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Electron-positron interaction in jellium

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The problem of a positron in jellium is solved in an approach involving self-consistent perturbation of a Jastrow-type state. The merits of this approach are the following: (1) The one-electron wave functions are allowed to be nonorthogonal, (2) the formalism is indifferent with regard to utilizing the Pauli exclusion principle, and (3) numerical calculations are shorter by a factor of the order of 100 in comparison with other theories. The first two points are of special importance in view of the difficulties encountered both by the Kahana formalism and the approach of Lowy and Jackson. The screening cloud obtained in this work reproduces quite well the recent results of Rubaszek and Stachowiak, as do the partial annihilation rates. A comparison with the results of other theories and with experiment is also made.

I. INTRODUCTION

The problem of electron-positron interaction in jellium, so important for investigations of metallic materials by positron annihilation, is still an open one (for details, see Ref. 1). While the electron density on the positron (measured experimentally as positron annihilation rate) is quite well understood theoretically and the results of theoretical calculations agree satisfactorily with each other and with experiment,[1,2] the annihilation probability of different electronic states is different depending on the theoretical approach, but none of the approaches seems to agree with measurements, although the Kahana formalism leads to results closest to experiment at least for alkalis.[1,3]

Of the theoretical approaches to the e^+-e^- interaction in jellium let us concentrate on the following three: (1) the approach of Kahana[4,1,3] (referred to as K in the following), (2) the approach of Lowy and Jackson[5,6] (LJ), and (3) the approach of Arponen and Pajanne[7] (AP). Each of these approaches leads to different partial annihilation rates (total momentum distributions of annihilation photon pairs). In our opinion the reason for that is the following: K and LJ use as an unperturbed state for the electron system the free electron state described by a Slater determinant of plane waves. The e^+-e^- interaction disturbs these plane waves. However, the way of computing the electron density distribution around the positron is different in both approaches. In K the interaction throws electrons out of the fully occupied Fermi sphere. In the LJ approach the Pauli exclusion principle in the usual form is neglected at least in part of the calculations on the basis of the argument that different electron eigenstates are orthogonal, so the Pauli exclusion principle is satisfied automatically at least if the positron recoil is neglected, with no additional constraints needed to be imposed on the solutions of the Schrödinger equation. As shown in Ref. 1, neither K nor LJ use orthogonal single-electron wave functions, so both approaches are approximate from that point of view. (Strictly speaking the LJ single-electron wave functions are orthogonal only insofar as the positron recoil is neglected.)

The AP approach is similar to K as far as it applies the Pauli exclusion principle in the usual form: no electron scattering is possible to states inside the Fermi sphere. The difference is that it uses as an unperturbed state of the electron system the random-phase-approximation (RPA) state instead of the free-electron state, taking into account in this way explicit electron-electron correlations. It has been shown by Boroński[8] that this is the reason for the difference of partial annihilation rates following from the two approaches. If one believes the suggestion of Carbotte and Kahana[9] that explicit electron-electron correlations of the Daniel-Vosko type have little effect on e^+-e^- annihilation, which occurs as if the electron distribution in momentum space had a rectangular shape, then the agreement of K (in the form of Ref. 1) with experiment, at least for low electron densities, is understandable. Note that taking into account the effect of the lattice could improve the agreement between experiment and the results following from a Kahanatype theory.[10]

In this work those assumptions of the K formalism against which LJ objected are avoided. Following K and LJ the wave function of the many-electrons–one-positron system is assumed in the form of a Slater determinant of single-electronic states scattering on the positron. Because of positron recoil the corresponding one-electron wave functions are not orthogonal. However, the unperturbed state is chosen in a different way than in previous approaches. Namely, we start from a Jastrow-type wave function describing electrons scattering on the positron in a state-independent approximation. A preliminary account of the basic assumptions has been given in Ref. 11. The origin of the approach comes from the theory of liquids in the form proposed for fermions by Zabolitzky.[12] This formalism has been adapted by Kallio *et al.*

(KPL) to the problem of charged impurities in jellium.[13,14] This last approach has been made much more effective by replacing in the Euler-Lagrange equation of KPL the electron-electron potential by the usual form used in the theory of metals.[2] The annihilation rates obtained in this way were in quite good agreement with experiment in the whole range of metallic densities. The formalism, however, does not allow one—for fundamental reasons—to compute the partial annihilation rates and hence the total momentum distribution of annihilation photons. This makes the approach of limited relevance for experimental applications.

Here the results of the computations of Gondzik and Stachowiak[2] yielding obviously a good first approximation to electron-positron correlation are used as an unperturbed state in a perturbative calculation of the eigenstate of the electron-liquid–one-positron system. The weakness of the nonorthogonality of the wave functions corresponding to different electron momenta allows one to compute the electron density distribution in spite of the nonorthogonality. The computation of the partial annihilation rates is now possible (Secs. VI and VII). These rates reproduce the enhancement factors obtained in Ref. 1 within the Kahana formalism but differ from the results of Lowy.[6]

One could ask about the relevance of theoretical results obtained for jellium as concerns applications to real metals. It is shown in Ref. 15 that the jellium annihilation characteristics are indeed a necessary ingredient of a theory of positron annihilation in real metals. So it is not appropriate to argue that it is not worthwhile to perform careful calculations for jellium, because the crystal lattice will alter our results anyway. Besides, jellium is also a material suited for experimental investigations if its behavior is simulated on the computer.

II. BASIC ASSUMPTIONS

The wave function of the jellium–one-positron system is assumed as a Slater determinant built of functions $\psi_{\mathbf{k}\sigma}(\mathbf{r}_e,\mathbf{r}_p)$. Here $\mathbf{r}_e$ and $\mathbf{r}_p$ are electron and positron coordinates, respectively. The electron spin index σ will be omitted unless necessary. The functions $\psi_{\mathbf{k}}$ describe the scattering of the electron plane wave on the screened positron and obey the equation (in Hartree atomic units)

$$[-\tfrac{1}{2}\nabla_e^2-\tfrac{1}{2}\nabla_p^2+V(|\mathbf{r}_e-\mathbf{r}_p|)]\psi_{\mathbf{k}}=\frac{k^2}{2}\psi_{\mathbf{k}} \ . \tag{2.1}$$

They are assumed as

$$\psi_{\mathbf{k}}(\mathbf{r}_e,\mathbf{r}_p)=w(|\mathbf{r}_e-\mathbf{r}_p|)\phi_{\mathbf{k}}(\mathbf{r}_e,\mathbf{r}_p) \ , \tag{2.2}$$

where the function $w(r)$ satisfies the equation (cf. Ref. 2)

$$[-\nabla^2+V_0(r)]w(r)=0 \ . \tag{2.3}$$

We set

$$\phi_{\mathbf{k}}(\mathbf{r}_e,\mathbf{r}_p)=\frac{1}{\sqrt{\Omega}}e^{i\mathbf{k}\cdot\mathbf{r}_e}+v_{\mathbf{k}}(\mathbf{r}_e,\mathbf{r}_p) \ , \tag{2.4}$$

where $v_{\mathbf{k}}$ is a small perturbation and Ω is the volume of the sample. In Ref. 2 the function $w(r)$ has the interpretation of square root of the electron density and satisfies the Euler-Lagrange equation (2.3) if one defines $V_0(r)$ according to the formula

$$V_0(r)=-\frac{1}{r}+\rho_0\int\frac{w^2(r')-1}{|\mathbf{r}-\mathbf{r}'|}d\mathbf{r}' +V_{\mathrm{xc}}[w^2(r)\rho_0]-V_{\mathrm{xc}}[\rho_0] \ . \tag{2.5}$$

The last term on the right-hand side of (2.5) follows from the requirement that the $W(r)$ potential in Refs. 13 and 14 (cf. also Gondzik and Stachowiak[2]) vanishes if the screening cloud around the positron disappears. The boundary condition

$$\lim_{r\Longrightarrow\infty}w(r)=1 \tag{2.6}$$

is imposed while $\rho_0=3/4\pi r_s^3$ is the density of the electron liquid. $V_{\mathrm{xc}}[\rho]$ is the exchange-correlation correction in the local density approximation. It was chosen in the form proposed by Hedin and Lundqvist.[16] Note that the function $w(r)$ defined by formula (2.2) no longer has the interpretation of the square root of the electron density.

Introducing (2.2) into (2.1) one gets, neglecting terms of higher order of smallness, the equation

$$\left[-\tfrac{1}{2}\nabla_e^2-\tfrac{1}{2}\nabla_p^2-\frac{k^2}{2}\right]\left[\frac{1}{\sqrt{\Omega}}e^{i\mathbf{k}\cdot\mathbf{r}_e}+v_{\mathbf{k}}(\mathbf{r}_e,\mathbf{r}_p)\right] =(\nabla_e\ln w)i\mathbf{k}\frac{1}{\sqrt{\Omega}}e^{i\mathbf{k}\cdot\mathbf{r}_e}-v(|\mathbf{r}_e-\mathbf{r}_p|)\frac{1}{\sqrt{\Omega}}e^{i\mathbf{k}\cdot\mathbf{r}_e} \ . \tag{2.7}$$

The terms in (2.7) belonging to the perturbative part of the new Hamiltonian

$$H'=-(\nabla_e\ln w)\nabla_e-(\nabla_p\ln w)\nabla_p+v(r) \ , \tag{2.8}$$

where

$$v(r)=V(r)-V_0(r) \tag{2.9}$$

are considered to be small. From (2.7) one gets

$$\left[-\tfrac{1}{2}\nabla_e^2-\tfrac{1}{2}\nabla_p^2-\frac{k^2}{2}\right]v_{\mathbf{k}}(\mathbf{r}_e,\mathbf{r}_p) =\frac{w'}{w}\frac{\mathbf{r}}{r}\frac{i\mathbf{k}}{\sqrt{\Omega}}e^{i\mathbf{k}\cdot\mathbf{r}_e}-\frac{1}{\sqrt{\Omega}}v(r)e^{i\mathbf{k}\cdot\mathbf{r}_e} \ . \tag{2.10}$$

