PHYSICAL REVIEW B VOLUME 23, NUMBER 4 15 FEBRUARY 1981

Exact solution of the Kahana equation for a positron in an electron gas

E. Boroński, Z. Szotek, and H. Stachowiak
Institute for Low Temperature and Structure Research, Polish Academy of Sciences, Plac Katedralny 1, 50-329 Wrocław, Poland
(Received 11 May 1978; revised manuscript received 24 June 1980)

It is pointed out that the spherical approximation used by Kahana when solving the Bethe-Goldstone equation for a positron in an electron gas is not satisfactory. In this paper the Kahana equation is treated as a two-dimensional integral equation and solved by expressing the electron-positron wave function as a series of Legendre polynomials. From the solution obtained in this way, the new values of the enhancement factors and total annihilation rates are computed. It is shown that the shape of the enhancement curve for large momenta differs from that obtained by Kahana. Moreover, the total screening charge and its distribution are found. These are analyzed and compared with equivalent distributions for $r_s = 2$, 3, and 4 obtained by Sjölander and Stott and also Arponen and Pajanne. The essential contribution of higher partial waves to the screening cloud neglected by previous authors is emphasized.

I. INTRODUCTION

It is well known that the angular-correlation measurements of positron annihilation quanta (ACPAQ) yield information about the momentum distribution of conduction electrons, and for this reason they are of direct interest for the study of the Fermi surface of metals and also of the electronic wave functions. However, in order to obtain the proper information about these quantities from experimental data, an appropriate theory of electron-positron interaction, at least for the jellium model, is necessary. Such a theory based on a Bethe-Goldstone–type equation for the two-particle electron-positron system was proposed by Kahana[1] in 1963. This equation was obtained by summing the infinite set of ladder diagrams for a static screened interaction. It is worthwhile to point out that this equation leads directly to the electron momentum dependence of the annihilation probability, which is very important for the interpretation of experimental data. Moreover, the values of the total annihilation probability obtained in the Kahana approach turn out to be in rather good agreement with experiment for $r_s \leq 4$ (r_s is the radius of a unit electron sphere). Unfortunately, as was shown by Crowell, Anderson, and Ritchie[2] the ladder approximation used by Kahana breaks down for $r_s \geq 5$, leading to divergent total annihilation rates in this region. Besides, as was pointed out by Bergersen,[3] the charge sum rule is violated in the Kahana treatment. It should be mentioned here that Carbotte,[4] adding some sets of diagrams to the ones included by Kahana, tried to remedy the overaccumulation of electronic charge around the positron to which the Bethe-Goldstone equation leads if the static random-phase approximation (RPA) is applied for the potential between an electron and a positron.

An alternative approach to this problem was proposed by Sjölander and Stott[5] based on a theory elaborated earlier by Singwi *et al.*[6] for the jellium model. It consists in computing in a self-consistent manner the electronic charge-density distribution around the positron. The values of the total annihilation rates calculated by Sjölander and Stott are in striking agreement with those of Kahana[1] and particularly Carbotte,[4] including the divergence at low densities (Fig. 1).

Bhattacharyya and Singwi[7] made an attempt to eliminate this incorrect behavior of the total annihilation probability for large r_s. They introduced into the formalism of Sjölander and Stott the effect of three-particle correlations (Bhattacharyya and Singwi call "three-particle correlations" the contributions from exchange and Coulomb correlations between the screening electrons). However, their theory turned out to be strongly dependent on a parameter which follows from the theory; however, a different value of it is chosen in order to get reasonable results in the low-density region. Moreover, their calculations and also those of Sjölander and Stott do not provide the momentum dependence of the annihilation probability that is so important for the interpretation of the experimental curves.

Recently Arponen and Pajanne[8] proposed a new approach to the problem of electron-positron interaction in jellium. Their approach is based on a self-consistent formalism in which the electron gas is described by a set of interacting bosons, representing collective excitations of the RPA state treated as the unperturbed state. From the exact Hamiltonian of the interacting electron gas Arponen and Pajanne kept, in addition to the positron kinetic energy and the electronic RPA energy, the most important electron-electron interaction terms beyond RPA i.e., terms of second order in the boson operators, including also contraction of higher-order terms responsible for the Fock

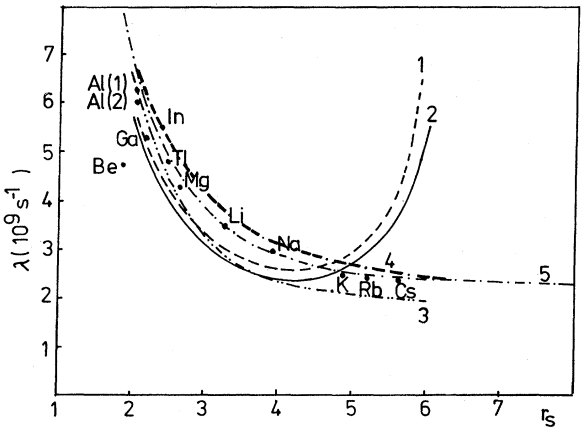


FIG. 1. Comparison of different theoretical annihilation rates with experimental results. Curve 1 is the Kahana result. Curves 2 and 3 represent the results of Sjölander and Stott, and Bhattacharyya and Singwi, respectively. Curve 4 is due to the calculations of Lowy and Jackson, and curve 5 is the result of Arponen and Pajanne. The circles show different experimental results.

and Hubbard self-energies), and for the electron-positron interaction they included terms up to the second order in boson operators. It should be pointed out that the enhancement factors obtained in this approach increase when the electron-positron pair momentum approaches the Fermi surface. Generally, they behave according to the Kahana formula

$$\epsilon(p) = a + bp^2 + cp^4 , \qquad (1.1)$$

but the ratios b/a and c/a decrease with increasing r_s, unlike the ones proposed by Kahana. One should remark that until now through experiment it has not been decided which of these two approaches gives the proper result.[9-13]

With regard to total annihilation rates, no divergence in the low-density region was found by Arponen and Pajanne. It is important to add here that just the inclusion of the electronic non-RPA correlation effects in the Hamiltonian was of paramount importance for obtianing nondivergent results for the total annihilation rates at large r_s.

