NUKLEONIKA 2010;55(1):3–8

ORIGINAL PAPER

Effect of electron-electron correlations on positron-electron momentum density distributions

Edward Boroński

Abstract. The calculations of the influence of the self-energy effects on the electron-positron (e-p) enhancement factors and the e-p momentum distributions are presented. The approach bases on the novel formulation of the Bethe--Goldstone (B-G) equation for the positron in an electron gas where the scattering of the electrons into the states below the Fermi surface due to the self-energy effects is allowed. This equation has been solved and the corresponding e-p enhancement factors and momentum distributions have been found. The agreement between the absolute values of the theoretical calculations and experimental data has improved noticeably.

Key words: positron annihilation • electronic structure • many-body physics

E. Boroński
Institute of Physics,
Opole University,
48 Oleska Str., 45-052 Opole, Poland,
Tel.: +48 77 452 7250, Fax: +48 77 452 7290,
E-mail: E.Boronski@uni.opole.pl

Received: 12 June 2009
Accepted: 8 October 2009

Introduction

One of the important methods of investigating the electronic structure of solid states is a study of angular correlation of positron annihilation quanta. In the last years some relatively complicated Fermi surfaces have been studied experimentally and interpreted with sophisticated formalisms [9].

The experimental angular correlation curves, however, cannot give directly the information about the electronic structure, as it is disturbed by the positron itself. The several effects play a role, namely electron--positron (e-p) correlation, still unrecognized in an inhomogeneous electron medium, and the influence of electron-lattice and positron-lattice interaction on this correlation. These effects have been studied with advanced approaches, however, mainly separately and the results (most from the theory of the positron in an electron gas) have been used in different ways to calculate e-p momentum densities. Such calculations still suffer from many difficulties, e.g. the absolute values and shapes of *ab initio* e-p momentum densities are often different from the corresponding reconstructions from the experimental curves. A progress towards incorporating all the above-mentioned effects into one theory has been made by Sormann *et al*. [13, 15], who proposed in a series of papers the Bloch-modified ladder (BML) approach describing in terms of Green functions the mutual scattering of electron and positron, as well as scattering of these particles on a crystal lattice. At present, this theory yields the best qualitative agreement with the experiment as concerns the features of the shape of the e-p momentum density curve.

However, serious simplifications have been done for the e-p potential in the lattice of a crystal, and finally, results are not self-consistent and absolute values of the enhancement of the electron density at the positron do not fit the experimental data. Moreover, the necessity of taking into account many effects connected with a real structure of a material and, at the same time, many body electron-positron (e-p) interaction makes such calculations terribly tedious and requiring a lot of computational time [13]. Therefore, some simpler approaches are still being applied as concerns the method of calculating the momentum distribution of e-p pair. One of the most popular is the local density approximation (LDA) in which the electron and positron states are calculated separately and their densities are used for the computation of the local value of the enhancement of electron densities due to e-p interaction. The unperturbed electron density is then multiplied by this enhancement. The formula itself for this enhancement is determined from many-body approaches for the positron in an electron gas [2, 4, 8].

One of the important points in the present knowledge, concerning the e-p momentum density distribution, is the influence of the electron-electron correlations on this distribution. In particular, since Carbotte's and Kahana [6] paper, the question has appeared about the so-called many-body tail in this distribution, confirmed in Compton experiments for simple metals [10]. In turn, in recent papers [14, 17] devoted to the reconstruction of the Fermi surface due to angular correlation of annihilation quanta the authors notice the importance of possible electron self-energy effects in the interpretation of the experimental data.

The purpose of this paper is to determine the momentum dependent enhancement factors (and the momentum distributions of the e-p pairs, which are the object of experimental studies) containing self-energy effects resulting from electron-electron (e-e) interaction. Whereas self-energy effects have been taken into account in the summation in the formula for e-p momentum distribution [17], they have never been applied to scattering rules when calculating the enhancement factors. Moreover, we present a simple approximation for the LDA formula for the e-p momentum distribution $R(p)$, that allows to take into account both the self-energy effects and the positron-lattice interaction within the enhancement factor. The results are presented in sections 'Results' and 'Conclusions'.

