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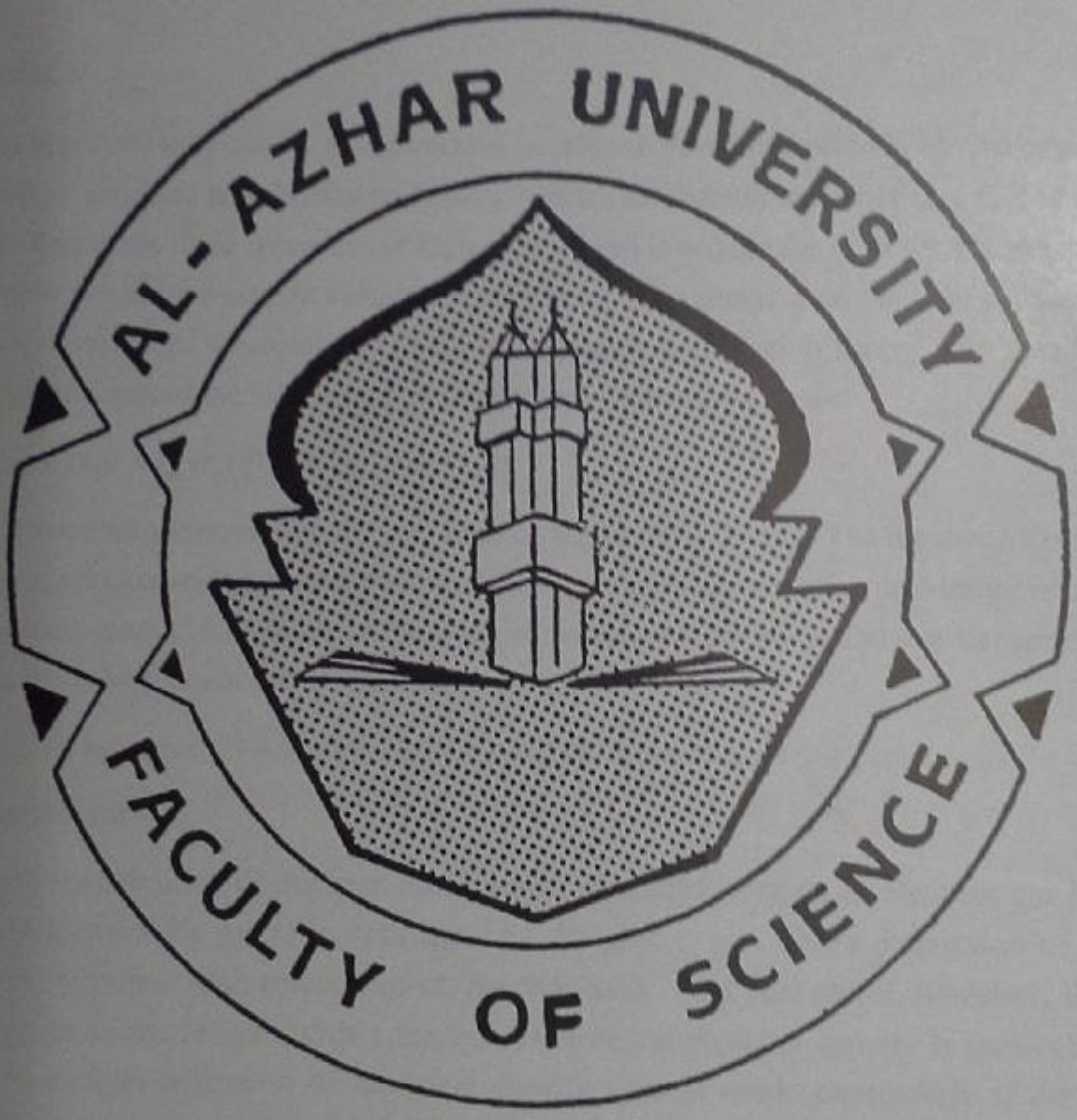

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POSITION ANNIHILATION CHARACTERISTICS IN AN ELECTRON GAS OF LOW AND HIGH DENSITIES

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Abstract

The approach to e^+ —— e^- interaction in jellium developed recently by Stachowiak[1] and used to calculate annihilation and characteristics for metallic densities ($2 \leq r_s \leq 6$) is applied to determine these quantities at high ($r_s < 2$) and low densities ($r_s > 6$). The results are reasonable for all investigated values of r_s. For $r_s \to 0$ the annihilation rates are compared to the exact asymptotic formulas of classical many-body perturbation theory. The results are presented in terms of the following formula for the enhancement factor:

$$\varepsilon (r_s, k/k_F) = \varepsilon_o (r_s) [1 + A (r_s) \gamma (k / k_F)]$$

