\},$$

$$\operatorname{Im} a_{-} = k \left\{ |a_{-}|^{2} - \frac{2(S+1)}{(2S+1)^{2}} |a_{+} - a_{-}|^{2}n(\omega) \right\},$$
(3)

 $n(\omega)$ is the Fermi distribution function.

Let us consider the function $u(^{[3,11]})$:

$$u = \frac{1 + 2ikA}{B} = 2ik \frac{(S+1)S_+ + SS_-}{S_+ - S_-}.$$
 (4)

Suhl has shown that

$$u(\omega + i\delta) - u(\omega - i\delta) = 2ik \operatorname{th} (\omega / 2T).$$
(5)

Bearing in mind that $u(\omega - i\delta) = u^*(\omega + i\delta)$ we get from (5)

$$u(\omega) = P(\omega) + \frac{1}{\pi} \int_{-E_F}^{\infty} \frac{k' d\omega'}{\omega' - \omega} \operatorname{th} \frac{\omega'}{2T}.$$
 (6)

 $P(\omega)$ is a rational function. We choose $P(\omega)$ in the same way as in^[2,3]. Carrying out calculations completely analogous to those in^[3], we get near the Fermi surface

$$u(\omega) = \frac{2p_0}{\pi g} - \frac{2p_0}{\pi} \left\{ \ln \frac{\pi T}{2\gamma E_F} + \Psi\left(\frac{1}{2} - \frac{i\omega}{2\pi T}\right) - \Psi\left(\frac{1}{2}\right) \right\}, \quad \text{Im } \omega > 0;$$

$$u(\omega) = \frac{2p_0}{\pi g} - \frac{2p_0}{\pi} \left\{ \ln \frac{\pi T}{2\gamma E_F} + \Psi\left(\frac{1}{2} + \frac{i\omega}{2\pi T}\right) - \Psi\left(\frac{1}{2}\right) \right\}, \quad \text{Im } \omega < 0;$$

$$\frac{1}{g} = \frac{\pi}{2p_0 b} \left[1 - \frac{4p_0 b}{\pi} (1 - \ln 2) + a_{+} a_{-} p_0^2 \right],$$

$$a_{+} = a + bS, \quad a_{-} = a - b(S + 1), \quad (7)$$

where Ψ is the logarithmic derivative of the Γ -function, $\ln \gamma = C = 0.577$.

It is convenient to introduce instead of u the dimensionless function

$$\Phi(\omega) = u / 2ik. \tag{8}$$

We have from (7) and (8) near the Fermi surface

$$\frac{i}{\pi} \left\{ -\frac{1}{g} + \ln \frac{\pi T}{2\gamma E_F} + \Psi \left(\frac{1}{2} - \frac{i\omega}{2\pi T} \right) - \Psi \left(\frac{1}{2} \right) \right\}, \quad \text{Im } \omega > 0;$$

$$\Phi = -\frac{i}{\pi} \left\{ -\frac{1}{g} + \ln \frac{\pi T}{2\gamma E_F} + \Psi \left(\frac{1}{2} + \frac{i\omega}{2\pi T} \right) - \Psi \left(\frac{1}{2} \right) \right\}, \quad \text{Im } \omega < 0.$$
(9)

One shows easily that on the real axis

$$\Phi = \frac{i}{\pi} \left\{ -\frac{1}{g} + \ln \frac{\pi T}{2\gamma E_F} + \frac{1}{2} \left[\Psi\left(\frac{1}{2} + \frac{i\omega}{2\pi T}\right) + \Psi\left(\frac{1}{2} - \frac{i\omega}{2\pi T}\right) - 2\Psi\left(\frac{1}{2}\right) \right] \right\} + \frac{1}{2} \operatorname{th} \frac{\omega}{2T}.$$
(10)

When $|\omega| \ll T$

 $\Phi =$

$$\Phi = \frac{i}{\pi} \left\{ -\frac{1}{g} + \ln \frac{\pi T}{2\gamma E_F} \right\}.$$
(11)

When $|z| \gg 1$, $\Psi(z) \approx \ln z$ so that when $|\omega| \gg T$

$$\Phi = \frac{i}{\pi} \left\{ -\frac{1}{g} + \ln \frac{\omega}{E_F} \right\} + \frac{1}{2}.$$
 (12)

From (4) and (8) we get easily the relation

$$\frac{S_+}{S_-} = \frac{\Phi + S}{\Phi - (S+1)}.$$
(13)

Moreover, using (2), (3), and (13), we find

$$|S_{\pm}|^{2} = \frac{(\operatorname{Im} \Phi)^{2} + \frac{1}{4}(2S + 1 \mp 2n)^{2}}{(\operatorname{Im} \Phi)^{2} + \frac{1}{4}[(2S + 1)^{2} - 4n(1 - n)]}.$$
 (14)

Expression (14) is the same as the analogous formula for η_{\pm}^2 obtained in^[3].