This last equation can be written in the form

$$\left[-\tfrac{1}{2}\nabla_e^2-\tfrac{1}{2}\nabla_p^2-\frac{k^2}{2}\right]v_{\mathbf{k}}(\mathbf{r}_e,\mathbf{r}_p) =[iW(r)k\cos\vartheta-v(r)]\frac{1}{\sqrt{\Omega}}e^{i\mathbf{k}\cdot\mathbf{r}_e} \ , \tag{2.11}$$

where

$$W(r)=\frac{1}{w}\frac{dw}{dr} \tag{2.12}$$

and ϑ is the angle between $\mathbf{k}$ and $\mathbf{r}=\mathbf{r}_e-\mathbf{r}_p$. $v_{\mathbf{k}}$ is assumed in the form

$$v_{\mathbf{k}}(\mathbf{r}_e,\mathbf{r}_p)=\sum_{\mathbf{k}_e,\mathbf{k}_p} A_{\mathbf{k}}(\mathbf{k}_e,\mathbf{k}_p)e^{i\mathbf{k}_e\cdot\mathbf{r}_e}e^{i\mathbf{k}_p\cdot\mathbf{r}_p} . \qquad (2.13)$$

Solving Eq. (2.11) in the Born approximation (cf. Ref. 17), one gets

$$v_{\mathbf{k}}(\mathbf{r}_e,\mathbf{r}_p)=\frac{1}{\Omega^{3/2}}\sum_{\mathbf{q}} A_{\mathbf{k}}(\mathbf{q})e^{i(\mathbf{k}+\mathbf{q})\cdot\mathbf{r}_e}e^{-i\mathbf{q}\cdot\mathbf{r}_p} , \qquad (2.14)$$

where

$$A_{\mathbf{k}}(\mathbf{q})=\frac{\Phi_1(q)k\cos\theta+\Phi_2(q)}{(\mathbf{k}+\mathbf{q})^2/2+q^2/2-k^2/2} , \qquad (2.15)$$

$$\Phi_1(q)=\frac{4\pi}{q^2}\int_0^\infty dr\, W(r)[\sin(qr)-qr\cos(qr)] , \qquad (2.16a)$$

$$\Phi_2(q)=-\frac{4\pi}{q}\int_0^\infty dr\, rv(r)\sin(qr) . \qquad (2.16b)$$

θ is the angle between **k** and **q**.

The wave function of the whole system can be written in the form

$$\Psi(\mathbf{r}_p;\mathbf{r}_1,\ldots,\mathbf{r}_N)=\prod_{i=1}^{N} w(|\mathbf{r}_i-\mathbf{r}_p|)\begin{vmatrix}\phi_{\mathbf{k}_1}(\mathbf{r}_1,\mathbf{r}_p) & \cdots & \phi_{\mathbf{k}_1}(\mathbf{r}_N,\mathbf{r}_p)\\ \phi_{\mathbf{k}_2}(\mathbf{r}_1,\mathbf{r}_p) & \cdots & \phi_{\mathbf{k}_2}(\mathbf{r}_N,\mathbf{r}_p)\\ & \cdots & \\ \phi_{\mathbf{k}_N}(\mathbf{r}_1,\mathbf{r}_p) & \cdots & \phi_{\mathbf{k}_N}(\mathbf{r}_N,\mathbf{r}_p)\end{vmatrix} . \qquad (2.17)$$

Setting

$$\mathbf{s}=\mathbf{r}_e-\mathbf{r}_p,\quad \mathbf{s}_i=\mathbf{r}_i-\mathbf{r}_p \qquad (2.18)$$

one can write

$$\phi_{\mathbf{k}}(\mathbf{r}_e,\mathbf{r}_p)=e^{i\mathbf{k}\cdot\mathbf{r}_p}\phi_{\mathbf{k}}(\mathbf{s}) , \qquad (2.19)$$

where

$$\phi_{\mathbf{k}}(\mathbf{s})=\frac{1}{\Omega^{1/2}}e^{i\mathbf{k}\cdot\mathbf{s}}+\frac{1}{\Omega^{3/2}}\sum_{\mathbf{q}} A_{\mathbf{k}}(\mathbf{q})e^{i(\mathbf{k}+\mathbf{q})\cdot\mathbf{s}} . \qquad (2.20)$$

The first factor on the right-hand side of (2.19) will give in (2.17) a factor

$$\exp[i(\Sigma\mathbf{k}_i)\cdot\mathbf{r}_p]=1 \qquad (2.21)$$

and can be omitted.[1,11,18] The wave function of the system can thus be written as

$$\Psi(\mathbf{s}_1,\ldots,\mathbf{s}_N)=\prod_{i=1}^{N} w(s_i)\begin{vmatrix}\phi_{\mathbf{k}_1}(\mathbf{s}_1) & \cdots & \phi_{\mathbf{k}_1}(\mathbf{s}_N)\\ \phi_{\mathbf{k}_1}(\mathbf{s}_1) & \cdots & \phi_{\mathbf{k}_2}(\mathbf{s}_N)\\ & \cdots & \\ \phi_{\mathbf{k}_N}(\mathbf{s}_1) & \cdots & \phi_{\mathbf{k}_N}(\mathbf{s}_N)\end{vmatrix} . \qquad (2.22)$$

Because of the smallness of the perturbative term in (2.20) the wave function Ψ in (2.22) is invariant with regard to switching from the set of functions ϕ_k to the set

$$\tilde{\phi}_{\mathbf{k}}(\mathbf{s})=\frac{1}{\Omega^{1/2}}e^{i\mathbf{k}\cdot\mathbf{s}}+v_{\mathbf{k}}(\mathbf{s})-v'_{\mathbf{k}}(\mathbf{s}) , \qquad (2.23)$$

where

$$v'_{\mathbf{k}}(\mathbf{s})=\frac{1}{\Omega^{3/2}}\sum_{\substack{\mathbf{q}\\ |\mathbf{k}+\mathbf{q}|<k_F}} A_{\mathbf{k}}(\mathbf{q})e^{i(\mathbf{k}+\mathbf{q})\cdot\mathbf{s}} \qquad (2.24)$$

(cf. Ref. 1). Note that the present way of applying the Pauli exclusion principle [formula (2.23)], because of the smallness of $v_{\mathbf{k}}$, is free of the deficiencies of the Kahana approach pointed at by LJ (cf. also Ref. 1).

III. FORMULAS FOR THE ELECTRON DENSITY

The electron density around the positron can be computed from the formula

$$\rho(\mathbf{s}_1)=N\frac{\int|\Psi|^2 d\tau_1}{\int|\Psi|^2 d\tau} , \qquad (3.1)$$

where

$$d\tau=\prod_{i=1}^{N} d\mathbf{s}_i,\quad d\tau_1=\frac{d\tau}{d\mathbf{s}_1} . \qquad (3.2)$$

We will use the full form $\psi_{\mathbf{k}\sigma}$ of the electron wave function remembering that

$$\psi^*_{\mathbf{k}+}\psi_{\mathbf{k}'-}=0 \qquad (3.3)$$

for any value of **k** and **k**′. The spatial part of $\psi_{\mathbf{k}\sigma}$ is defined of course as

$$\psi_{\mathbf{k}}(\mathbf{s})=w(s)\phi_{\mathbf{k}}(\mathbf{s}) . \qquad (3.4)$$

We will assume first that the $\psi_{\mathbf{k}}$ functions are orthogonal, i.e.,

$$\int \psi^*_{\mathbf{k}'\sigma}(\mathbf{s})\psi_{\mathbf{k}\sigma}(\mathbf{s})d\mathbf{s}=\delta_{\mathbf{k}\mathbf{k}'} . \qquad (3.5)$$

$|\Psi|^2$ can be written formally as

$$|\Psi|^2=\sum_{P'}(-1)^{P'}\prod_{i=1}^{N}\psi^*_{\mathbf{k}_i(P'2)\sigma_i(P'2)}(\mathbf{s}_i)\psi_{\mathbf{k}_i(P'1)\sigma_i(P'1)}(\mathbf{s}_i) , \qquad (3.6)$$

where P' is the total permutation characterizing a particular element of the sum in (3.6). After integration over $d\tau$ only those elements of the sum in (3.6) will remain, for which the equalities

$$\mathbf{k}_i(P'2)=\mathbf{k}_i(P'1),\quad \sigma_i(P'2)=\sigma_i(P'1) \qquad (3.7)$$

are simultaneously satisfied for all i's. The same will be true for integration over $d\tau_1$. This leads in (3.1) to the usual formula

$$\rho(\mathbf{s}_1)=2\sum_{|\mathbf{k}|<k_F}\psi^*_{\mathbf{k}}(\mathbf{s}_1)\psi_{\mathbf{k}}(\mathbf{s}_1) . \qquad (3.8)$$

In case of weak nonorthogonality of the wave functions $\psi_{\mathbf{k}\sigma}$, additional terms appearing in the denominator of (3.1) will be at least quadratic with regard to the parameter characterizing the nonorthogonality and will be omitted, since in this paper we will limit ourselves consequently to terms linear with regard to small parameters.

In the numerator of (3.1) additional terms will appear corresponding to permutations with regard to the order defined by Eqs. (3.7). These permutations consist of exchanging $\mathbf{k}_1(P'2)$ in (3.6) with one of the $(N/2)-1$ other possible values of the $\mathbf{k}$ vector. It is easy to see that each of the additional terms will be preceded by a minus sign. This leads to the following expression for the electron density:

$$\rho(\mathbf{s})=2\sum_{\mathbf{k}\ \mathrm{occ}}\psi^*_{\mathbf{k}}(\mathbf{s})\psi_{\mathbf{k}}(\mathbf{s})-2\sum_{\substack{\mathbf{k}\neq\mathbf{k}'\\ \mathrm{occ}}}A_{\mathbf{k}'\mathbf{k}}\psi^*_{\mathbf{k}'}(\mathbf{s})\psi_{\mathbf{k}}(\mathbf{s}) , \tag{3.9}$$

where

$$A_{\mathbf{k}'\mathbf{k}}=\int d\mathbf{s}'\,\psi^*_{\mathbf{k}}(\mathbf{s}')\psi_{\mathbf{k}'}(\mathbf{s}') . \tag{3.10}$$

