Influence of the zero motion of a positron on positron lifetime in a metal lattice due to higher Fourier components of its Bloch function

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Arponen and Pajanne suspected that the strong internal electric field of a real lattice decreases the contact density of electrons on the positron in comparison to expectations based on jellium calculations. In this work we propose an approach to this problem which indeed leads to decreasing annihilation rates of positrons in real metals. This is due to higher Fourier components of the Bloch function of the positron. With some probability the positron moves with regard to the electron gas. Owing to that the electron accumulation on this particle decreases. This improves agreement between theoretical and experimental annihilation rates in metals. However, because of the smallness of this effect the best agreement is still obtained if the Boroński-Nieminen formula is accepted for the electron-positron correlations in an electron gas. Consequences of this fact are discussed.

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I. INTRODUCTION

The problem of positron lifetime in metals has attracted considerable interest. A review of different approaches to this problem is given in Ref. 1.

It is known that e^+-e^- interaction in metals increases the contact density of electrons on the positron typically by one order of magnitude, decreasing the positron lifetime accordingly.

For an electron gas the annihilation rates (inverse of lifetime) depend on the electron density ρ_0 described usually by the r_s parameter defined in Hartree atomic units as

$$r_s = \left(\frac{3}{4\pi\rho_0}\right)^{1/3}. \tag{1}$$

They are obtained (in units of $10^9/s$) from the formula

$$\lambda(r_s) = \frac{12}{r_s^3} g(r_s, 0), \tag{2}$$

where $g(r_s, r)$ is the e^+-e^- correlation function at distance r from the positron.

Theoretical investigations of different authors led to several forms of the function $g(r_s, 0)$. The resulting annihilation rates are shown in Fig. 1. They differ by the assumptions introduced in order to obtain them. In Refs. 2 and 3 it was shown how important for the annihilation rates, especially for large values of r_s, is the dependence on the distance from a positron of e^--e^- correlations. The momentum dependence of electron scattering on the positron is also an effect which has been the subject of many investigations both theoretical and experimental. The calculations of Lantto[4] [forming the base of the Boroński-Nieminen[5] (BN) formula, Eq. (A3) in Ref. 5] assume a trial function which does not allow momentum dependence of electron-positron scattering nor dependence of e^--e^- correlations on the presence of the positron. This is why Lantto and co-workers[4,6,7] were unable to predict the momentum dependence of annihilation probabilities. This became possible only after introducing appropriate corrections in the wave function.[8,9] This does not mean that an effective dependence of e^--e^- correlations on the distance from the positron does not occur also in Lantto's approximations. However, it is not based on minimizing the mean value of the Hamiltonian with regard to any function parameter describing electron-electron correlations which would include the positron coordinates.

On the other hand, neither the Kohn-Sham-like ideas of Rubaszek *et al.*[3] or Stachowiak[8] nor the generalized Tamm-Dancoff approximation of Arponen and Pajanne[10] can be treated as absolute truth. Maybe the calculations of Lantto

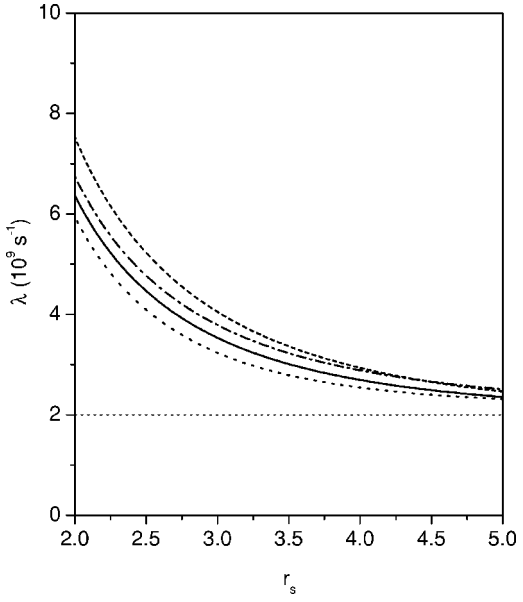

FIG. 1. Comparison of different formulas for the positron annihilation rate $\lambda(r_s)$ in an electron gas [dashed curve: Gondzik-Stachowiak (Ref. 2); dashed-dotted curve: Barbiellini *et al.* (Ref. 14); solid curve: Stachowiak *et al.* (Ref. 8); dotted curve: Boroński-Nieminen (Ref. 5)].

include some important contributions which are neglected in other approaches? It is worth to mention here the recent calculations of Apaja *et al.*[11] The authors assuming the trial wave function of Lantto improved his calculations by adding refinements to the Fermi-hypernetted-chain approximation.

The early results of Lantto[4] have been parametrized successively by Boroński and Nieminen,[5] and, as concerns his final results (cf. Ref. 6), by Sterne and Kaiser[12] and Puska *et al.*[13] The approach of Gondzik and Stachowiak[2] (based on the work of Kallio *et al.*[7]) benefits like the approach of Lantto of the achievements of the theory of liquids. It differs from the approach of Lantto by expressing electron-electron correlations and the electron-positron potential along the lines of the Kohn-Sham theory.

The correlation function parametrized by Barbiellini *et al.*[14] has been calculated by Arponen and Pajanne[10] (AP) after diagonalizing the Hamiltonian rewritten in terms of Sawada boson operators. This approach includes both momentum dependence of e^+-e^- scattering and positron influence on e^--e^- correlations. Let us mention that the calculations of Lowy and Jackson[15] and of Rubaszek and Stachowiak,[3] though using more traditional formalisms, led to practically the same annihilation rates as those of Arponen and Pajanne. The approach of Stachowiak[8] [perturbed hypernetted-chain approach (PHNC), see also the paper of Stachowiak and Lach[9] (SL) and Ref. 16] includes an additional effect, namely weak nonorthogonality of scattered one-electron wave functions (this problem was pointed out by Lowy and Jackson). This effect leads to a slight decrease of the contact density and contributes to lowering the annihilation rates.

