Enhancement of positron annihilation with core electrons

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A theoretical treatment is presented of the enhancement of positron annihilation with core electrons in a solid. A first estimate is obtained from the simple result for Coulomb scattering of a single positron-electron pair. For relative velocity v large compared to the Bohr velocity $v_0 = e^2/\hbar$ the enhancement is small, being given approximately by $\chi - 1 = \pi v_0/v$, where χ is the enhancement factor. Since core electrons typically have velocities much larger than v_0, the enhancement for core annihilation is expected to be small. Modifications due to the fact that the electron is embedded in a system of interacting electrons bound to an atomic nucleus are estimated from calculations partly for an electron gas of high density, and partly for a single electron closely bound to a nucleus. The enhancement is found to be similar to the result for a single, free electron but somewhat reduced in magnitude mainly due to the Pauli exclusion principle. Quantitative estimates of the small enhancement are derived for the core contribution to both the total and the momentum-dependent annihilation rates. The enhancements are much smaller than obtained in earlier treatments, and they lead to corrections for core annihilation which are significantly smaller than those derived from semiempirical estimates.

I. INTRODUCTION

Thermalized positrons in matter predominantly annihilate with outer electrons, owing to the high potential barriers close to nuclei. As a result, positron annihilation has become a useful tool in studies of, for instance, the momentum distribution of conduction electrons in metals.[1] This type of investigation relies to some extent on the possibility of subtracting the background of less frequent events corresponding to annihilation with core electrons. The correction for core contributions has been based either on empirical fitting procedures[2] or on theoretical predictions.

To calculate the annihilation probability per unit time one must evaluate the electron density at the position of the positron. The simplest estimate of this quantity is obtained on the basis of the independent particle model (IPM). Within this approximation the interaction between the charged particles is described through average fields only. In particular, the electron-positron correlation is neglected. In the case of outer electrons this correlation leads to a considerable increase in the electron density in the immediate vicinity of the positron, and the observed annihilation yields differ from the corresponding IPM values by enhancement factors as large as 10. The present paper is concerned with the calculation of enhancement factors pertaining to core annihilation rates. The generally accepted theoretical prediction, due to Carbotte and Salvadori,[3] gives an enhancement factor of the order of 3 for L-shell electrons in Al. This markedly disagrees with the results of a recent experiment by Lynn *et al.*,[4] in which the rare events from annihilation with high momentum core electrons in Al were isolated. The experimental spectra were satisfactorily reproduced by IPM calculations.

A new investigation of annihilation with core electrons is warranted on two counts. First, there is a lack of reliable information for core subtraction implied by the large discrepancy between calculated and observed core-enhancement factors. Second, annihilation spectra corresponding to electron momenta far beyond those of the outer electrons are now experimentally accessible. These spectra may well be worth studying in their own right. As indicated by Lynn *et al.*[4] these high momentum spectra should be superior to the conventional low momentum spectra for the characterization of vacancy-type defects in solids, provided that the spectra can be accounted for within the IPM, or that the enhancement, if important, can be estimated reliably.

For outer electrons the theoretical description of annihilation rates has been based on electron-gas

results.[1] In this paper the application of the electron-gas picture will be extended to the inner parts of the atoms, the electron cloud being represented locally by a free gas. Such a procedure, of Thomas-Fermi-type, is known to give useful results not only for atomic charge densities and potentials[5] but also for the energy loss of charged particles penetrating matter. In the latter case one uses the electron-gas picture to estimate the dynamic response of atomic electrons to a perturbation from an external charge. The atomic binding cannot be completely neglected, but it may be taken into account through a correction of the local plasma frequency which governs the response of a gas for low momentum transfers.[6] In contrast, for the evaluation of density enhancement at the position of a perturbing positive charge mainly the velocity distribution of the electrons is important, and one may hope for even better accuracy of estimates of Thomas-Fermi-type. This expectation is supported by the excellent results obtained by this type of calculation for the so-called shell corrections to the electronic stopping,[7,8] which are also determined by the velocity distribution. We have checked the accuracy of the momentum distribution for atomic electrons obtained with the local gas picture by comparing the momentum-dependent annihilation rates calculated within the IPM with atomic wave functions and with the plane-waves characteristic of the local gas picture. The high momentum tails arise from annihilation with core electrons and therefore directly reflect the momentum distribution of these electrons.