We consider first the zero temperature case. When T = 0 $|S_+|^2 = 1, \omega > 0$:

$$|S_{\pm}|^{2} = \frac{(\operatorname{Im} \Phi)^{2} + \frac{1}{4}(2S + 1 \mp 2)^{2}}{(\operatorname{Im} \Phi)^{2} + \frac{1}{4}(2S + 1)^{2}}, \quad \omega < 0.$$
(15)

The unitarity conditions (15) determine S_{\pm} apart from functions of modulus unity while Eq. (13) means that this function is the same for S_{\pm} and for S_{-} . Denoting it by $D_{S}(\omega)$ we get

$$S_{+} = \varphi_{S}(\omega) D_{S}(\omega),$$

$$S_{-} = \frac{\Phi - (S+1)}{\Phi + S} \varphi_{S}(\omega) D_{S}(\omega),$$

$$|D_{S}(\omega)|^{2} = 1.$$
(16)

We shall find $\varphi_{\rm S}$ for integral S. From (15) it is clear that

$$|S_+(S+1)|^2 = |S_-(S)|^{-2}$$
.

Moreover, we have from (16)

$$\varphi_{S+1}(\omega) = \frac{\Phi + S}{\Phi - (S+1)} \varphi_S^{-1}(\omega). \tag{17}$$

One shows easily that when S = 1 and 2 the unitarity condition (15) is satisfied by the functions

$$\varphi_1(\omega) = \frac{\Phi}{\Phi - 1}, \quad \varphi_2(\omega) = \frac{\Phi^2 - 1}{\Phi(\Phi - 2)}.$$
 (18)

From the recurrence relation (17) and (18) we get easily $\varphi_{\rm S}$ for any integral S:

$$\varphi_{S}(\omega) = \prod_{n=1}^{S} \frac{\Phi^{-1/2} + (-1)^{n-1} [S - n + \frac{1}{2}]}{\Phi^{-1/2} - (-1)^{n-1} [S - n + \frac{1}{2}]}.$$
 (19)

Equations (18) and (19) are the same as the corresponding equations obtained when the Chew-Low equations are solved.^[5,7].

We make some remarks. It is clear from (12) that when g < 0 the function Φ has a zero for $\omega = i\epsilon_0$ where

$$\varepsilon_0 = E_F \exp\left(-1 / |g|\right). \tag{20}$$

When g > 0 the function Φ has no zeroes near the Fermi surface (and just the region of energies $|\omega| \sim \epsilon_0$ is of interest to us).

It is clear from (18) that when g < 0 the function $\varphi_2(\omega)$ has a pole in the complex plane on the physical sheet; in a similar way it follows from (19) that all φ_S for even S will have the same pole. However, such a pole contradicts the spectral representation for the amplitudes.^[2] We must thus choose the unimodular function $D_S(\omega)$ such that this pole is eliminated. At the same time we also eliminate the zeroes of φ_S for odd S. Such an elimination of zeroes is not required by the presence of a spectral representation. However, the unitarity condition (1) depends analytically on S so that it is

natural to assume that the solution will also be analytical in S. In the Appendix we give such a solution (it gives the answer also for half-odd-integral S). For integral S near the Fermi surface we get when $|ka_t| \ll 1$

$$S_{+} = \varphi_{S} \frac{\omega + i\epsilon_{0}}{\omega - i\epsilon_{0}} \frac{1 + ika}{1 - ika}, \quad S = 2k + 1; \quad (21)$$
$$S_{+} = \varphi_{S} \frac{\omega - i\epsilon_{0}}{\omega + i\epsilon_{0}} \frac{1 + ika}{1 - ika}, \quad S = 2k.$$