Theory

The formula for the e-p momentum distribution $R(\boldsymbol{p})$ which relates to the experiment of angular correlation of annihilation quanta is the following

$$(1) \qquad R(\boldsymbol{p}) = \frac{\pi r_0^2 C}{\Omega} \sum_{\boldsymbol{k}} n_{\boldsymbol{k}} \left| \int_{\Omega} e^{-i\boldsymbol{pr}} \psi_{\boldsymbol{k}}^{\mathrm{ep}}(\boldsymbol{r},\boldsymbol{r}) d\boldsymbol{r} \right|^2$$

where $\boldsymbol{k}$ denotes all occupied states and $n_{\boldsymbol{k}}$ are the occupation numbers for the electrons. In the electron gas $n_k = \Theta(k_{\mathrm{F}} - k)$. The functions $\psi_{\boldsymbol{k}}^{\mathrm{ep}}(\boldsymbol{r}_-,\boldsymbol{r}_+)$ have to be orthogonal with respect to coordinates of both particles. For real metals, one often approximates the two-body wave function by a product of the Slater determinant of one-electron orbitals $\phi_{\boldsymbol{k}}^j(\boldsymbol{r})$ the positron wave function $\phi_+(\boldsymbol{r})$ and a factor γ which is, in general, a complicated functional of electron and positron wave function but approximately can be connected with the enhancement factor ε by the relation

$$(2) \qquad \gamma^2 = \varepsilon$$

where ε describes how the probability density of unperturbed electronic states changes due to e-p interaction. Then $R(\boldsymbol{p})$ reads

$$(3) \quad R(\boldsymbol{p}) = \frac{\pi r_0^2 C}{\Omega} \sum_{\boldsymbol{k},j} n_{\boldsymbol{k},j} \left| \int_{\Omega} e^{-i\boldsymbol{pr}} \gamma(\boldsymbol{k}, j, r_s(\boldsymbol{r})) \phi_{\boldsymbol{k}}^j(\boldsymbol{r}) \phi_+(\boldsymbol{r}) d\boldsymbol{r} \right|^2$$

where j is the band index; $n_{\boldsymbol{k},j}$ values may differ from 1 only due to lattice or temperature effects; r_s is the electron density parameter ($r_s = (3/(4\pi n_e))^{1/3}$).
In electron systems, however, there are self-energy effects that make the electron momentum distribution more complicated. Even for the interacting electron gas it exhibits non-rectangular character (Daniel-Vosko distribution) [7]. In our opinion the disagreement between $R(\boldsymbol{p})$ (Fig. 4 in Ref. [9]) and the experiment may, at least in part, result from neglecting the self-energy effects in formulas in the approach of Sormann *et al.* [14]. These effects should be taken into account directly in the formula for the $R(\boldsymbol{p})$ (see e.g. paper of Tang *et al.* [17] as well as in the two-body equation for the electron-positron wave function. The latter purpose can be done by the suitable change in the B-G equation for the electron-positron wave function $\chi(\boldsymbol{k},\boldsymbol{p})$. The $\chi(\boldsymbol{k},\boldsymbol{p})$ is the Fourier transform of the function $\chi_p(\boldsymbol{r}_-,\boldsymbol{r}_+)$ which relates to $\psi_p^{\mathrm{ep}}(\boldsymbol{r}_-,\boldsymbol{r}_+)$ in the following way (see e.g. [5])

$$(4) \qquad \Psi_p^{\mathrm{ep}}(\boldsymbol{r}_-,\boldsymbol{r}_+) = \frac{1}{\Omega} e^{i\boldsymbol{pr}_-} + \chi_p(\boldsymbol{r}_-,\boldsymbol{r}_+)$$

Our idea is to include the electron self-energy effects into the B-G equation by introducing appropriately the electron occupation numbers into the summation in this equation [5, 8].

$$(5) \quad \chi(\boldsymbol{k},\boldsymbol{p}) = \frac{a(r_s) V(|\boldsymbol{k}-\boldsymbol{p}|)}{p^2 + (\boldsymbol{k}-\boldsymbol{p})^2 - k^2} + \frac{a(r_s)}{p^2 + (\boldsymbol{k}-\boldsymbol{p})^2 - k^2} \cdot \sum_{\boldsymbol{q}} (1 - n_{\boldsymbol{q}}) V(|\boldsymbol{q}-\boldsymbol{p}|) \chi(\boldsymbol{q},\boldsymbol{p})$$

allowing electrons to be scattered with some probability to any states below and above the Fermi surface since there is a finite probability due to e-e interactions that these states are not occupied, and excluding the case when $\boldsymbol{k} = \boldsymbol{p}$. $V(|\boldsymbol{q} - \boldsymbol{p}|)$ is the Fourier transform of the e-p potential and $a(r_s)$ is a function of the electron density resulting from the change of units in the equation to k_F units [5].