The function γ indeed depends very little on the electron density. The functions $\varepsilon_o (r_s)$, $A (r_s)$ and $\gamma (k/k_F)$ describes the momentum dependence of the annihilation probability of a given electronic state as a function of the electron momentum. Let us remind that Kahana[7] expressed the enhancement factor in the form.

$$\varepsilon (r_s, k / k_F) = \alpha (r_s)^2 + b(r_s) (k / k_F)^4 + c (r_s) (k / k_F)$$

I. Introduction:

Most calculations of positron annihilation characteristics in an electron gas have been performed for metallic densities i.e. for $2 \leq r_s \leq 6$ (for a discussion of this problem, together with references cf. Stachowiak). In a real metal, however, there are regions in the lattice (within the core) where the electron density is particularly high. If an approximation of the local density type is used (particularly if the enhancement factor is introduced under the integral expressing the annihilation amplitude as was done for the first time by Daniuk et al (cf. also Refs.[3] and[4]), there is a need for annihilation characteristics in jellium for r_s even much lower than 2.

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Calculations of this kind have been presented by Rubaszek et al[5] in 1984. However, the computations performed within the kahana formalism were very laborious and self-consistency was achieved only partially (unlike in the computations performed later for metallic densities in Ref.[6].

The formalism developed in Ref.[1] being much more efficient allows to perform the computations fully self-consistently with low expenditure of manpower. These were performed for the values of r_s which were not considered in Ref[1] i.e. for $r_s < 2$ and $r_s > 6$.

II. COMMENTS ON THE FORMALISM:

The question was asked about the meaning of the approximations used in Refs. [7,6] and[1] in terms of perturbation theory.

The Kahana approach presented originally in Ref.[7] and reformulated in Ref.[6] relies on two main assumptions:

1) The unperturbed two particle state corresponds to free particles (one electron and the positron),

2) The approximation consists in taking account only of the infinite set of ladder diagrams where the rungs of the ladders mean the screened coulomb potential of interaction between the two particles. This leads to the Bethe-Goldstone equation from which for a given potential of interaction the scattering wave functions of the two particles can he computed.

The difference between Refs.[7] and[6] consists in the way of choosing the screened potential of interaction. From the solutions of the Bethe-goldstone equation one can compute the screening cloud distribution around the positron, and from there the screened Coulomb potential of interaction between the positron and the electrons. It is evident that the aposterioric potential obtained in this way should be equal to the aprioric potential assumed in the Bethe-Goldstone equation (self-consistency requirement).

Kahana used in the Bethe-Goldstone equation the static RPA (random-phase approximation) potential. This potential is self consistent only in a very limited sense. It would be strictly self consistent under the following circumstances:

1) Only the one rung ladder would be kept (Born approximation).

2) While computing the electron-electron potential only the Coulomb part would be included and the exchange-correlation omitted.

3) The positron should be assumed to have an infinite mass.

In Ref.[6] all these limitations are avoided: unlike in the original paper of Kahana[7] the Bethe-Goldstone equation is considered to be an equation not only for the two-particle wave functions, but also for the screened potential of interaction (The exchange-correlation correction is applied, however, in the local density approximation). An iteration procedure is developed which leads to a fully self-consistent potential. Owing to that one avoids both the divergence of the annihilation rate for low electron densities and its falling below the spin-averaged positronium value.

In Ref.[1] the assumptions of Kahana are replaced by the following ones:

1) The unperturbed state of the whole system is described by a Jastrow type trial function including already most of the electron-positron correlations. This state contains an adjustable function-parameter which was computed by Gondzik and Stachowiak[8] as the solution of a non-linear integro-differential equation. In the following we will refer to this approximation as to HNC (hypernetted- chain). We call Jastrow type trial function one in which tow-particle correlations do not depend on one- particle states.

2) The perturbation correction to the HNC state is computed in Born approximation and self-consistency achieved by solving an integro-differential equation. This approach will by referred to below as perturbed HNC (PHNC). The smallness of the perturbation makes the Born approximation reliable: as will be shown below, the annihilation characteristics obtained in this way are meaningful in the range of investigated densities of the electron gas ($0.1 \leq r_s \leq 25$). A similar statement could not be formulated in the case of Ref.[6] for lack of resources needed to perform appropriate calculations. Indeed the formalism of Ref.[1] makes the calculations shorter by a factor of the order of one handred in comparison with the approach used in Ref. 6. All the numerical results have been obtained using the same formalism as in Ref.[1].