While performing actual computations using Eq. (3.9) we will consider as small the factor $w^2(s)-1$, because it is limited in space and the term $v_{\mathbf{k}}$ arising from perturbation. Neglecting consequently terms of higher order of smallness we can write $\rho(\mathbf{s})$ in the form

$$\rho(\mathbf{s})=w^2(s)\rho_0+\delta\rho^3(\mathbf{s})-\delta\rho^1(\mathbf{s})-\delta\rho^2(\mathbf{s}) , \tag{3.11}$$

where

$$\delta\rho^1(\mathbf{s})=2\sum_{\substack{\mathbf{k}\neq\mathbf{k}'\\ \mathrm{occ}}}A^1_{\mathbf{k}'\mathbf{k}}\psi^*_{\mathbf{k}'}(\mathbf{s})\psi_{\mathbf{k}}(\mathbf{s}) , \tag{3.12a}$$

$$\delta\rho^2(\mathbf{s})=2\sum_{\substack{\mathbf{k}\neq\mathbf{k}'\\ \mathrm{occ}}}A^2_{\mathbf{k}'\mathbf{k}}\psi^*_{\mathbf{k}'}(\mathbf{s})\psi_{\mathbf{k}}(\mathbf{s}) , \tag{3.12b}$$

$$\delta\rho^3(\mathbf{s})=\frac{2w^2(\mathbf{s})}{\Omega^{1/2}}\sum_{\mathbf{k}\ \mathrm{occ}}[v_{\mathbf{k}}(\mathbf{s})e^{-i\mathbf{k}\cdot\mathbf{s}}+v^*_{\mathbf{k}}(\mathbf{s})e^{i\mathbf{k}\cdot\mathbf{s}}] , \tag{3.12c}$$

$$A_{\mathbf{k}'\mathbf{k}}=A^1_{\mathbf{k}'\mathbf{k}}+A^2_{\mathbf{k}'\mathbf{k}} , \tag{3.13}$$

$$A^1_{\mathbf{k}'\mathbf{k}}=\frac{1}{\Omega}\int d\mathbf{s}'[w^2(s')-1]e^{i(\mathbf{k}'-\mathbf{k})\cdot\mathbf{s}'} , \tag{3.14a}$$

$$A^2_{\mathbf{k}'\mathbf{k}}=\frac{1}{\Omega^{1/2}}\int d\mathbf{s}'[v_{\mathbf{k}'}(\mathbf{s}')e^{-i\mathbf{k}\cdot\mathbf{s}'}+v^*_{\mathbf{k}}(\mathbf{s}')e^{i\mathbf{k}'\cdot\mathbf{s}'}] . \tag{3.14b}$$

If the form (2.23) of the wave function is used in (3.9) and (3.10), $\rho(\mathbf{s})$ [or rather $\tilde{\rho}(\mathbf{s})$] can be written in the form

$$\tilde{\rho}(\mathbf{s})=w^2(\mathbf{s})\rho_0+\delta\tilde{\rho}^3(\mathbf{s})-\delta\tilde{\rho}^1(\mathbf{s})-\delta\tilde{\rho}^2(\mathbf{s}) , \tag{3.15}$$

where $\delta\tilde{\rho}^1$, $\delta\tilde{\rho}^2$, and $\delta\tilde{\rho}^3$ are given by formulas (3.12) where, however, the Pauli exclusion principle in the form of (2.23) and (2.24) has been applied to the wave functions $\psi_{\mathbf{k}}$.

One obtains

$$\begin{aligned}&\delta\tilde{\rho}^1(\mathbf{s})=\delta\rho^1(\mathbf{s}) ,\\ &\delta\tilde{\rho}^2(\mathbf{s})=0 ,\\ &\delta\tilde{\rho}^3(\mathbf{s})=\delta\rho^3(\mathbf{s})-\delta\rho'(\mathbf{s}) .\end{aligned} \tag{3.16}$$

One can show that

$$\delta\rho'(\mathbf{s})=\delta\rho^2(\mathbf{s}) . \tag{3.17}$$

So we have

$$\tilde{\rho}(\mathbf{s})=\rho(\mathbf{s}) . \tag{3.18}$$

Thus application of the Pauli exclusion principle in the form of (2.23) and (2.24) has no influence on the computed electron density distribution provided nonorthogonal terms are included according to Eq. (3.9).

In actual computations of $\rho(\mathbf{s})$ it is convenient to remark at the beginning that the electron density in $\mathbf{s}$ space is isotropic with regard to the origin of the coordinate system. So $\rho(\mathbf{s})$ is invariant with regard to averaging over all directions of $\mathbf{s}$. Such a preliminary operation greatly simplifies subsequent calculations. One gets

$$\delta\rho^1(s)=\frac{w^2(s)k_F^4}{4\pi^3 s}\int_0^\infty ds'\,s'[w^2(s')-1][f(k_F(s-s'))-f(k_F(s+s'))] , \tag{3.19}$$

where

$$f(x)=\frac{1}{x^2}\left[1-\frac{\sin(2x)}{x}+\frac{1-\cos(2x)}{2x^2}\right] , \tag{3.20}$$

$$\delta\rho^3(s)-\delta\rho^2(s)=\frac{w^2(s)}{2\pi^4 s}\int_0^\infty dq[\Phi_1(q)K_1(q)+\Phi_2(q)K_2(q)]\sin(qs) , \tag{3.21}$$

$$K_2(q)=\begin{cases}\dfrac{k_F^2}{2}\phi\left(\dfrac{q}{k_F}\right), & \text{for } \dfrac{q}{k_F}>2\\[2ex] \dfrac{k_F^2}{2}\zeta\left(\dfrac{q}{k_F}\right), & \text{for } \dfrac{q}{k_F}<2,\end{cases} \tag{3.22}$$

$$K_1(q)=\begin{cases}-\dfrac{k_F^3}{2}\left[\dfrac{q}{k_F}\phi\left(\dfrac{q}{k_F}\right)-\dfrac{4}{3}\right], & \text{for } \dfrac{q}{k_F}>2\\[2ex] -\dfrac{k_F^3}{2}\left[\dfrac{q}{k_F}\zeta\left(\dfrac{q}{k_F}\right)-\dfrac{q}{k_F}+\dfrac{1}{12}\left(\dfrac{q}{k_F}\right)^3\right], & \text{for } \dfrac{q}{k_F}<2,\end{cases} \tag{3.23}$$

$$\phi(x)=(1-x^2)\ln\left|\frac{1+1/x}{1-1/x}\right|+2x , \tag{3.24a}$$

$$\zeta(x)=\ln(1+x)-x^2\ln\left(2+\frac{2}{x}\right)+x+\frac{x^2}{2} . \tag{3.24b}$$

Note that the total electron density around the positron is expressed partly in terms of the unknown function $\Phi_2(q)$ defined by Eq. (2.16). This function in real space corresponds to the unknown correction $v(s)$ to the electron-positron potential. The computation of $v(s)$ will be the subject of the following section.

IV. COMPUTATION OF THE CORRECTED ELECTRON-POSITRON POTENTIAL

Let us write the Poisson-like equation (cf. Refs. 1 and 19)

$$\nabla^2\{V(s)-V_{\rm xc}[\rho(s)]\}=4\pi\{\delta(\mathbf{s})-[\rho(\mathbf{s})-\rho_0]\} \ . \tag{4.1}$$

$V_{\rm xc}(s)$ is the exchange-correlation correction which in Refs. 1 and 2 was taken in the local-density approximation

$$V_{\rm xc}(s)=V_{\rm xc}[\rho(s)]$$

and chosen in the form proposed by Hedin and Lundqvist.[16]

The "unperturbed" potential $V_0(s)$ from Ref. 2 satisfies the equation

$$\nabla^2[V_0(s)-V^0_{\rm xc}(s)]=4\pi\{\delta(\mathbf{s})-[w^2(s)-1]\rho_0\} \ . \tag{4.2}$$

Let us assume that the electron density distribution in our approach differs little from the one computed in Ref. 2, so the correlation correction does not depend on the small change of the electron density following from perturbing the hypernetted-chain (HNC) state of Ref. 2. In other words we assume

$$V_{\rm xc}[\rho(s)]=V^0_{\rm xc}(s) \ . \tag{4.3}$$

(Calculations without this assumption are performed in the Appendix). This leads for $v(s)$ to the equation

$$\nabla^2 v(s)=-4\pi[\rho(s)-w^2(s)\rho_0] \tag{4.4}$$

obtained from (4.1) and (4.2). Introducing in (4.4) $\rho(s)$ in the form (3.11) and taking account of (3.19) and (3.21), one obtains the equation

$$\pi^3 s\nabla^2 v(s)+2w^2(s)\int_0^\infty dq\ \Phi_2(q)K_2(q)\sin(qs)=L(s) \ , \tag{4.5}$$

where

$$L(s)=2w^2(s)\left[\frac{\pi k_F^4}{2}\int_0^\infty ds'\,s'[w^2(s')-1]\times[f(k_F(s-s'))-f(k_F(s+s'))]-\int_0^\infty dq\ \Phi_1(q)K_1(q)\sin(qs)\right] \ . \tag{4.6}$$

$L(s)$ can be easily computed numerically using the solution of Eq. (2.3) which was obtained in Ref. 2.

Equation (4.5) is an integrodifferential equation for $v(s)$. However, the unknown function appears both in coordinate space and in Fourier representation. It could seem that switching to Fourier representation would simplify the solution, reducing (4.5) to a Fredholm integral equation of the first kind. It is not so, however, probably because of the rapid oscillations of the kernel. In this situation we have to proceed the other way. We get, making use of (2.16),

$$\begin{aligned}F(s)&=\int_0^\infty \Phi_2(q)K_2(q)\sin(qs)dq\\&=-4\pi\int_0^\infty ds'\,s'v(s')\int_0^\infty dq\frac{K_2(q)}{q}\sin(qs)\sin(qs')\\&=-4\pi\int_0^\infty ds'\,K(s,s')s'v(s') \ ,\end{aligned} \tag{4.7}$$

where

$$\begin{aligned}K(s,s')&=\int_0^\infty dx\frac{K_2(k_Fx)}{x}\sin(sk_Fx)\sin(s'k_Fx)\\&=\tfrac{1}{2}\int_0^\infty dx\frac{K_2(k_Fx)}{x}\{\cos(|s-s'|k_Fx)-\cos[(s+s')k_Fx)]\}\\&=\frac{k_F^2}{4}[M(|s-s'|k_F)-M((s+s')k_F)] \ .\end{aligned} \tag{4.8}$$

So the kernel is expressed in terms of a universal function

$$M(a)=M_1(a)+M_2(a) \ , \tag{4.9}$$

where

$$M_1(a)=\int_0^2 dx\ m_1(x)\cos(ax) \ , \tag{4.10a}$$

$$M_2(a)=\int_2^\infty dx\ m_2(x)\cos(ax) \ , \tag{4.10b}$$

$$m_1(x)=\frac{1}{x}\ln(1+x)-x\ln\left|2+\frac{2}{x}\right|+1+\frac{x}{2} \ , \tag{4.11a}$$

$$m_2(x)=\left|\frac{1}{x}-x\right|\ln\left|\frac{1+1/x}{1-1/x}\right|+2 \ . \tag{4.11b}$$

The function $M(a)$ is shown in Fig. 1. Its main feature is a sharp peak at $a=0$ which extends up to about $a=2$.