A calculation of the electron density at the position of a positively charged particle in an electron gas is particularly simple for the high densities corresponding to atomic cores. The density enhancement is small, and a first-order perturbation treatment is sufficient. Furthermore, in the limit of high densities the screening of the Coulomb interaction becomes unimportant for calculations of scattering. The enhancement in this limit has been calculated by Kahana,[9] but we shall give a simple derivation based on the Born-approximation result for two-body scattering. Such a procedure, not relying on methods of field theory, is more transparent as regards the approximations involved. The momentum-dependent as well as the total enhancement are calculated both for a positron and for a very heavy positive particle (e.g., a proton). A comparison between these two cases elucidates some features of the results, in particular the role played by electron-electron exchange. The simpler case of an infinitely heavy positive particle also turns out to be useful for estimating the higher-order corrections which are important at lower densities. The electron-gas results for the enhancement may be applied in a straightforward manner in the local gas approximation to obtain a momentum-dependent enhancement for annihilation with atomic electrons, which can be used directly in the analysis of experiments.

For subtraction of the core contribution from total annihilation rates the enhancement for individual atomic shells is needed. Partly for this reason, the Thomas-Fermi-type treatment in which the atom is divided into regions with different density but not into shells with different binding is complemented with calculations using atomic orbitals for inner electrons. The enhancement corresponding to annihilation with core electrons should be insensitive to the structure of the solid, and thus the problem is reduced to an atomic one. For a single atom the calculation of enhancement is straightforward when Coulomb wave functions are used for the free electron and positron states. The problem is similar to that treated by Carbotte and Salvadori,[3,10,11] but since the complications introduced by the band structure of a solid are avoided, the calculations may be carried through without the crude approximations applied by these authors. It is then also possible to identify the approximation which led to their erroneous result of a very strong enhancement for core annihilation. In addition to supplementing the Thomas-Fermi-type results for the momentum-dependent enhancement, the atomic calculations provide a check of some of the approximations inherent in the free-gas model. In particular, it can be shown that although the existence of a potential barrier for the positron close to nuclei is crucial for the calculation of the annihilation yield from inner electrons, the barrier is not important for the evaluation of the corresponding enhancement factor. This is important for the application of the local gas picture, since here the effect of barrier penetration on enhancement is neglected.

II. BASIC FORMULAS

The annihilation of positrons in matter is dominated by processes which result in the emission of two γ rays. In this section we list a few basic formulas pertaining to this situation.

Consider a positron annihilating within a system of electrons. If $\hat{\phi}(\vec{x})$ and $\hat{\psi}(\vec{x})$ denote the positron and electron field operators, the probability per unit time for the emission of two γ rays with total momentum $\hbar\vec{q}$ within $\hbar^3 d^3\vec{q}$ is given by $\Gamma(\vec{q})\, d^3\vec{q}$, where[1,12]

$$\Gamma(\vec{q}) = \frac{r_0^2 \cdot c}{8\pi^2} \int\int d^3\vec{x}\, d^3\vec{y}\, e^{-i\vec{q}\cdot(\vec{x}-\vec{y})} \langle \hat{\psi}^+(\vec{y})\hat{\phi}^+(\vec{y})\hat{\phi}(\vec{x})\hat{\psi}(\vec{x})\rangle \quad . \tag{1}$$

Here c is the velocity of light and r_0 the classical electron radius. The expectation value is for the ground state, and the equation includes an average over spin directions.

A simple evaluation of the right-hand side of Eq. (1) leads to the following expression in terms of the antisymmetrized total wave function $\psi(\vec{r},\vec{r}_1,\vec{r}_2,\ldots,\vec{r}_N)$ for the system consisting of the positron with coordinates $\vec{r}$ and the electrons with coordinates $(\vec{r}_1,\vec{r}_2,\ldots,\vec{r}_N)$,

$$\Gamma(\vec{q}) = \frac{r_0^2 \cdot c}{8\pi^2} N \int d^3\vec{r}_2 \cdots \int d^3\vec{r}_N \left| \int d^3\vec{r}\, e^{-i\vec{q}\cdot\vec{r}} \psi(\vec{r},\vec{r},\vec{r}_2,\ldots,\vec{r}_N) \right|^2 . \tag{2}$$

As discussed in the Introduction, we shall be concerned with the evaluation of enhancements above the predictions of the independent particle model (IPM). For a positron with wave function ϕ annihilating in a system of electrons described by a Slater determinant of single-particle states ψ_i one obtains from Eq. (2)

$$\Gamma^{\mathrm{IPM}}(\vec{q}) = \frac{r_0^2 \cdot c}{8\pi^2} \sum_i \left| \int d^3\vec{r}\, e^{-i\vec{q}\cdot\vec{r}} \phi(\vec{r}) \psi_i(\vec{r}) \right|^2 . \tag{3}$$