III. HIGH DENSITIES:

The screening cloud distribution around the positron for $r_s < 2$ exhibits only quantitative changes in comparison with the results obtained for $r_s = 2$. Some of the distributions are shown in Fig. 1. [r_s = 1.5, 1.0, 0.7]. Note, however, that the difference between the results of HNC and PHNC increases with increasing density. So the assumption about the smallness of the perturbation becomes less and less convincing.

A mean of appreciating how reliable is the behavior of the solution for $r_s \to O$ is provided by the exact asymptotic formula of Arponen[9] for the annihilation rate obtained on ground of classic perturbation theory:

$$\lambda_A (r_s) = \frac{12}{3} \frac{}{r_s} [\, 1 + 1.23\, r_s + \text{higher terms} \,] \qquad (1)$$

The annihilation rates obtained in different approximations can be presented in the form.

$$\lambda_A (r_s) = \frac{12}{3} \frac{}{r_s} [\, 1 + C(r_s)\, r_s \,] \qquad (2)$$

where $C(r_s)$ should approach 1.23 as r_s goes to zero.

In Table I the values of $C(r_s)$ are collected for different approximations, not only HNC and PHNC, but also for two different approaches presented in Ref. 5. One in which the Kahana equation is solved with the original RPA potential and one in which an attempt is made to improve self-consistency by introducing an adjustable parameter in the potential.

All the approaches presented in table I behave regularly as $r_s \to o$ with some possible defect growing for $r_s < 0.2$. The value of $C(r_s)$ for small r_s compares reasonably in each case with the exact value 1.23 of Arponen. The best figures equal about 1.15 are provided by the approach using the Kahana formalism with adjusted RPA potential. However, the corresponding screening charge distribution is not self-consistent, so this agreement is of limited use as concerns determining the shape of the electronic cloud. It is also obvious that the static RPA potential used by Kahana is not a high density approximation between the positron and the electrons.

As concerns the present calculation, one should underline the following circumstances.

1) The character of the r_s dependence of λ is consistent with the Arponen formula.

2) The value of C(O) is equal 1.00 instead of 1.23.

3) Unlike in other approaches the present work provides also the screening cloud distribution [in other words- the whole e^+—— e^- correlation function g(r)].

4) The PHNC approach though based on the low density approximation works quite well even the limit of high densities.

As concerns partial annihilation rates at high densities, since the electron-positron interaction is weak, the main contribution to the annihilation of a particular

electronic state comes from the plane wave (free-particle) part of the electron wave function. And this part is the same for all electronic states. The difference comes from the scattering part of the wave function which is small at high densities. So for $r_s \to O$ the partial annihilation rate becomes the same for all electronic states. And such is the result of all calculations which have been performed. We express the momentum-dependent enhancement factor in the form proposed in Ref. 1. i.e.

$$\varepsilon (r_s, p) = \varepsilon_o (r_s) [1+A (r_s) \gamma (p/k_F)] \qquad (3)$$

where $\gamma (o) = o$ and $\gamma (1) = 1$. The behavior of $A(r_s)$ is shown in Fig. 2 for $r_s < 5$.

The function $\gamma (p/k_F)$ depend on the electron density, only slightly, as was pointed out already in Ref.[1]. We consider as characteristic for its behavior its value at $p = 0.8\ k_F$. This value is given in Table II for $0.1 \leq r_s \leq 25$. In Table II the results obtained in the present work are collected together with the figures found in Refs.[1,2,6] Remark the large plateau in $\gamma (0.8)$ occuring for metallic densities. Because of the importance of the enhancement factor $\varepsilon (r_s, p)$ for practical applications, we give also in Table II the values of $\varepsilon_o (r_s)$ and $A (r_s)$.

IV. LOW DENSITIES:

The screeing cloud distribution is shown in Fig. 3. for $r_s = 10$. Note that the difference between HNC and PHNC becomes smaller and smaller when r_s increases. This is an expression of the fact that NHC as a liquid theory approach is a low density approximation.

As concerns annihilation rates we found in HNC $\lambda = 2.07$ for $r_s = 8$ and 2.02 for $r_s = 10$, in PHNC $\lambda = 2.03$ and 2.01 respectively. For higher values of r_s we found some small fluctuations of the annihilation rate which we attribute to numerical errors e.g. for $r_s = 25$ λ is equal 2.06 in HNC and 2.02 in PHNC.

