

ON SOME EFFECTS CAUSED BY THE INTERACTION BETWEEN ELECTRONS IN METALS
WITH PARAMAGNETIC IMPURITIES

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Submitted May 17, 1968

Zh. Eksp. Teor. Fiz. 55, 1483–1497 (October, 1968)

The method for solving the problem of scattering of electrons by a point paramagnetic impurity is extended to the case of a finite size impurity. It is shown that the previously obtained formulas for the amplitude of scattering by a point center can be applied to the partial amplitudes $f_l(E)$, each of which has its own characteristic "Kondo" temperature T_1 . As a rule in real conditions the Kondo effect should be taken into account only for the wave with the maximal value of T_1 . The conductivity, thermoelectric power, thermal conductivity, and specific heat are then calculated. Simple limiting formulas are obtained, which are valid for low and high temperatures. In the case of "antiferromagnetic" interaction at $T \sim T_l$ the thermoelectric power possesses either a maximum or minimum, depending on the sign of the non-exchange part of the interaction: the specific heat possesses a maximum. At $T \rightarrow 0$ the conductivity is maximum and its magnitude is determined by the unitary limit of the cross section for the l -th partial wave. For any sign of the exchange interaction at $T \rightarrow 0$ the thermoelectric power is proportional to $(\ln T)^{-3}$, i.e., the contribution of impurities to these quantities is anomalously large. The equivalence of the formulas for the amplitude obtained in previous papers is demonstrated in the final part of the present paper.

1. INTRODUCTION

THE problem of scattering of electrons by a pointlike paramagnetic impurity was solved by Suhl and Wong^[1] and by the authors of the present article^[2-4] with the aid of a method based on the use of the analytic properties of the scattering amplitude and the unitarity conditions. The results obtained in this manner agree qualitatively well with a number of experiments^[5,6] and apparently are the most satisfactory from the theoretical point of view, since the expressions for the amplitude, obtained by other methods, clearly do not satisfy the unitarity condition (see, for example, ^[7,8] and ^[9]). At the same time, the notion of a pointlike impurity cannot be justified theoretically and, furthermore, it contradicts recent experiments by Daybell and Steyert^[10]. In the present paper, the results obtained in ^[3,4] are extended to include the case of an impurity of finite radius, and the contribution made by the impurities to the conductivity, thermal emf, thermal conductivity, and specific heat is calculated.

In the last part of the article we compare the expressions obtained in ^[1,3,4] for the amplitude and show that they are equivalent. It is shown incidentally that the scattering amplitude as a function of the exchange part of the interaction V_2 has an essential singularity at $V_2 = 0$; the fact that the amplitude is an even function of the energy is deduced and an expression, simpler than in ^[1], is derived for the amplitude; this expression may be useful for practical applications.

2. SCATTERING AMPLITUDE FOR A POTENTIAL OF FINITE RADIUS

We now generalize the method used in ^[1,4] to include an impurity of finite radius. It turns out here that the

problem can be formulated for each partial wave $f_l(E)$ with a specified value of the orbital angular momentum l in practically the same manner as it was formulated in the case of a pointlike center. Therefore the expression for each partial wave will have the same form as for a pointlike center.

To perform this program, we must obtain the unitarity conditions for the partial amplitudes $f_l(E)$ and clarify their analytic properties. We shall assume that the energy of interaction between the electrons and the impurity is given by

$$V(\mathbf{r}) = V_1(\mathbf{r}) + V_2(\mathbf{r})\mathbf{S}\boldsymbol{\sigma}, \quad (1)$$

where \mathbf{S} is the impurity spin, $\frac{1}{2}\boldsymbol{\sigma}$ the electron spin, and $V_{1,2}(\mathbf{r})$ differ from zero at $r \lesssim r_0$.

We shall also assume that to calculate the scattering amplitude we can use perturbation theory everywhere except in a narrow region of energy near the Fermi surface, due to the Kondo effect. The scattering amplitude can evidently be represented in the form

$$F(\vartheta, E) = A(\vartheta, E) + B(\vartheta, E)\mathbf{S}\boldsymbol{\sigma} = \sum_l (2l+1)P_l(\cos \vartheta)f_l(E),$$

$$f_l(E) = A_l(E) + B_l(E)\mathbf{S}\boldsymbol{\sigma}. \quad (2)$$

The unitarity conditions for $F(\vartheta, E)$, even in the case of simple potential scattering, are quite cumbersome and inconvenient (see ^[11]). At the same time, for the partial waves they have the simple form

$$\text{Im } f_l = k|f_l|^2. \quad (3)$$

We shall also use the unitarity conditions for f_l . In our case they have precisely the same form as the Suhl unitarity conditions for a pointlike center^[1,3]

$$\text{Im } A_l = k[|A_l|^2 + |B_l|^2 S(S+1)],$$

$$\text{Im } B_l = k[A_l B_l^* + A_l^* B_l - |B_l|^2(1-2n)] \quad (4)$$

or (if we introduce, in analogy with^[2,3], the amplitudes $\alpha_l^{(+)} = A_l + SB_l$ and $\alpha_l^{(-)} = A_l - (S + 1)B_l$)

$$\begin{aligned} \text{Im } \alpha_l^{(+)} &= k[|\alpha_l^{(+)}|^2 + 2S|B_l|^2 n], \\ \text{Im } \alpha_l^{(-)} &= k[|\alpha_l^{(-)}|^2 - 2(S + 1)|B_l|^2 n], \end{aligned} \quad (5)$$

where n is the Fermi distribution function. These formulas can be obtained by direct calculation, starting from the unitarity condition obtained in Appendix I of^[3] (the unitarity condition contained there has been written out for a pointlike center, but can be directly extended to the general case). The validity of (4) can also be verified without calculations, if it is recalled that the entire difference between the unitarity condition in our case and the case of simple potential scattering is connected with spins, and therefore the imaginary part of each partial amplitude should be expressed in terms of the same amplitude in the same manner as in the case of a pointlike center¹⁾.

We now proceed to determine the analytic properties of the amplitudes $f_l(E)$ as functions of the energy. We shall use throughout the retarded amplitudes introduced in^[3,12], since they are the only ones that have simple analytic properties and are of direct physical interest.

