THE SINGLE-PARTICLE APPROXIMATION AND ROLE OF MANY-PARTICLE STATES IN SCATTERING OF AN ELECTRON BY A PARAMAGNETIC IMPURITY

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The problem of scattering of a conductivity electron by a paramagnetic impurity (the Kondo effect) is solved by two methods: by decoupling the chain of the equation for the Green functions (Nagaoka) and by exploiting the analytic properties of the scattering amplitude and the unitarity conditions (Suhl, the author). Neither method, however, is sufficiently well founded. The present paper is dedicated to substantiation of the second method. The role of many-particle states under unitarity conditions is qualitatively investigated in the first part and it is shown that the role mainly consists in renormalization of the Kondo energy. It is also demonstrated that for large impurity spins the scattering amplitude found in the single-particle approximation is the major term in the expansion of the amplitude in inverse powers of the spin. The dynamic problem of electron scattering by a paramagnetic impurity is solved in the second part in the single-particle approximation, and it is shown that the single-particle solution previously obtained by means of the unitarity conditions is correct, i.e., the problem of the so-called CDD ambiguity is correctly solved. From the results obtained in the paper it follows, in particular, that the asymptotic formulas previously derived by the Suhl method for the temperature dependence of physical quantities (resistance, thermal e.m.f., thermal conductivity, and specific heat) are correct.

1. INTRODUCTION

AT the present time there are two distinct approaches to the question of the scattering of a conduction electron by a paramagnetic impurity. Nagaoka's approach[1,2], based on the decoupling of the chain of equations for the Green's functions, and the Suhl approach[3-7], which uses the unitarity conditions[1)]. Both approaches lead to the same expression for the non-exchange part of the scattering amplitude, from which follows the principal result of the theory. When the exchange interaction has a negative sign, the scattering amplitude on the Fermi surface reaches its maximum possible value (ik_F^{-1}), the so-called unitary limit, reliably confirmed by the experiments of Daybell and Steyert[10,11]). However, neither approach can be regarded as well founded from the theoretical point of view. Nagaoka's method employs essentially arbitrary decoupling of the system of equations, which can hardly be justified in any way. Suhl's approach is based on two assumptions, which also have to be justified. First, the many-particle intermediate states are discarded in the unitarity conditions. Second, in determining the scattering amplitude satisfying the unitarity conditions, in spite of a number of additional requirements (analytic properties, agreement with the perturbation-theory series at $E \gg E_F$), some leeway still remains and is eliminated with the aid of an additional assumption (the CDD ambiguity, for details see[4,5]). The question of many-particle states has been treated in a paper by the author[12], where it is shown that the role reduces in the main to a renormalization of the Kondo energy ϵ_0. The CDD ambiguity can be eliminated only by solving the dynamic problem that takes explicit account of the interaction energy, something not done in Suhl's method.

In this paper we consider first, from a somewhat different point of view than earlier, the question of many-particle states, and present qualitative considerations confirming the correctness of the result obtained in[12]. We then proceed to the question of elimination of the CDD ambiguity. As already noted, to this end it is necessary to solve a dynamic problem that makes explicit use of an expression for the interaction energy.

To this end, we decouple also the system of equations for the Green's functions, so as to make the solution automatically satisfy Suhl's single-particle unitarity conditions (this decoupling differs from that proposed by Nagaoka[1]). The solution of the equations obtained in this manner leads to an expression for the scattering amplitude; this expression coincides with that obtained earlier[4-7]. In other words, a correct solution of the single-particle problem was obtained in the cited papers (the equivalence of the results obtained in[4-7] has been demonstrated in[13]).

Thus, we succeed in justifying the two assumptions on which Suhl's method is based. The expression obtained by this method for the scattering amplitude is essentially the correct first approximation to the solution of the problem of the scattering of a conduction electron by a paramagnetic impurity. The refinements arising when account is taken of the many-particle states are discussed in[12] and at the end of the next section. This paper is a continuation of earlier papers[5,6,12] henceforth referred to as I, II, and III.

[1)] We do not concern ourselves with papers in which, besides electron scattering, is considered also the question of the causes of the occurrence of a localized impurity spin (see, for example, the review of Abrikosov [8] and the paper [9]).

2. ROLE OF MANY-PARTICLE INTERMEDIATE STATES

Just as in I and III, we shall consider an ideal electron gas at zero temperature, interacting with a point-like impurity via the potential

$$V(\mathbf{r}) = -4\pi(a+bR)\delta(\mathbf{r})\frac{\partial}{\partial r}r = V_1(\mathbf{r}) + V_2(\mathbf{r})R, \qquad (1)$$
$$R = (\mathbf{S}, \sigma).$$

In the case of non-exchange interaction (b = 0), the problem of scattering by such a potential can be solved exactly, and the delayed scattering amplitude has the same form as in the absence of a Fermi sphere:

$$F = a(1 - ika)^{-1}, \qquad (2)$$

where $k = \sqrt{E}$ (we use units in which $m = \frac{1}{2}$). The validity of (2) can be easily verified for example, by the method given in the book[14]; we shall derive this formula below by still another method. The amplitude (2) satisfies the usual single-particle unitarity condition:

$$\operatorname{Im} F = k|F|^2. \qquad (3)$$

The exchange interaction complicates the problem in two respects. First, inelastic scattering processes become possible (for example, an electron-hole pair is produced when the electron is scattered). Second, the electron and the hole are now scattered in different manners. This is due to the fact that the spin operators of these particles are different (the electron spin is $(\frac{1}{2})\sigma$, but the hole spin is $-(\frac{1}{2})\sigma^{T}$; for details see the authors paper[15]). The latter circumstance, in particular, leads to a change in the elastic part of the unitarity condition. Namely, if we neglect the many-particle intermediate states, then this condition takes the form (see I)

$$\operatorname{Im} A = k[|A|^2 + S(S+1)|B|^2],$$
$$\operatorname{Im} B = k[AB^* + A^*B - |B|^2\varepsilon(\xi)], \qquad (4)$$

where A and B are determined by the equation $F = A + BR$; $\xi = E - E_F$ and $\epsilon(\xi)$ is the sign function. The main feature of this expression is that the form of Im B depends on the sign of ξ.