It seems, then, that the behavior of a positron at rest in jellium is relatively well understood, though the problem of the optimal choice of a two-body electron-positron phenomenological equation is still open. The remark of Arponen and Pajanne that "... the problem of a light impurity in an electron gas cannot ultimately be reduced to a two-body problem, whatever effective interaction is used . . ." is not an answer, since belief in momentum conservation in the two-body electron-positron system is the basic assumption while applying angular correlation in studies of the electronic structure of metallic materials. So, we are of the opinion that the Kahana approach has a definite value, and it is worthwhile to elaborate on it in more detail than previous authors did. This approach, however, was criticized by Lowy and Jackson,[14] but these authors themselves hardly proposed a better solution, at least not for metallic densities. Their main objection against the Kahana theory concerned the way of including the Pauli exclusion principle. Since the Kahana equation is obtained by introducing the Pauli exclusion principle into the Schrödinger equation, they ask whether Kahana introduces superfluous restrictions concerning the wave function. Namely, he neglects the possibility of electrons scattering under the influence of the potential into empty places within the Fermi sea already left by other electrons scattered by the positron. The importance of this contribution is shown in the heavy-particle case by forming a new orthogonal set of eigenfunctions obtained from the Schrödinger equation without introducing Kahana's restrictions. For this reason, in order to obtain the wave function for an electron-positron pair, Lowy and Jackson used the half-shell Lippman-Schwinger equation with the electron-positron effective interaction. They solved this equation for several densities and obtained annihilation rates which were slightly higher than those obtained from experiment. However, they did not publish the momentum-dependent annihilation probabilities very often referred to in terms of enhancement factors. Nevertheless, it follows from the calculations we have performed according to their suggestions that the enhancement factor decreases with increasing electron momentum,[15] and this contradicts experimental results obtained for low[11,16] as well as for high electron densities, e.g., in aluminum.[13] So although Kahana's formalism has some drawbacks, so far it is the simplest one leading to increasing momentum-dependent enhancement factors. Of course the important objection against it is the lack of self-consistency. In order to achieve it, however, it is necessary to solve the Kahana equation more exactly than it has been up to now, and this is exactly the purpose of this paper. To be sure, as was mentioned before, Carbotte[4] tried to satisfy the displaced-charge sum rule, but our objection to his approach is that he should have used the exact solution of the Kahana equation instead of the spherically symmetrical approximation.

Moreover, the Kahana equation neglects exchange and Coulomb correlations between screen-

ing electrons. It was pointed out by Bhattacharyya and Singwi[7] that these effects effects play an important role in removing the divergence of the total annihilation rates in the low-density region. So it may be expected that after including in a self-consistent way electron-electron correlations into the Kahana formalism, the low-density divergence will disappear. Because of the above considerations and hoping that the Kahana approach could be a starting point in building the theory of positron annihilation in real metals, we share the opinion that the first necessary step of this program is done in this paper.

In Sec. II we present a set of integral equations for all partial waves, which should be solved in order to obtain the exact solution of the Kahana equation and describe the way of solving it. Section III is concerned with enhancement factors and total annihilation rates calculated using the exact solution of the Kahana equation. The results obtained in the spherically symmetrical approximation and those of Arponen and Pajanne are also presented for comparison. Then Carbotte's formula for the enhancement factor obtained after introducing Bergersen's so-called v_3 correction is briefly discussed, and its dependence on the higher-than-zero partial waves is demonstrated. Section IV is devoted to the computation of the total electron screening charge distribution around the positron. The results obtained using the exact solution of the Kahana equation are compared to those of Sjölander and Stott and also Arponen and Pajanne. The contribution of higher partial waves to the total electron density distribution around the positron is shown to be essential. Finally, in Sec. V we draw conclusions and give a short discussion of our results. Some preliminary results of this work have been published elsewhere[17-18] (cf. also Szotek[19] and Boroński[20]).

II. SOLUTION OF THE KAHANA EQUATION

The Kahana equation in k space has the form

$$\chi(\vec{p},\vec{k}) = a\frac{U(\vec{k}-\vec{p})}{k^2+(\vec{k}-\vec{p})^2-p^2} + \frac{a}{k^2+(\vec{k}-\vec{p})^2-p^2}\int_{|\vec{q}|\geq 1} d\vec{q}\; U(\vec{k}-\vec{q})\chi(\vec{p},\vec{q}) , \tag{2.1}$$

where momenta are expressed in units of p_F (p_F is the Fermi momentum). Here $a=\tau/8\pi^2=0.33\times r_s/8\pi^2$. $\chi(\vec{p},\vec{k})$ is the Fourier transform of the amplitude $\chi_{\vec{p}}(\vec{x}_e,\vec{x}_p)$ defined by the formula

$$\Psi_{\vec{p}}(\vec{x}_e,\vec{x}_p) = \frac{1}{V}e^{i\vec{p}\vec{x}_e} + \chi_{\vec{p}}(\vec{x}_e,\vec{x}_p) , \tag{2.2}$$

and $\Psi_{\vec{p}}(\vec{x}_e,\vec{x}_p)$ determines the wave function of the electron-positron pair corresponding to the initial electron momentum $\vec{p}$. Here $\vec{x}_e$ and $\vec{x}_p$ are electron and positron coordinates respectively. $U(\vec{k})$ is the Fourier transform of the effective potential of the electron-positron interaction. Generally, the solution of Eq. (2.1) can be expressed as a partial wave expansion

$$\chi(\vec{p},\vec{k}) = \frac{1}{k}\sum_{n=0}^{\infty} a_n\chi_n(p,k)\,P_n(\cos\vartheta) , \tag{2.3}$$

where P_n are Legendre polynomials, ϑ is the angle between $\vec{p}$ and $\vec{k}$, and $a_n=(2n+1)/2$. However, until now the Kahana equation has been solved only under very drastic assumptions which reduce this two-dimensional integral equation to a one-dimensional integral equation. [Kahana carried out an angular averaging of Eq. (2.1) over all directions of $\vec{p}$ and obtained a one-dimensional integral equation for $\chi(p,k)$. This way of calculating $\chi(p,k)$ will be further referred to as "spherical approximation."] Of course, the spherical approximation made in order to obtain in a simple way the solution of Eq. (2.1) is not valid for p close to p_F and must lead to an incorrect description of this region. So one should treat the problem more carefully, especially in the immediate neighborhood of the Fermi surface, and solve Kahana equation more exactly then was done by previous authors.