The results of Secs. IV–VII will be presented in terms of the momentum-dependent enhancement factor

$$F(\vec{q}) = \Gamma(\vec{q})/\Gamma^{\mathrm{IPM}}(\vec{q}) \tag{4}$$

and the average enhancement factor

$$\begin{aligned} \bar{F} &= \int d^3\vec{q}\, \Gamma(\vec{q}) \Big/ \int d^3\vec{q}\, \Gamma^{\mathrm{IPM}}(\vec{q}) \\ &= N \int d^3\vec{r}_2 \cdots \int d^3\vec{r}_N \int d^3\vec{r}\, |\psi(\vec{r},\vec{r},\vec{r}_2,\ldots,\vec{r}_N)|^2 \Big/ \sum_i \int d^3\vec{r}\, |\phi(\vec{r})\psi_i(\vec{r})|^2 . \end{aligned} \tag{5}$$

III. THOMAS-FERMI APPROXIMATION WITHIN THE IPM

As we shall see, the enhancement of positron annihilation relative to the IPM result depends mainly on the electron velocity distribution. Before considering the positron-electron correlation in an electron gas, with the aim of estimating the enhancement of positron annihilation with core electrons, we apply a Thomas-Fermi-type treatment to the calculation of momentum-dependent annihilation rates within the IPM. Since the high-momentum tail directly reflects the momentum distribution of inner electrons, this provides a check of the accuracy with which this distribution is reproduced by a Thomas-Fermi-type model.

In the Thomas-Fermi picture of the atom it is assumed that the electron cloud may be divided into volumes Ω small enough that the potential energy $V(r)$ of an electron is essentially constant over Ω and large enough that Ω contains several electrons. The electron states in Ω are described by plane waves,

$$\psi_\Omega(\vec{r}) = (\Omega)^{-1/2} e^{i\vec{k}\cdot\vec{r}}, \quad \vec{r} \in \Omega . \tag{6}$$

The states are filled in order of increasing momentum, reaching a local Fermi momentum $\hbar k_F(r)$, which is related to the local potential energy through

$$\hbar^2 k_F^2(r)/2m + V(r) = 0 , \tag{7}$$

where m is the electron mass.

For the thermalized positron the wave function may be determined by numerical integration of the Schrödinger equation with potential $|V(r)|$. The solution is obtained in the form of a spherically symmetric function, $(4\pi)^{-1/2} R_+(r)$, inside the Wigner-Seitz sphere for the solid under investigation. The contribution of the electrons in Ω to the momentum-dependent annihilation rate is then, according to Eq. (3), given by

$$\Gamma_\Omega(\vec{q}) = \frac{r_0^2 \cdot c}{4\pi^2} \sum_{\vec{k}} \left| \int d^3\vec{r}\, e^{-i\vec{q}\cdot\vec{r}} (4\pi)^{-1/2} R_+(r) \times (\Omega)^{-1/2} e^{i\vec{k}\cdot\vec{r}} \right|^2 . \tag{8}$$

With the assumption that for most electrons the quantity $\vec{k}\cdot\vec{r}$ varies rapidly within Ω while $R_+(r)$ remains essentially constant, we obtain

$$\Gamma_\Omega(\vec{q}) = \frac{r_0^2 \cdot c}{4\pi^2} \cdot \frac{\Omega}{4\pi} R_+^2(\vec{r}_\Omega), \quad \text{for } q \leq k_F(\vec{r}_\Omega) , \tag{9}$$

where $\vec{r}_\Omega$ specifies the position of Ω.

The total annihilation probability within the IPM is obtained by integration over $\vec{r}_\Omega$. Since the atomic density varies monotonically with r, the condition $q \leq k_F(r)$ may be replaced by an upper limit on the integral,

$$\Gamma^{\mathrm{IPM}}(q) = \frac{r_0^2 \cdot c}{4\pi^2} \int_0^{R(q)} dr\, r^2 R_+^2(r) ,$$

with

$$k_F(R(q)) = q . \tag{10}$$

The simple interpretation of this formula is that the momentum q is provided by the annihilating electron while the positron wave function, which does not contain high Fourier components, only provides a weighting function for the average over the momentum distribution of atomic electrons. As usual for a Thomas-Fermi-type estimate, the assumptions made in the derivation of Eq. (10) are only strictly fulfilled at very high atomic numbers, and for light atoms the accuracy of the estimate should be judged through its application.

The formula (10) has been applied to calculate the rates of positron annihilation in Al and Cu, and in Figs. 1(a) and 1(b) the results are compared with the rates calculated directly from Eq. (3) with atomic electronic wave functions. The agreement is good over several orders of magnitude in $\Gamma(q)$, and this indicates that in the region of interest the momentum distribution of the electrons is fairly well represented by the local gas picture.

IV. ENHANCEMENT IN DENSE ELECTRON GAS

For a positive particle in an electron gas the density enhancement at the position of the particle is determined by scattering of the electrons in the attractive screened Coulomb field. As will be shown in Sec. V A, in the limit of high densities the wavelength of an electron at the Fermi level is short compared to the screening length, and therefore an unscreened Coulomb potential may be used to calculate the scattering for most of the electrons. To obtain a first estimate of the enhancement, we consider the scattering of a single electron. The effect of exchange may then be studied by a consideration of the corresponding three-body problem.