It will be convenient in what follows to use a model in which the impurity is replaced by a gas of infinitely heavy impurities. In this case we have for the interaction energy, in place of (1),

$$V = \int dx\, dy\, \psi^+(x)\varphi^+(y)V(x-y)\varphi(y)\psi(x), \qquad (5)$$

where ψ and φ are the electron and impurity operators. This model is close to that proposed by Abrikosov[16] and makes it possible to use the ordinary Feynman diagram technique, whereas the Green's function of the impurity has the form $g(\omega) = (\omega + i\delta)^{-1}$; we shall show it dotted. The series of diagrams for the scattering amplitude is shown in Figs. 1 and 2. The analytic expression corresponding to each of these diagrams separately contains terms proportional to powers of the large logarithm $L = \ln(\xi E_F^{-1})$. Thus, for example, the upper diagrams of Fig. 1 contain L linearly. When b = 0, however L vanishes from the expression for the sum of these diagrams (the appearance of L in this sum at $b \neq 0$ is called the "Kondo

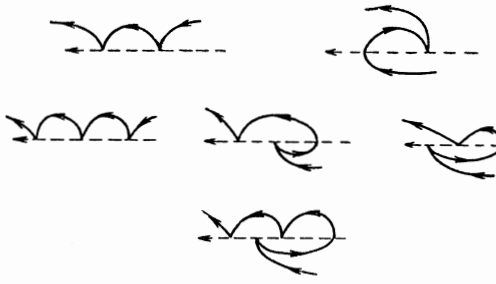

FIG. 1

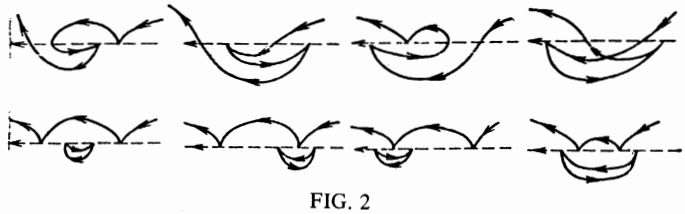

FIG. 2

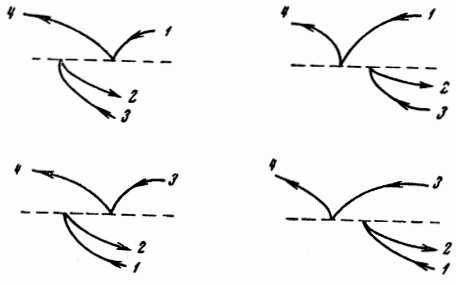

FIG. 3

effect"). From a comparison with (2) it is clear that such a vanishing of L at b = 0 should take place in all orders of perturbation theory.

Simultaneously, there should vanish the contribution made to F also by the many-particle intermediate states. The latter is physically connected with the fact that the scattering of an electron by an infinitely heavy spinless impurity must be elastic, i.e., is not accompanied by pair production. But without such a production no many-particle intermediate states can occur. This qualitative consideration is confirmed by a formal calculation. Let us consider, for example, the amplitude for the coalescence of two electrons and a hole into a single electron. The diagrams for this process in the lowest order of perturbation theory are shown in Fig. 3; they correspond to the following analytic expression (cf. III):

$$\tau^{(0)}_{\mu_4\mu_3\mu_2\mu_1} = -(4\pi)^2 \qquad (6)$$
$$\times\left\{\frac{f_{\mu_2\mu_3}f_{\mu_4\mu_1}}{E_1 - E_4 + i\delta} + \frac{f_{\mu_4\mu_1}f_{\mu_2\mu_3}}{E_3 - E_2 + i\delta} - \frac{f_{\mu_2\mu_1}f_{\mu_4\mu_3}}{E_3 - E_4 + i\delta} - \frac{f_{\mu_4\mu_3}f_{\mu_2\mu_1}}{E_1 - E_2 + i\delta}\right\},$$

where $f = a + bR$ and μ_i is the projection of the spin of the i-th particle. Particles 1, 3, and 4 are electrons $[E_{1,3,4} > E_F]$, and particle 2 is a hole $[E_2 < E_F]$. Therefore the denominators of the second and fourth curves do not vanish. Further, if the energy conservation law $E_1 + E_3 = E_2 + E_4$ is satisfied, then the first two terms combine into an expression proportional to the commutator $[f_{\mu_2\mu_3}, f_{\mu_4\mu_1}] = b^2[R_{\mu_2\mu_3}, R_{\mu_4\mu_1}]$; the same occurs also with the second pair of terms. Therefore, where the real coalescence process at

b = 0 we have $\tau^{(0)}_{1,3} = 0$. Obviously, this conclusion should hold also in the higher orders of perturbation theory; however, we shall not investigate this question in detail.

With the aid of (6) and the analogous expression for the electron decay amplitude we can easily write an expression for the contribution made to F by all the fourth-order diagrams containing in one of the intermediate states two electrons and a hole (Fig. 2):

$$F^{(0)}_{3\alpha'\alpha} = \frac{1}{2}\left(\frac{i}{(2\pi)^4}\right)^3 \int d^4p_1\, d^4p_2\, d^4p_3\, \tau^{(0)}_{\alpha'\mu_1\mu_2\mu_3}(p, p_1, p_2, p_3)$$

$$\times G(p_1)G(p_2)G(p_3)g(p - p_1 - p_3 + p_2)\tau^{(0)}_{\mu_3\mu_2\mu_1\alpha}(p_3, p_2, p_1, p)$$

$$= -\frac{1}{2(2\pi)^9}\int dp_1\, dp_2\, dp_3\, \vartheta_+(\xi_1)\vartheta_+(\xi_3)\vartheta_-(\xi_2)\frac{(\tau^{(0)}_{13}(\xi_i)\tau^{(0)}_{31}(\xi_i))_{\alpha'\alpha}}{\xi + \xi_2 - \xi_1 - \xi_3 + i\delta} \quad (7)$$

where $\xi_i = p_i^2 - E_F$, $\vartheta_+(\xi) = 1$ at $\xi > 0$ and $\vartheta_+(\xi) = 0$ when $\xi < 0$; $\vartheta_+ + \vartheta_- = 1$.

By virtue of the foregoing, the three-particle contribution to $\operatorname{Im} F^{(0)}_{3\alpha'\alpha}$ (and consequently also to $F^{(0)}_3$), obtained for the denominator in (7) is replaced by a δ-function, vanishes at b = 0.

A similar situation takes place also in the case of diagrams with a larger number of particles in the intermediate states, since at lower order of perturbation theory the amplitude for the coalescence of n particles can be represented in the form of a sum of terms, each of which is proportional to the $(n-1)2^{-1}$-fold commutator of the quantities s. This is easy to verify by noting that the amplitude of the coalescence of n particles is obtained by writing down the expression for the diagrams of Fig. 4 (the circle denotes the amplitude of coalescence of n - 2 particles), and then antisymmetrizing the obtained expression over all electrons and holes present in the initial state.