Now Eq. (4.5) takes the form

$$\pi^3 s\nabla^2 v(s)-2\pi k_F^2 w^2(s)\int_0^\infty ds'\,\mathcal{K}(s,s')s'v(s')=L(s) \ . \tag{4.12}$$

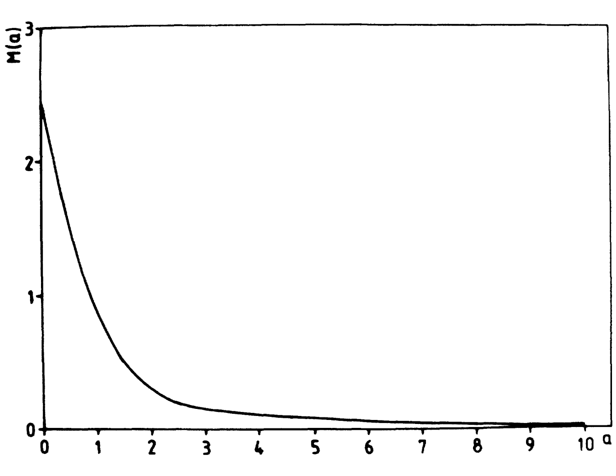

FIG. 1. The $M(a)$ function.

Switching to the function

$$Z(s)=sv(s) \tag{4.13}$$

and capitalizing on the spherical symmetry of the problem, we get finally the equation

$$\pi^3 Z''(s)-2\pi k_F^2 w^2(s)\int_0^\infty ds'\,\mathcal{K}(s,s')Z(s')=L(s) , \tag{4.14}$$

where

$$\mathcal{K}(s,s')=M(|s-s'|k_F)-M((s+s')k_F) . \tag{4.15}$$

Since Eq. (4.14) contains a derivative, the problem of boundary conditions arises.

At $s=0$, Eq. (4.14) takes the form

$$Z''(s)=\lambda s , \tag{4.16}$$

where λ is a constant. This is due in part to the relation

$$\mathcal{K}(0,s')=0 \tag{4.17}$$

following from (4.15). So for small s we have

$$Z(s)=\tfrac{1}{6}\lambda s^3+C_1 s+C_2 . \tag{4.18}$$

The constant of integration C_2 vanishes, since owing to (4.13) it would correspond to a point charge at $s=0$ different from the charge of the positron. And this is the first boundary condition.

For large s the function $L(s)$ on the right-hand side vanishes. The main part in the integral in (4.14) comes from the first term in (4.15). If $Z(s)$ is a slowly varying function in this interval, (4.14) takes the form

$$\pi^3 Z''(s)-2\pi k_F^2\langle M\rangle Z(s)=0 , \tag{4.19}$$

where

$$\langle M\rangle=\int_0^\infty M(|s-s'|k_F)ds' . \tag{4.20}$$

The solution is

$$Z(s)=Ae^{as}+Be^{-as} ,$$

where (4.21)

$$a=k_F\sqrt{2\pi\langle M\rangle} .$$

If one assumes that $Z(s)$ vanishes for $s>s_N$, this corresponds to choosing $A=0$ in (4.21). In this way a consistent boundary condition is imposed at infinity.

Equation (4.14) is solved using algebra. A set of points $s_1,\ldots,s_N$ is chosen ($s_1=0$) and the integral (as well as the derivative) in (4.14) expressed in terms of the $N-1$ unknown quantities $Z(s_2),\ldots,Z(s_N)$. In this way one obtained $N-2$ equations for $s=s_3, s_4,\ldots,s_N$. Additional equations are obtained from (4.18):

$$Z(s_2)=\tfrac{1}{6}\lambda s_2^3+C_1 s_2 , \tag{4.22a}$$

$$Z(s_3)=\tfrac{1}{6}\lambda s_3^3+C_1 s_3 . \tag{4.22b}$$

This makes N equations for $N+1$ unknown quantities. Finally we complete the set with the equation

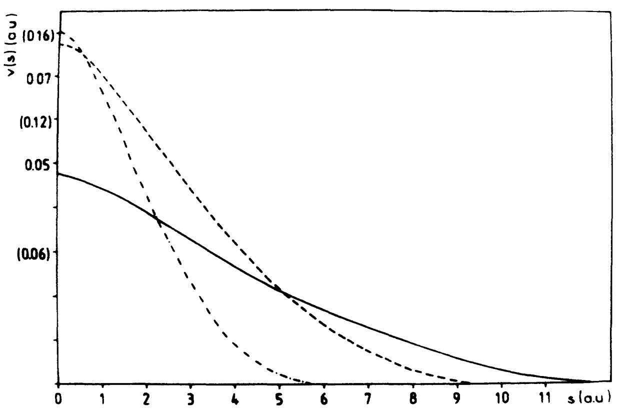

FIG. 2. The $v(s)$ function as obtained from Eq. (4.14) (dashed-dotted line for $r_s=2$, dashed line for $r_s=4$, solid line for $r_s=6$). Note that the vertical scale is different for different values of r_s. The scale for $r_s=2$ is indicated in parentheses.

$$\pi^3\lambda=\lim_{s\to 0}\left[\frac{L(s)}{s}+2\pi k_F^2 w^2(0)\int_0^\infty ds'\frac{\mathcal{K}(s,s')}{s}Z(s')\right] . \tag{4.23}$$

The function $Z(s)$ obtained in this way is quite stable with regard to different choices of the set of points $s_1,\ldots,s_N$, unlike other approaches we tried. The function $v(s)$ following from these calculations is shown in Fig. 2 for different electron densities. It is visible that the approach used in this work is a low density approximation as is usual in the theory of liquids. This conclusion follows from the fact that for $r_s=6$ the correction to the electron-positron potential introduced by the perturbation is smaller than for $r_s=2$ and $r_s=4$.

If one resigns from the assumption (4.3) (cf. the Appendix) one obtains the functions $v(s)$ shown in Fig. 3. Comparison between Figs. 2 and 3 shows that the differences

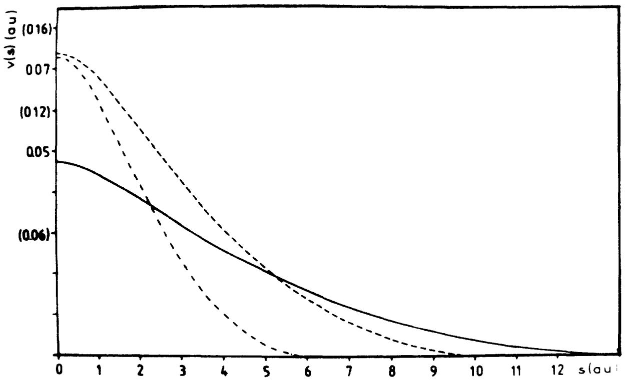

FIG. 3. The same as in Fig. 2, but the curves have been obtained from solving Eq. (A13).

between the two cases are negligible. The values of $v(s)$ are small, thus confirming that the approach used in Ref. 2 gives a good first approximation to the solution of the problem.

V. SCREENING CLOUD DISTRIBUTION AND POSITRON LIFETIME

The density correction $\delta\rho(s)$ [cf. Eqs. (A1) and (A2)] can be written with the help of (3.19), (3.21), and (4.6) in the form

$$\delta\rho(s)=-\frac{1}{4\pi^4 s}\left[L(s)+2\pi k_F^2 w^2(s)\int_0^\infty ds'\mathcal{K}(s,s')\times Z(s')\right]. \qquad (5.1)$$

So the electron density $\rho(s)$ can be computed from the solutions of Eqs. (4.14) or (A13).

First we compute the electron density on the positron

$$\rho(0)=w^2(0)\rho_0+\delta\rho(0) \qquad (5.2)$$

which yields the positron annihilation rate $\lambda(r_s)$—a measurable quantity. It is known that all the existing theories lead at high metallic electron densities to annihilation rates slightly higher than the ones observed experimentally (cf. Refs. 1, 2, and 10). That is, the theoretical annihilation rate obtained by different authors for $r_s=2$ oscillates between 6.8×10^9 s^{-1} (Ref. 7) and 7.6×10^9 s^{-1} (Ref. 20), while the experimental value measured for Al ($r_s=2.07$) by Schaefer and Banhart[21] amounts to 6.13×10^9 s^{-1}.

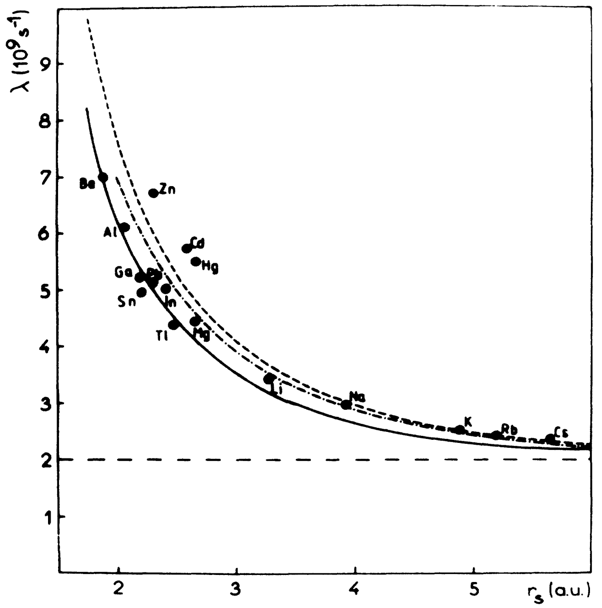

FIG. 4. Annihilation rates λ for different values of r_s. The upper curve was obtained from Ref. 2, the middle one from Ref. 1, and the lower curve from the present work. The straight dashed line corresponds to spin-averaged positronium. The solid circles show the experimental results as collected in Ref. 22.

In this work the annihilation rate at $r_s=2$ has been found equal to 6.48×10^9 s^{-1} (if one uses Eq. (A13), Eq. (4.14) yields 6.58×10^9 s^{-1}). In general our annihilation rates, as can be seen from Fig. 4 are appreciably lower than the ones following from HNC (Ref. 2) and the ones obtained on the ground of the Kahana approach.[1] This follows probably from the fact that the nonorthogonality of the wave functions is taken into account [Eq. (3.9)], so their contribution to the total density is smaller than would follow from the usual formula (3.8). The theoretical results for the annihilation rates obtained in this paper (as well as those calculated in Refs. 1 and 2) are compared to the experimental values for real metals listed by Seeger *et al.*[22] Only simple metals are included since only those could be hoped to exhibit a jelliumlike behavior. It is visible that the lower curve in Fig. 4 shows the best agreement with experiment. It should be kept in mind that while determining r_s for real metals only conduction electrons were taken into account. The electrons from inner levels will contribute to increase the annihilation rates. Splitting the contribution into core and conduction electrons is, however, difficult and impossible without taking account of the electronic structure. In principle, adding inner electrons will increase the annihilation rate, so the values for jellium must lie below the experimental points. In Fig. 4 this is particularly visible for metals of the second group having completely filled shallow d shells contributing appreciably to the annihilation rate (Zn,Cd,Hg). The experimental rates for these metals lie high above the simplistic theoretical predictions. For the other metals the agreement between the results of this work and experiment is very good.