Although the analytic properties of $f_l(E)$ could be formulated directly, we shall first illustrate them with the aid of the first two terms of the perturbation-theory series. For simplicity we confine ourselves to the case $T = 0$, which is perfectly immaterial for what follows. In the second order of perturbation theory we can easily obtain for the scattering amplitude the formula

$$\begin{aligned} -4\pi F_{\alpha\alpha}(\theta, E) &= V_{\alpha\alpha}(\mathbf{q}) + \frac{1}{(2\pi)^3} \int_{p > k_F} d\mathbf{p} \frac{V_{\alpha\beta}(\mathbf{k}' - \mathbf{p}) V_{\beta\alpha}(\mathbf{p} - \mathbf{k})}{E_p - E - i\delta} \\ &+ \frac{1}{(2\pi)^3} \int_{p < k_F} d\mathbf{p} \frac{V_{\beta\alpha}(\mathbf{k} - \mathbf{p}) V_{\alpha\beta}(\mathbf{p} - \mathbf{k}')}{E_p - E - i\delta}. \end{aligned} \quad (6)$$

Here \mathbf{k} and \mathbf{k}' are the electron momenta before and after scattering, α and α' are the corresponding electron spin projections, $\mathbf{q} = \mathbf{k} - \mathbf{k}'$, and $V(\mathbf{q})$ are the Fourier components of the potential (1). We use a system of units in which the electron mass is $m = 1/2$.

The dependence on the energy E in (6) occurs in two ways. First, the denominators in the second-order terms depend on the energy, and second, the Fourier components of the potential depend on the energy, since they contain the momenta \mathbf{k} and \mathbf{k}' which are related to E by the equation $k^2 = k'^2 = E$. The dependence on the energy of the denominators is the same as in the case of a pointlike center, and leads to a cut along the positive part of the real axis in the E plane (Fig. 1). It is obvious that this cut will occur also for the amplitudes $f_l(E)$.

Let us determine now which singularities of $f_l(E)$ are due to the dependence of the Fourier components of the potential on E . We consider first the first term $V(\mathbf{q})$ and clarify the resultant situation using as an example a screened Coulomb interaction (Yukawa-type potential). Let $V(\mathbf{r}) = V_0 r^{-1} e^{-\alpha r}$, and then $V(\mathbf{q}) = 8\pi V_0 (q^2 + \alpha^2)^{-1}$, and we have

$$V_l(E) = \frac{1}{4\pi} \int d\Omega P_l(\cos\theta) \frac{8\pi V_0}{q^2 + \alpha^2} = 4\pi V_0 \int_{-1}^1 \frac{dx P_l(x)}{2E(1-x) + \alpha^2}. \quad (7)$$

The integral in the right side of this equation defines a function of the complex variable E ; this function is regular on the plane with a cut along the real axis from the point $E_0 = -\alpha^2/4$ to $-\infty$ (see Fig. 1; the cut exists for those values of E at which the denominator of the integrand vanishes at any value of x from the integration region).

It can be shown (see, for example^[13]) that the second-order terms in (6) lead to a cut along the negative axis of the real axis, starting at the point $E_1 = -\alpha^2$, and the terms of higher order lead to more remote cuts. Potentials of another type also lead to cuts when $E \leq 0$, although apparently there exists at present no general proof of this fact. A detailed analysis of the properties of the functions $F_l(E)$ for $E < 0$ is not needed, however, since all the singularities in this region lie far from the point $E = E_F$ and do not play any role whatever in our problem.

Taking all the foregoing into account, it can be stated that $f_l(E)$ is regular on the entire plane of the complex variable E with cuts along the real axis from zero to infinity and from a certain $E_0 \leq 0$ to $-\infty$ (left-hand cut); in addition, $f_l(E)$ can have, when $E < 0$, poles corresponding to real bound states, designated by crosses in Fig. 1.

We note one more interesting consequence of (6). Retaining only the large logarithm in the second-order approximation of perturbation theory, we can represent the partial amplitude near the Fermi surface in the form

$$\begin{aligned} -4\pi f_l(E) &\approx V_{1l}(E_F) + V_{2l}(E_F) S\sigma + \frac{V_{2l}^2(E_F) k_F}{2\pi^2} \int_0^{E_F} \frac{dE'}{E' - E - i\delta} S\sigma \\ &\approx V_{1l}(E_F) + V_{2l}(E_F) \left(1 + \frac{1}{2\pi^2} V_{2l}(E_F) k_F \ln \frac{E - E_F}{E_F} \right) S\sigma. \end{aligned} \quad (8)$$

It follows from this formula that for each partial wave there exists its own characteristic "Kondo" energy:

$$\epsilon_l = E_F \exp\left(-\frac{1}{|g_l|}\right), \quad g_l = -\frac{2\pi^2}{k_F V_{2l}(E_F)}, \quad (9)$$

near which there begin phenomena due to the Kondo effect. In exactly the same manner as for a pointlike center, the case of greatest interest is that of negative $g_l(V_{2l}(E_F)) > 0$, "antiferromagnetic" interaction). Since the argument of the exponential in (9) is large, even a small change of $V_{2l}(E_F)$ (on the order of 20–30%) can change ϵ_l by one order of magnitude. On the other hand, the agreement, with a high degree of accuracy, of two different $V_{2l}(E_F)$ is not very probable. Therefore, the experimental situation should be such as if the Kondo effect were to take place for one partial wave. The interesting situation, when this is not the case, will be discussed briefly later.

As already noted, the unitarity conditions and the

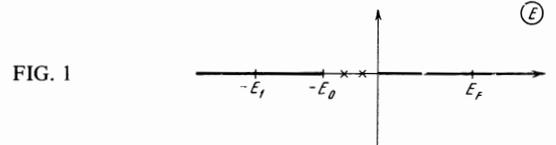


FIG. 1

¹⁾In expressions (4) and (5) we neglect the contributions made to $\text{Im} f_l$ by the many-particle intermediate states, just as done previously in^[1-3]. The validity of this procedure will be demonstrated elsewhere.

analytic properties of the partial amplitudes $f_l(E)$ practically coincide with the corresponding properties of the amplitude for the pointlike center. We can therefore write immediately an expression for $f_l(E)$, using the previously obtained results^[3,4].