When $b \neq 0$, the situation becomes much more complicated and, as shown in III, the three-particle contribution to $\operatorname{Im} F^{(0)}_3$ is proportional to the infinite integral

$$\int_0^{\xi} d\xi_1 \int_0^{\xi-\xi_1} d\xi_3 (\xi - \xi_1)^{-2} = \int_0^1 \frac{dx}{x}. \quad (8)$$

Obviously, there should exist a mechanism that eliminates this infinity. Its nature is very simple. In higher orders of perturbation theory there appear in place of f total vertex parts of the interaction of the electron with the impurity (see Fig. 5). As a result we get in place of (6)

$$\tau_{\mu_4\mu_3\mu_2\mu_1} = -(4\pi)^2\left\{\frac{\Gamma_{\mu_2\mu_3}(\xi_2, 0, \xi_3, \xi_1 - \xi_4)\Gamma_{\mu_4\mu_1}(\xi_4, \xi_1 - \xi_4, \xi_1, 0)}{\xi_1 - \xi_4 + i\delta}\right.$$

$$\left. + \frac{\Gamma_{\mu_4\mu_1}(\xi_4, 0, \xi_1, \xi_3 - \xi_2)\Gamma_{\mu_2\mu_3}(\xi_2, \xi_3 - \xi_2, \xi_3, 0)}{\xi_3 - \xi_2 + i\delta} - (1 \rightleftarrows 3)\right\}; \quad (9)$$

we have left out here the two terms obtained from those written out by permuting the particles 1 and 3. The divergence (8) is due to the fact that (6) has poles

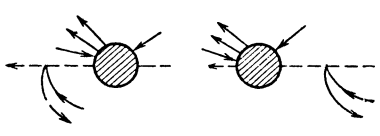

FIG. 4

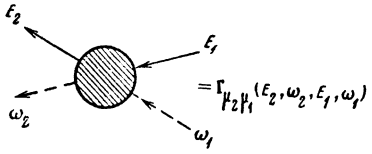

FIG. 5

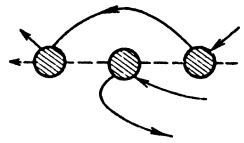

FIG. 6

at $\xi_4 = \xi_{1,3}$. Similar poles are present also in (9). Now, however, the residues of these poles are equal to zero. Indeed, if for example $E_1 = E_4$, then $E_2 = E_3 = E_F$. The functions Γ contained in (9) are then transformed into $F(E_F)$ and the residue turns out to be

$$-(4\pi)^2[F_{\mu_2\mu_3}(E_F), F_{\mu_4\mu_1}(E_F)] = -(4\pi)^2 B^2(E_F)[R_{\mu_2\mu_3}, R_{\mu_4\mu_1}].$$

However, from the results of I (see also III and[13]) it follows that $B \sim \ln^{-1}\xi$ when $\xi \to 0$, i.e., $B(E_F) = 0$[2].

Further, if the function Γ tends to $F(E_F)$ like the reciprocal power of the logarithm of one of its arguments (it does not matter which argument!), then it can be readily verified that the three-particle contribution to Im F turns out to be of the order of $\ln^{-3}\xi$ as $\xi \to 0$, (cf. III). Such a contribution is negligibly small, since, as follows from I, the single-particle contribution at small ξ has the form $c + d\ln^{-1}\xi + e\ln^{-2}\xi$.[3] But expression (9) does not account for the entire pole part of the amplitude of coalescence of three particles into one. Thus, for example, it is easy to verify that the diagram of Fig. 6 also has a pole character. The next step in the iteration procedure with respect to the number of particles taking part in the scattering was made in III. All the three-particle intermediate states were discarded in the expression for the amplitude τ_{13} for the coalescence of three particles into one. The result was an integral equation for τ_{13}, the solution of which has the form $\tau_{1,3} = -(4\pi)^2 B(E_1)B(E_3)f(E_4 + i\delta)$, the function f having the same poles as before, and the residues at these poles being, apart from the sign, the same commutators R.[4] Obviously, such a solution has all the above-described properties necessary in order for the three-particle contribution to F to be small.

One more step in the iteration procedure with respect to the number of participating particles should consist in allowance for the two- and three-particle states in the equation for τ_{13} and simultaneously for the five-particle states in the expression for Im F, and to investigate the latter it is again necessary to use the single-particle approximation.

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[2] The equality $B(E_F) = 0$ is due to the presence of $\epsilon(\xi)$ in expression (4) for ImB. Indeed, reconstructing B from ImB with the aid of the dispersion integral, we find immediately that $B \sim B(E_F)|^2 \ln\xi$ when $\xi \to 0$, which in turn contradicts the expression for ImA (infinities of different order appear on the right and on the left).

[3] The factor $\epsilon(\xi)$ in the expression ImB appears also in the three-particle term. This is connected with the fact that the spin of the hole is $-(1/2)\sigma^T$, and therefore the amplitude for the coalescence of a pair and a hole differs from (9) in that the spin indices are permuted.

[4] It can be shown that the equation for τ_{13} leads to a unitarity condition that takes into account only single-particle intermediate states. To the contrary, when account is taken of the symmetry with respect to permutation of the particles 2 and 4, these conditions yield an equation for τ_{13} (the general properties of the unitarity conditions for inelastic processes are discussed in [17,18]).

Just as in the case of τ_{13}, it can be shown that

$$\tau_{15} \sim B(E_1)B(E_3)B(E_5)\frac{[[R_{\mu_4\mu_1}, R_{\mu_2\mu_3}], R_{\mu_4\mu_5}]c(\xi_i)}{(\xi_1-\xi_6)(\xi_5-\xi_4)}+\ldots, \quad (10)$$

where $c(\xi_i)$ at the pole is a constant, and the unwritten terms are obtained from the written one by antisymmetrization with respect to the particles and poles present in the initial state (see III). The corresponding contribution to Im F as $\xi \to 0$ turns out to be of the order of $\ln^{-4}\xi$, i.e., it is small compared with the three-particle contribution.