Certainly, this *ad hoc* procedure introduces the self-energy effects in this meaning that if one replaced the free propagators $G_e^0(\boldsymbol{k},\omega)$ in the equation for the two-body e-p Green function [8] by the quasi-particle propagators $G_e(\boldsymbol{k},\omega)$ the "dressed" in self-energy diagrams propagators would be linked to the occupation numbers $n_{\boldsymbol{k}}$ by the renormalization factors Z_k and a correction $f(\boldsymbol{k},\omega)$ (see e.g. [11]). Since the exact evaluation of the suitable self-energy terms within the two-body equation seems only hardly tractable, we decided for

an approximation presented above: to apply directly some known formulas for the occupation numbers to the Goldstone equation for the e-p wave function, i.e. by changing appropriately the summation rules over the momenta of the scattered electron. Then, the corresponding formula for $\gamma(\boldsymbol{p},\boldsymbol{r}_s)$ reads

$$\gamma(\boldsymbol{p},r_s)=1+\sum_{\boldsymbol{q}}(1-n_{\boldsymbol{q},r_s})\chi(\boldsymbol{q},\boldsymbol{p},r_s) \tag{6}$$

and, with the use of Eq. (2), the momentum dependent enhancement factor can be calculated from Eq. (6). The annihilation rate λ can be determined from

$$\lambda=\sum_{\boldsymbol{p}}R(\boldsymbol{p})=\pi r_0^2 c\int_{\Omega}d\boldsymbol{r}\sum_{\boldsymbol{k}}n_{\boldsymbol{k}}\left|\psi_{\boldsymbol{k}}^{\mathrm{ep}}(\boldsymbol{r},\boldsymbol{r})\right|^2 \tag{7}$$

For the electron gas the momentum distribution of e-p pairs is

$$R(p)=n_p\,\varepsilon(p) \tag{8}$$

and the formula (7) for the electron gas transforms into

$$\lambda=\pi r_0^2 c\sum_{\boldsymbol{p}}n_{\boldsymbol{p}}\varepsilon(\boldsymbol{p}) \tag{9}$$

The occupation numbers $n_{\boldsymbol{p}}$ can be calculated within the random phase approximation (RPA) according to the prescription in [6]:

$$n_{\boldsymbol{p}}=\Theta(p_{\mathrm{F}}-p)+P_e(\boldsymbol{p}) \tag{10}$$

where

$$P_e(\boldsymbol{p})=i\int\frac{d\omega}{2\pi}\frac{i}{V}\sum_{\boldsymbol{q}}\int\frac{d\varepsilon}{2\pi}u(\boldsymbol{q},\varepsilon)(G_e^0(\boldsymbol{p},\omega))^2\cdot G_e^0(\boldsymbol{p}-\boldsymbol{q},\omega-\varepsilon) \tag{11}$$

where $u(\boldsymbol{q},\varepsilon)$ is the e-p interaction dynamic potential in the RPA approximation. In order to solve the two-dimensional integral Eq. (5) we can expand the following function into Legendre polynomials

$$g(\boldsymbol{k},\boldsymbol{p})\overset{\mathrm{def}}{=}\chi(\boldsymbol{k},\boldsymbol{p})(p^2+(\boldsymbol{k}-\boldsymbol{p})^2-k^2)=\sum_l g_l(k,p)P_l(\cos(\vartheta)) \tag{12}$$

where ϑ is the angle between $\boldsymbol{k}$ and $\boldsymbol{p}$. Then, we get the following set of equations for the $g_n(k,p)$.