A. Two-particle scattering

The positive particle with charge e is given an arbitrary mass M, as a comparison between the cases

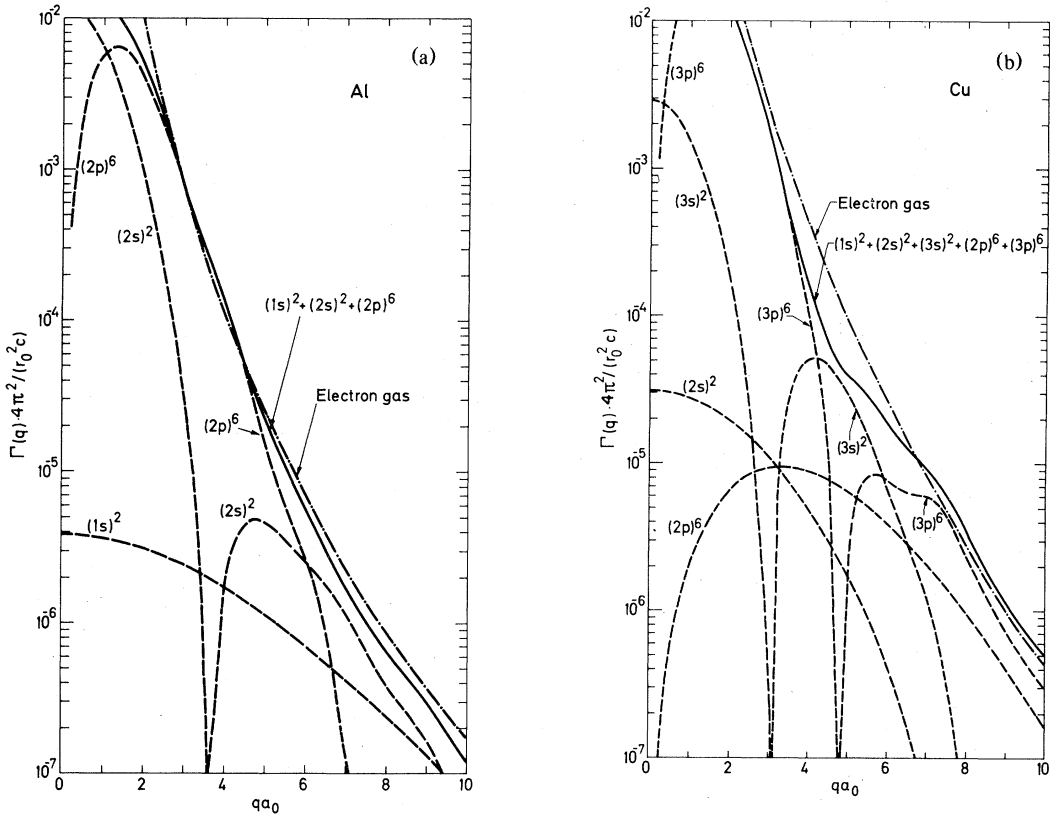

FIG. 1. (a) Independent-particle annihilation rates for Al, obtained from Eq. (3) and from the electron-gas formula (10). Electron and positron wave functions were calculated from the Schrödinger equation with overlapping atomic potentials obtained from Clementi wave functions. The electron potential included Slater exchange. The length a_0 is the Bohr radius $a_0=\hbar^2/(me^2)$. The contributions from individual electron orbitals are shown, and their sum is compared to the results from the local gas approximation. (b) Similar to Fig. 1(a), but for annihilation in Cu. For the configuration $(1s)^2$, which is not included in the figure, one finds $\Gamma(q=0)\cdot 4\pi^2/(r_0^2\cdot c)=6.6\times 10^{-9}$.

$M=m$ and $M\to\infty$ will prove useful later on. Since the enhancement is expected to be small in the cases under investigation, the Coulomb attraction between the two particles can be treated as a perturbation. Denoting the quantization volume by V and letting coordinates $\vec{r}$ and $\vec{r}_1$ refer to the positive and negative particles of momentum $\hbar\vec{k}_0$ and $\hbar\vec{k}_1$, respectively, we obtain to first order for the wave function

$$\psi(\vec{r},\vec{r}_1)\simeq\psi_0(\vec{r},\vec{r}_1)+\delta\psi(\vec{r},\vec{r}_1)$$
$$=V^{-1}e^{i\vec{k}_0\cdot\vec{r}}e^{i\vec{k}_1\cdot\vec{r}_1}$$
$$+V^{-1}\sum_{\vec{k}\neq\vec{0}}\frac{4\pi e^2}{k^2}\left(\frac{\hbar^2k^2}{2m_r}+\hbar\vec{k}\cdot(\vec{v}_1-\vec{v}_0)\right)^{-1}$$
$$\times V^{-1}e^{i(\vec{k}_0-\vec{k})\cdot\vec{r}}e^{i(\vec{k}_1+\vec{k})\cdot\vec{r}_1}\ . \qquad (11)$$

Here the reduced mass $m_r=mM/(m+M)$ and the velocities $\vec{v}_0$ and $\vec{v}_1$ of the unperturbed particles have been introduced.