Let us consider further the three-particle contribution to the equation for τ_{13}. It can be represented schematically in the form

$$\int d^4p_1\, d^4p_2\, d^4p_3\, \tau_{13}G(p_1)G(p_2)G(p_3)g(k_4-p_1-p_3+p_2)\tau_{33}, \quad (11)$$

where τ_{33} is the amplitude for the scattering of three particles. If we integrate this formula with respect to p_{0i}, then we obtain an expression having a structure

$$\int d\xi_1\, d\xi_2\, d\xi_3\, \tau_{13}\frac{\rho(\xi_1,\xi_2,\xi_3,\xi_4)}{\xi_4-\xi_1-\xi_3+\xi_2}\tau_{33}, \quad (12)$$

where ρ is a function of the order of unity, limiting the region of integration with respect to ξ_i. The amplitude τ_{33} is the same analytic function of the variables ξ_i as τ_{15}, but the signs of the imaginary parts of its arguments are different (an analogous connection between τ_{13} and τ_{22} is discussed in detail in III). Owing to this circumstance, τ_{33} differs from (10) by terms having the form of products of δ-functions of $\xi_i - \xi_k$ by the amplitudes of F and τ_{13}, making it possible to estimate the value of the expression (12) and to verify that in the worst case the three-particle contribution to τ_{13} as $\xi \to 0$ is of the same order as the single-particle contribution. Analogous estimates are obtained also in other cases and do not change the conclusion that the contribution to Im F from the many-particle states can be neglected at small values of ξ.

We have thus clarified the role of the many-particle states at small values of ξ, when the equation $B \sim \ln^{-1}\xi$ holds. According to I and III, in the single-particle approximation,

$$|B|^2=\left(\frac{\pi}{2k_F}\right)^2\left[\left(\ln\frac{|\xi|}{\epsilon_0}\right)^2+\frac{\pi^2}{4}(2S+1)^2\right]^{-1}, \quad (13)$$

where ϵ_0 is the Kondo energy and $|\xi| \ll E_F$. Therefore the region of small ξ is the region where $\ln(\epsilon_0/|\xi|) \gg 1$. If $|\xi| \sim \epsilon_0$, then the contribution of the many-particle states to Im F is no longer small. By virtue of the weak decrease of $|B|$ when $\xi > \epsilon_0$, it remains noticeable in the entire region $\epsilon_0 < \xi < E_F$. The contribution of the many-particle states becomes small again only when $\xi \gtrsim E_F$ and formula (13) no longer is valid and B is small ($B \sim b$).

It is shown in III that the three-particle contribution to Im B can be represented, with logarithmic accuracy, in the form $k_F|B|^2\gamma(\xi)\epsilon(\xi)$, where $\gamma(\xi)$ is a function practically constant in the region $\epsilon_0 < \xi < E_F$. This form of the three-particle contribution leads in the main only to a renormalization of the Kondo energy, i.e., to a replacement of ϵ_0 by $\epsilon_1 > \epsilon_0$. Following such a replacement, all the asymptotic formulas for A and B (see III and[13]) remain unchanged, and a three-particle correction arises only in the next higher terms of the expansion of the amplitudes in powers of $(\ln|\xi|/\epsilon_0)^{-1}$. This means, in particular, that the limiting formulas of[13] for the temperature dependence of the physical quantities (resistance, thermal emf, thermal conductivity, and specific heat) are valid.

The iteration procedure considered by us is additionally justified in the case of large $S(S \gg 1)$. Indeed, according to (13), $|B| \leq [(2S+1)k_F]^{-1}$, i.e., it is small at large S (this does not mean that the exchange part of the scattering amplitude is small; since F = A + BR, the second term is of the order of unity). It follows from the foregoing that τ_{13} is of the order of the product of the two B by the commutator of the operators R, i.e., a quantity of the order of S^{-1}. Therefore allowance for the three-particle terms is equivalent to calculation of the corrections for F. At first glance, the corresponding terms may yield corrections of the order of S^{-2} to the principal expression. However, owing to the pole character of τ_{13}, the three-particle term in Im F contains a poorly-converging integral and the correction turns out to be of the order of S^{-1} (for more details see III). In exactly the same manner, the five-particle terms lead to corrections of the order of S^{-2}, etc. It should be noted that inasmuch as the smallness of the many-particle terms is due mainly to the factors B, it can be assumed that the actual result is an expansion in powers of $(2S+1)^{-1}$, and the solution of the problem in the single-particle approximation yields the principal term of this expansion.

3. SINGLE-PARTICLE APPROXIMATION

As already noted in the Introduction, the solution based on the single-particle unitarity condition is not unique, and it is necessary to solve a dynamic problem that employs explicitly an expression for the interaction energy. At the same time, in our approach it is very difficult to obtain an equation for F on the basis of the ordinary methods of summing Feynman diagrams, since the same diagram can yield both a single-particle and a many-particle contribution to Im F. We therefore use the device of decoupling the equations for the Green's functions. This decoupling was carried out in such a way, that the obtained equations lead automatically to the single-particle unitarity condition. The corresponding decoupling method will be called the single-particle approximation. It was already used in II to prove Suhl's unitarity conditions at finite temperatures. However, in view of its importance for what follows, we shall consider this approximation here anew.

We introduce, as usual, the retarded single-electron Green's function

$$G_{\alpha'\alpha}^{M'M}(x,y)=-i\vartheta(x_0-y_0)\langle M'|\{\psi_{\alpha'}(x),\psi_\alpha^+(y)\}|M\rangle, \quad (14)$$

where M and M′ are the projections of the impurity spin. We write this function in the energy representation in the form of a sum over the intermediate states:

$$G_{E\alpha'\alpha}^{M'M}(x,y)=-\sum_n\left\{\frac{\langle M'|\psi_{\alpha'}(x)|n\rangle\langle n|\psi_\alpha^+(y)|M\rangle}{E_n-E-i\delta}-\frac{\langle M'|\psi_\alpha^+(y)|n\rangle\langle n|\psi_{\alpha'}(x)|M\rangle}{E_n+E+i\delta}\right\}; \quad (15)$$

Here the intermediate states are characterized by definite numbers of electrons and holes in the incident

wave (in the scattered waves these number can be different). We shall take into account below only the single-particle states (containing one electron or one hole).