Introducing (2.3) into Eq. (2.1) we obtain the infinite system of integral equations

$$\chi_n(p,k) = \frac{n}{2n+1}\frac{p}{k}\chi_{n-1}(p,k) + \frac{n+1}{2n+1}\frac{p}{k}\chi_{n+1}(p,k) + \frac{\tau}{4\pi k}U_n(p,k) + \frac{\tau}{2\pi k}\int_1^{\infty} dq\; qU_n(k,q)\chi_n(p,q) \tag{2.4}$$

(for $n=0,1,2,\ldots$), where

$$U_n(p,k) = \int_{-1}^{1} U(p,k,x)P_n(x)dx . \tag{2.5}$$

However, because of the weak convergence of the expansion (2.3) caused by the singularity of $\chi(\vec{p},\vec{k})$ when $\vec{p}$ tends to $\vec{k}$, solving Eqs. (2.4) is not the best way of obtaining the partial waves $\chi_n(p,k)$. A more appropriate way is solving the following equation:

$$g(\vec{p},\vec{k}) = aU(\vec{p}-\vec{k}) + a\int_{|\vec{q}|\geq 1} d\vec{q}\; U(\vec{k}-\vec{q})\frac{g(\vec{p},\vec{q})}{q^2+(\vec{q}-\vec{p})^2-p^2} , \tag{2.6}$$

where

$$g(\vec{p},\vec{k}) = [k^2+(\vec{k}-\vec{p})^2-p^2]\chi(\vec{p},\vec{k}) . \tag{2.7}$$

The above function is slowly varying when $\vec{p}$ tends to $\vec{p}_F$ and exhibits only a weak anisotropy. It has the advantage to have no singularity at $\vec{p}=\vec{k}$, so the expansion of $g(\vec{p},\vec{k})$ into partial waves consists of a few terms only. Thus expanding it and also the other functions in (2.6) according to Legendre polynomials, we obtain the infinite system of integral equations

$$g_n(p,k)=aU(p,k)+\frac{2\pi a}{p}\int_1^\infty dq\, qU_n(k,q)\left[\sum_{m=0}^{\infty} a_m g_m(p,q) P_{m,n^<}\left(\frac{q}{p}\right) Q_{m,n^>}\left(\frac{q}{p}\right)\right], \tag{2.8}$$

where $Q_n(x)$ are Legendre functions of the second kind, and $m,n^<$ $(m,n^>)$ means the smaller (bigger) index from the two. The relation between the functions $\chi_n(p,k)$ and $g_n(p,k)$ is given as

$$\chi_n(p,k)=\frac{1}{p}\sum_m a_m g_m(p,k) P_{m,n^<}\left(\frac{k}{p}\right) Q_{m,n^>}\left(\frac{k}{p}\right). \tag{2.9}$$

Equation (2.8) is solved by iteration. U_m are taken as zero approximations for g_m, i.e.,

$$g_m^{(0)}(p,k)=U_m(p,k) \quad \text{for } m=0,1,2,\ldots,n_g .$$

The quantity n_g limiting the number of equations in (2.8) depends on the initial electron momentum p. We found that it suffices to take $n_g=3$ for $|\vec{p}|<0.8p_F$, and $n_g=6$ for $|\vec{p}|$ close to p_F. Then using the above approximation we solve Eq. (2.8) for $g_0(p,k)$ and obtain $g_0^{(1)}(p,k)$. Generally, the consecutive approximations $g_n^{(i)}$ of g_n are obtained as a result of computing the right-hand side of the equation

$$g_n^{(i)}(p,k)=aU(p,k)+\frac{2\pi a}{p}\int_1^\infty dq\, qU_n(k,q)\left[a_0 g_0^{(i)}(p,q)P_0\left(\frac{q}{p}\right)Q_n\left(\frac{q}{p}\right)+a_1 g_1^{(i)}(p,q)P_1\left(\frac{q}{p}\right)Q_n\left(\frac{q}{p}\right)+\cdots\right.$$
$$\left.+a_n g_n^{(i-1)}(p,q)P_n\left(\frac{q}{p}\right)Q_n\left(\frac{q}{p}\right)+\cdots+a_{n_g} g_{n_g}^{(i-1)}(p,q)P_n\left(\frac{q}{p}\right)Q_{n_g}\left(\frac{q}{p}\right)\right], \tag{2.10}$$

where $i=1,2,3,\ldots$; $n=0,1,2,\ldots,n_g$. The system of equations (2.10) is solved until the condition

$$\left|\frac{g_n^{(i)}(p,k)-g_n^{(i-1)}(p,k)}{g_n^{(i)}(p,k)}\right|<10^{-6}$$

is satisfied, and then it is assumed that

$$g_n(p,k)=g_n^{(i)}(p,k) .$$

It is necessary to add that, when solving Eqs. (2.10) in order to account properly for the behavior of g_n when k is close to the Fermi momentum, the k points between p_F and $1.2p_F$ were chosen according to the logarithmic scale and their number increased when p approached the Fermi surface.

Our calculations were performed on the computer ODRA 1305 for the static RPA and the exponential screening (ES) potentials (the latter was proposed by Stachowiak[21] and it is in better agreement with the RPA potential than the Yukawa potential) for $r_s=2$, 3, and 4, and several momenta p chosen in the range $0-0.9999p_F$. These potentials expressed in units of p_F are, respectively,

$$U_{s\mathrm{RPA}}(k)=\frac{4\pi}{k^2\{1+(\tau/k^3)[k+(1-0.25k^2)\ln|(k+2)/(k-2)|]\}}, \tag{2.11}$$

$$U_{\mathrm{ES}}(k)=4\pi\frac{8\tau+k^2}{(4\tau+k^2)^2} . \tag{2.12}$$

The wave functions $\chi_n(p,k)$ obtained in this way were used for calculating the enhancement factors, the total annihilation probabilities, and the screening charge distribution around the positron. The results presented in this paper correspond to the case when the static RPA potential is used in the Kahana equation.