$$g_n(k,p)=a(r_s)V_n(k,p)+\frac{2\pi a(r_s)}{p}\int_0^{\infty}dq(1-n(q))qV_n(q,k)\cdot\left[\sum_{m=0}^{\infty}\frac{2m+1}{2}g_m(q,p)P_{m,n<}\left(\frac{q}{p}\right)Q_{m,n>}\left(\frac{q}{p}\right)\right] \tag{13}$$

where $P_{m,n<}$ and $Q_{m,n>}$ are Legendre functions of the second kind and $m,n>(m,n<)$ means that the greater (less) from both the numbers should be taken. The suitable linear combination of the $g_n(k,p)$ and Legendre polynomials gives the requested function $\chi(\boldsymbol{k},\boldsymbol{p})$. If one takes into account that the positron in a real metal is scattered on a crystal lattice, there will be different contribution to the annihilation rate λ and $R(\boldsymbol{p})$ from the several Fourier components of the positron wave function. The e-p correlation function and the corresponding enhancement factor depend on the reciprocal lattice vectors as well. This effect can be estimated by considering the screening of the particle moving through the electron gas [16], i.e. $\gamma(\boldsymbol{k},\boldsymbol{G},r_s)$ will be obtained by a solution of Eq. (5) not only for positron momentum equal to 0 but also if the initial positron momentum is $\boldsymbol{G}$. Then

$$R(\boldsymbol{p})=\frac{\pi r_0^2 c}{\Omega}\cdot\sum_{\boldsymbol{k}}n_{\boldsymbol{k}}\left|\sum_{\boldsymbol{G}}b_{\boldsymbol{G}}\int_{\Omega}e^{-i(\boldsymbol{p}-\boldsymbol{G})\boldsymbol{r}}\gamma(\boldsymbol{k},\boldsymbol{G},r_s(\boldsymbol{r}))\phi_{\boldsymbol{k}}(\boldsymbol{r})d\boldsymbol{r}\right|^2 \tag{14}$$

where $b_{\boldsymbol{G}}$ are the coefficients of the Fourier expansion of the positron wave function $\phi_+(\boldsymbol{r})$. This, in general, leads to a smaller total enhancement factor.

Results

Using the formulas (10) and (11) we calculated the occupation numbers $n_{\boldsymbol{p}}$ for $r_s=2,3,4,5,6$. Then, we solved the set of Eqs. (13) iteratively according to a scheme presented in [5]. The e-p potential was assumed at the moment in the RPA approximation, though we realize that it cannot be reasonable for $r_s>4$. Taking this potential in this preliminary calculation makes, however, an easy comparison to the earlier similar calculations based on the Bethe-Goldstone equation, possible. Certainly, the e-p potential have to be calculated self-consistently (see Ref. [12]). The new element in this procedure, making some difficulties in comparison to the scheme in Ref. [5], was to calculate the integrals at $\boldsymbol{q}=\boldsymbol{p}$. The discontinuities that appear at these points arise because of the energetic denominator in Eq. (5). This have been performed by the evaluation of the principal values of the integrals at these points. The enhancements (as defined by Eq. (2)), the momentum distributions and annihilation rates were calculated with the formulas (6), (8) and (9), respectively. The values of $n_{\boldsymbol{p}}$ determined above have been used.

The example enhancement factor resulting from our calculations for $r_s=2$ is presented in Fig. 1a (full squares). It is shown together with the enhancement corresponding to the conventional calculations presented in [5] that has been got for the same potential (RPA). The difference is that the new one contains self-energy effects of e-e correlations. It is slightly higher than the old one, especially at p_{F}, however, for $p>p_{\mathrm{F}}$ it is finite and, beside the maximum at $p\cong p_{\mathrm{F}}$, slowly goes down to zero. The tail for $p>p_{\mathrm{F}}$ corresponds to scattering of the electron from the states from above the Fermi surface to any states below and above the Fermi momentum. The characteristic feature of the momentum dependence of the enhancement calculated on the basis of Eq. (5) is that it exhibits a maximum just above the Fermi surface. This reflects a large susceptibility of the excited electrons to participate in screening of the positron. The number of such electrons is, however, small and finally the $R(\boldsymbol{p})$ given by the formula (8) exhibits only relatively small tail (Fig. 1b). This tail can still be