The positron annihilation rates for jellium have been the subject of many calculations (cf. Ref. 23). Most of them yield too high values of the annihilation rate. Low values can be obtained easily as demonstrated in Refs. 1 and 2 if one neglects electron-electron correlations (e.g., Kahana[4]) or take them into account incorrectly (Kallio *et al.*[13,14]). This work seems to be the first which leads to correct values of the annihilation rate (especially for $r_s<4$) while treating correctly electron-electron correlations.

Note that simple approaches such as HNC or cusp condition and rule of charge conservation[2,13,14] are likely to lead to a roughly correct estimation of the annihilation rate, but yield screening charge distributions markedly different from the ones obtained using more elaborate theories.

The screening cloud distribution is shown in Fig. 5 for different electron densities and compared as well with the original results of Gondzik and Stachowiak[2] as with the distributions of Rubaszek and Stachowiak.[1] The curves obtained in this work reproduce quite well the general behavior of the curves of Ref. 1. The accumulation of screening charge in the immediate neighborhood of the positron is, however, a little smaller, corresponding to a somewhat lower annihilation rate.

VI. DERIVATION OF THE FORMULA FOR THE PARTIAL ANNIHILATION RATE

The amplitude of annihilation of an electron of momentum **k** with creation of a pair of photons with total momentum **p** is given as the matrix element connecting the initial state and the final state in the following way:

$$E_{\mathbf{k}}(\mathbf{p})=\frac{A}{\Omega^{1/2}}\int d\tau\,\Psi_{\mathbf{k}}^{*}(\mathbf{r}_2,\ldots,\mathbf{r}_N)\times e^{-i\mathbf{p}\cdot\mathbf{r}_1}\Psi(\mathbf{r}_1;\mathbf{r}_1,\ldots,\mathbf{r}_N)\ , \tag{6.1}$$

where

$$d\tau=\prod_{i=1}^{N}d\mathbf{r}_i\ , \tag{6.2}$$

$\Psi(\mathbf{r}_p;\mathbf{r}_1,\ldots,\mathbf{r}_N)$ is the wave function of N electrons and one positron in their ground state, $\Psi_{\mathbf{k}}(\mathbf{r}_2,\ldots,\mathbf{r}_N)$ is the wave function of $N-1$ electrons filling the Fermi sphere with a hole in the occupation number for momentum **k**. Ψ is a Slater determinant consisting of $\psi_{\mathbf{k}}$ functions (2.2) while $\Psi_{\mathbf{k}}$ is also a Slater determinant but constructed out of plane waves.

Formally we can write $E_{\mathbf{k}}(\mathbf{p})$ as a sum:

$$E_{\mathbf{k}}(\mathbf{p})=A\int d\tau\sum_{P'}(-1)^{P'}\frac{e^{-i\mathbf{p}\cdot\mathbf{r}_1}}{\Omega^{1/2}}w_0\phi_{\mathbf{k}_1(P'1)\sigma_1(P'1)}(\mathbf{r}_1,\mathbf{r}_1)\prod_{i=2}^{N}\frac{e^{-i\mathbf{k}_i(P'2)\cdot\mathbf{r}_i}}{\Omega^{1/2}}\sigma_i(P'2)\psi_{\mathbf{k}_i(P'1)\sigma_i(P'1)}(\mathbf{r}_i,\mathbf{r}_1)\ . \tag{6.3}$$

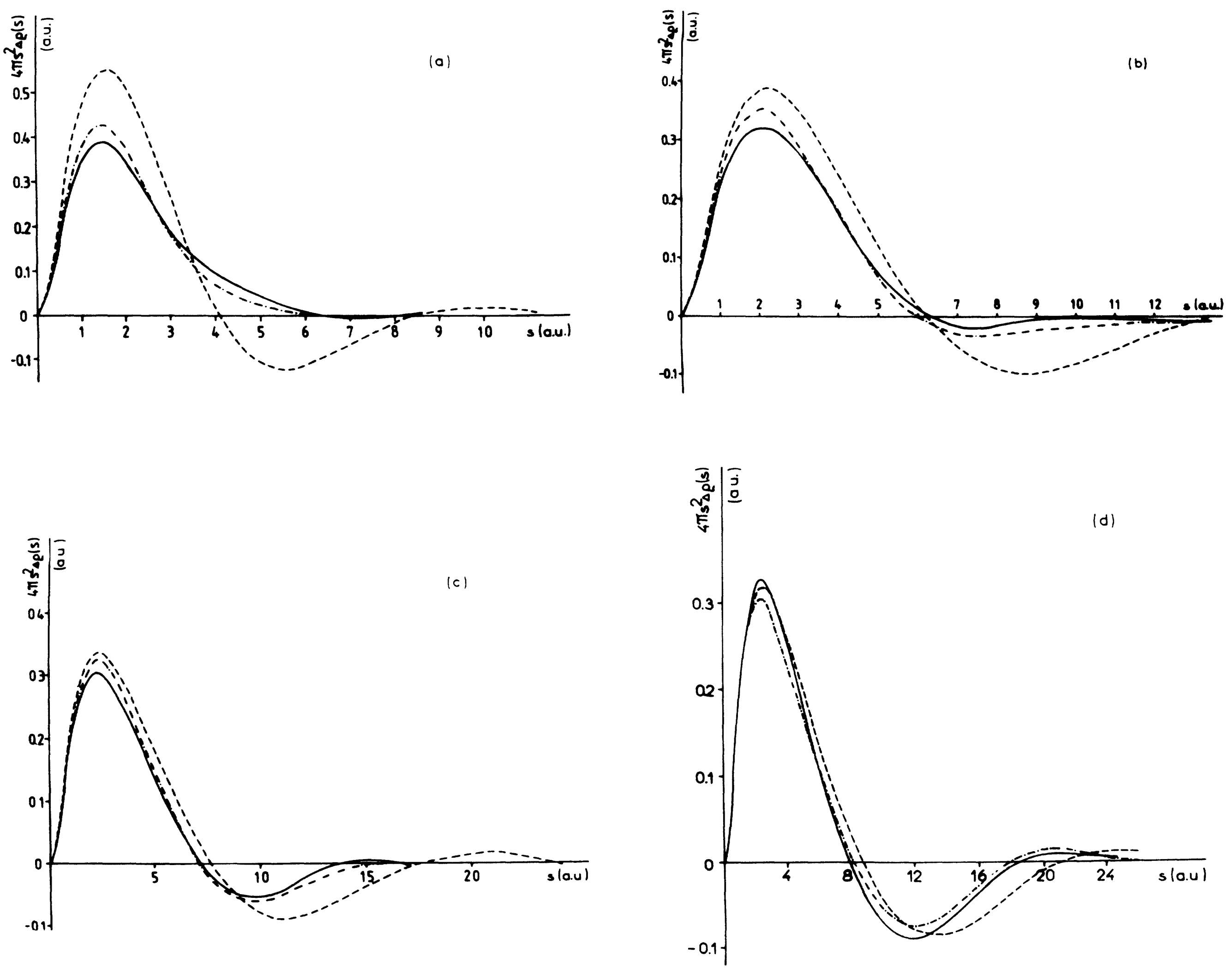

FIG. 5. The screening cloud distribution $4\pi s^2\Delta\rho(s)$ (a) for $r_s=2$, (b) for $r_s=4$, (c) for $r_s=6$, and (d) for $r_s=8$. The dashed curves were obtained from Ref. 2, the dashed-dotted curves from Ref. 1, and the solid curves from the present work.

We set of course

$$w_0=w(0),\quad \sigma_+\sigma_+=\sigma_-\sigma_-=1,\quad \sigma_+\sigma_-=0\ . \tag{6.4}$$

P' is the total permutation characterizing a particular element of the sum in (6.3). $\mathbf{k}_i\ (P'1)$, for example, is the value of the momentum associated with the $\mathbf{r}_i$ coordinates in the $\psi_\mathbf{k}$ factor in the product occurring in (6.3).

Let us introduce the function $C(\mathbf{k}_i,\mathbf{k}_j)$:

$$\begin{aligned}C(\mathbf{k}_i,\mathbf{k}_j)&=\int d\mathbf{r}_i\frac{e^{-i\mathbf{k}\cdot\mathbf{r}_i}}{\Omega^{1/2}}\psi_{\mathbf{k}_j}(\mathbf{r}_i,\mathbf{r}_1)\\&=\delta_{\mathbf{k}_i\mathbf{k}_j}+\frac{1}{\Omega}e^{i(\mathbf{k}_j-\mathbf{k}_i)\cdot\mathbf{r}_1}\left[\int d\mathbf{r}[w(r)-1]e^{i(\mathbf{k}_j-\mathbf{k}_i)\cdot\mathbf{r}}\right.\\&\qquad\left.+A_{\mathbf{k}_j}(\mathbf{k}_i-\mathbf{k}_j)\right]\ .\end{aligned} \tag{6.5}$$

We will consider as small the quantity $w(r)-1$ because it is limited in space and the quantity $v_\mathbf{k}$ which is a perturbation, and neglect consequently terms of second order and higher in these quantities. So the dominant term in $E_\mathbf{k}(\mathbf{p})$, which will be called $E^0_\mathbf{k}(\mathbf{p})$, comes from the permutations fulfilling the relations

$$\mathbf{k}_i(P'1)=\mathbf{k}_i(P'2),\quad \sigma_i(P'1)=\sigma_i(P'2)\quad\text{for every } i>1\ . \tag{6.6}$$

They impose the condition

$$\mathbf{k}_1(P'1)=\mathbf{k}\ . \tag{6.7}$$

We get from (6.3)

$$E^0_\mathbf{k}(\mathbf{p})=A(N-1)!\prod_{i=2}^{N}C(\mathbf{k}_i,\mathbf{k}_i)\int d\mathbf{r}_1\frac{e^{-i\mathbf{p}\cdot\mathbf{r}_1}}{\Omega^{1/2}}w_0\phi_\mathbf{k}(\mathbf{r}_1,\mathbf{r}_1)\ . \tag{6.8}$$

From (6.5) we have

$$C(\mathbf{k}_i,\mathbf{k}_i)=1+\frac{4\pi}{\Omega}\int_0^\infty dr\, r^2[w(r)-1]\ . \tag{6.9}$$

Setting

$$\gamma=4\pi\int_0^\infty dr\, r^2[w(r)-1],\quad N=\rho_0\Omega \tag{6.10}$$

we have

$$\Gamma_N=\prod_{i=1}^{N}\left[1+\frac{\rho_0\gamma}{N}\right]=\left[1+\frac{\rho_0\gamma}{N}\right]^N=e^{\rho_0\gamma}\ . \tag{6.11}$$

From (2.4) and (2.14) we have

$$\phi_\mathbf{k}(\mathbf{r}_1,\mathbf{r}_1)=\frac{1}{\Omega^{1/2}}\left[1+\frac{1}{\Omega}\sum_\mathbf{q}A_\mathbf{k}(\mathbf{q})\right]e^{i\mathbf{k}\cdot\mathbf{r}_1}\ . \tag{6.12}$$

Introducing (6.11) and (6.12) into (6.8) we get

$$E^0_\mathbf{k}(\mathbf{p})=A(N-1)!\frac{e^{\rho_0\gamma}}{1+\dfrac{\rho_0\gamma}{N}}w_0\left[1+\frac{1}{\Omega}\sum_\mathbf{q}A_\mathbf{p}(\mathbf{q})\right]\delta_{\mathbf{kp}}\ . \tag{6.13}$$

Let us find now other permutations giving a substantial contribution to $E_\mathbf{k}(\mathbf{p})$.