Most calculations of positron lifetimes in metals use the BN formula for the correlation function. Obviously it gives the best agreement with experiment, though the lifetimes obtained by using it in computations are still a little shorter than measured. All calculations use such simplifying approaches as the local density approximation (LDA) (Ref. 17) or the weighted density approximation (WDA).[18] Barbiellini *et al.* used the generalized gradient approach (GGA) (Ref. 14) and the annihilation rates of Arponen and Pajanne.[10] However, Mijnarends *et al.*[19] showed that using LDA and the annihilation rates of Puska *et al.*[13] would lead to a better agreement with experiment, at least in Al (in fact, the formula of Puska *et al.*[13] is equivalent to the BN formula). From the paper of Mitroy and Barbiellini[20] it also follows that the annihilation rates of Arponen and Pajanne (called LDA in their paper) are too high. For more comments, see the Appendix.

The deficiencies of the Jastrow-type trial function used by Lantto made us skeptical as concerns the formula of Boroński and Nieminen. Developing a first-principles approach to e^+-e^- interaction in inhomogeneous systems[21–25] we tried in vain to find an effect which would decrease the annihilation rates in comparison to expectations based on calculations concerning the electron gas. The present work is devoted to studies of the possible influence of the zero motion of the positron in a metal lattice on its screening and annihilation rate. Arponen and Pajanne wrote (in Sec. 6.3 of Ref. 10): "One expects the strong internal electric field of a real lattice to suppress the electron-positron correlations much in the same way as the Stark effect decreases the electron density at the positron in a positronium atom. This effect, which decreases the experimental annihilation rates in comparison with the jellium model, has never been described in a realistic way."

The present paper points at a possible mechanism leading to such an effect. However, we did not find any analog of the Stark effect which consists of an external field acting on an electron bound to a positive charge. In the present work an external periodic field modulates the ground-state wave function of the positron. The screening of the nonzero Fourier components of this wave function is influenced by the finite velocity of the positron with regard to the electron gas. This decreases the electron density on the positron and consequently the annihilation rate. In earlier works we considered an analog of chemical bonding.[22,23] Collectivization of core electrons by the nucleus and the positron gives rise to an attractive term in the positron potential which increases its density in the core region where the electron density is high. This leads to increase the annihilation rate. Perhaps the gauge field theory formalism proposed by Arponen and Pajanne[26] could throw an additional light on this problem.

The ground-state wave function of the positron is modulated by the lattice in such a way that the positron is expelled from the atomic cores. Developing this wave function into a Fourier series needs introducing components of nonzero wave vectors corresponding to a moving positron. From our works published a couple of years ago[27,28] it follows that in the case of a proton moving in an electron gas the contact density decreases with increasing momentum. Treatment of a moving positron interacting with the electron gas is a difficult problem. This is why we replace the positron by a heavy particle of charge $1/2$ of the electronic charge showing at the same time why such an approach is legitimate. We show that at rest the contact density of electrons on this particle does not differ much from that for a positron in the whole range of metallic electron densities.

Such an approach to a positron in an electron gas makes it possible to extend on the positron the formalism used in the case of a proton moving in an electron gas and compute the influence of the modulation of the positron wave function by the lattice on the annihilation rates.

II. THE POSITRON AS A HEAVY PARTICLE

In this first calculation of the effect of the modulation of the positron wave function on the screening we will adopt the simplest and less sophisticated approach. Benefitting of the achievements of the theory of liquids interpreted according to Ref. 7 Gondzik and Stachowiak[2] proposed to write the Euler-Lagrange equation for the density amplitude w around a positron in jellium in the form

$$[-\nabla^2 + V_0(\mathbf{r})]w(\mathbf{r}) = 0 \tag{3}$$

or (after dividing the above equation by 2)

$$\left(-\frac{1}{2}\nabla^2 + \tilde{V}(\mathbf{r})\right)w(\mathbf{r}) = 0, \tag{4}$$

where the Coulomb part of the effective potential $\tilde{V}_c(\mathbf{r})$ satisfies the Poisson equation

$$\nabla^2 \tilde{V}_c(\mathbf{r}) = \frac{1}{2}[-4\pi\Delta\rho(r) + 4\pi\delta(\mathbf{r})]. \tag{5}$$

In the above approximation [called after Kallio *et al.* hypernetted-chain (HNC),[7] according to the terminology of the theory of liquids] the positron can be considered as a heavy particle of charge $1/2$ apart from the fact that the screening charge $\Delta\rho$ also appears with a coefficient $1/2$.

Let us try to find to what extent the positron can be described as a heavy particle also when applying the Kohn-Sham formalism instead of HNC.