For the density enhancement we obtain

$$\chi=|\psi(\vec{r},\vec{r})|^2/|\psi_0(\vec{r},\vec{r})|^2$$
$$\simeq 1+\frac{2}{V}\sum_{\vec{k}\neq\vec{0}}\frac{4\pi e^2}{k^2}\left(\frac{\hbar^2k^2}{2m_r}+\hbar\vec{k}\cdot(\vec{v}_1-\vec{v}_0)\right)^{-1}\ . \qquad (12)$$

As expected, only the relative velocity enters in Eq. (12). The problem is in fact more naturally treated in the center-of-mass reference frame, but for the purpose of generalizing to the many-body problem for an electron gas, we stay in the laboratory frame. Without loss of generality we may set $v_0=0$, and by direct evaluation we obtain

$$\chi(k)-1=\frac{\pi e^2}{\hbar v}\ , \qquad (13)$$

where $\hbar k$ and v now denote the momentum and velocity of the electron. It is a remarkable feature of this formula that the enhancement factor is independent of mass for fixed relative velocity. This result is not restricted to the Born limit but is retained in an exact treatment of the scattering of two particles interacting through a Coulomb field. The exact value of the enhancement is given later [Eq. (31)]. It will be noted that the enhancement for two-body scattering has not been denoted by the symbol F introduced in Sec. II for the momentum-dependent enhancement. The reason is that there is an important distinction between the two quantities in the corresponding many-body problem.

B. Average enhancement for $M\to\infty$

For a positive particle in an electron gas the evaluation of enhancement factors is complicated by exchange effects, but for a particle of infinite mass the situation is simple. In this case all the electron orbitals are solutions to the same one-particle Schrödinger equation, and are therefore automatically orthogonal. The average electron density at a point $\vec{r}$, represented by the sum of one-particle operators $\sum_i\delta(\vec{r}-\vec{r}_i)$, is then the same whether calculated from a simple product wave function or from the Slater determinant of the orbitals in the product function. By averaging Eq. (13) over the velocities of the electrons within the Fermi sphere, one obtains for the average enhancement $\bar{F}$ in the limit of high density n,

$$\bar{F}-1=\frac{3\pi}{2}\frac{e^2}{\hbar v_F}=2.455r_s,\quad r_s\to 0\ , \qquad (14)$$

where v_F is the Fermi velocity and r_s the usual density parameter,

$$r_s=\left(\frac{4\pi}{3}a_0^3n\right)^{-1/3}\ ,$$

$a_0=\hbar^2/me^2$ being the Bohr radius.

As was noted already, the two-body enhancement factor is mass independent and one might therefore expect that the formula (14) would apply for arbitrary mass M of the positive particle in the high-density limit where screening can be neglected. To see that this is in fact not true, we need only study a system containing two (identical) electrons interacting with the positive particle.

C. Three-particle scattering and exchange

For simplicity we neglect the Coulomb interaction between the two electrons. It is straightforward to show that to first order it influences neither the total nor the momentum-dependent enhancement. With an obvious generalization of the notation used above, the following expression is then obtained to first order for the enhancement of the electron density at the position of the positive particle,

$$\bar{F}-1=\frac{1}{2}\left[\frac{2}{V}\sum_{\substack{\vec{k}\neq\vec{0}\\ \vec{k}\neq\vec{k}_2-\vec{k}_1}}\frac{4\pi e^2}{k^2}\left(\frac{\hbar^2k^2}{2m_r}+\hbar\vec{k}\cdot(\vec{v}_1-\vec{v}_0)\right)^{-1}+\frac{2}{V}\sum_{\substack{\vec{k}\neq\vec{0}\\ \vec{k}\neq\vec{k}_1-\vec{k}_2}}\frac{4\pi e^2}{k^2}\left(\frac{\hbar^2k^2}{2m_r}+\hbar\vec{k}\cdot(\vec{v}_2-\vec{v}_0)\right)^{-1}\right]\ . \qquad (15)$$

In general, this result is different from the average of the two-particle enhancement factors, given by Eq. (12), since the summation over momentum transfers is restricted in Eq. (15). The restriction arises from the exchange

term, which must be subtracted from the corresponding direct term. The presence of an exchange term in the expectation value of a sum of one-particle operators, $\sum_i \delta(\vec{r}-\vec{r}_i)$, originates in the nonorthogonality, to first order, of the orbitals $\psi_i+\delta\psi_i$. In the special case $M\to\infty$, (i.e., $m_r=m$) these orbitals are orthogonal and the two exchange terms in Eq. (15) cancel. For antiparallel electron spins the exchange term of course vanishes.