From (6.5) it is visible that if $\mathbf{k}_i\neq\mathbf{k}_j$, $C(\mathbf{k}_i,\mathbf{k}_j)$ is small. Let us call P_0 the permutations satisfying the relations (6.6). The permutations P_1, which are equivalent to P_0 except that for some particular values of i and $j>1$ we have

$$\mathbf{k}_i(P_11)=\mathbf{k}_j(P_01),\quad \mathbf{k}_j(P_11)=\mathbf{k}_i(P_01)\ , \tag{6.14}$$

give in (6.3) a contribution quadratic in the small parameter. So a substantial contribution will arise only from permutations P_2 differing from P_0 uniquely through the relations

$$\mathbf{k}_1(P_21)=\mathbf{k}_i(P_01),\quad \mathbf{k}_i(P_21)=\mathbf{k}_1(P_01)\ , \tag{6.15}$$

where i lies in the interval from 2 to $N/2$.

These permutations give in $E_\mathbf{k}(\mathbf{p})$ the contribution

$$E_{\mathbf{k}_1}(\mathbf{p})=-A(N-1)!\frac{e^{\rho_0/\gamma}}{\left[1+\dfrac{\rho_0\gamma}{N}\right]^2}\sum_{\mathbf{k}_i\neq\mathbf{k}_1}\frac{1}{\Omega}\int d\mathbf{r}_1 e^{-i\mathbf{p}\cdot\mathbf{r}_1}w_0\left[1+\frac{1}{\Omega}\sum_q A_{\mathbf{k}_i}(\mathbf{q})\right]e^{i\mathbf{k}_i\cdot\mathbf{r}_1}C(\mathbf{k}_i,\mathbf{k}_1)\ . \tag{6.16}$$

Neglecting terms of higher order of smallness we get with the help of (6.5)

$$\Delta E_{\mathbf{k}_1}(\mathbf{p})=-A(N-1)!\frac{e^{\rho_0\gamma}}{\left[1+\dfrac{\rho_0\gamma}{N}\right]^2}\frac{1}{\Omega}\sum_{\mathbf{k}_i\neq\mathbf{p}}w_0\left[\int d\mathbf{r}\,[w(r)-1]e^{i(\mathbf{p}-\mathbf{k}_i)\cdot\mathbf{r}}+A_\mathbf{p}(\mathbf{k}_i-\mathbf{p})\right]\delta_{\mathbf{pk}_1}\ . \tag{6.17}$$

So in this approximation (unlike in AP) the total momentum of annihilation photons is equal to the momentum of the annihilating electron. Owing to (6.3), (6.13), and (6.17) we can write the amplitude of annihilation with emission of a pair of photons with momentum $\mathbf{p}$ in the form

$$E(p)=C[E^0(p)-\Delta E(p)]\ , \tag{6.18}$$

where

$$E^0(p)=1+\frac{1}{\Omega}\sum_q A_\mathbf{p}(\mathbf{q})\ , \tag{6.19}$$

$$\Delta E(p)=\frac{1}{\Omega}\sum_{\mathbf{k}\neq\mathbf{p}}\int d\mathbf{r}[w(r)-1]e^{i(\mathbf{p}-\mathbf{k})\cdot\mathbf{r}}+\frac{1}{\Omega}\sum_{\substack{\mathbf{q}\\|\mathbf{p}+\mathbf{q}|<k_F}}A_{\mathbf{p}}(\mathbf{q})\ . \tag{6.20}$$

If we assume $w(r)=1$ and the e^+-e^- interaction is weak, (6.18) becomes identical to the corresponding formula of Kahana. Switching from summation to integration we get from (6.19) and (6.20)

$$\begin{aligned}E'(p)&=\frac{1}{\Omega}\sum_{\mathbf{k}}\int d\mathbf{r}[w(r)-1]e^{i(\mathbf{p}-\mathbf{k})\cdot\mathbf{r}}\\&=\frac{2}{\pi p}\int_0^\infty dr[w(r)-1]\frac{\sin(k_Fr)-k_Fr\cos(k_Fr)}{r^2}\sin(pr)\ ,\end{aligned} \tag{6.21}$$

$$\begin{aligned}\Delta\mathcal{B}(p)&=\frac{1}{\Omega}\sum_{\substack{\mathbf{q}\\|\mathbf{p}+\mathbf{q}|>k_F}}A_{\mathbf{p}}(\mathbf{q})\\&=\frac{1}{4\pi^2}\left[\int_{k_F-p}^{k_F+p}dq\left\{\Phi_1(q)\left[\frac{(p+q)^2-k_F^2}{2p}+\frac{q^2}{p}\ln\left[\frac{k_F^2+q^2-p^2}{2q(p+q)}\right]\right]-\Phi_2(q)\frac{q}{p}\ln\left[\frac{k_F^2+q^2-p^2}{2p(p+q)}\right]\right\}\right.\\&\qquad\left.+\int_{k_F+p}^\infty dq\left\{\Phi_1(q)q\left[2-\frac{q}{p}\ln\left[\frac{q+p}{q-p}\right]\right]+\Phi_2(q)\frac{q}{p}\ln\left[\frac{q+p}{q-p}\right]\right\}\right]\ .\end{aligned} \tag{6.22}$$

$E(p)$ is now equal:

$$E(p)=1+\Delta\mathcal{B}(p)-E'(p)\ . \tag{6.23}$$

The relative enhancement factor is obtained from the formula

$$\epsilon(p)=\frac{E^2(p)}{E^2(0)}\ . \tag{6.24}$$

VII. RESULTS FOR PARTIAL ANNIHILATION RATES AND DISCUSSION

The function $\epsilon(p)$ obtained from formula (6.24) depends of course on the electron density. We can write it as $\epsilon(r_s,p)$ and present it in the form

$$\epsilon(r_s,p)=1+A(r_s)\gamma\left[\frac{p}{k_F}\right]\ . \tag{7.1}$$

The values of $A(r_s)$ and $\gamma(p/k_F)$ are given in Table I and compared to the analogical results obtained in Ref. 1 (cf. also Rubaszek[24]) within the Kahana formalism. The curves $\epsilon(r_s,p)$ obtained in the present work are a little more steep, although the agreement between them and that of Refs. 1 and 24 is generally very good. The curves $\gamma(p/k_F)$ depend very little on the electron density, as anticipated by formula (7.1), however there is a slight difference between them and those of the above-

TABLE I. Annihilation characteristics for jellium: comparison of the results of Rubaszek and Stachowiak (Refs. 1 and 24) and of the present work. The values of $\gamma(p/k_F)$ are given on top. The index R refers to Refs. 1 and 24 and the index S refers to the present work [as follows from solving Eq. (A13)]. $\lambda(r_s)$ is the annihilation rate divided by 10^9 s^{-1}.

r_s / p/k_F	2_R	4_R	6_R	2_s	4_S	6_S
0.1	0.0036	0.0032	0.0032	0.0035	0.0022	0.0017
0.2	0.0179	0.0159	0.0144	0.0203	0.0181	0.0171
0.3	0.0430	0.0383	0.0335	0.0488	0.0453	0.0435
0.4	0.0789	0.0702	0.0638	0.0901	0.0854	0.0825
0.5	0.1272	0.1164	0.1069	0.1462	0.1403	0.1364
0.6	0.1918	0.1786	0.1675	0.2200	0.2136	0.2088
0.7	0.2796	0.2648	0.2536	0.3164	0.3106	0.3055
0.8	0.3996	0.3876	0.3812	0.4454	0.4419	0.4378
0.9	0.5842	0.5805	0.5821	0.6312	0.6320	0.6303
0.95	0.7258	0.7305	0.7321	0.7665	0.7697	0.7695
0.99	0.9140	0.9218	0.9266	0.9297	0.9323	0.9326
1.00	1.00	1.00	1.00	1.00	1.00	1.00
$A(r_s)$	0.558	0.627	0.627	0.6900	0.7725	0.7198
$\rho(0)$	0.1392	0.0575	0.0435	0.1290	0.0530	0.0425
$\epsilon_0(r_s)$	3.791	12.31	31.55	3.2750	10.4694	28.8931
$\lambda(r_s)$	6.99	2.89	2.19	6.48	2.66	2.14

mentioned papers.

Referring to what was mentioned already in the Introduction, the situation can be summarized as follows.

We dispose of four independent calculations of the partial annihilation rates for jellium (cf. also Maldague[25]). Three of them neglect explicit three-particle correlations (E3PC): Refs. 1, 6, and the present work. One approach takes them into account (AP).[7]

Here we define explicit three-particle correlations in the following way. Let us write the exact wave function of the system as $\Psi_{\mathrm{ex}}(\mathbf{r}_p;\mathbf{r}_1,\ldots,\mathbf{r}_N)$ different from the wave function $\Psi(\mathbf{r}_p;\mathbf{r}_1,\ldots,\mathbf{r}_N)$ of Eq. (2.17), this last imposing some constraints on the wave function. Changing the values of $\mathbf{r}_i$ for $i>1$ we get the fluctuations in $\Psi_{\mathrm{ex}}(\mathbf{r}_1;\mathbf{r}_1,\ldots,\mathbf{r}_N)$ which do not occur in $\Psi(\mathbf{r}_1;\mathbf{r}_1,\ldots,\mathbf{r}_N)$. These fluctuations will of course affect the annihilation characteristics. In particular, since the wave function cannot be constructed anymore out of two-particle functions, all the calculations of the previous section become impossible.