For our purposes it is most convenient to use the expression for the amplitude derived in^[4]. We now present the corresponding formulas, in which the approximate equalities will hold only near the Fermi surface. Some more general formulas and a comparison of the expressions presented below with the results of other works^[1,3] are given at the end of the article. Thus,

$$\begin{aligned} a_l^{(\pm)} &= \frac{1}{2ik} (S_l^{(\pm)} - 1), \quad S_l^{(-)} = S_l^{(+)} \frac{\Phi_l - S - 1}{\Phi_l + S}, \\ A_l &= \frac{1}{2S+1} [(S+1)a_l^{(+)} + S a_l^{(-)}] = \frac{1}{2ik} \left(S_l^{(+)} \frac{\Phi_l}{\Phi_l + S} - 1 \right), \\ B_l &= \frac{1}{2ik} \frac{S_l^{(+)}}{\Phi_l + S}. \end{aligned} \quad (10)$$

These formulas are exact. All the amplitudes are expressed in terms of two functions Φ_l and S_l^+ , for which we have

$$\begin{aligned} \Phi_l &\approx \frac{i}{\pi} \left[-\frac{1}{g_l} + I(\zeta) \right] + \frac{1}{2} \operatorname{th} \frac{\zeta}{2T}, \\ I(\zeta) &= 2k_F \int_{-\zeta}^{\infty} \frac{dk' n(\zeta')}{\zeta' - \zeta} \approx \ln \frac{\pi T}{8E_F \gamma} + \operatorname{Re} \psi \left(\frac{1}{2} + \frac{\zeta i}{2\pi T} \right) - \psi \left(\frac{1}{2} \right) \\ &= \frac{1}{2} \ln \frac{\zeta^2 + (\pi T)^2}{16E_F^2} + \int_0^{\infty} dt e^{-t\zeta} \left(\frac{1}{t} - \frac{e^t}{e^t - 1} \right) \cos \frac{\zeta t}{2\pi T}, \end{aligned} \quad (11)$$

where $\zeta = E - E_F$ and it is assumed that $|\zeta| \ll E_F$. Further

$$\begin{aligned} S_l^{(+)} &= \exp(2i\nu_l^{(+)} + 2i\Psi_l) \frac{K(\Phi_l)}{K_0(\Phi_l)}, \\ K(\Phi_l) &= \frac{\Gamma[1/2(S+1+\Phi_l)] \Gamma[1/2(S+1-\Phi_l)]}{\Gamma[1/2(S+\Phi_l)] \Gamma[1/2(2+S-\Phi_l)]}. \end{aligned} \quad (12)$$

Here $\nu_l^{(+)}$ is the phase of scattering (with total spin $J = S + 1/2$) by potential (1) without the "Kondo effect." In the Born approximation $\exp(2i\nu_l^{(+)}) \approx 1 + 2ik_F a_l^{(+)}(E_F)$, where $a_l^{(+)}(E_F)$ is a corresponding Born scattering amplitude, we have

$$K_0(\Phi_l) \approx K(\Phi_l^{(0)}), \quad \Phi_l^{(0)} = -\frac{i}{\pi g_l} + \frac{1}{2}. \quad (13)$$

This formula is discussed later, in Sec. 4. Finally,

$$\begin{aligned} 2i\Psi_l &= \frac{k}{2\pi i} \int_0^{\infty} \frac{dE'}{k'(E' - E - i\delta)} \ln \frac{\eta_{+t^2}}{|K|^2}, \\ \eta_{+t^2} &= \frac{(\operatorname{Im} \Phi_l)^2 + (S + 1/2 - n)^2}{(\operatorname{Im} \Phi_l)^2 + (S + 1/2)^2 - n(1-n)}. \end{aligned} \quad (14)$$

Using (11) and (12), we can show that when $|\zeta| \gg T$ we get $|K|^2 = \eta_{+l}^2$. Consequently, the function Ψ_l vanishes when $T = 0$.

3. ANALYSIS OF THE AMPLITUDE IN LIMITING CASES, AND CALCULATION OF THE CONDUCTIVITY, THERMAL EMF, THERMAL CONDUCTIVITY, AND SPECIFIC HEAT

It is well known that the expression for the amplitude depends strongly on the sign of the interaction constant

g_l . If $g_l > 0$, then $|\Phi_l| \gg 1$, and since we assume that $|g_l| \ll 1$, we also get $|\Phi_l^{(0)}| \gg 1$. Therefore all the expressions that enter in (10)–(14) can be expanded in powers of Φ_l^{-1} and $\Phi_l^{(0)-1}$. In the expansion of $K(\Phi_l)$, it is convenient to represent this quantity, using the well known properties of the Γ functions^[14], in the form

$$K(\Phi_l) = \frac{\Gamma[1/2(S+1+\Phi_l)] \Gamma[1/2(-S+\Phi_l)]}{\Gamma[1/2(S+\Phi_l)] \Gamma[1/2(-S+1+\Phi_l)]} \operatorname{tg} \frac{\pi}{2} (\Phi_l - S). \quad (15)$$

The expansion of the first factor of this formula in powers of Φ_l^{-1} can be readily obtained with the aid of the asymptotic expression for the Γ functions^[14], while $\tan[(\pi/2)(\Phi_l - S)] = -i$ with exponential accuracy.

Further, $2i\Psi_l$ is of the order of Φ_l^{-4} and can be neglected; as a result we get

$$\begin{aligned} S_l^{(+)} &\approx (1 + 2ik_F a_l) \left(1 + \frac{S}{\Phi_l} + \frac{1}{2} \frac{S(S+1)}{\Phi_l^2} \right), \\ A_l &\approx a_l + \frac{S(S+1)}{4ik_F \Phi_l^2} (1 + 2ik_F a_l), \\ B_l &\approx \frac{1}{2ik_F \Phi_l} (1 + 2ik_F a_l) \left(1 + \frac{S(S+1)}{2\Phi_l^2} \right) \approx \frac{1}{2ik_F \Phi_l}. \end{aligned} \quad (16)$$

Here $a_l = a_l^{(+)}(E_F) - S b_l(E_F)$ is the spin-independent part of the Born scattering amplitude. At negative g_l in the temperature region $T \sim \epsilon_l$, the quantity $|\Phi_l| \lesssim 1$ and the amplitude can be determined only with the aid of numerical integration. On the other hand, the expansion in powers of Φ_l^{-1} is possible only when $T \gg \epsilon_l$ and when $T \ll \epsilon_l$ or, more precisely, if the following condition is satisfied²⁾

$$|g_l(T)| \ll 1, \quad g_l(T) = \frac{g_l}{1 - g_l \ln(T/E_F)} = \frac{1}{\ln(T/T_l)}. \quad (17)$$