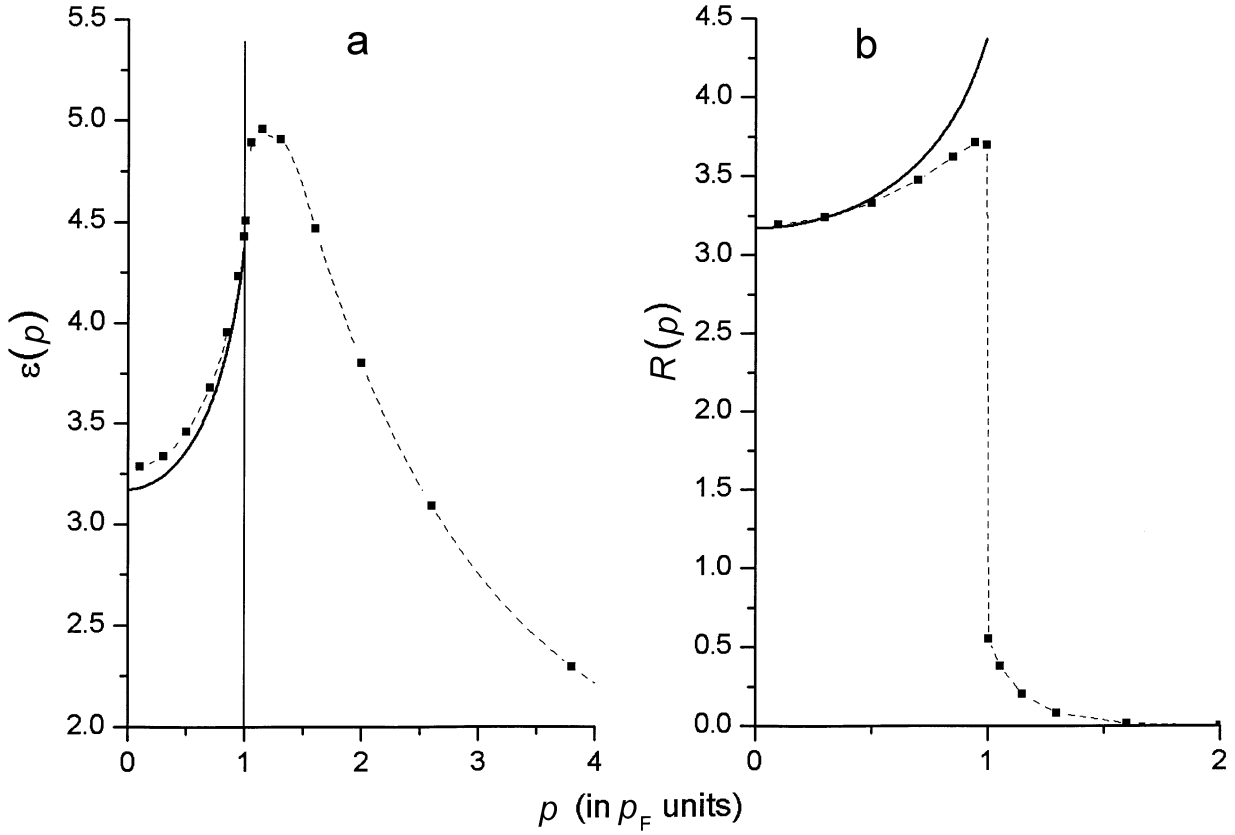

Fig. 1. a – The enhancement $\varepsilon(p)$ for $r_s = 2$ (dotted line with squares), the conventional (Kahana type) enhancement (solid line); b – the $R(p)$ according to calculations in this work (dotted line with squares), the conventional $R(p)$ for the electron gas (solid line).

reduced if taking into account Carbotte's calculations [6] concerning the cancellation of the contributions from electron and positron self-energies for $p > p_F$. The example of such a reduced tail for $r_s = 4$ is presented in Fig. 2 by full squares and can be compared to the tail before this reduction (dotted line).

The enhancement factors may also be defined as a following relation [1] (relative momentum enhancement factors)

$$\varepsilon(p) = R(p) / R(0) \tag{15}$$

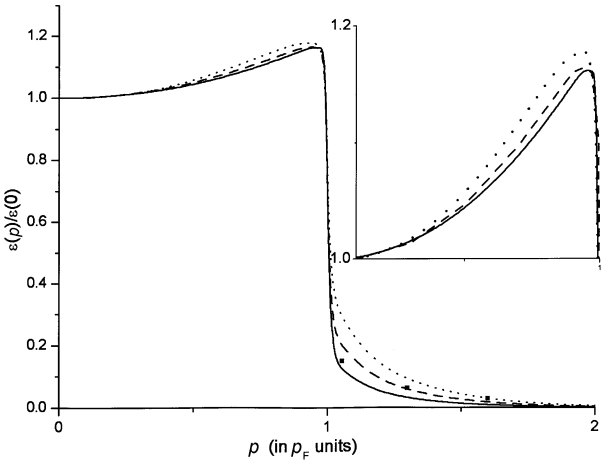

Fig. 2. Relative enhancement factors for $r_s = 2, 3, 4$. $r_s = 2$ (solid line), $r_s = 3$ (dashed line), $r_s = 4$ (dotted line). The reduced tail for $r_s = 4$ (full squares according to [6]) to be compared to dotted line. Upper-right corner: magnified part of the figure.