The results of K (Ref. 1) and LJ (Ref. 6) for $\epsilon(r_s,p)$ are different. This could be attributed to some of the deficiencies of the Kahana approach, namely to the unjustified form of the Pauli exclusion principle and to treating nonorthogonal functions as orthogonal. It should be pointed out that the present approach *is different from the Kahana approach* as formulated by us in Ref. 1. Indeed, it avoids the assumptions which have been criticized by Lowy and Jackson.[5] And since it takes care of the nonorthogonality of the wave functions, it is still further from Kahana than the approach of these last authors. In spite of that it leads to results for $\epsilon(r_s,p)$ which are quite close to those obtained within K, being at that time quite distant from those proposed by Lowy.[6] In this situation the values of $\epsilon(r_s,p)$ given in Ref. 6 should be treated as unexpected. It should be concluded that partial annihilation rates obtained while neglecting E3PC are well under control, and this is the main result of this work.

As concerns the work of Arponen and Pajanne,[7] it comes out quite unexpectedly[8] that their partial annihilation rates can be obtained from those of Ref. 1 by replacing the rectangular momentum distribution of the electrons by the RPA distribution. So from the point of view of E3PC the work of AP in spite of its sophistication and complexity is quite trivial: it just corresponds to replacing the rectangular momentum distribution of free electrons by the RPA distribution of pure jellium, i.e., explicit three-particle correlations are approximated by the appropriate two-particle electron-electron correlations.

As concerns experiment, if one interprets the results as corresponding to jellium of the appropriate electron density, one comes to the conclusion that for low electron densities ($r_s \geq 4$), $\epsilon(r_s,p)$ is well described by theories neglecting E3PC (cf. Refs. 1, 3, and 24) while AP gives good predictions for high electron densities ($r_s=2$). Figure 6 taken from Ref. 1 visualizes the situation. Usually much importance is attached to alkalis because they are believed to be the most similar to jellium among real metals. In this case, however, it seems that their agreement with theories neglecting E3PC is due to the low-electron-density characteristic for them, especially if one observes that the agreement is better for potassium and rubidium and worse for lithium, sodium being intermediary. Such a situation agrees with the point of view that theories neglecting E3PC are a low density approximation. This can be understood if one considers the wave function of the system in the form (2.17): two-particle systems consisting of one electron and the positron are separated out of the whole sample and their wave function obeys Eq. (2.1). Such an approximation becomes convincing if the electrons are far from each other, i.e., their density is small. The approach of AP on the other side is perturbative, so it holds rather for high electron densities. In this way we come to the preliminary conclusion that we still do not dispose of a theory which would hold for intermediate densities. Some additional light on this problem is shed in the paper of Carbotte and Kahana,[9] where the authors found reasons why the many-body tail in the RPA electron momentum distribution (states with momentum higher than the Fermi momentum[26]) should be deenhanced. This effect is visibly not accounted for in the AP approach, while in the remaining theories the electron momentum distribution is arbitrarily assumed to be rectangular.

It is of course quite hypothetical to identify real metals with jellium of the appropriate electron density. As concerns this problem, we rather share the point of view represented by Daniuk *et al.*[15] who proposed to use a local-density approximation based on the Thomas-Fermi treatment of the electron gas in a real metal: the annihilation characteristics are defined locally and correspond

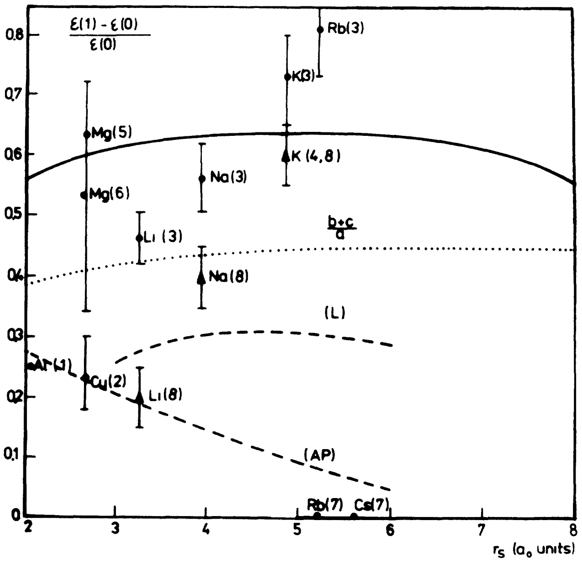

FIG. 6. Relative enhancement factors from Ref. 1 on the Fermi surface (solid line) compared with their biparabolic analogue $(b+c)/a$. The dashed curve denoted (AP) corresponds to the results of Ref. 7 for $(b+c)/a$ and the one denoted (L) to the values extracted from Ref. 6. $\epsilon(1)$ denotes here the relative enhancement factor on the Fermi surface. For details and references see Refs. 1 and 35.

to the properties of jellium having a density equal to the local density of the electrons in the absence of the positron. So the properties of the e^+-e^- interaction in jellium are a necessary ingredient of the theory of positron annihilation in real metals. We believe, and this is confirmed by experiment[15,27–31] (cf. also Kontrym-Sznajd and Šob[32]), that the periodic character of the e^+-e^- interaction is the leading effect of the lattice on the annihilation characteristics (the effect of the Bloch character of the electrons[33,34] also deserves of course careful studies). As the result of this periodicity, we get an additional decrease of the contribution of inner electrons to the annihilation. This follows from the formula proposed by Daniuk *et al.*[15] for the amplitude of annihilation of an electron in state (k,n) with emission of quanta with total momentum **p**:

$$A^{\epsilon}_{\mathbf{k}n}(\mathbf{p}) \simeq \int \{\epsilon_{\mathrm{enh}}[r_s(r), X_{\mathbf{k}n}(\mathbf{r})]\}^{1/2} \psi_{\mathbf{k}n}(\mathbf{r}) \psi_+(\mathbf{r}) e^{-i\mathbf{p}\cdot\mathbf{r}} d\mathbf{r} \; . \tag{7.2}$$

Here, $X_{\mathbf{k}n}(\mathbf{r})$ is the local "momentum" of the electron at $\mathbf{r}$:

$$X_{\mathbf{k}n}(\mathbf{r}) = \{2[E_{\mathbf{k}n} - V(\mathbf{r})]\}^{1/2} \tag{7.3}$$

while the local "Fermi momentum" is equal:

$$p_F(\mathbf{r}) = \{2[E_F - V(\mathbf{r})]\}^{1/2} \; . \tag{7.4}$$

$V(\mathbf{r})$ is the lattice potential, E_F is the Fermi energy, $E_{\mathbf{k}n}$ is the energy of the state $(\mathbf{k},n)$, and $r_s(\mathbf{r})$ is the local value of r_s:

$$r_s(\mathbf{r}) = [\tfrac{4}{3}\pi \rho_e(\mathbf{r})]^{-1/3} \; , \tag{7.5}$$

where $\rho_e(\mathbf{r})$ is the local density of the electrons in the absence of the positron. Tunneling is neglected, i.e., circumstances when the kinetic energy is negative are treated as corresponding to zero kinetic energy. $\epsilon_{\mathrm{enh}}(r_s,p)$ is the true partial annihilation rate determined by the enhancement. Note that unlike in the case of jellium the relative annihilation rates given by Eqs. (6.24) and (7.1) are not sufficient to compute the amplitude of annihilation according to formula (7.2). ϵ_{enh} is expressed by the relative annihilation rate ϵ through the formula

$$\epsilon_{\mathrm{enh}}(r_s,p) = \epsilon_0(r_s)\epsilon(r_s,p) \; , \tag{7.6}$$

where $\epsilon_0(r_s)$ is a normalization factor which can be computed from the electron density on the positron given by formula (5.2) if one keeps in mind that the e^+-e^- attraction increases the density of the p-momentum state on the positron by a factor $\epsilon_{\mathrm{enh}}(r_s,p)$. The values of ϵ_0 are given in Table I. The behavior of ϵ_{enh} is shown in Fig. 7 for $r_s = 2$ and $r_s = 6$. It is obvious that the enhancement decreases when the electron density increases, so the contribution to the annihilation of electrons localized in regions of high electron density is smaller than would follow from the independent-particle model. This is the physical reason why application of formula (7.2) improves the agreement between theory and experiment, or in other words allows one to reproduce the experimental data without additional fitting parameters, which would take care of the relative contribution of conduction electrons on one side and core and d electrons on the other.

Formula (7.2) was first applied to zinc[15] ($r_s = 2.30$). This first application showed that the values of ϵ_{enh} obtained within the Kahana formalism are more momentum dependent than the experimental values. This was confirmed by later works.[28] Also, the theoretical annihilation rate was too high.

In this situation one is tempted to propose a phenome-

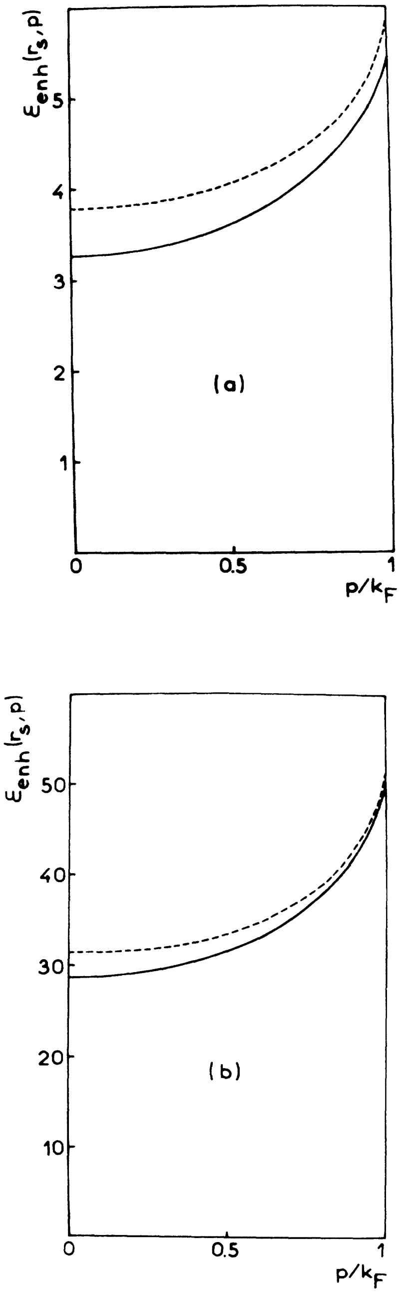

FIG. 7. $\epsilon_{\mathrm{enh}}(r_s,p)$ for (a) $r_s = 2$ and (b) $r_s = 6$. The upper curves show the results of Refs. 1 and 24, the lower curves those of the present work.

nological formula for $A(r_s)$ [cf. Eq. (7.1)]:

$$A(r_s)=a+br_s \ , \tag{7.7}$$

which would hold for metallic densities with $a=0$ and $b=0.13$. Note, however, that magnesium ($r_s=2.65$) agrees surprisingly well with theories neglecting E3PC, while zinc ($r_s=2.30$) does not.[28] So it is not definitely clear whether the residual disagreement between theory and experiment is due to neglecting E3PC or to an oversimplified treatment of the influence of the lattice on the e^+-e^- interaction.