III. ENHANCEMENT FACTORS

The enhancement factor is defined by the formula

$$\epsilon(p)=\frac{|\Psi_{\vec{p}}(\vec{x}_e,\vec{x}_p)|^2}{|\Psi^0_{\vec{p}}(\vec{x}_e,\vec{x}_p)|^2}\Bigg|_{\vec{x}_e=\vec{x}_p}, \tag{3.1}$$

where $\Psi^0_{\vec{p}}(\vec{x}_e,\vec{x}_p)$ is the wave function of a noninteracting electron-positron pair, and $\Psi_{\vec{p}}(\vec{x}_e,\vec{x}_p)$ is the solution of the Kahana equation. This quantity characterizes the distortion of the electron wave function by the positron. It gives information about the relation between the electron momentum distribution obtained from the positron annihilation studies and the real one. Therefore knowledge of the enhancement factor is necessary for a proper interpretation of the experimental data in terms of Fermi surface, wave functions, occupation numbers, and electron density.

The most striking conclusion is that Kahana and also other authors have never tried to solve the Bethe-Goldstone equation for larger electron momenta p, namely, for p greater than $0.9p_F$, even in the spherical approximation. They assumed that the formula(1.1) describing the electron momentum dependence of the enhancement factor, proposed by Kahana on the basis of the spherical solution of the Bethe-Goldstone equation for three electron momenta only ($p=0$, 0.5, and 0.75 in units of p_F), is valid in the whole region between 0 and p_F. However, our computations that were performed using both the exact and spherical solutions of the Kahana equation [for potentials (2.11) and (2.12)] led us to the conclusion that it is impossible to describe properly the behavior of the enhancement factor by so simple a formula, and without solving the set (2.10). This can be easily seen from Figs. 2 and 3.

In Fig. 2 we present the relative enhancement factor as a function of the initial electron momentum p, calculated on the basis of the exact solution (curve 1) in comparison with the curve following from both the exact solution and the formula (1.1) (curve 2). Here the results obtained according to the formula (1.1) using the parameters a, b, and c calculated on the basis of the spherical solution (curve 3), and those of Arponen and Pajanne[8] (curve 4) are also given. As can be seen, the slopes of these curves are quite different, and the values of the enhancement factor calculated using the exact solution of Eq. (2.1), presented in Table I, differ appreciably for large momenta p from those obtained according to the formula (1.1) with parameters a, b, and c calculated from the solution of the set (2.10) (curve 2), and moreso from those represented by curve 3. It seems to us, however, when com-

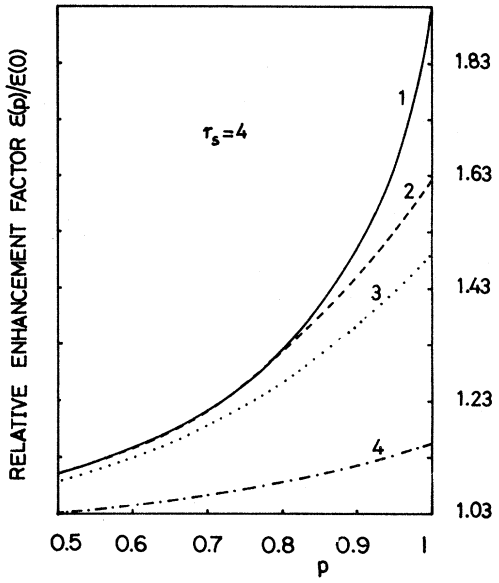


FIG. 2. Relative momentum-dependent enhancement factors. Curve 1 refers to the results obtained using the exact solution of the Kahana equation. Curve 2 was obtained according to the formula (1.1) using the parameters a, b, and c calculated on the basis of the exact solution. Curve 3 refers to the enhancement factors obtained using both the spherical solution and the formula (1.1) and curve 4 represents the results of Arponen and Pajanne.

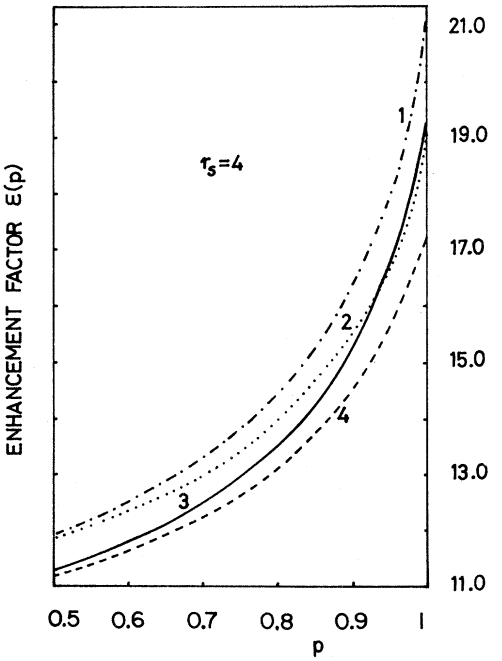


FIG. 3. Momentum-dependent enhancement factors. Curves 1 and 2 were obtained according to the formula (3.1) using the exact solution of the Kahana equation and the spherical one, respectively. Curves 3 and 4 were calculated according to the Carbotte formula (3.4) based on the same solutions as previously.

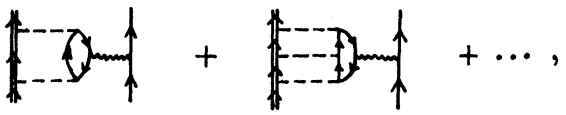
TABLE I. Values of the enhancement factors calculated according to the formula (3.1) from the exact solution of Eq. (2.1) using the static RPA potential.