The corresponding expansion in the region of high temperatures ($-g_l(T) \ll 1$) leads, just as in the case when $g_l > 0$, to formulas (16), while at low temperatures ($g_l(T) \ll 1$) we have

$$\begin{aligned} S_l^{(+)} &\approx -(1 + 2ik_F a_l) \left(1 + \frac{S}{\Phi_l} + \frac{1}{2} \frac{S(S+1)}{\Phi_l^2} \right) \\ A_l &\approx \frac{i}{k_F} - a_l - \frac{S(S+1)}{4ik_F \Phi_l^2} (1 + 2ik_F a_l), \\ B_l &\approx -\frac{1}{2ik_F \Phi_l}. \end{aligned} \quad (18)$$

The minus sign in the expression for $S_l^{(\pm)}$ is the result of the fact that

$$\operatorname{tg} \frac{\pi}{2} (S - \Phi_l) \left[\operatorname{tg} \frac{\pi}{2} (S - \Phi_l^{(0)}) \right]^{-1} \approx -1.$$

The non-exchange part of the amplitude A_l is now close to the maximum possible value $1/k_F$; this result was also noted many times earlier^[2-4].

It is easy to generalize the results to include the case when the potential $V_1(\mathbf{r})$ is large and the Born approximation is not applicable to it, and $V_2(\mathbf{r})$ is small as before. It turns out here that in the limiting cases under consideration, when $|\zeta| \ll E_F$, we have

²⁾The numerical factor of the order of unity under the logarithm sign in (17) cannot be determined within the framework of the present theory, since we use the Born approximation outside the region of the Kondo effect. For a pointlike center, this follows from the formulas for g [2,3]. Therefore T_l and ϵ_l are also determined only in order of magnitude. Below, we should consider these quantities as well as u_l , as phenomenological parameters.

$$A_l \approx \frac{1}{2ik_F} \left[\frac{1 + ik_F \bar{a}_l}{1 - ik_F \bar{a}_l} \left(1 + \frac{S(S+1)}{\Phi_l^2} \right) - 1 \right], \quad (19)$$

where $\lambda = 1$ when $g_l > 0$ and $\lambda = -1$ when $g_l < 0$, and the quantities \bar{a}_l are connected with the amplitude $A_l^{(0)}$ of scattering by the potential V_l by the equation $A_l^{(0)} \approx \bar{a}_l(1 - ik_F \bar{a}_l)^{-1}$. Here g_l must depend on V_l and must therefore be regarded as phenomenological parameters. We shall henceforth not use formula (19).

We can now proceed to calculate the experimentally observed physical quantities. To this end we use the following formulas^[15]:

$$\begin{aligned} \Sigma &= -\frac{e^2 N}{n_0 k_F} L_0, \quad Q = -\frac{1}{|e|T} \frac{L_1}{L_0}, \\ \kappa &= -\frac{e^2 N}{n_0 k_F T} \left(L_2 - \frac{L_1^2}{L_0} \right), \quad L_n = \int d\xi^n \frac{\partial n}{\partial \xi} \frac{1}{\sigma_{tr}}. \end{aligned} \quad (20)$$

Here Σ is the electric conductivity, Q the thermoelectric power, κ the thermal conductivity, N the conduction electron density, n_0 the impurity density, e the electron charge, and σ_{tr} the transport cross section of the collisions, defined by the formula

$$\begin{aligned} \sigma_{tr} &= \int |\bar{a}_l \Omega (1 - \cos \theta) \sigma(\theta) \\ &= 4\pi \sum_l \{ (2l+1) [|A_l|^2 + S(S+1) |B_l|^2] \\ &\quad - 2l \operatorname{Re} [A_l \bar{A}_{l+1} + S(S+1) B_l \bar{B}_{l+1}] \}. \end{aligned} \quad (21)$$

As already noted, the Kondo effect should be manifest only in one partial wave. If this is indeed the case in a wave with a certain l , then, by separating from σ_{tr} the term containing the amplitudes with this l , we obtain $\sigma_{tr} = \sigma_{tr}^{(K)} + \sigma_{tr}^{(0)}$, where

$$\begin{aligned} \sigma_{tr}^{(K)} &= 4\pi(2l+1) \{ |A_l|^2 + S(S+1) |B_l|^2 - 2 \operatorname{Re} [A_l \bar{A}_{l+1} + S(S+1) B_l \bar{B}_{l+1}] \\ &\approx 4\pi(2l+1) \{ |A_l|^2 + S(S+1) |B_l|^2 - 2 [\bar{A}_l \operatorname{Re} A_{l+1} + S(S+1) \bar{B}_l \operatorname{Re} B_{l+1}] \}, \end{aligned} \quad (22)$$

$\sigma_{tr}^{(0)}$ is that part of σ_{tr} which does not contain the amplitudes with the selected l , and

$$\begin{aligned} \bar{A}_l &= \frac{1}{2l+1} (lA_{l-1} + (l+1)A_{l+1}), \\ \bar{B}_l &= \frac{1}{2l+1} (lB_{l-1} + (l+1)B_{l+1}). \end{aligned} \quad (23)$$

The approximate equality in the right side of (22) takes place in the Born approximation, when \bar{A}_l and \bar{B}_l are real.

Now, using (11), (16), (18), (20), (22), and (23), we can easily obtain the following formulas for the conductivity:

$$\begin{aligned} \Sigma &= -\frac{e^2 N}{n_0 k_F} \left\{ \sigma_{tr}^{(0)} + 4\pi(2l+1) \left[a_l^2 - 2\bar{A}_l a_l \right. \right. \\ &\quad \left. \left. + \frac{S(S+1)\pi^2 g_l^2}{4k_F^2(1-g_l \ln(T/E_F))^2} (1 + 4k_F^2 a_l \bar{A}_l) - \frac{2\bar{B}_l b_l S(S+1)}{1-g_l \ln(T/E_F)} \right] \right\}^{-1}, \end{aligned} \quad (24)$$

when $g_l > 0$ or $-g_l(T) \ll 1$ and

$$\begin{aligned} \Sigma &= -\frac{e^2 N}{n_0 k_F} \frac{1}{\sigma_{tr}^{(0)} + \sigma_{tr}^{(m)}} \left\{ 1 + \frac{\sigma_{tr}^{(m)}}{\sigma_{tr}^{(0)} + \sigma_{tr}^{(m)}} \left[k_F^2 a_l (a_l - 2\bar{A}_l) \right. \right. \\ &\quad \left. \left. + \frac{S(S+1)\pi^2}{4(\ln(T_l/T))^2} (1 + 4a_l \bar{A}_l k_F^2) - \frac{\bar{B}_l b_l k_F^2}{\ln(T_l/T)} \right] \right\}, \end{aligned} \quad (25)$$