When g > 0 there are no poles or zeroes in $\varphi_S(\omega)$ so that factors such as $(\omega - i\epsilon)(\omega + i\epsilon)^{-1}$ do not appear. In that case we get for $|ka_{\pm}| \ll 1$

$$S_{+} = \varphi_{S} \frac{1 + ika}{1 - ika} \,. \tag{22}$$

From Eqs. (2) and (13) we get easily the following expressions for the scattering amplitudes

$$A = \frac{1}{2ik} \left\{ \frac{\Phi}{\Phi + S} S_{+}(\Phi) - 1 \right\},$$

$$B = \frac{1}{2ik} \frac{S_{+}(\Phi)}{\Phi + S}.$$
 (23)

Let us consider in more detail the case S = 1, a = 0. When g < 0 we get from Eqs. (12), (18), (21), and (23)

$$A = \frac{1}{2ik} \left\{ \frac{(z + \frac{1}{2i\pi g})^2}{(z + \frac{1}{2i\pi g})^2 + (\pi g)^2} \frac{\omega + i\varepsilon_0}{\omega - i\varepsilon_0} - 1 \right\},$$

$$B = b \frac{z + \frac{1}{2i\pi g}}{(z + \frac{1}{2i\pi g})^2 + (\pi g)^2} \frac{\omega + i\varepsilon_0}{\omega - i\varepsilon_0}$$
(24)

When g > 0

$$A = b \frac{i\pi g}{(z + 1/2i\pi g)^2 + (\pi g)^2},$$

$$B = b \frac{z + 1/2i\pi g}{(z + 1/2i\pi g)^2 + (\pi g)^2}, \quad z = 1 - g \ln(\omega/E_F).$$
(25)

When g>0 we have $|z|\gg g$ in the whole energy range, so that in this case

$$A = \frac{i\pi g}{z^2} \quad b, \qquad B = \frac{b}{z} \tag{26}$$

Equation (26) is the same as the result obtained by Abrikosov.^[12] The scattering cross section is equal to

$$\sigma = 4\pi \{ |A|^2 + S(S+1) |B|^2 \} = 8\pi b^2 / |z|^2.$$
(27)

It is clear that one obtains the same result also when g < 0, $|\omega| \gg \epsilon_0$. When g < 0 and $|\omega| \ll \epsilon_0$ we have again $|z| \gg g$; we get from (24), expanding in $g|z|^{-1}$

$$A = \frac{i}{p_0} - \frac{i\pi g}{|z|^2} b, \quad B = -\frac{b}{z}, \quad \sigma = \frac{4\pi}{p_0^2}.$$
 (28)

Let us now consider the region $g<0,\,\omega\sim\varepsilon_0.$ We note that for negative g we can write the quantity z in the form

$$z = -g \ln (\omega / \varepsilon_0). \tag{29}$$

When $|\omega - \epsilon_0| \ll \epsilon_0$ we can expand the logarithm in a power series: $z = -g(\omega - \epsilon_0)/\epsilon_0$. Then we have

$$A = \frac{1}{2ip_0} \left\{ \frac{(\omega - \varepsilon_0 - i\pi\varepsilon_0/2)^2}{(\omega - \varepsilon_0 - i\pi\varepsilon_0/2)^2 + (\pi\varepsilon_0)^2} \frac{\omega + i\varepsilon_0}{\omega - i\varepsilon_0} - 1 \right\}$$
$$B = -\frac{\pi}{2p_0} \frac{\varepsilon_0(\omega - \varepsilon_0 - i\pi\varepsilon_0/2)}{(\omega - \varepsilon_0 - i\pi\varepsilon_0/2)^2 + (\pi\varepsilon_0)^2} \frac{\omega + i\varepsilon_0}{\omega - i\varepsilon_0}$$
(30)

For $\omega = \epsilon_0$ we get, for instance,

$$A = \frac{3i-1}{6p_0}, \quad B = -\frac{1}{3p_0}, \quad \sigma = \frac{2\pi}{p_0^2}.$$
 (31)

We turn now to a discussion of finite temperatures. When $T \neq 0$ the function φ_S does not satisfy the unitarity condition (14). We shall show, however, that in the case when $|1 - g \ln (\pi T/2\gamma E_F)| \gg g$, φ_S up to terms of order $g^4[1 - g \ln(\pi T/2\gamma E_F)]^{-4}$ satisfies the unitarity condition and Eqs. (21) and (22) give the solution of the problem with the only correction that we must substitute ϵ_1 for ϵ_0 , where $i\epsilon_1$ is the root of the equation $\Phi = 0$ for finite T. We put

$$S_{+} = \varphi_{\mathcal{S}}(\omega) M_{\mathcal{S}}(\omega) D_{\mathcal{S}}(\omega), \quad |D_{\mathcal{S}}|^{2} = 1.$$
(32)