In Eq. (3) the potential is labeled with a zero in order to indicate that it is self-consistent only in HNC approximation. According to Ref. 2 it is expressed as

$$V_0(\mathbf{r}) = -\frac{1}{r} + \int d\mathbf{r}' \frac{w^2(r') - \rho_0}{|\mathbf{r} - \mathbf{r}'|} + V_{\mathrm{HL}}\{w^2(r)\} - V_{\mathrm{HL}}\{\rho_0\}, \tag{6}$$

where $V_{\mathrm{HL}}\{\rho\}$ is the exchange-correlation correction in the form proposed by Hedin and Lundqvist.[29]

In Kohn-Sham formalism the wave function of an electron gas in presence of a heavy positron is described by a Slater determinant of one-electron functions $\psi_{\mathbf{k}}(\mathbf{r})$ consisting of plane waves scattering on the positron and obeying the equation

$$\left(-\frac{1}{2}\nabla^2 + \frac{1}{2}V(\mathbf{r})\right)\psi_{\mathbf{k}}(\mathbf{r}) = \frac{k^2}{2}\psi_{\mathbf{k}}(\mathbf{r}), \tag{7}$$

where

$$V(\mathbf{r}) = V_0(\mathbf{r}) + v(\mathbf{r}), \tag{8}$$

$$v(\mathbf{r}) = \int d\mathbf{r}' \frac{\rho(r') - w^2(r')}{|\mathbf{r} - \mathbf{r}'|} + V_{\mathrm{HL}}\{\rho(r)\} - V_{\mathrm{HL}}\{w^2(r)\}. \tag{9}$$

$\rho(r)$ is the Kohn-Sham density distribution of electrons.

Choosing the Z-axis parallel to the $\mathbf{k}$ vector we can express the wave function $\psi_{\mathbf{k}}(\mathbf{r})$ in the form of a series in Legendre polynomials,

$$\psi_{\mathbf{k}}(\mathbf{r}) = \sum_{l=0}^{\infty} R_l(k,r) P_l(\cos\vartheta), \tag{10}$$

where ϑ is the angle between $\mathbf{k}$ and $\mathbf{r}$.

Asymptotically (i.e., outside the range of interaction of the positron) R_l takes the form[30]

$$R_l(k,r) = A_l[\cos\delta_l(k) j_l(kr) - \sin\delta_l(k) n_l(kr)], \tag{11}$$

where δ_l are phase shifts and j_l and n_l are the spherical Bessel functions.

Assuming that only the first partial waves are scattered we can write the wave function $\psi_{\mathbf{k}}(\mathbf{r})$ in the form

$$\psi_{\mathbf{k}}(\mathbf{r}) = \frac{1}{\sqrt{\Omega}}\left\{ e^{i\mathbf{kr}} + \sum_{l=0}^{l_M} (2l+1) i^l \beta_l(k,r) P_l(\cos\vartheta) \right\}, \tag{12}$$

where

$$\beta_l(k,r) = e^{i\delta_l(k)} b_l(k,r) - j_l(kr) \tag{13}$$

and b_l is defined by the formula

$$R_l(k,r) = (2l+1) i^l e^{i\delta_l(k)} b_l(k,r). \tag{14}$$

Ω is the volume of the sample. l_M is the maximal value of l chosen in the calculations.

$\rho(r)$ is obtained from the expression

$$\rho(r) = 2\sum_{\mathbf{k}\ occ} \psi^*_{\mathbf{k}}(\mathbf{r})\psi_{\mathbf{k}}(\mathbf{r}). \tag{15}$$

which finally leads to the formula

$$\rho(r) = \rho_0 + \frac{1}{\pi^2}\sum_{l=0}^{l_M}(2l+1)\int_0^{k_F} k^2 dk[b_l^2(k,r) - j_l^2(kr)], \tag{16}$$

where k_F is the Fermi vector.

Let us apply in Eq. (7) the potential $V_0(r)$ obtained from Eq. (3). Then, following the routine method of iteration, the potential $V_1(r)$ is obtained from Eqs. (8) and (9) as

$$V_1(r) = V_0(r) + \alpha v_0(r), \tag{17}$$

where α is smaller than 1 (e.g., equal to 0.2). In general, in successive iterations we use the potential

$$V_{n+1}(r) = V_n(r) + \alpha[V_0(r) + v_n(r) - V_n(r)], \tag{18}$$

where

$$v_n(\mathbf{r}) = \int d\mathbf{r}' \frac{\rho_n(r') - w^2(r')}{|\mathbf{r} - \mathbf{r}'|} + V_{\mathrm{HL}}\{\rho_n(r)\} - V_{\mathrm{HL}}\{w^2(r)\}. \tag{19}$$

$\rho_n(r)$ is the electron density following from Eq. (7) with the potential $V_n(r)$. The total screening cloud, i.e.,

$$S_n = \int d\mathbf{r}[\rho_n(r) - \rho_0], \tag{20}$$

should be equal to one electronic charge. Some complications occur because S_n in successive iterations is not neccessarily equal to 1. For this reason we decided to renormalize $\rho_n(r)$ before using it in Eq. (19). This is accomplished by adding to $\rho_n(r)$ a term of the form

$$\Delta\rho_n(r) = A_n e^{-r} \tag{21}$$

such that the renormalized screening cloud S'_n satisfies the equation

$$S'_n - 1 = \beta(S_n - 1) \tag{22}$$

where β is a constant smaller than 1 chosen in such a way as to facilitate achieving self-consistency. Calculations continue until self-consistency is reached. The criterion for self-