where $\sigma_{tr}^{(m)} = 4\pi(2l+1)/k_F^2$. This formula is valid when

$g_l(T) \ll 1$, i.e., in the low temperature region at $g_l < 0$. Expressions (24) and (25) generalize the previously obtained results for s-scattering^[3]. It follows from (25) that when $T \rightarrow 0$ the resistance $\rho = \Sigma^{-1}$ increases by an amount close to $\sigma_{tr}^{(m)}/n_0 k_F/e^2 N$. Such an increase of the resistance is the maximum possible from the point of view of the unitarity conditions, since $\sigma_{tr}^{(m)}$ is the unitary limit for the partial cross section. In this connection, we call attention to recent experiments by Daybell and Steyert^[5,10], who investigated the resistance of copper with slight additions of iron and chromium. In the first case (Cu + Fe) they observed an increase of the resistance, corresponding to the unitary limit for s-scattering, and in the second case (Cu + Cr) an increase corresponding to five unitary limits for s-scattering. In this case, apparently, the Kondo effect takes place in the d wave.

We note also that, owing to the interference of waves with different l , the deviation of Σ from the limiting value at $T = 0$ is proportional to $(\ln T)^{-1}$, and not to $(\ln T)^{-2}$, as for pure s scattering^[3]. It may be that it is precisely this interference effect which explains the qualitatively different character of the approach of the resistance to the limiting value in the two cases considered in^[5,10].

Assume now that the Kondo effect takes place in two partial waves, i.e., the temperatures T_{l_1} and T_{l_2} lie in the experimentally attainable region. We confine ourselves to the case when $g_{l_1} < 0$ and $g_{l_2} < 0$. If $|l_1 - l_2| > 1$, then the corresponding waves do not interfere and the contribution from them to the resistance is simply the sum of the contributions from each of the waves. On the other hand, if $l_2 = l_1 + 1$, then the interference becomes appreciable.

The corresponding behavior of the resistance can be easily obtained from the expression for σ_{tr} (21). Thus, if $T_{l_1} \gg T_{l_2}$, then in the region $T_{l_1+1} \ll T \ll T_{l_1}$ the increase of the resistance is proportional to $4\pi(2l_1+1)/k_F^2$, and then, with decreasing temperature, the resistance decreases if $l_1 \neq 0$, and increases if $l_1 = 0$, reaching a limit proportional to $8\pi/k_F^2$, i.e., so to speak the unitary limit with $l = 1/2$. On the other hand, if $T_{l_1+1} \gg T_{l_1}$, then the magnitude of the intermediate maximum is larger and is proportional to $2l_1 + 3$, and the limiting value at $T = 0$ is the same as before.

We proceed to calculate the thermoelectric power. Usually at low temperatures in metals, it is positive and small (proportional to T/E_F). We shall now show that in the region of the Kondo effect this is not the case. In the calculations we shall systematically discard the small terms proportional to T/E_F . As follows from (20), to calculate the thermoelectric power it is necessary to separate from σ_{tr} the part that is odd in ξ . In the limiting cases considered by us, this can be readily done by using (11), (16), and (18), after which we can easily obtain the following formulas:

$$Q = -\frac{S(S+1)k_F\pi^2}{8\pi|e|\sigma_{tr}} \left(\frac{g_l}{1-g_l \ln(T/E_F)} \right)^2 \left[2k_F a_l \bar{B}_l + \frac{\pi g_l (\bar{A}_l - a_l)}{1-g_l \ln(T/E_F)} \right] \quad (26)$$

when $g_l > 0$ or $g_l < 0$, but $-g_l(T) \ll 1$, and

$$Q = \frac{S(S+1)k_F\pi^2}{8|e|\sigma_{tr}} \frac{1}{(\ln(T_l/T))^2} \left[2k_F a_l \bar{B}_l + \frac{\pi(\bar{A}_l - a_l)}{\ln(T_l/T)} \right], \quad (27)$$

If $g_l(T) \ll 1$. In these formulas $\sigma_{tr} = (n_0 k_F / e^2 N) \Sigma$ is the magnitude of the transport cross section at $\xi = 0$. We note that the thermoelectric power is absent if the amplitudes a_l and \bar{A}_l are equal to zero, or, what is the same, the nonexchange part of the interaction V_1 is equal to zero. This statement holds true also when $T \sim T_l$, as follows from the evenness of A_l and B_l which was deduced in Sec. 4, and agrees with the numerical calculations in^[1].

Further, the first term in (26) and (27) is small (it contains the additional small factor $k_F \bar{B}_l$) and therefore, with the exception of the region of very low temperatures, it can be neglected. If $g_l < 0$, then Q has the same sign, which coincides with the sign of $A_l - a_l$ at both high and low temperatures. $|Q|$ increases with decreasing temperature in the former case, and decreases in the latter thus indicating that Q has a maximum (if $\bar{A}_l - a_l > 0$), or a minimum (if $\bar{A}_l - a_l < 0$) at $T \sim T_l$. This behavior agrees qualitatively with experiment^[6,15] and with the results of the numerical calculations in^[1]. Finally, if the sign of $a_l \bar{B}_l$ is opposite to the sign of $\bar{A}_l - a_l$, then the thermoelectric power should reverse sign in the region of very low temperatures.

Let us now calculate the thermal conductivity. As follows from the results obtained above for Q , the second term in the definition (20) of the thermal conductivity κ is proportional to $g_l^4(T)$ and can therefore be neglected; as a result we get the Wiedemann-Franz law

$$\kappa = \frac{\pi^2}{3e^2} T \Sigma. \quad (28)$$

To conclude this section, let us analyze the specific heat. The contribution to the system energy from the pointlike impurities is determined by the formula^[9]

$$\Delta E = \frac{n_0}{\pi} \int_{-E_F}^{\infty} d\xi n(\xi) \frac{\xi}{k} \text{Re} A(\xi). \quad (29)$$

In the case of an impurity of finite radius, Eq. (29) should contain the quantity $A(0, \xi)$, as can be readily verified by considering, for example, the first terms of the perturbation-theory series. Expressing $\text{Re} A$ in terms of $\text{Im} A$ with the aid of the dispersion integral^[1,3], we obtain³⁾

$$\Delta E = -\frac{n_0}{\pi^2} \int_{-E_F}^{\infty} d\xi \text{Im} A(\xi) \int_{-E_F}^{\infty} \frac{d\xi' \xi' n(\xi')}{k'(\xi' - \xi)}. \quad (30)$$

It follows from this formula that $\Delta E < 0$, inasmuch as $\text{Im} A > 0$, and, as can be readily verified, the integral with respect to ξ' is positive for all ξ .