The corresponding figures are presented in Fig. 2 for $r_s = 2, 3, 4$. The annihilation rates for $r_s = 2, 3, 4, 5, 6$ are presented in Fig. 3. They are lower than the rates obtained when neglecting self-energy effects. For comparison, the rates of Arponen and Pajanne approach [2] and with the Boroński-Nieminen formula (BN) [4] (recent Monte Carlo calculations [3] give similar results) are shown. For $r_s > 4$ our rates, however, start to diverge, due to the inconsistency caused by the too simplified e-p potential.

Finally, we solved the Eq. (13) for $r_s = 2.66$. This value of r_s corresponds to the effective electron density in magnesium (for simplicity we assumed the fcc

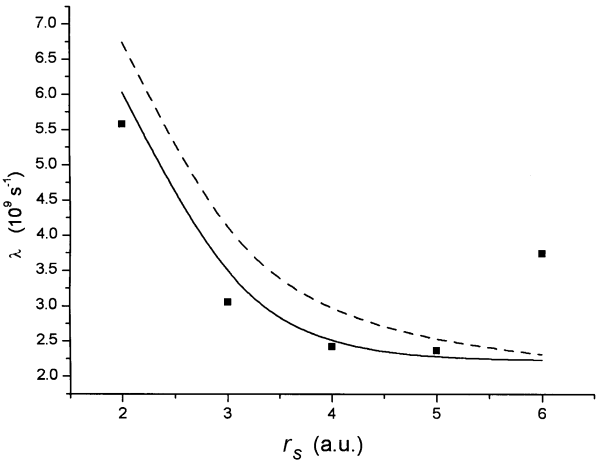

Fig. 3. Annihilation rates vs. r_s. The results of this work (full squares), Boroński and Nieminen [4] (solid line), Arponen and Pajanne [2] (dashed line).