We shall not consider the quantity S₋ since S₋ is connected with S_{+} by Eq. (13). From (32) and (14) we have

$$|M_{s}|^{2} = \frac{(\operatorname{Im} \Phi)^{2} + \frac{1}{4}(2S+1-2n)^{2}}{(\operatorname{Im} \Phi)^{2} + \frac{1}{4}[(2S+1)^{2} - 4n(1-n)]} |\varphi_{s}|^{-2}.$$
 (33)

Moreover, as $in^{[1-3]}$, we put

$$M_{s} = \exp (2i\Psi_{s}),$$

$$\Psi_{s} = -\frac{k}{4\pi} \int_{-E_{\pi}}^{\infty} \frac{d\omega'}{k'(\omega'-\omega)} \ln |M_{s}|^{2}.$$
(34)

We choose the function $\boldsymbol{D}_{\!\boldsymbol{S}}$ from the same considerations as in the case T = 0.

One shows easily that when the temperature increases the zero of the function $\Phi(\omega)$ approaches the point $\omega = 0$ along the imaginary axis and at some temperature

$$T_c = 2\gamma \varepsilon_c / \pi \tag{35}$$

vanishes. We put for g < 0, $T < T_c$

$$S_{+}(S) = M_{S}\varphi_{S} \frac{\omega + i\epsilon_{1}}{\omega - i\epsilon_{1}} \frac{1 + ika}{1 - ika}, \quad S = 2n + 1;$$

$$S_{+}(S) = M_{S}\varphi_{S} \frac{\omega - i\epsilon_{1}}{\omega + i\epsilon_{1}} \frac{1 + ika}{1 - ika}, \quad S = 2n.$$
(36)

Here $i\epsilon_1$ is the root of the equation $\Phi = 0$. When g < 0, $T > \, T_{\mathbf{C}}$ and also when g > 0

$$S_{+} = M_{S}\varphi_{S} \frac{1 + ika}{1 - ika}.$$
(37)

The analysis of Eqs. (36) and (37) for arbitrary ω and T is difficult. We consider again some particular cases. Let us consider $M_S(\omega)$ for S = 1. From (10), (14), (18), and (34) we have

$$\Psi_{i} = -\frac{k}{4\pi} \int_{-E_{F}}^{\infty} \frac{d\omega'}{k'(\omega'-\omega)} \ln\left[\frac{(\operatorname{Im}\Phi)^{2} + \frac{1}{4}(1+2n)^{2}}{(\operatorname{Im}\Phi)^{2} + \frac{1}{4}(1-2n)^{2}} \times \frac{(\operatorname{Im}\Phi)^{2} + \frac{1}{4}(3-2n)^{2}}{(\operatorname{Im}\Phi)^{2} + \frac{1}{4}(9-4n(1-n)]}\right].$$
(38)

It is clear that when $|\omega| \gg T$ the integrand vanishes so that the integration is only over the region $|\omega| \lesssim T$ but it is clear from (11) that we may assume that Φ in that range of energies is equal to

$$\Phi = -\frac{i}{\pi} \frac{1-gL}{g}, \quad L = \ln \frac{\pi T}{2\gamma E_F}.$$
 (39)

Let us consider the case when $|1 - gL| \gg |g|$ which occurs for g > 0 for all temperatures and when g < 0when $T\gg T_{\rm c}$ and $T\ll T_{\rm c}.$ One then sees easily that

$$|M_1|^2 = 1 + O\left[\left(\frac{g}{1-gL}\right)^4\right].$$
 (40)

Thus, when $|1 - gL| \gg |g|$ the value of Ψ_S is zero up to terms of order $g^4(1 - gL)^{-4}$. We shall neglect these small quantities and assume M_1 to be equal to unity. The same result is also abtained for arbitrary S. As a result we get for $|1 - gL| \gg |g|$ Eqs. (36) and (37) with M_S replaced by unity.