The behavior of $A(r_s)$ characterizing the momentum dependence of the enhancement is obtained. The values of $\lambda (0.8)$ which define the shape of the enhancement are given in Table II together with the values of $\varepsilon_o (r_s)$ and $A(r_s)$.

It is well known that in the low density limit the ground state corresponds to the negative positron. This means that the positron is surrounded by an electronic cloud containing two electronic charges. The cloud screening this object should consist in total of an electron deficiency corresponding to one electronic charge. In terms of Friedel oscillations this corresponds to an overaccumulation of electrons in the immediate neighbourhood of the positron followed by an electron deficiency at higher distances. In the case of Ps in vacuum the amount of overscreening is, of course, equal to unity. Note, however, that the present formalism assumes at the very beginning the absence of bound states.

Table (1)

The values of C (r_s) in different approaches, C_G refers to HNC, C_{SL} to PHNC, C_R and C_{RPA} to Ref.5, C_{RPA} was obtained when solving the Bethe-Goldstone equation with the static RPA potential, C_R from an attempt to reach self-consistency .

r_s	C_G	C_{SL}	C_R	C_{RPA}
2.0	2.03	1.64	1.62	1.47
1.8	1.91	1.55	-	-
1.5	1.76	1.41	1.39	1.27
1.3	1.68	1.32	-	-
1.0	1.57	1.21	1.22	1.12
0.9	1.54	1.18	-	-
0.7	1.51	1.12	1.15	1.06
0.5	1.48	1.06	1.14	1.03
0.3	1.53	1.00	1.15	1.02
0.2	1.58	1.00	1.19	1.03
0.1	1.77	1.01	1.39	1.07

Table (2)

Over screening of the positron (as defined in the paper) in different approaches, AP refers to Ref. 11, R to Ref. 6 and SL to the present work

r_s	AP	R	SL
4	0.02	0.13	0.07
6	0.12	0.27	0.21
8	0.26	0.41	0.33
10	–	–	0.41
15	–	–	0.48
20	–	–	0.67