Further, as shown in II, we can use plane waves to calculate the matrix elements contained in (15), since the part of the wave function describing the scattering decreases far from the impurity and its contribution to the matrix element vanishes when the volume of the system tends to infinity (the final result, from which follows the unitarity condition, confirms the correctness of this statement). Therefore the intermediate states can be regarded as the states of the free particles at the instant of time $t = -\infty$, and we have (compare with I and II):

$$\langle M'|\psi_{\alpha'}(x)|n\rangle = \langle M'|\psi_{\alpha'}(x)a_{k\beta}^{+}(t=-\infty)|M_1\rangle$$
$$= \frac{1}{\sqrt{V}}\int dz\, e^{ikz}\langle M'|\psi_{\alpha'}(x)\psi_{\beta}^{+}(z, z_0=-\infty)|M_1\rangle$$
$$= \int d^4z e^{ikz} G_{\alpha'\beta}^{M'M_1}(x,z)\left(-i\frac{\partial}{\partial z_0}-H_0\right), \qquad (16)$$

where $k > k_F$ and $H_0 = -\nabla^2$. Analogously we have

$$\langle n|\psi_{\alpha'}(x)|M\rangle = \frac{1}{\sqrt{V}}\int d^4z e^{ikz} G_{\alpha'\beta}(x,z)\left(-i\frac{\partial}{\partial z_0}-H_0\right), \quad k<k_F;$$
$$\langle n|\psi_{\alpha}^{+}(y)|M\rangle = \frac{1}{\sqrt{V}}\int d^4z e^{-ikz}\left(i\frac{\partial}{\partial z_0}-H_0\right) G_{\beta\alpha}^{+M_1M}(z,y), \quad k>k_F; \qquad (17)$$
$$\langle M'|\psi_{\alpha}^{+}(y)|n\rangle = \frac{1}{\sqrt{V}}\int d^4z e^{-ikz}\left(i\frac{\partial}{\partial z_0}-H_0\right) G_{\beta\alpha}^{+M'M_1}(z,y), \quad k<k_F,$$

where G^+ is the advanced Green's function. Substituting these formulas in (15), we obtain

$$G_E(x,y) = -\frac{1}{(2\pi)^3}\int \frac{dk\, dz_1\, dz_2}{E'-E-i\delta}\{G_{E'}(x,z_1)(E'-H_{01})(E'-H_{02})$$
$$\times G_E^{+}(z_2,y) + \vartheta_-(\xi')[(G_{E'}^{T}(x,z_1)(E'-H_{01})(E'-H_{02})G_{E'}^{+T}(z_2,y))^T$$
$$- G_{E'}(x,z_1)(E'-H_{01})(E'-H_{02})G_{E'}^{+}(z_2;y)]\}, \qquad (18)$$

where $E' = k^2$. As shown in II, in the case of a point-like center the Green's function is of the form

$$G_E(x,y) = G_{0E}(x-y) - 4\pi G_{0E}(x) F G_{0E}(y),$$
$$G_{0E} = -\frac{1}{4\pi x}e^{ikx}. \qquad (19)$$

Substituting these formulas in (18) and recognizing that $R^2 = S(S+1) - R$ and $R^{T^2} = S(S+1) + R^T$, we arrive after simple calculations to the inequality

$$e^{ik(x+y)}F_E = \frac{1}{2\pi i}\int_0^{\infty}\frac{dE'}{E'-E-i\delta}\{e^{ik'(x+y)}F_{E'} - e^{-ik'(x+y)}F_{E'}^{+}$$
$$+ e^{ik'(x-y)}[F_{E'}^{+} - F_{E'} + 2ik'(F_{E'}F_{E'}^{+} + 2R\vartheta_-(\xi')|B_{E'}|^2)]\}. \qquad (20)$$

Since the scattering amplitude F_E is an analytic function of the energy with a cut along the positive part of the real axis, with $F^+(E) = F(E - i\delta)$, the first two terms in the right side of (20) are transformed into an integral over a contour encompassing this cut. This contour integral can be readily obtained and is exactly equal to the expression on the left side of (20). The remaining integral is equal to zero for all E, provided only that the integrand vanishes, i.e., if the following equation is satisfied

$$F - F^{+} = 2ik[FF^{+} + 2R\vartheta_-(\xi)|B|^2], \qquad (21)$$

which is the single-particle unitarity condition (formulas (4) are obtained from it immediately by substituting $F = A + BR$)[5].

4. EQUATIONS OF MOTION IN SINGLE-PARTICLE APPROXIMATION

In this section we employ the single-particle approximation to decouple the chain of equations for the Green's function. We first write out all the equations that will be used in the following. To save space, we write all the equations in the energy representation, and the corresponding determinations of the Green's function in the time representation. Thus, using (1), we obtain

$$(E-H_0)G_E(x,y) = \delta(x-y) + V_1(x)G_E(x,y) + V_2(x)\Gamma_E(x,y),$$
$$\Gamma_{\alpha'\alpha}^{M'M}(x,y) = -i\vartheta(x_0-y_0)\langle M'|\{R_{\alpha'\beta}\psi_{\beta}(x), \psi_{\alpha}^{+}(y)\}|M\rangle; \qquad (22a)$$
$$(E-H_0)\Gamma_E(x,y) = R\delta(x-y) + [V_1(x) - V_2(x)]\Gamma_E(x,y)$$
$$+ S(S+1)V_2(x)G_E(x,y) - 4\pi b\Lambda_E(x,y),$$
$$\Lambda_{\alpha'\alpha}^{M'M}(x,y) = -i\vartheta(x_0-y_0)\langle M'|\{K_{\alpha'\mu}(x_0)\psi_{\mu}(x), \psi_{\alpha}^{+}(y)\}|M\rangle, \qquad (22b)$$
$$K_{\alpha'\mu}(x_0) = [R_{\alpha'\mu}, \psi_{\rho}^{+}(0,x_0)R_{\rho\sigma}\psi_{\sigma}(0,x_0)],$$
$$\Lambda_E(x,y)(E-H_0) = C(x,y) + \Lambda_E(x,y)V_1(y) + \Phi_E(x,y)V_2(y),$$
$$C_{\alpha'\alpha}^{M'M}(x,y) = \langle M'|\{K_{\alpha'\mu}(0)\psi_{\mu}(x,0), \psi_{\alpha}^{+}(y,0)\}|M\rangle, \qquad (22c)$$
$$\Phi_{\alpha'\alpha}^{M'M}(x,y) = -i\vartheta(x_0-y_0)\langle M'|\{K_{\alpha'\mu}(x_0)\psi_{\mu}(x), \psi_{\nu}^{+}(y)R_{\nu\alpha}\}|M\rangle.$$