The remaining calculations are completely analogous to the corresponding calculations performed at zero temperature. We give some of the formulae for the amplitudes for a = 0 in some particular cases. When $T \ll |\omega|$, we obtain, of course, Eqs. (24)-(28). When $T \gg |\omega|$ we get when g > 0 or g < 0, but $T \gg T_c$

$$A = b \frac{i\pi g}{(1 - gL)^2}, \quad B = \frac{b}{1 - gL}.$$
 (41)

When g < 0 and $T \ll T_c$ ($|\omega| \ll T \ll T_c \sim \epsilon_1$)

$$A = \frac{i}{p_0} - b \frac{i\pi g}{(1 - gL)^2}, \quad B = -\frac{b}{1 - gL}.$$
 (42)

A comparison of the results obtained in the present paper with the results of^[3] can most conveniently be made by the method used by the author in^[8]. Repeating verbatim the calculations made in^[8] one shows easily that the results of the present paper are the same as those obtained in^[3]. However, our formulae are appreciably simpler while the method of solving the problem which is proposed in the present paper is very convenient to generalize to the case of superconductivity, as we shall do in the near future.

In conclusion the author expresses his gratitude to S. V. Maleev for a large number of interesting discussions.

APPENDIX

All considerations in the Appendix will be given for the zero-temperature case. Let us consider the function, which has a structure very close to the corresponding function in^[6]:

$$K_{s}(\Phi) = \Gamma\left(\frac{1+S}{2} + \frac{\Phi}{2}\right)$$

$$\times \Gamma\left(\frac{1+S}{2} - \frac{\Phi}{2}\right) / \Gamma\left(\frac{S}{2} + \frac{\Phi}{2}\right) \Gamma\left(1 + \frac{S}{2} - \frac{\Phi}{2}\right).$$
(A.1)

Bearing in mind the explicit form of Φ one shows easily that $K_{S}(\Phi)$ satisfies the condition of unitarity for $S_{\scriptscriptstyle +}$ and therefore differs from $S_{\scriptscriptstyle +}$ by a unimodular factor. In contrast to φ_S the functions K_S has no poles in the complex plane on the physical sheet. Indeed, $K_S(\Phi)$ has a pole when $\Phi = \pm (2n + S + 1)$ where n is an integer; at the same time it follows from the explicit form of Φ that $\Phi \pm (2n + S + 1)$ has no zeroes for complex values of the energy. On the other hand, $K_{S}(\Phi)$ is an analytical function of S. For integral S the function $K_{S}(\Phi)$ can be expressed in terms of elementary functions:

$$\begin{split} K_S(\Phi) &= \varphi_S(\Phi) \operatorname{tg} {}^{1/_2} \pi \Phi, \quad S = 2k; \\ K_S(\Phi) &= -\varphi_S(\Phi) \operatorname{ctg} {}^{1/_2} \pi \Phi, \quad S = 2k+1. \end{split} \tag{A.2}$$
 For S = 1, 2 we get

$$K_1(\Phi) = -\frac{\Phi}{\Phi - 1} \operatorname{ctg} \frac{\pi \Phi}{2}, \qquad (A.3)$$
$$K_2(\Phi) = \frac{\Phi^2 - 1}{\Phi(\Phi - 2)} \operatorname{tg} \frac{\pi \Phi}{2}.$$

Using Eq. (12) for Φ at zero temperature one shows easily that $\tan(\pi\Phi/2)$ is a unimodular function. To determine S_{+} we must take into account that far from the Fermi surface S+ must have the usual form $(1 + ika_{+})(1 - ika_{+})^{-1}$. We determine S₊ as follows:

$$S_{+} = \frac{K_{S}(\Phi)}{K_{S}(\Phi_{0})} \frac{1 + ika_{+}}{1 - ika_{+}}, \quad \Phi_{0} = -\frac{i}{\pi g} + \frac{1}{2}.$$
 (A.4)

One shows easily that $K_S(\Phi_0)$ is unimodular; $K_S(\Phi_0)$ is

introduced in order that far from the Fermi surface the expression obtained goes over into the solution for $E_F = 0$.

Bearing in mind that $|g| \ll 1$ one gets easily from (12) and (A.4)

$$\operatorname{tg} \frac{\pi \Phi}{2} \operatorname{ctg} \frac{\pi \Phi_0}{2} = 1, \quad g > 0,$$
$$\operatorname{tg} \frac{\pi \Phi}{2} \operatorname{ctg} \frac{\pi \Phi_0}{2} = \frac{\omega - i\varepsilon_0}{\omega + i\varepsilon_0}, \quad g < 0.$$
(A.5)

The terms dropped in (A.5) are of order $\exp(-|g|^{-1})$, i.e., they are exponentially small. One obtains from (A.2) to (A.5) easily Eqs. (22) and (21) of the main text.

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Translated by D. ter Haar 170