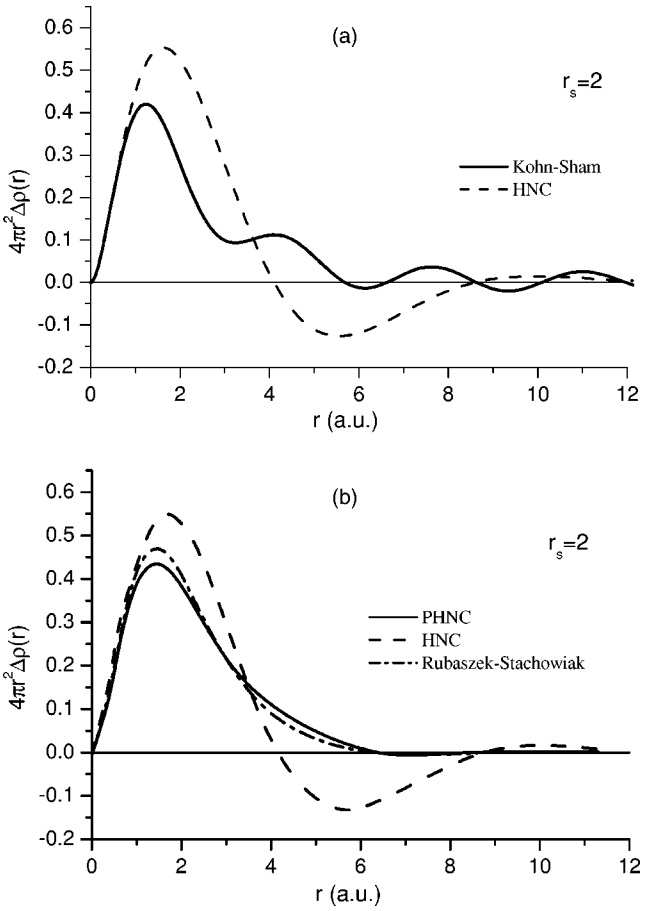

FIG. 2. (a) The screening cloud distribution $4\pi r^2\Delta\rho(r)$ around a heavy positron for $r_s=2$. The dashed curves correspond to HNC approximation, the full curve has been obtained in this work. (b) The screening cloud distribution according to HNC (dashed curve), PHNC (full curve), and from Ref. 3 (dashed-dotted curve).

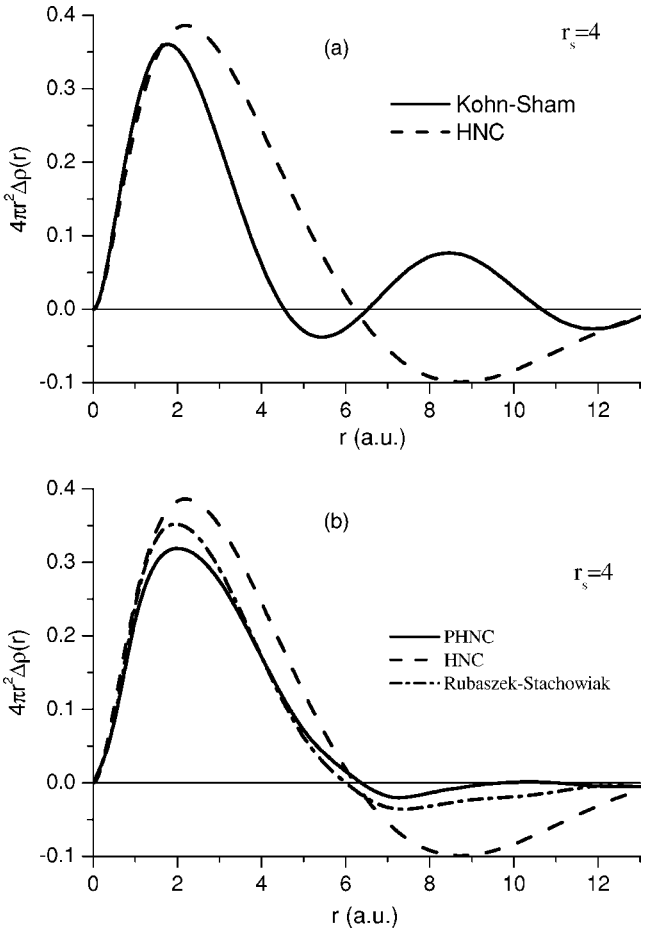

FIG. 3. The same as in Fig. 2 but for $r_s=4$.

consistency is vanishing of $V_{n+1}-V_n$ and simultaneous smallness of $S_{n+1}-1$ and S_n-1. Note that because of Friedel oscillations the value of the total screening cloud oscillates with the maximal value of r taken into account in calculations. Increasing this value improves the results only to a limited degree because of increasing numerical errors. In comparison to analogous calculations which we performed for an Li atom in an electron gas, the requirements concerning l_M are rather high. In our calculations it was necessary to use l_M equal at least 3. We were able in this way to get self-consistent solutions up to $r_s=4.5$. Assuming that actual positron screening in an electron gas is given by perturbed HNC calculations,[8,9] we can see how the screening of a heavy positron reproduces the screening of a real one. Let us remark that within the approach of Gondzik and Stachowiak[2] a heavy positron is equivalent to a real one. In Figs. 2 and 3 we find the screening cloud around a heavy positron in Kohn-Sham approximation compared to the HNC result obtained according to the approach of Ref. 2. We show also the corresponding quantities obtained according to PHNC,[8] and according to the self-consistent solution of the Bethe-Goldstone equation.[3] The corresponding curves are quite similar except that Friedel oscillations occur in the screening of a heavy positron which obviously are smeared out in the case of a light positron because of its recoil. Remark also that the screening of a heavy positron reproduces better the results of Ref. 3 than those of PHNC. This is due to assuming in the approach proposed by Kahana[31] exact orthogonality of one-electron wave functions. This assumption has been criticized by Lowy and Jackson.[15] In PHNC this assumption is avoided. The annihilation rates are for metallic densities a little higher for a heavy positron in Kohn-Sham approximation than according to HNC, while in SL (PHNC) they are a little lower. They are given in Table I. The correlation functions $g(r_s,r)$ are shown in Fig. 4 for $r=0$ and compared to the predictions of RPA and of the asymptotic formula of Arponen[32] for small r_s,

$$g(r_s,0) = 1 + 1.23r_s. \tag{23}$$

III. SCREENING OF A MOVING HEAVY POSITRON

We can now apply the results of Sec. II to the screening of a moving heavy positron.