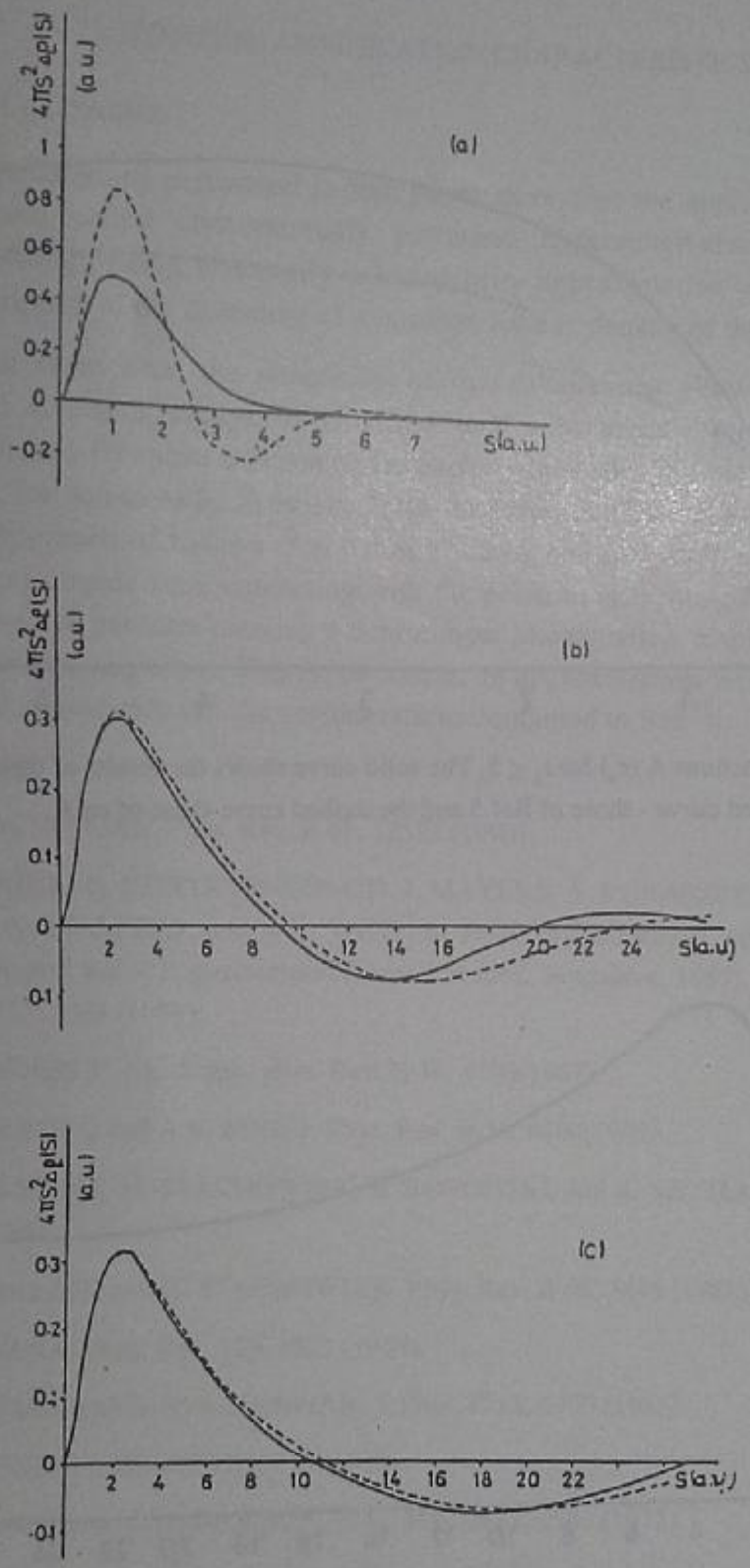

Fig. (1): The screening cloud distribution $4\pi S^2 \Delta\rho$ (S) (a) for r_s =1.5 (b) for r_s =1.0 (c) for r_s = 0.7. The dashed curves are obtained form, Ref. 8 and the solid curves from, the present works.

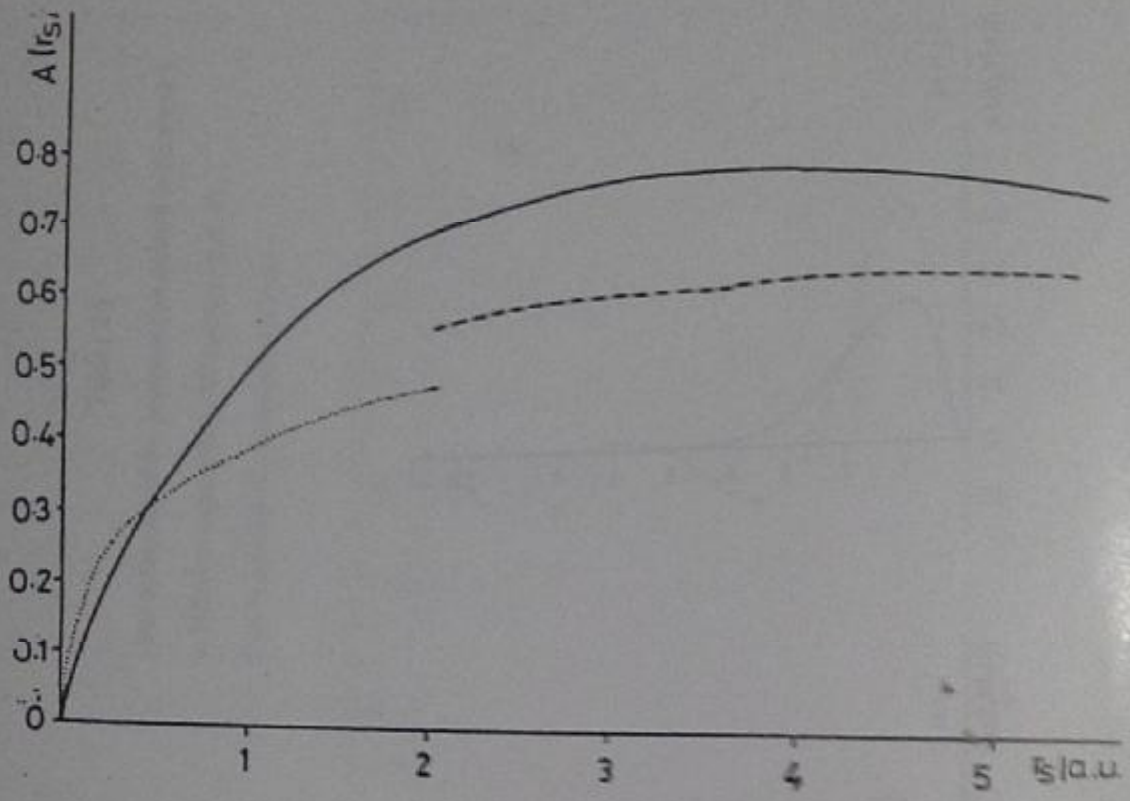

Fig. (2): The functions A (r_s) for $r_s \leq 5$, The solid curve shows the results of the present work the doted curve - those of Ref.5 and the dashed curve-these of ref.6