D. Average enhancement for arbitrary mass

The formula (15) may be directly generalized to the case of N electrons with parallel spins, described by a Slater determinant,

$$\bar{F}-1=\frac{1}{N}\sum_{|\vec{k}'|<k_F}\frac{2}{V}\sum_{|\vec{k}'+\vec{k}|>k_F}\frac{4\pi e^2}{k^2}\left(\frac{\hbar^2k^2}{2m_r}+\frac{\hbar^2\vec{k}\cdot\vec{k}'}{m}\right)^{-1} . \tag{16}$$

This result, applicable for an electron gas of high density, was first derived by Kahana[9] for the case of $M=m$, with a correction for screening included. It turns out that for pure Coulomb scattering the evaluation of Eq. (16) can be carried rather far analytically, and one obtains

$$\bar{F}-1=\left(\frac{3\pi}{2}\frac{e^2}{\hbar v_F}\right)\cdot\left\{\frac{2}{\pi^2}\left[\int_0^{(1+\beta)^{-1}}\frac{dz}{z}\log\left|\frac{1+z}{1-z}\right|+\int_0^{1-\beta}\frac{dz}{z}\log\left|\frac{1+\gamma z}{1-z}\right|\right]\right\} , \tag{17}$$

where $\beta=m/M$ and $\gamma=(M+m)/(M-m)$. The enhancement is here written as a product of two terms, the first of which depends on the gas density only, and not on the mass of the positive particle. The mass dependence is given by the second factor, which for $M\to\infty$ approaches unity such that the result (14) is obtained. For the case $M=m$ the mass-dependent factor is equal to 0.5. Hence, for a positron in a high-density gas, the average enhancement factor for positron annihilation is given by

$$\bar{F}-1=\frac{3\pi}{4}\frac{e^2}{\hbar v_F}=1.228r_s . \tag{18}$$

E. Momentum-dependent enhancement

Having noted the particular simplicity of the limit $M\to\infty$ in the calculation of the average enhancement $\bar{F}$ in an electron gas of high density, one might expect the corresponding momentum-dependent enhancement factor to be given by Eq. (13) in this limit. However, once again exchange invalidates the simple expectation.

As above, we consider two noninteracting electrons scattered by a positive particle of mass M, and for simplicity we immediately set $v_0=0$. The annihilation rate $\Gamma(\vec{q})$, given by Eq. (2), reduces to

$$\Gamma(\vec{q})=2\frac{r_0^2\cdot c}{8\pi^2}\int d^3\vec{r}_2\left|\int d^3\vec{r}\,e^{-i\vec{q}\cdot\vec{r}}\psi(\vec{r},\vec{r},\vec{r}_2)\right|^2 . \tag{19}$$

As expected, we find that to first order $\Gamma(\vec{q})$ vanishes unless $\vec{q}=\vec{k}_1$ or $\vec{q}=\vec{k}_2$, and we obtain for two electrons with parallel spins

$$\Gamma(\vec{q}=\vec{k}_1)=\frac{r_0^2\cdot c}{8\pi^2}\left[1+\frac{2}{V}\sum_{\substack{\vec{k}\neq\vec{0}\\ \vec{k}\neq\vec{k}_2-\vec{k}_1}}\frac{4\pi e^2}{k^2}\left(\frac{\hbar^2k^2}{2m_r}+\frac{\hbar^2\vec{k}\cdot\vec{k}_1}{m}\right)^{-1}\right] . \tag{20}$$

The result of the direct process, the annihilation of an electron with momentum $\hbar\vec{k}_1$, is reduced by the exchange process, the annihilation of an electron with momentum $\hbar\vec{k}_2$ together with a replacement of the momentum $\hbar\vec{k}_1$ by $\hbar\vec{k}_2$ for the other electron.