The main difference between screening a heavy positron and a proton lies in the Poisson equation (5) which for a proton would have the form

TABLE I. The electron-positron correlation function in different approaches. The figures labeled HNC and Kohn-Sham have been obtained in this work. SL indicates the numerical results obtained (using PHNC) in Ref. 9 while BN follows from the formula for $g(r_s,0)$ proposed in Ref. 5.

r_s	HNC	Kohn-Sham	SL	BN
0.1	1.176	1.117	1.097	1.138
0.2	1.318	1.236	1.196	1.277
0.3	1.458	1.360	1.346	1.413
0.5	1.746	1.631	1.529	1.672
0.7	2.052	1.937	1.782	1.921
0.9	2.393	2.282	2.058	2.169
1.	2.577	2.473	2.212	2.295
1.3	3.192	3.122	2.715	2.698
1.5	3.658	3.623	3.111	3.002
1.8	4.455	4.498	3.786	3.535
2.	5.061	5.173	4.287	3.958
2.5	6.875	7.242	5.872	5.330
3.	9.201	9.956	7.988	7.283
3.5	12.147	13.394	10.719	9.978
4.	15.845	17.646	14.187	13.578
4.5	20.412	22.531	17.724	18.241

$$\nabla^2 V = -4\pi\Delta\rho + 4\pi\delta(\mathbf{r}). \tag{24}$$

So for a moving heavy positron in an electron gas the screening charge distribution $\Delta\rho(r)$ in random-phase approximation (RPA) should be

$$\Delta\rho(\mathbf{r}) = \frac{1}{(2\pi)^3}\int d\mathbf{q}\frac{(1/2)J(k_F,q,k_0t)e^{-i\mathbf{qr}}}{q^2+(1/2)J(k_F,q,k_0t)}, \tag{25}$$

where $\mathbf{k}_0$ is the wave vector of the heavy positron, $t=\cos\vartheta$ where ϑ is the angle between $\mathbf{q}$ and $\mathbf{k}_0$, while for a proton we would have

$$\Delta\rho(\mathbf{r}) = \frac{1}{(2\pi)^3}\int d\mathbf{q}\frac{J(k_F,q,k_0t)e^{-i\mathbf{qr}}}{q^2+J(k_F,q,k_0t)}. \tag{26}$$

$$J(k_F,q,k_0t) = \frac{2k_F}{\pi} + \frac{1}{\pi q}\left\{[k_F^2-(q+2k_0t)^2/4]\ln\left|\frac{q+2k_0t+2k_F}{q+2k_0t-2k_F}\right| + [k_F^2-(q-2k_0t)^2/4]\ln\left|\frac{q-2k_0t+2k_F}{q-2k_0t-2k_F}\right|\right\}. \tag{27}$$

IV. NUMERICAL DETERMINATION OF $\Delta\rho(0)$

We are interested mainly in the contact density of electrons on the positron, since this quantity determines the positron annihilation rate which is an observable. The integral in Eq. (25) is computed as usual as

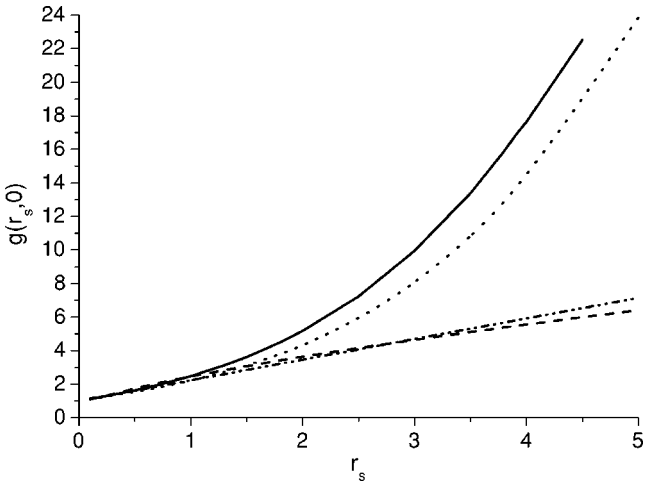

FIG. 4. The electron-positron correlation function $g(r_s,0)$ in Kohn-Sham approximation as obtained in this paper (full curve), according to PHNC (dotted curve) and according to RPA (dashed curve). The straight dash-dot-dot line corresponds to the asymptotic behavior for small r_s according to the formula of Arponen (Ref. 32).

$$\Delta\rho(0) = \frac{1}{2\pi^2}\int_0^\infty q^2 dq F(k_F,k_0,q), \tag{28}$$

where

$$F(k_F,k_0,q) = \int_0^1 dt\frac{\tilde{J}}{q^2+\tilde{J}} \tag{29}$$

and $\tilde{J}=(1/2)J$.