Let us calculate now the contribution of the impurity to the thermal conductivity. It is evident that $\Delta C = d\Delta E/dT = \Delta E'$. In the expression for ΔC , the term containing n' can be neglected, since it depends on the odd part of $\text{Im} H_l$, which has a small factor $k_F a$ (see the end of the next section). To calculate $\text{Im} A'_l$, we cannot use expressions (16) and (18). Thus, with the aid of (16) we arrive, for ΔC in the lowest order in $g_l(g_l^3)$, at an expression proportional to the quantity

$$\int_{-E_F}^{\infty} d\xi \int_{-E_F}^{\infty} d\xi' \frac{\xi' n(1-n)}{T^2(\xi' - \xi)} \int_{-E_F}^{\infty} \frac{d\xi'' \xi'' n(\xi'')}{k''(\xi'' - \xi)} \sim T. \quad (31)$$

We shall show below that the main contribution to ΔC is made by terms which do not contain the factor T and are proportional to g_l^4 . Obviously they cannot be determined from (16). To calculate $\text{Im} A'_l$ it is most convenient to use the formulas from^[3] (see formula (35) in the next section). The calculation of $\text{Im} A'_l$ gives rise to terms proportional to $\eta'_\pm \cos 2\delta_\pm$ and $\delta'_\pm \sin 2\delta_\pm$ ($\delta_\pm = \nu_\pm + \text{Re } \varphi_\pm$). The contribution made by the terms with η'_\pm to $\text{Im} A'_l$ is proportional to $g_l^4 n'$.

The terms δ'_\pm lead to a small contribution to ΔC (they give rise to terms proportional to (31) or to analogous small integrals, or else proportional to g_l^5), except for the case $g_l < 0$, $g_l(T) \ll 1$, when a term

$$-\frac{\pi}{2} \frac{n_0 S(S+1) g_l^4}{(1-g_l \ln(T/E_F))^4} \int_{-\infty}^{\infty} \frac{d\xi}{\xi} \frac{(2S-1) \sin 2\delta_+ + (2S+3) \sin 2\delta_-}{2S+1} = \frac{\pi^2 c}{2(\ln(T_l/T))^4}, \quad (32)$$

having the same order of magnitude as the contribution from the terms with η'_\pm , arises. As a result we have for $g_l > 0$ and for $g_l < 0$ but $-g_l(T) \ll 1$

$$\Delta C = \frac{\pi^2 S(S+1) n_0 g_l^4}{2(1-g_l \ln(T/E_F))^4} (2l+1), \quad (33)$$

and for $g_l < 0$ but $g_l(T) \ll 1$

$$\Delta C = \frac{\pi^2}{2} \frac{S(S+1) n_0}{\ln^4(T_l/T)} (2l+1) [c-1]. \quad (34)$$

Here c is a constant determined by the equality (32). It should obviously be larger than unity.

The term $c-1$ in (34) is due to the contribution made to $\text{Im} A'_l$ by terms containing $\eta'_\pm \cos 2\delta_\pm$, inasmuch as in the case under consideration $\cos 2\delta_\pm \approx -1$. The existence of a maximum of ΔC when $g < 0$ is apparently confirmed by experiment^[6], and was also predicted earlier^[8,9], but the cited papers did not contain limiting formulas such as (33) and (34), from which it follows that when $T \rightarrow 0$ the impurity specific heat is much larger than the electronic specific heat.

4. ANALYSIS OF THE EXPRESSION FOR THE AMPLITUDE. COMPARISON OF RESULTS OF DIFFERENT INVESTIGATIONS

We shall demonstrate the equivalence of the expressions obtained in^[1,3,4] for the amplitudes. We start with the comparison of the results of^[3] and^[4]. We shall henceforth omit the subscript l from all the quantities. It is sufficient to demonstrate the equivalence of the expressions for $S^{(\pm)}$, since $S^{(+)}$ and $S^{(-)}$ are connected by the simple relation (10), which is a consequence of the unitarity condition^[2,3]. In^[3] we obtained the following expression for $S^{(\pm)}$

$$S^{(\pm)} = \exp\{2i(\nu_\pm + \varphi_\pm)\}, \\ 2i\varphi_\pm = \frac{k}{2\pi i} \int_0^\infty \frac{dE'}{k'(E' - E - i\delta)} \ln \eta_{\pm}^2(E'), \\ \eta_{\pm}^2 = \frac{(\text{Im } \Phi)^2 + (S + 1/2 \mp n)^2}{(\text{Im } \Phi)^2 + (S + 1/2)^2 - n(1-n)}. \quad (35)$$

Here ν_\pm is the scattering phase shift in the absence of

³⁾Strictly speaking, (30) should contain a term, which is immaterial for our purposes, proportional to the Born amplitude $V_1(0)$.

the Kondo effect in the case of a pointlike center, given by (see^[2,3]) $\nu_{\pm} = \tan^{-1}ka_{\pm}$, where a_{\pm} is a constant. The function Φ is connected with the function $u = B^{-1}(1 + 2ikA)$, introduced in^[2,3], by the equality $2ik\Phi = u$. By virtue of the unitarity of (4), $u(E + i\delta) - u(E - i\delta) = 2ik[1 - 2n(E)]$ and therefore u is given by

$$u(E) = P(E) - \frac{2E}{\pi k_F} I(E) + ik, \quad I(E) = 2k_F \int_0^{\infty} \frac{dk'n(E')}{E' - E}. \quad (36)$$

Here $P(E)$ is a function that is regular on the complex E plane with a cut along the negative part of the real axis, the same as for the scattering amplitude (Fig. 1).