Before we undertake to decouple this system, we derive from it a number of exact relations. Taking into account (19) and the fact that $V_{1,2}(x) \sim \delta(x)$, we obtain from (22a) and (22b)

$$\Gamma_E(x,y) = RG_{0E}(x-y) + \gamma_E(x)G_{0E}(y). \qquad (23)$$

Further, since

$$-4\pi\frac{\partial}{\partial x}xG_{0E}(x)|_{x=0} = ik,$$

we have

$$(1-ika)F = f + b\gamma_E(0), \quad \gamma_E(0) = \frac{\partial}{\partial x}x\gamma_E(x)|_{x=0}, \qquad (24)$$

whence follows formula (2) at $b = 0$. The operators ψ and ψ^+ decrease and increase, respectively, the number of particles in the system by unity. Therefore $\Lambda = 0$ when $E_F = 0$, and from (22b), (23), and (24) we obtain

$$\gamma_E(x) = -4\pi RFG_{0E}(x), \quad \gamma_E(0) = ikRF,$$
$$F = f(1-ikf)^{-1}. \qquad (25)$$

In the general case we seek γ in the form

$$\gamma_E(x) = -4\pi RFG_{0E}(x) + Fw_E(x). \qquad (26)$$

Substitution of this formula in (24) yields

$$F = f[1 - ikf - bw_E(0)]^{-1}, \qquad (27)$$

and, by virtue of the single-particle unitarity condition (21),

$$w_E(0) - w_E^{+}(0) = \frac{4ikR\vartheta_-f|B|^2}{bFF^{+}}. \qquad (28)$$

Further, it follows from (19), (22b), and (23) that Λ can be written in the form:

[5] We have assumed here that when $E < 0$ the function F has no poles corresponding to bound states. If such poles exist, then it is necessary to add in (15) and (18) the terms corresponding to them, which also cancel out completely as a result of the contour integration.

$$\Lambda_E(\mathbf{x}, \mathbf{y}) = Fq_E(x)G_{0E}(y) \tag{29}$$

and by virtue of (23) Eq. (22b) takes the form

$$(E - H_0)w_E(x) = -4\pi[\tilde{f}w_E(0)\delta(\mathbf{x}) + bq_E(x)], \tag{30}$$

where $\tilde{f} = a - b(1 + R)$; we note that $f\tilde{f} = a^2 - ab - S(S+1)b^2 = a_+a_-$ is a c-number; here $a_\pm$ are the Born amplitudes of scattering of an electron in states with total angular momentum $J = S \pm 1/2$. Finally, from (22c) and (29) it follows that

$$\begin{gathered}(1 - ika)Fq_E(x) = c(x) - 4\pi b\langle 0|_L(\mathbf{x}, \mathbf{y})|_{y=0}, \\ C(\mathbf{x}, \mathbf{y}) = c(\mathbf{x})\delta(\mathbf{y}).\end{gathered} \tag{31}$$

The function $c(x)$ is expressed in exact manner in terms of the scattering amplitude. This is done with the aid of the usual commutation relations for the operators ψ and ψ^+, and calculations similar to those contained in the paper of Nagaoka[1]. As a result we obtain the formula

$$\begin{gathered}c(x) = \frac{fi}{\pi}\int_0^{E_F} dE[G_{0E}(x)Q(E) - G_{0E}^*(x)Q^+(E)], \\ Q(E) = \frac{1}{b}\left[(1 + ikA) - \frac{A}{\tilde{f}}\right].\end{gathered} \tag{32}$$

We have now written out all the exact relations that follow from (22), and we should proceed to decouple this system. We shall do this in accordance with the scheme described in Sec. 3. Just as $\langle M|\psi|n\rangle$ was connected with G, we shall connect $\langle M|R\psi|n\rangle$ with Γ, $\langle M|K\psi|n\rangle$ with Λ, etc. We therefore omit all the intermediate calculations and present immediately the final expressions. Thus, by decoupling the function Γ, we arrive at the equation

$$\begin{aligned}\gamma_E(x)e^{iky} = \frac{1}{2\pi i}\int_0^\infty \frac{dE'}{E' - E - i\delta}\Big\{e^{ik'y}\gamma_{E'}(x) - e^{-ik'y}\Big[\gamma_{E'}(x) \\ - \frac{e^{ik'x} - e^{-ik'x}}{x}RF_{E'}^+ - 2ik'\gamma_{E'}(x)F_{E'}^+ \\ - 2RB_{E'}^*\vartheta_-\left(\frac{e^{ik'x} - e^{-ik'x}}{x} + 2ik'\gamma_{2E'}(x)\right)\Big]\Big\}.\end{aligned} \tag{33}$$

Here γ_2 is defined by the equation $\gamma = \gamma_1 + R\gamma_2$; the symbols 1 and 2 have the same meaning in all the 16 formulas. Equation (33) can be satisfied only if the expression in the curly brackets is equal to $\gamma_{E'}^+(x)$. From this condition we obtain the following formulas for the jumps of γ and w:

$$\begin{aligned}\gamma_E(x) - \gamma_E^+(x) = 2ik\Big\{\Big[\frac{\sin kx}{kx}R + \gamma_E(x)\Big]F^+ \\ + 2R\vartheta_-B^*\Big[\frac{\sin kx}{kx} + \gamma_{2E}(x)\Big]\Big\},\end{aligned} \tag{34a}$$

$$w_E(x) - w_E^+(x) = \frac{4ikRB^*\vartheta_-}{F^+}\left\{\frac{\sin kx}{kx} + \left[\frac{e^{ikx}}{x} + w_{2E}(x)\right]\tilde{F}\right\}, \tag{34b}$$

where $\tilde{F} = A - B(1 + R)$, and just as in the case when f and $\tilde{f}$, we have $F\tilde{F} = A^2 - AB - S(S+1)B^2$. From (34b), using (27), we can obtain formula (28), which is equivalent, as we have seen, to the unitarity conditions (4).

The decoupling of Λ leads only to an expression for the jump of q, which we shall obtain in a different manner, by analyzing (31).