These computations need some care because of the singularities appearing in the integral (28) at some values of $\kappa=k_0/k_F$. This is due to vanishing of the denominator. In Fig. 5 we show for $r_s=2$ and three values of κ the curves in the plane (q,t) corresponding to the equation

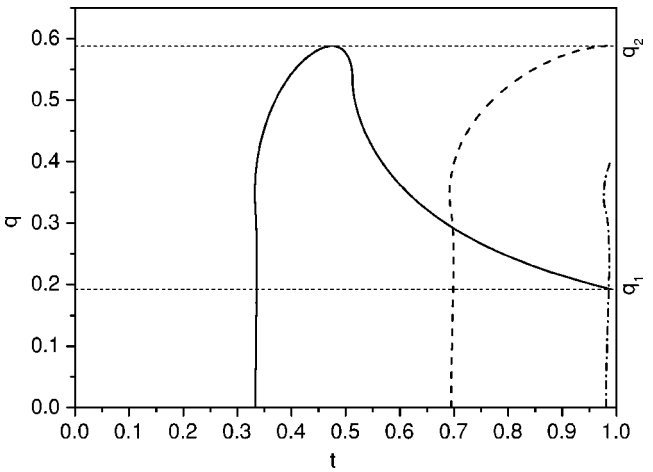

FIG. 5. Curves of singularities for $r_s=2$. The solid curve corresponds to $\kappa=2.5$, the dashed curve to $\kappa=1.2$ and the dashed-dotted curve to $\kappa=0.85$. The values of q_1 and q_2 are indicated for $\kappa=2.5$.

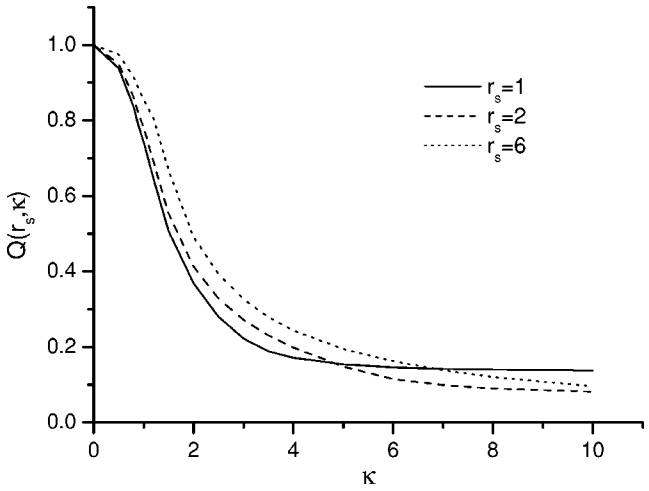

FIG. 6. The function $Q(r_s,\kappa)$ for r_s=1, 2, and 6.

$$q^2 + J/2 = 0. \tag{30}$$

The integral in Eq. (28) is understood as the principal value. Singularities appear, however, in F for q equal q_1 and q_2, as indicated in Fig. 5.

The singularity at q_1 has the form

$$F(q) \sim \ln|q - q_1| \tag{31}$$

while at q_2

$$F(q) \sim -\frac{1}{\sqrt{q - q_2}} \text{ for } q > q_2. \tag{32}$$

For $q < q_2$ $F(q)$ behaves regularly.

The quantity of interest is the dependence of $\Delta\rho(0)$ on κ and r_s. It is described by the function $Q(r_s,\kappa)$ defined as

$$Q(r_s,\kappa) = \frac{\Delta\rho(r_s,\kappa,0)}{\Delta\rho(r_s,0,0)}. \tag{33}$$

The κ dependence of $Q(r_s,\kappa)$ is shown in Fig. 6 for several values of r_s.

V. COMPUTATION OF THE POSITRON ANNIHILATION RATE

We will use the local-density approximation for the positron annihilation rate in order to study the effect of positron zero motion on the observed values of positron lifetime (computations supporting the LDA approach are given in Refs. 22 and 23).

In a homogeneous electron gas we have for the annihilation rate λ_0 in units of $10^9/s$ the formula

$$\lambda_0 = 16\pi\rho_0\, g(r_s,0). \tag{34}$$

In the subsequent formulas we shall use the values of $g(r_s,0)$ corresponding to the three approaches belonging to (i) Boroński and Nieminen,[5] (ii) Stachowiak *et al.*,[8,9] (iii) Arponen and Pajanne.[10,14] In a metal lattice while neglecting the effect of positron motion we have for the annihilation rate λ_1 the formula

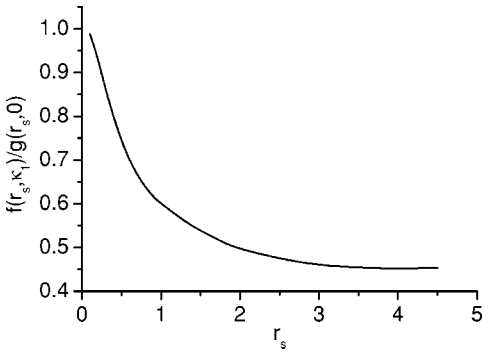

FIG. 7. The function $f(r_s,\kappa_1)/g(r_s,0)$ vs r_s for the lowest nonzero momentum component κ_1 [cf. Eq. (42)].

$$\lambda_1 = 16\pi \int d\mathbf{r}\rho(\mathbf{r})g[r_s(\mathbf{r}),0]\phi(\mathbf{r})^2, \tag{35}$$

where $\phi(\mathbf{r})$ is the positron wave function and $\rho(\mathbf{r})$ is the local value of the electron density.

Let us develop $\phi(\mathbf{r})$ into the Fourier series

$$\phi(\mathbf{r}) = \sum_{\mathbf{l}} a_{\mathbf{l}} e^{\mathbf{i}\mathbf{l}B\mathbf{r}}. \tag{36}$$

The probability P_l of finding the positron in the momentum state $|\mathbf{l}B|$ is

$$P_l = \frac{n_l|a_{\mathbf{l}}|^2}{\sum_{\mathbf{n}}|a_{\mathbf{n}}|^2}, \tag{37}$$

where n_l is the number of reciprocal-lattice vectors of absolute value equal $|\mathbf{l}B|$.