In order to check this problem, it would be useful to perform a careful study of the experimental partial annihilation rates in those among the simple metals which have not yet been investigated in sufficient detail. The disagreement between theory and experiment in this regard is the most striking in zinc and cadmium, for which the positron lifetime does not agree with jellium predictions (unlike for magnesium). So the next step in elucidating this problem should be 2D-ACAR studies (referring to Fig. 4) of Be, Al, Ga, Pb, In, and Tl.

Finally let us point out that according to the formalism presented in this paper, solving the problem of a positron in jellium for a particular electron density consists simply of solving the nonlinear integrodifferential equation (2.3) for $w(r)$ and then the linear integrodifferential equation (4.14) [or (A13)] for $Z(s)$. So the computations need approximately one hundred times less computer time than those of Ref. 1.

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APPENDIX

Let us write the density $\rho(s)$ (3.11) in the form

$$\rho(s)=\rho_G(s)+\delta\rho(s) \ , \tag{A1}$$

where

$$\begin{aligned}&\rho_G(s)=w^2(s)\rho_0 \ ,\\ &\delta\rho(s)=\delta\rho^3(s)-\delta\rho^1(s)-\delta\rho^2(s) \ .\end{aligned} \tag{A2}$$

Owing to the smallness of $\delta\rho(s)$ we can write $V_{\text{xc}}(s)$ [Eq. (4.1)] as

$$V_{\text{xc}}[\rho]=V_{\text{xc}}[\rho_G]+\left.\frac{dV_{\text{xc}}}{d\rho}\right|_{\rho=\rho_G}\delta\rho \ . \tag{A3}$$

According to Hedin and Lundqvist,[16]

$$V_{\text{xc}}[\rho]=-3\alpha\left[\frac{3}{8\pi}\rho\right]^{1/3} , \tag{A4}$$

where

$$\alpha=\frac{2}{3}\left[1+Ar_s\ln\left[\frac{B+r_s}{r_s}\right]\right] ,$$

$$A=0.036\,831, \quad B=21 \ . \tag{A5}$$

Replacing (4.3) by (A3) [of course we have $V_{\text{xc}}[\rho_G]=V^0_{\text{xc}}(s)$] we get instead of (4.4) the equation

$$\nabla^2[v(s)-v_{\text{xc}}(s)]=-4\pi[\rho(s)-w^2(s)\rho_0] \ , \tag{A6}$$

where

$$v_{\text{xc}}(s)=\left.\frac{dV_{\text{xc}}}{d\rho}\right|_{\rho_G(s)}\delta\rho(s)=f_{\text{xc}}(s)\delta\rho(s) \ . \tag{A7}$$

We have

$$f_{\text{xc}}(s)=-\frac{2}{3}\left[\frac{2\pi}{3}\right]^{1/3}\left[\frac{1}{r_s(s)}+\frac{AB}{r_s(s)+B}\right]r_s^3(s) \ , \tag{A8}$$

where

$$r_s(s)=\left[\frac{3}{4\pi}\right]^{1/3}[w^2(s)\rho_0]^{-1/3} \ . \tag{A9}$$

Using formulas (3.19), (3.21), (4.6), and (A2) we can write

$$\pi^3 s\nabla^2 v_{\text{xc}}(s)=-\frac{1}{4\pi}\frac{d^2}{ds^2}\left[f_{\text{xc}}(s)L(s)+2\pi f_{\text{xc}}(s)w^2(s)k_F^2\int_0^\infty ds'\,\mathcal{K}(s,s')s'v(s')\right] \ . \tag{A10}$$

From (A6) and (A10) we get the equation

$$\pi^3 Z''(s)-2\pi k_F^2 w^2(s)\int_0^\infty ds'\,\mathcal{K}(s,s')Z(s')+\tfrac{1}{2}k_F^2\frac{d^2}{ds^2}\left[f_{\text{xc}}(s)w^2(s)\int_0^\infty ds'\,\mathcal{K}(s,s')Z(s')\right]=\Lambda(s) \ , \tag{A11}$$

where

$$\Lambda(s)=L(s)-\frac{1}{4\pi}\frac{d^2}{ds^2}[f_{\text{xc}}(s)L(s)] \tag{A12}$$

and the notation (4.13) is adopted.

It is convenient to separate out in (A11) the term following from differentiating the discontinuity of the derivative of $\mathcal{K}(s,s')$ at $s=s'$. In this way one gets finally the equation

$$\pi^3 Z''(s)+k_F^3 M'(0)f_{\text{xc}}(s)w^2(s)Z(s)-2\pi k_F^2\int_0^\infty ds'\left[w^2(s)\mathcal{K}(s,s')-\frac{1}{4\pi}\frac{\overline{d^2}}{ds^2}[f_{\text{xc}}(s)w^2(s)\mathcal{K}(s,s')]\right]Z(s')=\Lambda(s) \ , \tag{A13}$$

where the bar over the derivative means that it does not include the discontinuity at $s=s'$.

While solving Eq. (A13) it is important to note that the asymptotic form of $Z(s)$ for $s \Longrightarrow 0$ is equal:

$$Z(s)=\tfrac{1}{2}\lambda_2 s^2+C_1 s \tag{A14}$$

thus differing from the form (4.22) which holds when the assumption (4.3) is accepted.

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[1] A. Rubaszek and H. Stachowiak, Phys. Rev. B **38**, 3846 (1988).

[2] J. Gondzik and H. Stachowiak, J. Phys. C **18**, 5399 (1985).

[3] A. Rubaszek and H. Stachowiak, Phys. Status Solidi B **124**, 159 (1984).

[4] S. Kahana, Phys. Rev. **129**, 1622 (1963).

[5] D. N. Lowy and A. D. Jackson, Phys. Rev. B **12**, 1689 (1975).

[6] D. N. Lowy, Phys. Rev. B **26**, 60 (1982).

[7] J. Arponen and E. Pajanne, Ann. Phys. (N.Y.) **121**, 343 (1979); J. Phys. F **9**, 2359 (1979).

[8] E. Boroński, in Proceedings of the Eighth International Conference on Positron Annihilation, Gent, 1988 (unpublished).

[9] J. P. Carbotte and S. Kahana, Phys. Rev. **139**, A213 (1965).

[10] J. Gondzik and H. Stachowiak, Cryst. Res. Technol. **22**, 1511 (1987).

[11] H. Stachowiak, Helv. Phys. Acta **61**, 415 (1988).

[12] J. G. Zabolitzky, Phys. Rev. B **22**, 2353 (1980).

[13] A. Kallio, P. Pietiläinen, and L. Lantto, Phys. Scr. **25**, 943 (1982).

[14] P. Pietiläinen and A. Kallio, Phys. Rev. B **27**, 224 (1983).

[15] S. Daniuk, G. Kontrym-Sznajd, J. Mayers, A. Rubaszek, H. Stachowiak, P. A. Walters, and R. N. West, in *Positron Annihilation,* edited by P. C. Jain, R. M. Singru, and K. P. Gopinathan (World Scientific, Singapore, 1985), pp. 43 and 279; J. Phys. F **17**, 1365 (1987).

[16] L. Hedin and B. I. Lundqvist, J. Phys. C **4**, 2064 (1971).

[17] L. I. Schiff, *Quantum Mechanics* (McGraw-Hill, New York, 1955).

[18] H. Stachowiak and E. Boroński, Acta Phys. Polon. A **59**, 213 (1981).

[19] H. Stachowiak, Phys. Status Solidi B **52**, 513 (1972).

[20] C. H. Leung, M. J. Stott, and C. O. Almbladh, Phys. Lett. A **57**, 26 (1976).

[21] H. E. Schaefer and F. Banhart, Phys. Status Solidi A **104**, 263 (1987).

[22] A. Seeger, F. Banhart, and W. Bauer, in *Positron Annihilation,* edited by L. Dorikens-Vanpraet, M. Dorikens, and D. Segers (World Scientific, Singapore, 1989), p. 275.

[23] J. Arponen and E. Pajanne, in Ref. 15, p. 21.

[24] A. Rubaszek, Ph.D. thesis (in Polish), Polish Academy of Sciences, Wrocław, 1986 (unpublished).

[25] P. F. Maldague, Phys. Rev. B **21**, (1979).

[26] E. Daniel and S. Vosko, Phys. Rev. **120**, 2041 (1960).

[27] T. Jarlborg and A. K. Singh, Phys. Rev. B **36**, 4460 (1987).

[28] G. Kontrym-Sznajd and J. Majsnerowski, Solid State Commun. **70**, 593 (1989) and private communication.

[29] S. Daniuk, G. Kontrym-Sznajd, J. Majsnerowski, M. Šob, and H. Stachowiak, J. Phys. Condens. Matter **1**, 6321 (1989).

[30] A. Rubaszek and J. Lach, Surf. Sci. **211/212**, 227 (1989).

[31] A. Rubaszek and J. Lach, J. Phys. Condens. Matter **1**, 9243 (1989).

[32] G. Kontrym-Sznajd and M. Šob, J. Phys. F **18**, 1317 (1988).

[33] J. P. Carbotte and A. Salvadori, Phys. Rev. **162**, 290 (1967).

[34] H. Sormann, P. Nowak, P. Kindl, and W. Puff, in *Positron Annihilation,* edited by P. G. Coleman, S. C. Sharma, and L. M. Diana (North-Holland, Amsterdam, 1982), p. 218; H. Sormann, Phys. Status Solidi B **142**, K45 (1987); H. Sormann, in Ref. 22, p. 272.

[35] A. Rubaszek and H. Stachowiak, J. Phys. F **15**, 231 (1985).