The formula may immediately be generalized to the case of N electrons with parallel spins, described by a Slater determinant, and we arrive at an expression for the momentum-dependent enhancement factor for a dense electron gas with Fermi momentum k_F,

$$F(\vec{q})-1=\frac{2}{V}\sum_{\substack{\vec{k}\neq\vec{0}\\ |\vec{q}+\vec{k}|>k_F}}\frac{4\pi e^2}{k^2}\left(\frac{\hbar^2k^2}{2m_r}+\frac{\hbar^2\vec{k}\cdot\vec{q}}{m}\right)^{-1}, \quad \text{for } q<k_F . \tag{21}$$

To first order the annihilation rate $\Gamma(\vec{q})$ vanishes for $q > k_F$. The result (21) will be discussed and applied later (Secs. V and VII). At this point we merely emphasize that the exchange effect reflected in the restriction on momentum transfers in Eq. (21) is crucial for the determination of $F(\vec{q})$. In fact, if exchange is neglected, one arrives at an enhancement given by the function $\chi(\vec{k}=\vec{q})$ in Eq. (13), which decreases for increasing q and diverges in the limit $q \to 0$. In contrast, as shown later for the case $M = m$, the formula (21) leads to a function $F(q)$ which increases with q and diverges at the Fermi surface, $q \to k_F$.

It will be noted that by summing Eq. (21) over momenta q one can recover the expression for $\bar{F}$ in Eq. (16). We should also note here that the expression appearing in Ref. 9 which corresponds to our Eq. (16) was derived with a dynamically screened potential rather than with the static Coulomb potential. For a dynamic potential, the summand in the expression for $\bar{F}$ is no longer directly identifiable with the momentum-dependent enhancement factor $F(q)$.

We have several reasons for presenting this rederivation of some of the results of Ref. 9 at some length. First, we find an elementary treatment, not relying on methods of field theory, more transparent as regards the approximations involved. Second, we have attempted to elucidate the origin of the spectacular difference between the shape of the momentum dependence as obtained from Eq. (21) and from simple expectations based on formulas like (13). Finally, the generalization of Kahana's formula to a positive particle of arbitrary mass will find useful applications below.

V. SCREENING AND NONLINEARITY

In Sec. IV we have treated the electron gas in the limit of high density, where pure Coulomb scattering in the Born limit suffices to calculate the electron-positron correlation. We ultimately want to apply the results to annihilation within atomic cores but although the electron density is high in these regions, corrections to the simple limiting results may be of significance. In this section we estimate the two most important corrections due to screening of the electron-positron interaction and deviations from the linear treatment. Since the corrections are expected not to be very large for the electron densities of interest, simple estimates should suffice.

A. Screening

For a positive particle of infinite mass at rest in an electron gas, screening can easily be introduced into the description. Free electrons are scattered by an average static potential which, within the Thomas-Fermi description, is determined from the Poisson equation and the requirement that the single particle energy at the Fermi level be independent of position [cf. Eq. (7)]. At high gas densities the induced charge density is a small correction and a point charge e of infinite mass gives rise to an exponentially screened Coulomb potential,

$$V(r) = -\frac{e^2}{r} e^{-r/a} , \tag{22}$$

where

$$a = \left(\frac{\pi a_0}{4k_F}\right)^{1/2}, \quad a_0 = \frac{\hbar^2}{me^2} . \tag{23}$$

In the formulas for annihilation rates, such as Eqs. (16) and (21), this simply leads to a replacement of the Coulomb potential by a screened potential,

$$\frac{4\pi e^2}{k^2} \to \frac{4\pi e^2}{k^2 + a^{-2}} . \tag{24}$$

In the limit of very high densities the screening length a becomes long compared to the wavelength k_F^{-1}, and the enhancement approaches that of a pure Coulomb field.

Kahana[9] obtained the average enhancement at high densities from a series expansion of the free electron-positron Green's function, with an effective dynamic interaction potential equal to the Coulomb potential $4\pi e^2/k^2$ divided by Lindhard's longitudinal dielectric function $\epsilon(k, \omega)$. His final average enhancement factor, obtained after an integration over ω, is given by Eq. (16) with the replacement

$$\frac{4\pi e^2}{k^2} \to \frac{4\pi e^2}{k^2} \times \left|\epsilon\left(k, \omega = \frac{\hbar}{2m}[(\vec{k}+\vec{k}')^2 - k'^2]\right)\right|^{-2} . \tag{25}$$

A numerical evaluation of the formula (16) with the replacements (24) and (25) shows that the two estimates of screening do, in fact, give the same results in the limit $M \to \infty$. In Table I the average enhancement as a function of r_s is represented in terms of

TABLE I. Values of $\bar{I}(r_s)$ from Eq. (26) in the limit $M \to \infty$. The second and third columns correspond to the replacements (24) and (25), respectively, in Eq. (16). The fourth column is obtained from Eq. (27).

r_s	$\bar{I}(r_s)$	$\bar{I}(r_s)$	$\bar{I}(r_s)$
10^{-5}	2.43	2.43	2.44
10^{-3}	2.39	2.39	2.41
10^{-2}	2.31	2.31	2.33
10^{-1}	2.08	2.06	2.10
1	1.51	1.53	1.59

the slowly varying quantity $\bar{I}(r_s)$, defined through the relation

$$\bar{F}-1=r_s\bar{I}(r_s) \quad . \tag{26}$$

At high densities $\bar{I}(r_s)$ approaches the constant value determined by Eq. (14), and thus the deviation from this value at lower densities is a direct measure of the importance of screening.