Now, taking into account that in a metal the probability P_l is different from zero for $\mathbf{l} \neq \mathbf{0}$, owing to the interaction of the positron with the lattice, we introduce the following expression for the annihilation rate:

$$\lambda_2 = 16\pi\sum_l P_l \int d\mathbf{r}\rho(\mathbf{r})|\phi(\mathbf{r})|^2 f[r_s(\mathbf{r}),\kappa_l(\mathbf{r})]. \tag{38}$$

According to the principle applied in this work of adopting the simplest approximation, we assume that in an electron gas the correlation factor for a positron of momentum $|\mathbf{l}B|$ is

$$f(r_s,\kappa_l) = 1 + [g(r_s,0) - 1]Q(r_s,\kappa_l), \tag{39}$$

where

$$\kappa_l(\mathbf{r}) = \frac{|\mathbf{l}B|}{k_F(\mathbf{r})} \tag{40}$$

and

$$k_F(r) = [3\pi^2\rho(r)]^{1/3}. \tag{41}$$

Q is defined by Eq. (33).

The relation $f(r_s,\kappa_1)/g(r_s,0)$ vs r_s for the smallest different from zero reciprocal-lattice vector κ_1 is shown in Fig. 7. κ_1 in the case of monovalent fcc metals is

TABLE II. Positron lifetimes (in ps) in metals from the first and second group, and for Al. The experimental values (Ref. 40) are given in the second column. Some more recent experimental data (Ref. 41) are labeled with an asterisk. The next column contains the results of Puska (Ref. 39). The next three columns present the results of LMTO-ASA calculations of Rubaszek *et al.* (Ref. 36) (from Table V in Ref. 36). Then six columns present our FLAPW results: Note that the 9th, 10th, and 11th columns contain the results of calculations taking into account the smaller enhancement due to the nonzero momentum of the positron. The last column presents the contribution (in %) of the higher components in the Fourier expansion of the positron wave function of the corresponding metals.

Metal	Expt.	Puska BN	AR(LMTO-LDA)			This work (FLAPW-LDA)			This work (hp)			% high
			BN	SL	AP	BN	SL	AP	BN	SL	AP	comp.
Li	291	305	300	284	260	298	275	258	300	277	260	1.7
Na	338	337	328	323	291	328	308	294	332	312	294	2.7
K	397	387	367	373	331	368	352	332	375	359	338	4.2
Rb	406	396	377	388	342	377	364	343	385	372	351	4.6
Cs	418	407	389	409	357	388	377	355	398	386	364	6.5
Al	163	166	163.4	155.4	145	162.3	152	143.9	165.9	155.3	147.2	5.3
Cu	110, 118*	106	104.6	102.9	97	105	101	97.4	107.8	103.4	101	5.6
Ag	131, 136*	120	119.1	116.6	109	121	115	111	126	120	116	7.4
Au	117	107	106.0	104.2	98	110	105	101	115	110	106	8.7

$$\kappa_1 = 3^{1/2}\left(\frac{2}{3}\pi\right)^{1/3} = 2.216. \tag{42}$$

We performed calculations of positron lifetimes in a few metals (Li, Na, K, Rb, Cs, Al, Cu, Ag, Au) according to Eqs. (35) and (38). Both valence and core electrons were treated on equal footing, i.e., we used the LDA approximation to the Fermi momentum as given in Eq. (41). We made sure to omit transition metals for which we could not apply the above approach since the *d* shells are not completely filled with electrons. In this situation we have to allow for participation in the screening of the positron of electron states belonging to the partially filled *d* bands. As pointed out in Refs. 23 and 33 this could result in deviations of the annihilation rate from the LDA predictions. The results are shown in Table II. The electronic structure was determined according to the FLAPW (full potential linearized augmented plane wave) code WIEN95.[34] The electron densities and potentials obtained in this way were used to calculate the positron wave functions according to the finite difference method (the appropriate code was based on the ATSUP code of Puska[35]). Three correlation functions were tried in the computations: the one of Boroński and Nieminen (BN),[5] the one of Arponen and Pajanne[10] as parametrized by Barbiellini *et al.*,[14] and the one of Stachowiak and Lach (SL).[9] The results are compared to those of Rubaszek *et al.*[36] who applied the self-consistent linearized muffin-tin orbital method (LMTO) within the atomic-spheres approximation (ASA) for determining the electronic structure and the BN, SL, and AP correlation functions (τ_1^{LDA} in Table V of Ref. 36). The differences between the corresponding calculations for positron lifetimes within FLAPW and LMTO are almost negligible, however, it is worthwhile to remember the conclusions of Šob *et al.*[37] if the electronic structure is calculated at different assumptions. Note that Ref. 36 is devoted mainly to developing the approach labeled weighted density approximation (WDA).

The last column of Table II shows the probability $1-P_0$ (in %) of observing the positron in a state corresponding to a nonzero reciprocal-lattice vector (NRV). It is sufficient to take into account the momenta belonging to the first star of reciprocal-lattice vectors. The contribution corresponding to the momenta belonging to the second star is negligible, only for Ag and Au it is slightly bigger than 1%.

The first conclusion one can draw from the results presented in Table II is that the BN formula describes the experimental results better than the alternative expressions (AP and SL). This should be treated as an experimental fact, since the BN figures reproduce in principle the results of Lantto[6] which are based on maybe too crude approximations. Obviously, we still do not fully understand e^+-e^- interaction even in an electron gas.

Recently Mitroy and Barbiellini[20] compared results of different approaches like LDA, symmetrized LDA (SLDA), IPM, GGA, and the two-component approach of Boroński and Nieminen with direct calculations for molecules containing a positron, effectuated using the stochastic variational method (SVM). Such calculations can be considered as a benchmark. In the case when LDA and SLDA approaches give identical results (i.e., the positron density is everywhere smaller than electron density) the jellium annihilation rates of Arponen and Pajanne used in their paper lead to too high annihilation rates in the corresponding molecules (particularly LiPs and NaPs). Applying the annihilation rates of Boroński and Nieminen (eventually of Stachowiak and Lach[9]) would decrease these values. It is surprising that these authors did not perform this attempt to improve the agreement of their results with experiment.