	Enhancement factor $\epsilon(p)$		
p	$r_s=2$	$r_s=3$	$r_s=4$
0.05	3.425	6.067	10.954
0.1	3.430	6.079	10.974
0.2	3.451	6.125	11.084
0.3	3.487	6.206	11.274
0.4	3.540	6.326	11.564
0.5	3.613	6.495	11.964
0.6	3.712	6.725	12.524
0.7	3.846	7.038	13.304
0.8	4.034	7.488	14.454
0.9	4.322	8.196	16.334
0.945	4.520	8.691	17.694
0.99	4.843	9.509	20.004
0.994 5	4.895	9.642	20.394
0.999	4.962	9.813	20.884
0.999 45	4.971	9.835	20.944
0.999 9	4.982	9.862	21.024

paring curves 1 and 2, that the deviation of the enhancement factor calculated using the exact solution from the behavior described by the formula (1.1), is mainly due to the lack of self-consistency in the Kahana approach. Our preliminary considerations show that the overaccumulation of electronic charge around a positron particularly influences the enhancement factors for momenta close to the Fermi momentum. Removing this excess of charge decreases the values of the enhancement factor mainly in this region, making the momentum dependence weaker. Therefore one can expect that if self-consistency in the Kahana approach is achieved, curve 1 (see Fig. 2) will probably approach curve 2. However, the difference between curves 2 and 3 is still considerable, meaning that the exact solution of Eq. (2.1) is significant for describing properly the behavior of the enhancement factor following from the Kahana equation in the immediate neighborhood of the Fermi surface. Moreover, it is necessary to add that the differences between the values of the enhancement factor calculated using the exact solution and the spherical one increase with increasing r_s.

Of course, we share the opinion that the problem of the real behavior of the enhancement factor with respect to the initial electron momentum p is still open. It can be said, however, that the Kahana equation leads to the enhancement factors presented in Table I instead of those computed by Kahana.[1]

With regard to the Carbotte correction to the Kahana approach we have found that the formula for the total enhancement factor, derived by him after including the infinite set of diagrams



(3.2)

in order to ensure that the displaced-charge sum rule was satisfied, depends on the value of all partial waves. Indeed, inserting (2.3) into Carbotte's formula

$$\epsilon(p)=1+\frac{\tau}{8\pi^2}\int d\vec{m}\,\frac{U(\vec{m}-\vec{p})}{m^2+(\vec{m}-\vec{p})^2-p^2}+2\int d\vec{m}\,L(\vec{m}-\vec{p})\chi^{(2)}(\vec{p},\vec{m})+\int d\vec{m}\,d\vec{m}'\chi(\vec{p},\vec{m})L(\vec{m}-\vec{m}')\chi(\vec{p},\vec{m}')\,, \tag{3.3}$$

where

$$\chi^{(2)}(\vec{p},\vec{m})=\chi(\vec{p},\vec{m})+\frac{\tau\pi}{(2\pi)^3}\,\frac{U(\vec{m}-\vec{p})}{m^2+(m^2+(\vec{m}-\vec{p})^2-p^2}\,,$$

one gets

$$\epsilon(p)=1+\int_1^\infty m\,dm\left[\frac{\tau}{2\pi p}\int_{m-p}^{m+p}\frac{\rho d\rho U(\rho)}{m^2+\rho^2-p^2}[1-L(\rho)]+4\pi\sum_{n=0}^{\infty}a_n\left(L_n(m,p)\chi_n(p,m)+\pi\chi_n(p,m)\int_1^\infty dm'\,m'L_n(m,m')\chi_n(p,m')\right)\right]. \tag{3.4}$$

Here

$$L_n(m,m')=\int_{-1}^{1}dx\,L(m,m',x)P_n(x)\,, \tag{3.5}$$

and

$$L(\rho)=\rho^2/(\rho^2+\tau\{1+(\tfrac{1}{2}\rho)(1-0.25\rho^2)\times\ln[(\rho+2)/(\rho-2)]^2\})\,.$$

So, it is obvious now that Carbotte should have

TABLE II. Annihilation rates obtained from the momentum-dependent enhancement factor.

	Annihilation rate (10^9 s^{-1})			
	Spherical solution		Exact solution	
r_s	Formula (3.1)	Formula (3.4)	Formula (3.1)	Formula (3.4)
2	5.774	5.585	5.870	5.640
3	3.172	3.007	3.240	3.069
4	2.617	2.453	2.697	2.551

used the exact solution of the Kahana equation while taking into account Bergersen's objection. Indeed, if the total screening charge is not computed properly, how can we know to what extent Kahana approach is not self-consistent? Let us remark at this point that Kahana's enhancement factor depends only on the zero-partial wave. Besides, it is worthwhile to note that the method of solving the Kahana equation presented in this paper allows us to determine the zero-partial wave better, than is possible in the spherical approximation.

The difference between the enhancement factors calculated according to the Carbotte formula using either several partial waves, or only the spherical solution of Eq. (2.1), are presented in Fig. 3 (curve 3 and 4). Here the enhancement factors obtained according to formula (3.1) based on both the exact solution (curve 1) and the spherical one (curve 2) are also presented for comparison. Of course, the contribution of higher partial waves to the enhancement factor is particularly important for momenta close to the Fermi momentum and also for lower densities.

In contrast to the enhancement factors, the total annihilation rates do not change as much when taking into account higher partial waves. This is shown in Table II. For comparison we present the values obtained using the enhancement factors computed according to the Carbotte formula and also according to (3.1) either for several partial waves or for the spherical solution.

The main conclusion of these calculations, with respect to enhancement factors, is that formula (1.1) proposed by Kahana on the basis of the spherical approximation for $p \leq 0.75 p_F$ does not describe properly the behavior of the enhancement factor in the immediate neighborhood of the Fermi surface.

IV. DENSITY DISTRIBUTION OF SCREENING ELECTRONS AROUND A POSITRON

In Sec. II the method of calculating electron-positron wave functions has been presented. The functions obtained in this way will be used now for computing the screening charge distribution around the positron. It is well known that the Kahana approach leads to an overaccumulation of screening charge around the positron. This overaccumulation, of course, affects the annihilation rates and the enhancement factors, as has been mentioned in Sec. III. Knowledge of the screening cloud distribution, however, may be of great importance for improving the Kahana method. Such a distribution may be used subsequently for investigating the behavior of a positron in real metals.