By carrying out the decoupling in this equation, we arrive at the formula

$$\begin{aligned}(1 - ika)Fq_E(x) = c(x) + \frac{b}{2\pi i}\int_0^\infty \frac{dE'}{E' - E - i\delta}\Big\{\Big[\frac{e^{ik'y} - e^{-ik'y}}{y}R \\ + 2ik'\gamma_{E'}^+(y)\Big]Fq_{E'}(x) + 2R\vartheta_-[Fq_{E'}(x)]_2 \cdot \\ \times\Big[\frac{e^{ik'y} - e^{-ik'y}}{y} + \gamma_{2E'}^+(y)\Big]\Big\}\Big|_{y=0}.\end{aligned} \tag{35}$$

We shall show below that at large E the quantity q is a constant and $F = ik^{-1}$. Therefore as $E \to \infty$ the integrand decreases slowly, and it is impossible to interchange the order of the integration and the transition to the limit as $y = 0$. With the aid of (34a) (more accurately, with the aid of an equivalent formula obtained from (34a) by circuiting around the point $E = 0$ or by decoupling the function $\Gamma' = -i\vartheta\langle\{\psi, \psi^+R\}\rangle$), we can represent formula (35) in the form

$$\begin{aligned}(1 - ika)Fq_E(x) = c(x) + \frac{b}{2\pi i}\int_0^\infty \frac{dE'}{E' - E - i\delta}\{[\gamma_{E'}(y)q_{E'}(x) \\ - \gamma_{E'}^+(y)q_{E'}^+(x) - \gamma^+(y)(q_{E'}(x) - q_{E'}^+(x))]|_{y=0} \\ + 4ik'R\vartheta_-[(Fq_{E'}(x))_2 - Bq_{E'}(x)(1 + \gamma_{2E'}^+(0))]\}.\end{aligned} \tag{36}$$

To transform this equation further, it is necessary to take into account the fact that q and w may have poles, i.e., terms of the type $r(E_0 - E)^{-1}$. In this case, by virtue of (27), the poles of $w_E(0)$ coincide with the zeroes of F. It follows further from (36) and (34a) that the position of the poles does not depend on x (this can be easily verified by assuming the contrary), and finally the poles of q and w coincide by virtue of (30). We separate from q the pole part q_p and take into account the fact that, by virtue of (26) and (27), we have at the pole $\gamma(y) = -fw(y)(bw(0))^{-1}$. Then, after simple transformations we obtain

$$\begin{aligned}[(1 - ika)F - b\gamma_E(0)]q_E(x) = c(x) + fq_{pE}(x) \\ + \frac{b}{2\pi i}\int_0^\infty \frac{dE'}{E' - E - i\delta}\Big\{-\gamma_{E'}^+(y)[\bar{q}_{E'}(x) - \bar{q}_{E'}^+(x)]\Big|_{y=0} \\ + 4ik'R\vartheta_-[1 + \gamma_{2E'}^+(0)]Fq_{2E'}(x)\Big\},\end{aligned} \tag{37}$$

where $\bar{q}$ is the non-pole part ($q = q_p + \bar{q}$). We now take (24) into account; as a result of simple transformations we obtain

$$q_E(x)|_{E\to\infty} = q_0(x) \equiv c(x)/f, \tag{38a}$$

$$q_E(x) - q_E^+(x) = \frac{4ikR\vartheta_-B^*F}{F^+}q_{2E}(x), \tag{38b}$$

These equations are fully equivalent to (35). Together with (30), (34b), and (4) they are the basic equations of the single-particle approximation.

5. SOLUTION OF SINGLE-PARTICLE EQUATIONS

We first describe the method used to obtain the solution. Starting from (30) and (38), we calculate w(x) and compare its jump with (34b). As a result we obtain an expression relating w(0) with A, and forming together with (27) a closed system of nonlinear integral equations for the scattering amplitude. The solution of this system should automatically satisfy the unitarity conditions (4). However, as shown in I, the determination of an amplitude satisfying these conditions reduces to a determination of two functions of relatively simple form, in the choice of which there remains a definite leeway (the CDD ambiguity).

Thus, the solution of the equations for F should reduce to a determination of these functions. The latter can be easily done, since it turns out that it suffices for this purpose to have two factors: a decrease of w(0) as $E \to \infty$, and the absence of other zeroes of B from the physical sheet, with the exception of the point $E = E_F$.

It thus follows from (30) that

$$w_E(x) = -4\pi\left\{\tilde{f} w_E(0)\delta(x) + b\int dy\, G_{0E}(x-y) q_E(y)\right\}. \quad (39)$$

For an analysis of this equation it is necessary to know the coordinate dependence of q(x). We shall seek q(x) in the form

$$q_E(x) = q_0(x) + q_{20}(x)\lambda_E; \quad (40)$$

This expression does not contradict formulas (38), from which, in particular, it is possible to find the jump of λ. Substituting (40) in (39) and taking (32) into account, we obtain after simple calculations

$$w_E(x) = -4\pi\{[\tilde{f} w_E(0) + b(D_E + \lambda_E D_{2E})]G_{0E}(x) - b[H_E(x) + \lambda_E H_{2E}(x)], \quad (41a)$$

$$D_E = \frac{i}{\pi}\int_0^{E_F} \frac{dE'}{E' - E - i\delta}(Q_{E'} - Q_{E'}^+), \quad (41b)$$

$$H_E(x) = \frac{i}{\pi}\int_0^{E_F} \frac{dE'}{E' - E - i\delta}[Q_{E'}G_{0E'}(x) - Q_{E'}^+ G_{0E'}(x)]. \quad (41c)$$

The function G_{0E} has a cut from zero to infinity, and all the remaining functions in (41) have cuts from zero to E_F. Consequently, the coefficient of G_{0E} should be zero, and therefore

$$w_E(x) = 4\pi b[H_E(x) + \lambda_E H_{2E}(x)], \quad (42a)$$

$$w_E(0) = 4\pi b[H_E(0) + \lambda_E H_{2E}(0)] = -\frac{b}{\tilde{f}}(D_E + \lambda_E D_{2E}). \quad (42b)$$

We now calculate the jump (42a) and substitute it in (34b), as a result of which we obtain

$$2b\frac{e^{ikx}}{x}(Q + Q_2\lambda^+ - Q^+ - Q_2^+\lambda^+) + 4\pi bi(Q^+ + Q_2^+\lambda^+)\frac{\sin kx}{x} + 4\pi b H_2(x)(\lambda - \lambda^+) = \frac{4ikB^*R}{F^+}\left[\frac{\sin kx}{kx} + \frac{e^{ikx}}{x}F + w_{2E}(x)F\right], \quad (43)$$

with $0 < E < E_F$. The last terms on the right and on the left are equal, as can be readily verified by calculating the jump of λ and using Eq. (42b). Formula (43) is valid for all x, and therefore

$$Q^+ + Q_2^+\lambda^+ = \frac{B^*R}{bF^+}, \quad (44a)$$

$$Q + Q_2\lambda^+ + Q^+ + Q_2^+\lambda^+ = \frac{2ikB^*RF}{bF^+}. \quad (44b)$$

Equation (44a) contains functions that are defined on one (lower) edge of the cut, and consequently, by virtue of the uniqueness of the analytic continuation, this equality is valid on the entire physical sheet. Therefore, using (32), we obtain from (44a)

$$\lambda_E = \tilde{f} w_E(0). \quad (45)$$

Further, taking (4) into account, it is easy to show that formula (44b) is an identity. From (45) and (42) it follows that

$$w_E(0) = -bD_E\tilde{f}^{-1}(1 + bD_{2E})^{-1}, \quad (46a)$$

$$w_E(0) = -4\pi b H_E(0)[1 - 4\pi b\tilde{f} H_{2E}(0)]^{-1}. \quad (46b)$$

By virtue of (32), Eq. (46a) gives the connection between w(0) and A. Formulas (46a) and (46b) yield two different expressions for w(0) and it is necessary to demonstrate their equivalence. To this end, we equate the right sides of these formulas and reduce them to a common denominator. The numerators of the expression obtained in this manner are analytic functions which have no singularities other than are cut from zero to E_F, and decrease when $E \to \infty$. For such functions to be equal, it suffices for their jumps to be equal. That these jumps are indeed equal can be verified with the aid of rather prolonged but straightforward calculations, which will not be presented here.