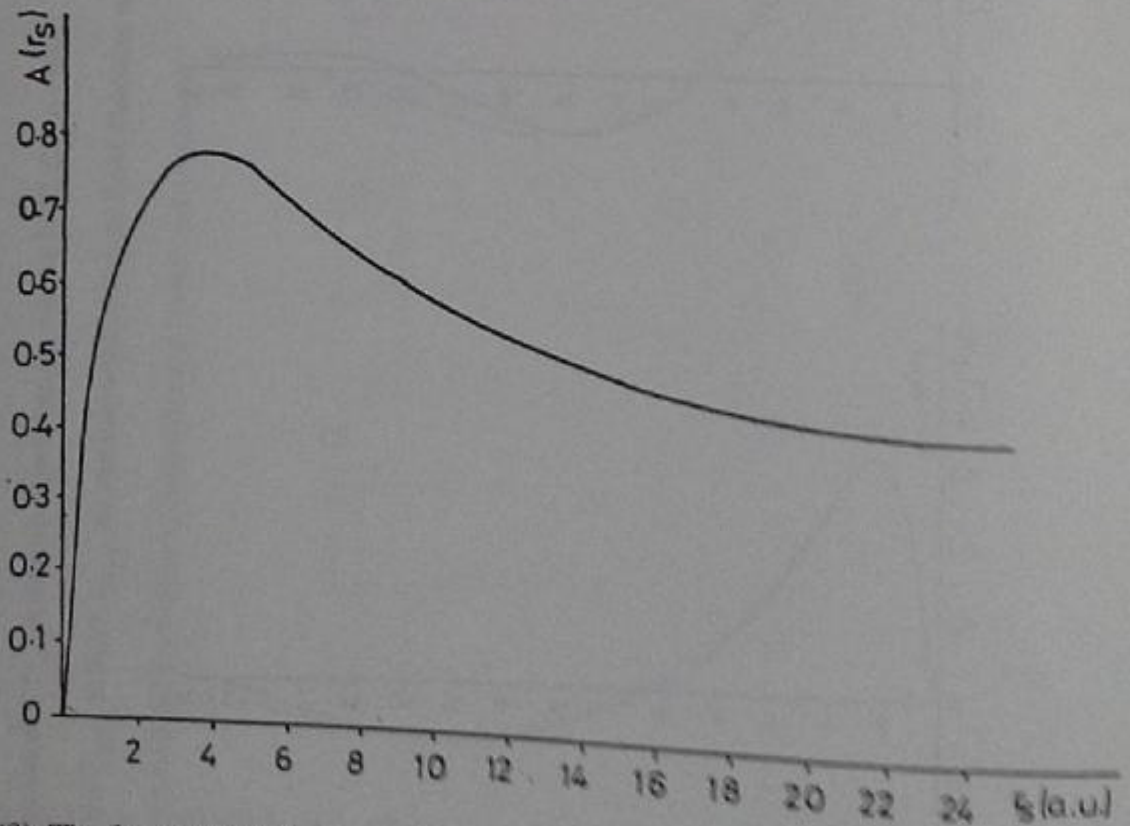

Fig. (3): The function A (r_s) for $r_s \leq 25$.

V. CONCLUSIONS:

The calculations performed in this paper show that the approach developed in Ref. 1 and called conventionally perturbed hypernetted-chain approximation (PHNC) though being essentially a low-density approximation provides a reasonable description of the screening of a positron for any density of the electron gas.

At the same time the simplicity of the calculations allows to obtain self-consistent screening charge distributions (and subsequently reliable annihilation characteristics) for those electron densities for which this has not been done previously, i.e. for non metallic densities. Note, however, that the PHNC approach shares with the approach of Kahana[7,6] and that of Lowy and Jackson[10,11] a common feature ; the electronic state interacting with the positron is separated out of the whole system, the two particles obeying a Schrodinger like equation. Explicit three particle correlations are neglected. This is, of course, an approximation which can influence the results appreciably (cf. the considerations contained in Ref.[1].

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