Applying formula (2.2), the contribution to the screening cloud around a positron of the electron state determined by the momentum $\vec{p}$ may be expressed as

$$2\left|\Psi_{\vec{p}}(\vec{x}_e,\vec{x}_p)\right|^2 = 2\left|\frac{1}{V}e^{i\vec{p}\vec{x}_e} + \chi_{\vec{p}}(\vec{x}_e,\vec{x}_p)\right|^2$$

$$= \frac{2}{V^2}\left(1 + 2\sum_{\vec{k}>\vec{p}_F}\chi(\vec{p},\vec{k})\cos[(\vec{p}-\vec{k})\vec{r}]\right.$$

$$\left. + \sum_{\vec{k},\vec{k}'>\vec{p}_F} e^{i(\vec{k}-\vec{k}')\vec{r}}\,\chi(\vec{p},\vec{k})\,\chi(\vec{p},\vec{k}')\right),$$

where $\vec{r} = \vec{x}_e - \vec{x}_p$ and the factor of 2 is due to spin.

The screening charge distribution $\Delta\rho(r)$ around a positron can be obtained after integrating (4.1) over the positron coordinates $\vec{x}_p$ and summing over the initial momenta $p < p_F$. Since the distribution is isotropic, it is possible to average (4.1) over all directions of $\vec{r}$. Expanding all functions in (4.1) into Legendre polynomials, depending on the angle between $\vec{k}$, $\vec{k}'$, and $\vec{p}$, and switching from summation to integration, one obtains

$$\Delta\rho(r) = \frac{8}{\pi}\int_0^{p_F} dp\; p^2 \sum_n a_n[j_n(pr) + \pi K_n(p,r)]K_n(p,r)\;, \tag{4.2}$$

where

$$K_n(p,r) = \int_{p_F}^{\infty} dk\; k\chi_n(p,k)j_n(kr)\;, \tag{4.3}$$

and $j_n(x)$ are spherical Bessel functions of order n. This result is based on the formula (see Boroński[20])

$$\int_{-1}^{1} dx\,\frac{\sin[(p^2-k^2-2pkx)^{1/2}r]}{(p^2-k^2-2pkx)^{1/2}}P_n(x) = 2rj_n(pr)j_n(kr)\;. \tag{4.4}$$

The expression (4.2) was used for calculating values of the electron density at distances from the positron between 0 and $12p_F^{-1}$. Since the functions χ_n, for n greater than the order of the set of equations, are not known exactly, we have limited the

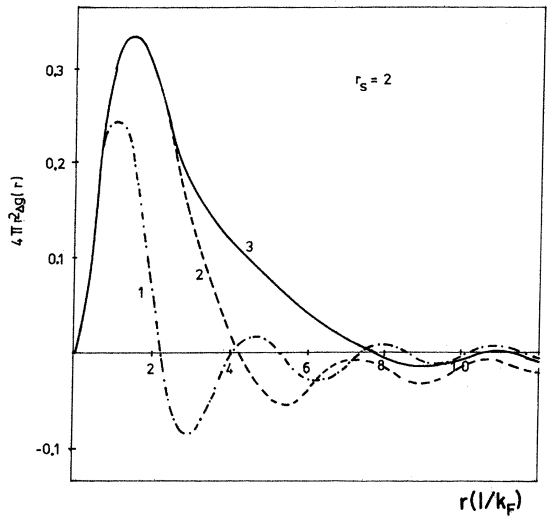


FIG. 4. Total electron-density distribution around the positron for $r_s=2$. Curves 1, 2, and 3 indicate the contributions obtained when including in the computations one, three, and six partial waves, respectively.

number of partial waves in (4.2) and have taken into consideration only six of them. With regard to possible, similar calculations in the future, it may be interesting to note that the contribution to the electron density coming from the nonlinear [i.e., containing $\chi(\vec{p},\vec{k})\chi(\vec{p},\vec{k}')$] term in (4.1) is very small for $r > 9p_F^{-1}$, and we can neglect it in this region.

In Figs. 4–6 we can see that taking into account higher partial waves is of essential importance for obtaining the correct screening charge distribution, especially for $r \sim 2p_F^{-1}$. The differences between curve 1 which results from the Kahana equation in the spherical approximation and curve 3 are very large in the range $r \geq p_F^{-1}$.

Of course, for $r=0$ only the s wave gives a nonzero contribution. For larger distances the contributions of partial waves with n differing by one are close in magnitude. Therefore many partial waves must be taken into account in the total screening cloud distribution. For greater distances they compensate each other to such an extent that we do not observe any Friedel oscillations in the total distribution of the screening charge.

The total electron charge contained inside a sphere of radius r is given by

$$Q(r) = 4\pi \int_0^r \Delta\rho(r)\, r^2 dr \ . \tag{4.5}$$

Curves showing this dependence for $r_s=2$, 3, and

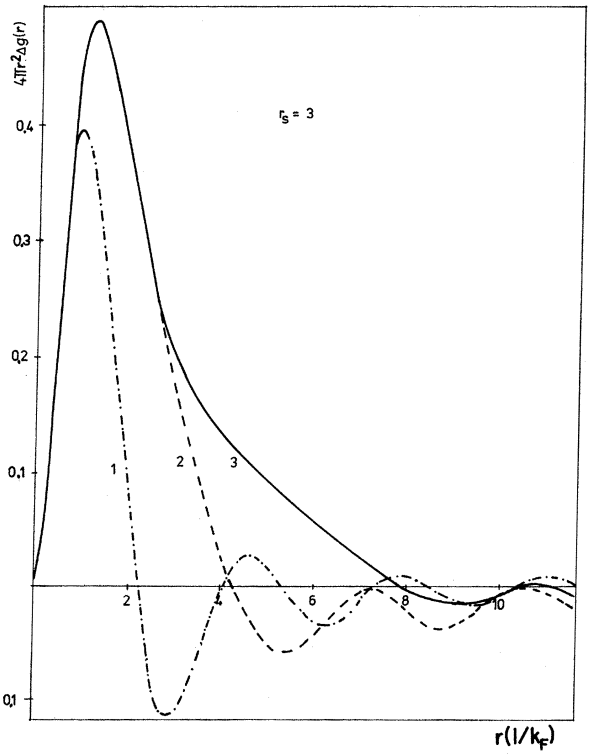


FIG. 5. Total electron-density distribution around the positron for $r_s=3$. Curves 1, 2, and 3 refer to the results obtained when including in the computations one, three, and six partial waves, respectively.