Further, from (41a), taking into account formulas (27), (29), (41b), and (32), we obtain

$$1 + bD_{2E} = \frac{ba_+a_-}{Ba_+a_-}, \quad (47a)$$

$$bD_{2E} = -\frac{2b}{a_+a_-\pi}\int_0^{E_F}\frac{dE'\,\mathrm{Im}\,A}{E' - E - i\delta}, \quad (47b)$$

where $\alpha_\pm$ are the amplitudes for the scattering of the electron in states with total angular momentum $J = S \pm 1/2$.

By virtue of (4), $\mathrm{Im}\,A > 0$, making it possible to clarify completely the question of the zeroes of the left part of (47a), i.e., the poles of w(0). Indeed, for real E lying outside the region $0 < E < E_F$, the integral in (47b) is a monotonic function of E, and is negative when $E > E_F$ and positive when $E < E_F$. Therefore the left side of (47a) has not more than one real zero, and the region where the zero is located (if it exists), depends on the sign of the quantity $(a_+a_-)^{-1}b$. Further, it is easy to verify that at complex value of A the imaginary part of the integral differs from zero and therefore there are no complex zeroes. We note also that the denominator in (46b) depends on the total angular momentum J ($\tilde{f}_\pm = a_\mp$), and therefore only one of the functions $w_\pm(0)$ can have a pole, and consequently, by virtue of (27), only one of the amplitudes $\alpha_\pm$ can vanish.

It follows immediately from the foregoing that B has on the physical sheet only one zero at $E = E_F$. In fact, the left side of (47a) becomes infinite only at the point $E = E_F$ (there is no infinity at zero, since $\mathrm{Im}\,A \sim k$). Therefore when $E \neq E_F$ the zero of B should coincide with the zero of one of the amplitudes $\alpha_\pm$, which is impossible, since $B \sim \alpha_+ - \alpha_-$, and the zeroes of $\alpha_\pm$ do not coincide. We note also that $w_E(0) \sim E^{-1}$ as $E \to \infty$. We are now in the position to prove the correctness of the results of I. To this end, we write out all the formulas we need:

$$\alpha_\pm = \frac{1}{2ik}[e^{2i(\nu_\pm + \varphi_\pm)} - 1], \quad (48a)$$

$$2i\varphi_\pm = \frac{k}{2\pi i}\int_0^{E_F}\frac{dE'}{k'(E' - E - i\delta)}\ln\frac{|u + 2ik'R_\pm|^2}{|u|^2 + 4k'^2S(S+1)}, \quad (48b)$$

$$R_+ = S, \quad R_- = -S - 1,$$

$$1 + 2ikA = Bu, \quad (48c)$$

$$u - u^* = 2ik\varepsilon(\xi), \quad (48d)$$

$$B = e^{2i(\nu_+ + \varphi_+)}(u + 2ikR_+)^{-1} = e^{2i(\nu_- + \varphi_-)}(u + 2ikR_-)^{-1}. \quad (48e)$$

In these expressions the arbitrary functions are $\nu_\pm$ or one of these functions and the rational part of u (for details see I and[13]). Eq. (48d) determines u accurate to a rational function, and when $\xi \to 0$ we have $u \sim \ln \xi$. In (48c) the left side is bounded, and B has no zeroes except the point $E = E_F$. Therefore the rational part of u cannot have any poles (CDD poles!). i.e., it is a polynomial that can be readily determined with the aid of (27) if account is taken of the fact that w_E decreases as $E \to \infty$. As a result we obtain

$$u = \frac{1 + a_+ a_- E}{b} - \frac{2}{\pi} \int_0^{E_F} \frac{dE' k'}{E' - E - i\delta} + ik, \qquad (49)$$

which is the expression used in I.

Further, $\exp(2i\varphi_\pm)$ has no zeroes. Therefore, by virtue of (48e), the functions $\exp(2i\nu_\pm)$ should have zeroes that coincide with the zeroes of $z_\pm = u + 2ikR_\pm$, and cannot have others. But the zeroes of $z_\pm$ were obtained in the Appendix of I. They exist only if $a_\pm > 0$, and lie on the negative part of the real axis ($E_\pm^{(0)} \approx -a_\pm^{-2}$; we recall that on the physical sheet $\mathrm{Im}\sqrt{E} > 0$). On the other hand, according to I,

$$\exp(2i\nu_\pm) = \frac{1 + ika'_\pm - \sum a'_\pm R_\pm^{(n)} (E_\pm^{(n)} - E)^{-1}}{1 - ika'_\pm - \sum a'_\pm R_\pm^{(n)} (E_\pm^{(n)} - E)^{-1}}, \qquad (50)$$

where $a'_\pm \approx a_\pm$; $R_\pm^{(n)} \geq 0$ and $E_\pm^{(n)}$ are real. It is necessary first to have all $R_\pm^{(n)}$ equal to zero, for otherwise, as can be readily verified, (50) will have complex zeroes. Then, by suitable choice of $a'_\pm$, it is possible to make the zeroes of (50) coincide with the zeroes of $z_\pm$. If $z_\pm$ have no zeroes, then $a'_\pm$ can be readily determined by comparing the values obtained from (48) and (27) for $\alpha_\pm$ as $E \to \infty$. It turns out here that $\alpha'_\pm$ differ from $\alpha_\pm$ by small terms of order $(k_F \alpha_\pm)^2$. We note also that $\nu_\pm$ can be determined also directly from (48e) and (49) by a method close to that used in the Appendix of I and in[13], but this will not be done here.

The results can be readily generalized to the case of finite temperatures if the Fermi distribution function is introduced in place of all the encountered limitations of the region of variation of E.

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