It is shown in^[2,3] that in the case of a pointlike center

$$P(E) = \frac{1}{b} (1 + a_+ a_- E) - \frac{4k_F}{\pi}, \quad (37)$$

where $a_+ = a + bS$, $a_- = a - b(S + 1)$, a and b are the non-exchange and exchange parts of the Born scattering amplitude⁴⁾. It is easy to show with the aid of perturbation theory that in the general case, when $E \approx E_F$, we have $P(E) \approx -4\pi/V_2(E_F)$.

We shall now show that

$$e^{2i\varphi_+} = K(\Phi)K_0^{-1}(\Phi)e^{2i\psi}, \quad (38)$$

where K , K_0 , and Ψ are determined by equalities (12)–(14). Using (35), we can write

$$2i\varphi_+ = \frac{k}{2\pi i} \int_0^{\infty} \frac{dE'}{k'(E' - E - i\delta)} \ln \frac{\eta_+^2}{|K|^2} + \frac{k}{2\pi i} \int_0^{\infty} \frac{dE' \ln |K|^2}{k'(E' - E - i\delta)}. \quad (39)$$

The first term in the right side of this equality is exactly equal to $2i\psi$. Further, recognizing that $\Phi(E + i\delta) = \Phi^*(E - i\delta)$ and that the same property is possessed by the function $K(\Phi)$, we get

$$\begin{aligned} \frac{k}{2\pi i} \int_0^{\infty} \frac{dE' \ln |K|^2}{k'(E' - E - i\delta)} &= \frac{k}{2\pi i} \int_C \frac{dE' \ln K}{k'(E' - E - i\delta)} \\ &= \ln K(E) + \frac{k}{2\pi i} \int_{C_1} \frac{dE' \ln K}{k'(E' - E)}, \end{aligned} \quad (40)$$

where the contours C and C_1 are shown in Fig. 2. The contour C_1 encompasses all the singular points of the function $\ln K(E')$, lying on the physical sheet off the positive part of the real axis. These singular points coincide with the poles of the Γ -functions, which enter in definition K (12), and with the start of the left cut of the function $P(E)$. The function $I(E)$ which enters in the definition of Φ is large only when $E \approx E_F$, and can be neglected for other E . Therefore the poles of the Γ -functions can be of two types. The first includes the poles near the Fermi surface, due to the compensation of the large quantities $4\pi/V_2$ and $2EI/\pi k_F$. It is easy to show that there are no such poles.

The poles of the second type lie far from the Fermi surface and the function I can be neglected in their determination in the first approximation. The integral in (40) can be represented in the form of a sum of integrals along the contours C_2 and C_1' , where the contour C_2 encloses the left-hand cut (Fig. 2), and C_1' all the singular points $\ln K$ due to the poles of the Γ -functions. The

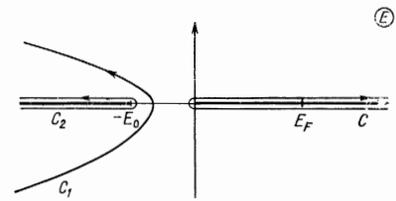


FIG. 2

integral along the contour C_1' can be readily determined by integrating by parts (see the appendix of^[2]):

$$\begin{aligned} \frac{k}{2\pi i} \int_{C_1'} \frac{dE' \ln K(E')}{k'(E' - E)} &= \frac{1}{2\pi i} \int_{C_1'} dk' \left(\frac{1}{k' - k} - \frac{1}{k' + k} \right) \ln K(E') \\ &= \frac{1}{2\pi i} \left[\ln \frac{k' - k}{k' + k} \ln K(E') \right]_{\text{circuit along } C_1'} - \int_{C_1'} dk' \ln \frac{k' - k}{k' + k} \frac{1}{K(E')} \\ &\quad \times \frac{dK(E')}{dE'} = \sum_p \ln \frac{k_p - k}{k_p + k} - \sum_z \ln \frac{k_z - k}{k_z + k}. \end{aligned} \quad (41)$$

Here k_p and k_z are respectively the poles and zeroes of $K(E)$ on the physical sheet.

Thus, by virtue of (39) and (41), we have for $e^{2i\varphi_+}$ an equation similar to (38), where, however, $K_0^{-1}(\Phi)$ ($K_0(\Phi)$ is defined by formula (13)) is replaced for the time being by the factor

$$K_1^{-1}(\Phi) = e^{2i\psi} \prod_p \frac{k_p - k}{k_p + k} \prod_z \frac{k_z + k}{k_z - k}, \quad 2i\psi = \frac{k}{2\pi i} \int_{C_2} \frac{dE' \ln K(E')}{k'(E' - E)}. \quad (42)$$

The product $K_1^{-1}(\Phi)K(\Phi)$ is obviously so constructed that it has no zeroes or poles on the physical sheet, nor does it have a left-hand cut, in full agreement with the properties of the function $\exp(2i\varphi_+)$. Further, it is obvious that $K_1(\Phi) \approx K(\Phi_0)$, since, as we have already noted, k_p and k_z lie far from the Fermi surface and can be computed, in first approximation, with the aid of Φ_0 ⁵⁾; the same, of course, pertains also to the function $2i\psi$. Therefore the function determined by the equality (42) can be chosen as $K_0(\Phi)$ which enters in (38) and (12). We note also that when $V_2 \rightarrow 0$ ($b \rightarrow 0$), the quantity $S^{(*)}$ (and consequently also the scattering amplitude) has as a function of V_2 an essential singularity, thus explaining the entirely different character of the behavior of the amplitude at $V_2 > 0$ and $V_2 < 0$. This statement is a direct consequence of the formulas (12), (38), and (42) given above, if we recognize that k_p , k_z , and γ can be represented in the form of a series in powers of V_2 . The latter statement can be readily verified, for example, in the case of a pointlike center.

We shall now show that our results are equivalent to those of Suhl and Wong^[1]. We confine ourselves here only to the case of a pointlike center. The formulas obtained for A and B in^[1] at $T > T_K$ are

$$A = \frac{1}{2ik} (e^{2i\psi} R - 1), \quad B = \frac{1}{2ib\Phi} e^{2i\psi} R,$$

$$R = \exp \left\{ \frac{k}{2\pi i} \int_0^{\infty} \frac{dE'}{k'(E' - E - i\delta)} \ln \frac{|\Phi|^2}{|\Phi|^2 + S(S + 1)} \right\}. \quad (43)$$

Here $e^{2i\psi}$ is a unimodular function of the energy with a

⁴⁾We disregard here the possibility that the function P may have poles at $E \approx E_F$ (the CDD ambiguity)^[1-3]. The same pertains also to $\exp(2i\psi)$.