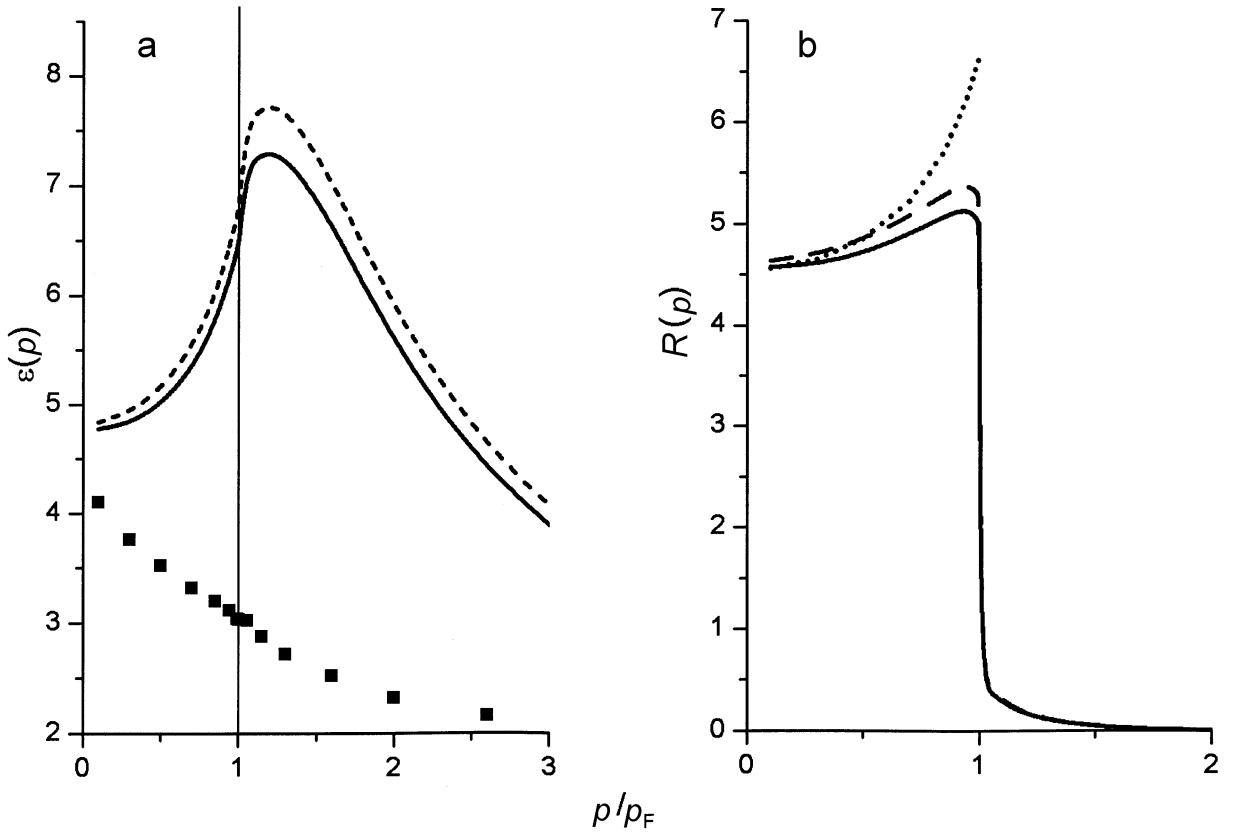

Fig. 4. a – The enhancement $\varepsilon(p)$ for $r_s = 2.66$ for the lowest non-zero Fourier component of positron wave function (squares). It corresponds to $G = 2.21$ (monovalent fcc metal). The enhancement for the zero Fourier component (dashed line). The total enhancement (solid line); b – the total $R(\boldsymbol{p})$ (solid line), without taking into account the positron lattice interaction (dashed line), without positron-lattice interaction and self-energy effects (dotted line).

structure). Our aim was to compare the momentum distribution based on the present calculations (Eqs. (13) and (14)) with that in Fig. 4 of the paper of Sormann *et al.* [14]. The results of calculations according to the formula (14) are presented in Fig. 4 and 5. In Fig. 4a the enhancement $\varepsilon(p)$ for the lowest non-zero momentum component ($G = 2.21$) of the positron wave function is shown (full squares). This is slowly decreasing function for any electron momenta. The total enhancement function is adequately less than the enhancement calculated at the assumption that only zero momentum Fourier component is considered, i.e. if there is no scattering of the positron on a crystal lattice. This behaviour of the enhancement ε makes the corresponding curve of $R(p)$ in Fig. 4b lower and increasing more slowly when approaching p_F. In order to compare our results to those plotted in Fig. 4 of Sormann *et al.* [14], we have smeared out our final curve to follow the experimental resolution FWHM = 0.1.

Conclusions

Annihilation rates behave reasonably for $r_s \leq 5$. They are smaller than the corresponding rates calculated in [5] and the rates based on Boroński Monte Carlo calculation [3] (or Boroński-Nieminen formula [4]). However, we expect that as soon as the self-consistency is achieved, which is planned in the next project, they will get slightly higher and reasonable for all values of r_s. Our enhancements for $p < p_F$ are slightly higher than those calculated without taking the self-energy effects into account. The values of these enhancements extend, however, to the momenta greater than p_F and slowly diminish. Consequently, the values of momentum distributions are smaller than the old ones, their increase with the momentum is weaker, and they

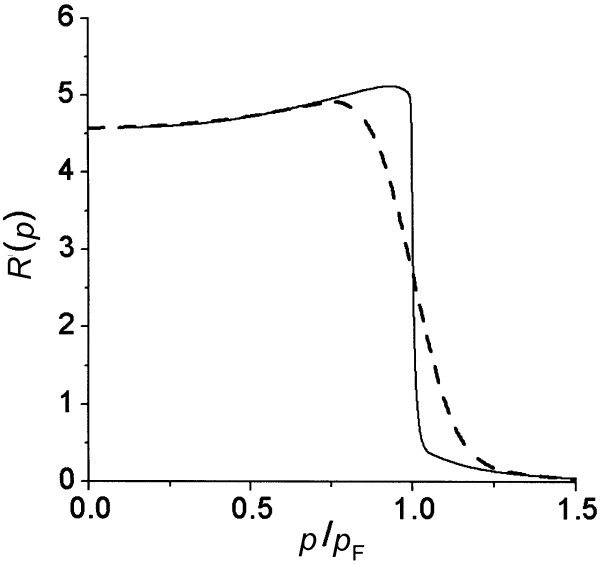

Fig. 5. The results of this work for $R(p)$ (solid line) for $r_s = 2.66$ (self-energy effects and positron lattice interaction are taken into account). The $R(p)$ (dashed line) after smearing with FWHM = 0.1. The curves on this plot can be compared to the results of Sorman and Kontrym-Sznajd [9] (Fig. 4) for Mg.