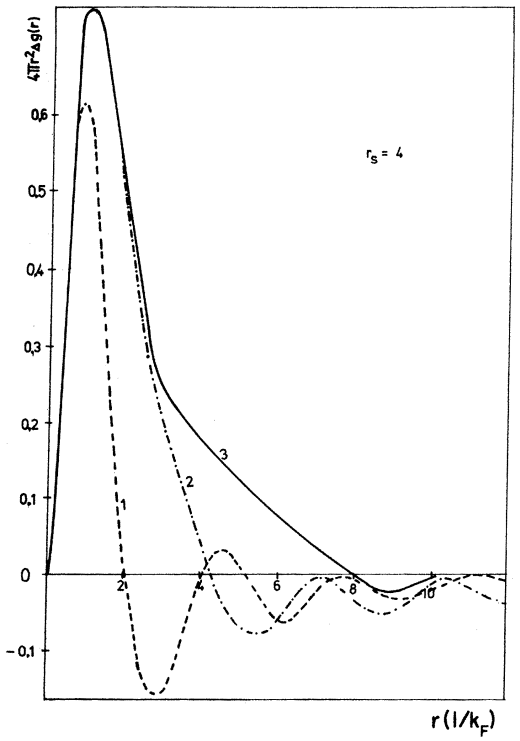


FIG. 6. Total electron-density distribution around the positron for $r_s=4$. Curves 1, 2, and 3 are due to the contributions obtained when one, three, and six partial waves are included in the computations, respectively.

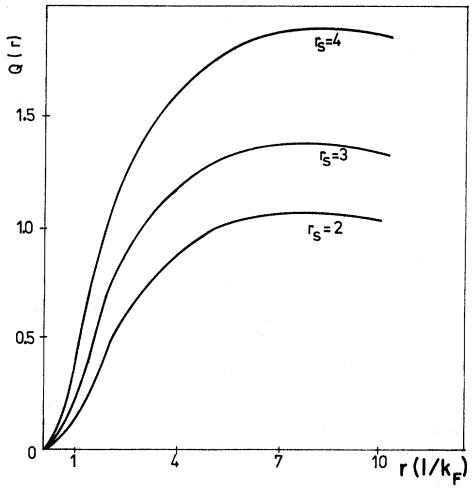


FIG. 7. Dependence of the total electron screening charge on the distance from the positron for $r_s=2$, 3, and 4.

4, and obtained when six partial waves were taken into account, are presented in Fig. 7.

The Kahana equation can be self-consistent only if the total screening charge is equal to one electronic charge. However, it is easy to see that we have a considerable excess of screening charge for all values of r_s, and if we were to take into account all partial waves, this charge would be still bigger. The radii of spheres containing an electron charge equal to one for $r_s=2$, 3, and 4 are, respectively, 5.7, 3.4, and 2.0 (in units of p_F^{-1}).

Now let us compare the electron density distribution around the positron with that around a heavy particle given by three (s, p, and d) partial waves and computed by Stachowiak[23] in the RPA approximation. One can clearly see (Fig.8) that the contribution of higher-than-s partial waves to the screening of a heavy particle is considerably smaller than in the case of a positron. This follows from the fact that the positron recoils during the interaction with the electron. This effect causes the mixing of all partial waves as shown by expression (2.8). For a heavy particle the states

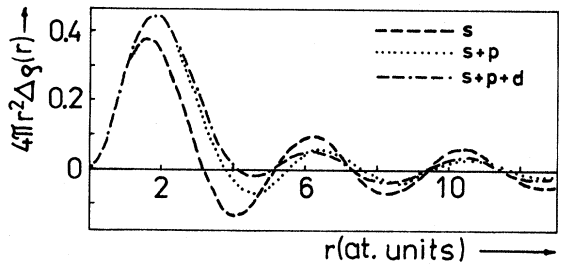


FIG. 8. Contributions of different partial waves to the screening cloud around a positive heavy particle (p_F = 0.75).

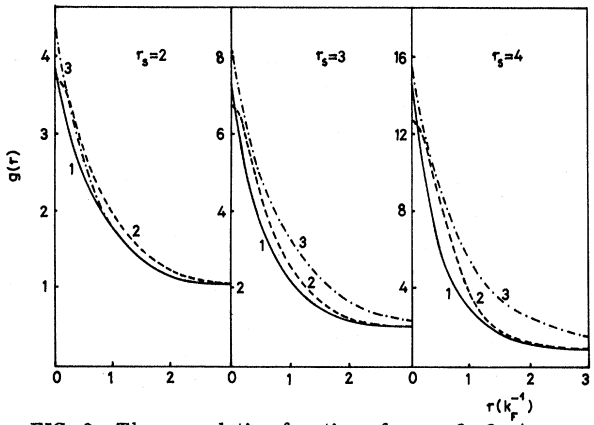


FIG. 9. The correlation functions for $r_s=2$, 3, 4. Curves 1, 2, and 3 indicate the results obtained in this work, by Sjölander and Stott, and by Arponen and Pajanne, respectively.

corresponding to different values of the angular momentum participate in the scattering independently.

It may be very interesting to compare the results for the correlation function

$$g(r)=1+3\pi^2\Delta\rho(r) \tag{4.6}$$

with those obtained for small distances by Sjölander and Stott[5] (SS) and also recently by Arponen and Pajanne[8] (AP) (see Fig.9). One can see that in the region where the attractive interaction is strong, namely for $r\to 0$, our curves run between the curves of SS and AP. In this region the curves of SS show, however, a rounding off in shape while from quantum-mechanical considerations it follows that the correlation function should have a cusp as in our results and those of AP (cf. Lebeda and Schrader[22]). For greater distances the agreement between the results of this work and the AP curves is good for high electron densities, but for high r_s the curves of AP tend to run above our curves and those of SS.

It should be added that for larger distances our distributions are affected by some numerical errors caused mainly by too small a number of partial waves included in the consideration. On the other hand, it is possible that the convergence of the partial-wave series would be better with appropriately changing the effective potential in the Bethe-Goldstone equation and taking into account correlations between screening electrons in a self-consistent way.