⁵⁾In the case of a pointlike center, k_p and k_z are of the order of a^{-1} , and the corrections to them are of the order of $k_F^{-3}ab$.

cut from zero to infinity, assuming complex-conjugate values on different edges of the cut, and approximately equal to $1 + 2ika$. The function Φ is related to the function F introduced in^[1] by the equality $\Phi = -(2\pi ikF)^{-1}$. T_K is the temperature above which in the function Φ there are no zeroes on the physical sheet ($T_K = T_0$). Obviously, such zeroes can occur only when $g < 0$.

When $T < T_K$, formulas (43) are not applicable, since B acquires a pole on the physical sheet, contradicting the spectral representation for this quantity^[2,3,12]. A method for analytically continuing (43) with respect to temperature, making it possible to get around this difficulty, was proposed in^[1]. As a result, very complicated expressions were obtained for A and B , whose analysis is possible only with the aid of numerical integration. In^[2,3], owing to a more successful choice of the initial amplitudes (α_+ in lieu of A and B), the foregoing difficulty did not arise at all. We shall now indicate an analytic continuation in the temperature by a method simpler than in^[1]. Recognizing that $\Phi(E + i\delta) = \Phi^*(E - i\delta)$ when $T > T_K$, we have

$$\begin{aligned} \frac{k}{2\pi i} \int_0^\infty \frac{dE' \ln |\Phi|^2}{k'(E' - E - i\delta)} &= \frac{k}{2\pi i} \int_C \frac{dE' \ln \Phi}{k'(E' - E - i\delta)} \\ &= \ln \Phi + \frac{k}{2\pi i} \int_{C'} \frac{dE' \ln \Phi}{k'(E' - E)} \end{aligned} \quad (44)$$

where the contour C is indicated in Fig. 2, and the contour C' encompasses the zeroes of Φ lying on the physical sheet at $E < 0$. With the aid of this expression, we can rewrite (43) in the form

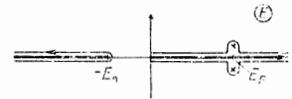
$$\begin{aligned} A &= \frac{1}{2ik} \left(e^{2i\nu} \frac{\Phi}{D} - 1 \right) \quad B = \frac{e^{2i\nu}}{2ik} \eta^{-1} \\ D &= \exp \left\{ \frac{k}{2\pi i} \int_0^\infty \frac{dE' \ln [|\Phi|^2 + S(S+1)]}{k'(E' - E - i\delta)} \right\} \\ \nu &= \nu - \frac{k}{4\pi} \int_{C'} \frac{dE' \ln \Phi}{k'(E' - E)} \end{aligned} \quad (45)$$

It is evident that B now has no pole on the physical sheet at $T < T_K$. These formulas effect the analytic continuation in the temperature from $T > T_K$ to $T < T_K$. The point $T = T_K$ is not a singular point of the amplitude. The mechanism of this continuation can be readily understood by starting from the following considerations. When $T > T_K$, the zeroes of Φ lie on the unphysical sheet. When $T = T_K$ they go on the real axis, and when $T < T_K$ they go over to the physical sheet. By the same token, they deform the integration contour C as shown in Fig. 3, where the positions of the zeroes are marked by crosses. The result of the contour integration remains unchanged and leads to formulas (45).

We note an important consequence of formulas (43). The function R can be represented in the form $R = \eta e^{2i\delta}$. In the integral that determines R , the integration region near the Fermi surface is important. In this region $|\Phi|^2$ is an even function of $E' - E_F$. It is easy to show that if we neglect the corrections of the order ζ/E_F , then η is an even function and δ an odd function of ζ . Recognizing that $e^{2i\nu} \approx 1 + 2ika$, we obtain

$$\begin{aligned} \text{Im } A &\approx \frac{1}{2k_F} (1 - \eta \cos 2\delta + ak_F \eta \sin 2\delta), \\ \text{Re } A &\approx \frac{\eta}{2k_F} (\sin 2\delta + k_F a \cos 2\delta). \end{aligned} \quad (46)$$

FIG. 3



From this we get, taking into account the definition of Φ (11), the properties of evenness of A and B , which we used in Sec. 3. Since the point $T = T_K$ is not a singular point of the amplitude, these properties remain in force also when $T < T_K$.

It remains to demonstrate the equivalence of (45) and our results. To this end, we compare the expression for B in (10) and (45). Recalling the definitions of Φ , $S^{(*)}$, and η^2 , we readily obtain the equality

$$\begin{aligned} \exp \{2i(\nu + \nu_+)\} &= \frac{1}{\Phi + S} \exp \left\{ \frac{k}{2\pi i} \int_0^\infty \frac{dE' \ln |\Phi + S|^2}{k'(E' - E - i\delta)} \right\} \\ &= \exp \left\{ \frac{k}{2\pi i} \int_{C''} \frac{dE' \ln (\Phi + S)}{k'(E' - E - i\delta)} \right\}. \end{aligned} \quad (47)$$

Here the contour C'' encompasses the zeroes of $\Phi + S$, lying on the physical sheet when $E < 0$ (for details concerning these zeroes see^[2]). With the aid of (45) and (47) we can determine the function ν which enters in the Suhl and Wong solution in terms of the function ν_+ , and vice versa.

The solution of the problem on the basis of the properties of analyticity and unitarity is in principle non-unique. It contains certain simple auxiliary functions, which must be determined from additional considerations. In our case these are P and ν_+ , in^[2,3] these are ν_+ and ν_- , and in^[1] these are P and ν . We determine these functions by starting from the requirement that our formulas go over, outside the region of the Kondo effect, into the formulas of the perturbation theory. Suhl and Wong did this somewhat differently, so that their formulas go beyond the scope of perturbation theory when $|\zeta| \gg T_K$, and therefore, in particular, in their formulas T_K depends on V_1 , although at sufficiently small V_1 their formulas practically coincide with ours. Actually, however, when $T_K \ll E_F$, the scattering amplitude depends only on two parameters, determined by the values of the auxiliary functions at $E = E_F$. In our case these are the parameters $a_I(E_F)$ and $g_I(E_F)$ (\bar{V} and \bar{J} in the notation of Suhl and Wong). These are the parameters that should be used to compare theory with experiment.

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Translated by J. G. Adashko

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