exhibit some tails. The enhancement factors increase when approaching the Fermi momentum and this is the important argument for the validity of this approach. The next argument supporting this approach is the increase of these factors with r_s, the feature contrasting with the result of Arponen and Pajanne. This was a weak point of their theory [1]. Of course, such a behaviour of our momentum distributions does not exclude that for some real metals with strongly localized electrons in atomic cores these distributions could be decreasing with increasing momentum.

The e-p momentum distributions calculated for $r_s = 2.66$ (Fig. 5) can be compared to the distributions (Ref. [9], Fig. 4) reconstructed on the basis of the experimental data. The agreement between the absolute values of the theoretical calculations and experimental data has improved noticeably, in particular, if positron scattering on the crystal lattice and the experimental resolution ($\sigma = 0.1$) were taken into account. This is a very important result of including some features of the crystal structure directly into the enhancement factor. One realizes that such calculations of self-energy effects even for the electron gas are only preliminary, since the RPA is only the first step to achieve the correct occupation numbers. For real metals, the prescription for such calculations with the use of spectral functions is given in, e.g. the paper of Tang *et al*. [17]. Moreover, Eq. (5) should be solved self-consistently with taking the xc potential into account [12]. Certainly, a lot of tests have to be done for real metals. Fortunately, the computations can be made literally in seconds since the numerical code is quite effective.

References

1. Arponen J, Pajanne E (1979) Angular correlation in positron annihilation. J Phys F 9:2359–2376
2. Arponen J, Pajanne E (1979) Electron liquid in collective description. III. Positron annihilation. Ann Phys 121:343–389
3. Boroński E (2006) Positron-electron annihilation rates in an electron gas studied by variational Monte Carlo simulation. Europhysics Lett 75:475–482
4. Boroński E, Nieminen RM (1986) Electron-positron density functional theory. Phys Rev B 34:3820–3831
5. Boroński E, Szotek Z, Stachowiak H (1981) Exact solution of the Kahana equation for a positron in an electron gas. Phys Rev B 23:1785–1795
6. Carbotte JP, Kahana S (1965) Positron annihilation in an interacting electron gas. Phys Rev A 139:213–222
7. Daniel E, Vosko S (1960) Momentum distribution of an interacting electron gas. Phys Rev 120:2041–2044
8. Kahana S (1963) Positron annihilation in metals. Phys Rev 129:1622–1628
9. Kontrym-Sznajd G (1990) Three-dimensional image reconstruction with application in positron annihilation. Phys Status Solidi A 117:227–240
10. Kontrym-Sznajd G, Samsel-Czekala M, Pietraszko A (2002) Electron momentum density in yttrium. Phys Rev B 66:155110–155121
11. Mattuck RD (1967) A guide to Feynman diagrams in the many-body problem. McGraw-Hill Publishing Co, Ltd, London. Chapter 11, §3
12. Rubaszek A, Stachowiak H (1988) Self-consistent solution of the Kahana equation for a positron in an electron gas. Phys Rev B 38:3846–3855
13. Sormann H (1996) Influence of lattice effects on the electron-positron interaction in metals. Phys Rev B 54:4558–4581
14. Sormann H, Kontrym-Sznajd G (2006) Many-body effects on the electron-positron momentum density in simple and transition metals: comparison with positron annihilation spectroscopy data. Phys Rev B 73:75111-1-11
15. Sormann H, Puff W (1985) Momentum dependent enhancement factors in alkali metals. In: Jain PC, Singru RM (eds) Proc of the 7th Int Conf on Positron Annihilation, January 1985, New Delhi, India. World-Scientific, Singapore, pp 161–163
16. Stachowiak H, Boroński E (2005) Influence of the zero motion of a positron on positron lifetime in a metal lattice due to higher Fourier components of its Bloch function. Phys Rev B 71:245107-1-9
17. Tang Z, Nagai Y, Inoue K *et al*. (2005) Self energy correction to momentum-density distribution of positron--electron pairs. Phys Rev Lett 94:106402-1-4