The case of lithium has already been treated in detail in recent works.[22,23,25,38] The amplitude of NRV components is small and their influence on the annihilation rate negligible. In Ref. 23 it is shown, based on many-body calculations, that the total positron annihilation rate in lithium can be obtained using the local-density approximation for the interaction. The positron wave function on the other hand is affected by an attraction term in the effective interaction of the positron and

the nucleus due to collectivization of core electrons by the two positive charges. This leads to a decrease of the positron lifetime in comparison to the local-density approximation amounting to about 5 ps. This improves agreement with experimental data.

Comparing our BN lifetimes with the corresponding results of Puska[39] we observe a marked difference for alkalis heavier than lithium. We do not understand the reasons for this discrepancy since our self-consistent FLAPW results are almost the same as those of Rubaszek *et al.*[36] calculated self-consistently within the LMTO (LDA) method and yet we used the numerical code of Puska[35] for calculating the positron wave function (ATSUP). The computations of the positron wave function were performed on different meshes (up to $112\times112\times112$ points) in order to control the accuracy of the calculation. Moreover, we have tested the accuracy of calculations for Cs using the atomic superposition method. The calculations have been performed subsequently for the meshes of $66\times66\times66$, $82\times82\times82$, $112\times112\times112$, $134\times134\times134$ points within the elementary cell. The overall relative change in annihilation rates was $\sim1\times10^{-6}$.

It may be worthwhile to point out here that the results for positron lifetimes of the WDA calculations of Rubaszek *et al.*[36] for heavier alkali metals such as Rb and Cs are quite far from the experimental values. However, in contrast to LDA results which are lower, the WDA lifetimes are markedly higher than experimental ones (similarly for Cu, Ag, Au). It is obvious that the problem of lifetimes in real metals needs further studies.

Our calculations [according to Eqs. (35) and (38)] for noble metals reproduce quite well the experimental results [note that the annihilation rate for NRV is, approximately, only half of that for a positron at rest (cf. Fig. 8)]. For Al, despite that the contribution of higher Fourier components to the positron function is considerable, the difference between the enhancements corresponding to zero and first nonzero reciprocal-lattice vectors is less than in the case of Cu, Ag, and Au (cf. Fig. 6). This is due to the higher value of the Fermi momentum in comparison to the length of these vectors.

VI. CONCLUSIONS

An approach to e^+-e^- interaction in an electron gas called heavy positron model has been developed. It is shown that the screening of such a particle in an electron gas reproduces quite well the screening of a real positron. The approach to the screening of a moving proton developed in earlier papers[27,28] is then applied to a heavy positron. In this way it was possible to compute the dependence of the contact density of electrons on the positron as a function of its momentum.

In a crystal lattice the positron is expelled from the core region, so its ground-state Bloch function includes a substantial contribution of higher momentum components. This factor reduces the annihilation rate of positrons in a metal since the accumulation of electrons on a moving positron is smaller than for a positron at rest. Its influence on the annihilation rate is thus opposite to that of other effects considered up to now. This effect helps to reduce the gap between theory and experiment in this field.

As we have seen previously[19,22] (cf. also Refs. 23–25), the local-density approximation to e^+-e^- interaction describes quite well (at least in lithium) the behavior of the annihilation rate even in an inhomogeneous electron gas.

The effect due to higher momentum components of the positron wave function is small (in lithium negligible). Though it improves agreement between theory and experiment, the best agreement is still obtained if the Boroński-Nieminen formula for the electron-positron correlation function in an electron gas is assumed.

The annihilation rates computed by Arponen and Pajanne,[10] by Rubaszek and Stachowiak[3] (ARS), and by Stachowiak and Lach[9] are too high as compared to experiment if the local-density approximation (to e^+-e^- correlations) is adopted. The works of Barbiellini *et al.*,[14] Mijnarends *et al.*,[19] as well as our calculations mentioned above show that going beyond the local-density approximation does not change this conclusion. The ARS annihilation rates remain higher than the experimental ones. The formula of Boroński and Nieminen still gives the best description of the experiment.

Since this last formula parametrizes (at least for metallic densities) the results of the approach of Lantto of which the deficiencies have been pointed out in the Introduction (cf. also the Monte Carlo calculations of Fraser[42]), this shows that we still do not fully understand e^+-e^- interaction even in an electron gas. More precisely, in order to get better agreement between theory and experiment calculations concerning e^+-e^- interaction in an electron gas must be improved.

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APPENDIX

Mitroy and Barbiellini[20] find that LDA-type approximations give overestimates of annihilation rates in positron-atom systems whereas the two-component density-functional theory (TC-DFT) of Boroński and Nieminen[5] underestimates systematically the enhancement factor for large interparticle separations. Our comments to these conclusions are the following.

In undefected metals the electron density n_- is always greater than $|\psi_+|^2$, so this remark is maybe not very relevant as concerns the present work. However, we would like to make here the following statement.

We do not consider TC-DFT as an ideal approach, quite the contrary, we appreciate the success of the SLDA approximation proposed by Mitroy and Barbiellini. Nevertheless, our opinion is that the superiority of SLDA over TC-DFT is largely due to the inexact results calculated by Lantto for $n_+=n_-$ and $n_+=\frac{1}{2}n_-$ (see, e.g., pp. 3822 and 3823 in Ref. 5).

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