V. CONCLUSIONS

The Kahana approach to the problem of electron-positron interaction in an electron gas is the simplest one relatively well confirmed, for $r_s\leq 4$, by most of the experimental work done until

recently. It is necessary to point out that the enhancement factor arising from the Kahana equation increases when approaching the Fermi momentum, and this is the main argument for the validity of this approach. This increase of the enhancement factor in the Kahana formalism arises from the energy denominator in Eq. (2.1) vanishing when p tends to k, this is possible only when p approaches the Fermi momentum.

The results of Arponen and Pajanne[8] also show an increase of the enhancement factor; however, the ratios b/a and c/a of the respective parameters in the formula (1.1) decrease when r_s increases, and this is quite opposite to the results of Kahana. With regard to experimental work done until recently, it does not answer exactly which theory gives proper results. Because of that and the very complicated formalism of Arponen and Pajanne, we are of the opinion that the Kahana equation still has an important significance for understanding the behavior of a positron in metals. Therefore, it is most striking that although starting from 1963 this equation was solved in many papers, its exact solution has not been obtained. However, as was mentioned before, this exact solution leads to a considerably stronger increase of the enhancement factor when approaching the Fermi momentum. Besides, the values of the enhancement factor turn out to be somewhat larger than it follows from Kahana's solution. As concerns experimental confirmation of this high increase we share the opinion that it would require more experimental investigations in this direction, the more so since the results of Arponen and Pajanne (see Fig. 2) show a remarkable difference as compared to Kahana-type calculations. Of course, the problem of the validity of the Kahana equation itself is still open (Arponen and Pajanne[8]). So, the results available up to now within the Kahana formalism are not definitive. However, we do not consider as very serious the objection that it is not self-consistent, nor does it include electron-electron correlations, since an appropriate improvement can be introduced into it.

The exact solution of the Kahana equation has also allowed us to compute the screening charge distribution around the positron. This distribution, as was pointed out long ago,[3] is not self-consistent. However, the very possibility of calculating it shows the proper way to reach self-consistency by choosing a suitable potential.

It is worthwhile to add that we have also obtained the enhancement factors and the charge distributions corresponding to the Kahana equation for ES potential (2.12). These results seem to be better and more consistent than those obtained for the static RPA potential, but in order to compare them with those of previous authors, only results obtained using the static RPA potential are presented here. Moreover, we also performed calculations according to the suggestions of Lowy and Jackson[14] (i.e., neglecting the Pauli projector operator in the Bethe-Goldstone equation), but the distribution of the screening charge turned out to be much worse than that obtained on the basis of the Kahana equation. Therefore we are of the opinion that it is encouraging that the exact solution of the Kahana equation allows one to continue studies toward achieving self-consistency and including correlations between the screening electrons in the sense of Bhattacharyya and Singwi.[7]

ACKNOWLEDGMENTS

The authors wish to thank Dr. J. Arponen and Dr. E. Pajanne for helpful and constructive remarks concerning present calculations.

[1]S. Kahana, Phys. Rev. 129, 1622 (1963).
[2]J. Crowell, V. E. Anderson, and R. H. Ritchie, Phys. Rev. 150, 243 (1966).
[3]B. Bergersen, Ph.D. thesis, Brandeis University, 1964 (unpublished).
[4]J. P. Carbotte, Phys. Rev. 155, 197 (1967).
[5]A. Sjölander and M. J. Stott, Phys. Rev. B 5, 2109 (1972).
[6]K. S. Singwi, M. P. Tosi, R. H. Land, and A. Sjölander, Phys. Rev. 176, 589 (1968).
[7]P. Bhattacharyya and K. S. Singwi, Phys. Rev. Lett. 29, 22 (1972).
[8]J. Arponen and E. Pajanne, J. Phys. F 9, 2359 (1979); J. Phys. C 12, L161 (1979); Ann. Phys. 121, 343 (1979).
[9]J. J. Donaghy and A. T. Stewart, Phys. Rev. 164, 396 (1967).
[10]J. A. Arias–Limonta and P. G. Varlashkin, Phys. Rev. B 1, 142 (1970).
[11]S. M. Kim and A. T. Stewart, Phys. Rev. B 11, 2490 (1975).
[12]D. R. Gustafson and J. D. Willenberg, Phys. Rev. B 13, 5193 (1976).
[13]J. Mader, S. Berko, H. Krakauer, and A. Bansil, Phys. Rev. Lett. 37, 1232 (1976).
[14]D. N. Lowy and A. D. Jackson, Phys. Rev. B 12, 1689 (1975).
[15]H. Stachowiak and E. Boroński, in *Positron Annihilation, Proceedings of the Fifth International Conference on Positron Annihilation*, edited by R. R. Hasiguti and K. Fujiwara (The Japan Institute of Metals, Sendai,

1979).
[16]H. Stachowiak, Phys. Stat. Solidi 41, 599 (1970).
[17]E. Boroński, Z. Szotek, and H. Stachowiak, in *Positron Annihilation, Proceedings of the Fifth International Conference on Positron Annihilation*, edited by R. R. Hasiguti and K. Fujiwara (The Japan Institute of Metals, Sendai, 1979), p. 297.
[18]H. Stachowiak and Z. Szotek, in *Proceedings of the 9th Annual International Symposium on Electronic Structure of Metals and Alloys, Gaussig, East Germany 1979*, edited by P. Ziesche (Technische Universität, Dresden, 1979).
[19]Z. Szotek, Ph.D. thesis, Institute for Low Temperature and Structure Research, Polish Academy of Sciences, Wrocław, 1976 (unpublished).
[20]E. Boroński, Ph.D. thesis, Institute for Low Temperature and Structure Research, Polish Academy of Sciences, Wrocław, 1977 (unpublished).
[21]H. Stachowiak, Phys. Status Solidi 52, 313 (1972).
[22]C. F. Lebeda and D. M. Schrader, Phys. Rev. 178, 24 (1969).
[23]H. Stachowiak, Bull. Acad. Pol. Sci. Math. Astron. Phys. 24, 535 (1976).