In the derivation of the modification (25), the contribution to $\bar{F}$ from plasmon excitations is omitted. The increase in density at the position of a positive particle of infinite mass may, however, be evaluated directly within the dielectric description, and one obtains for the density enhancement

$$\bar{F}=\tfrac{3}{2}\int_0^\infty dx\, x^2[1-\epsilon^{-1}(x,0)], \quad M\to\infty \quad . \tag{27}$$

Here no distinction is made between single-particle and plasmon excitations, i.e., the expression (27) contains the total enhancement within the dielectric description. In Table I it is seen that $\bar{F}$ derived from Eq. (27) agrees closely with the enhancement determined from single-particle scattering alone. This result supports the conclusion of Kahana,[9] who estimated the contribution from plasmon excitations to be small.

For the subsequent application of electron-gas results to the atomic case it is important that single-particle excitations determine the enhancement effects at high densities. The reason is that in the application to an atom the collective features, characterized by the local plasma frequency, have to be modified to take into account the binding force. For example, this effect is important in calculations of the stopping power for high-velocity particles penetrating matter.[6] As we have seen, a similar complication does not arise in the calculation of positron annihilation with core electrons. The enhancement is determined by the velocity distribution of the electrons and not by the restoring forces.

We shall now consider a positive particle of finite mass, in particular a positron, $M=m$. Because of the recoil of the positive particle, a static potential is not strictly applicable. In spite of this, the simple screened potential (24) does lead to accurate enhancement factors for the gas densities of interest. This is seen from Table II, which gives a comparison of average enhancement factors obtained with Kahana's expression (25) and with the Yukawa potential represented by (24). Again, the results are presented in terms of the function $\bar{I}(r_s)$ introduced in Eq. (26). With the static approximation (22), the momentum-dependent enhancement factors are obtained from Eq. (21) with the replacement (24), and the results for a positron are given in Fig. 2 for a number of r_s values. In analogy to Tables I and II, the results are presented in terms of the function

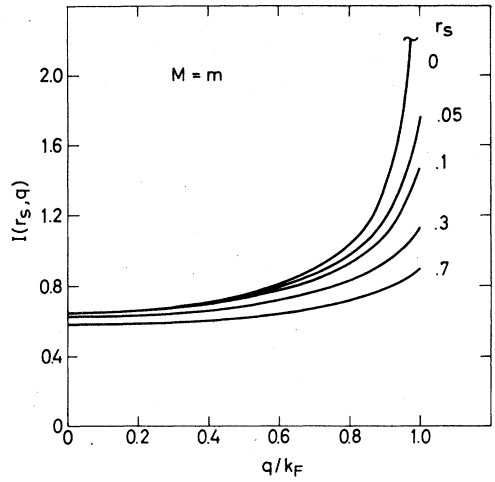

FIG. 2. $I(r_s,q)$ for a positron at the gas densities characterized by the r_s values given in the figure. The momentum $\hbar q$ is given in units of the Fermi momentum $\hbar k_F$. The function $I(r_s,q)$ is introduced in Eq. (28), and the evaluation is based on Eq. (21) with the replacement (24).

$I(r_s,q)$ introduced through the relation

$$F(q)-1=r_sI(r_s,q) \quad . \tag{28}$$

In contrast to the enhancement corresponding to a two-body collision, the enhancement in a gas is an increasing function of q. In the Coulomb limit, $r_s\to 0$, the enhancement factor even diverges logarithmically for $q\to k_F$. The increase in $F(q)$ close to the Fermi momentum is, however, considerably reduced for r_s values corresponding to typical core electron densities, $10^{-1}<r_s<1$. This was to be expected, since screening mainly affects small momentum transfers, and owing to the Pauli principle such momenta can only be imparted to electrons close to the Fermi surface. We conclude this discussion of screening by mentioning that for positron annihilation in an electron gas of a much lower density a static scattering potential has been found to provide reasonably accurate values for the momentum-dependent enhancement factor.[13]

TABLE II. Values of $\bar{I}(r_s)$ from Eq. (26) for $M=m$. The second and third columns correspond to the replacements (24) and (25), respectively, in Eq. (16).

r_s	$\bar{I}(r_s)$	$\bar{I}(r_s)$
10^{-5}	1.22	1.22
10^{-3}	1.19	1.18
10^{-2}	1.12	1.13
10^{-1}	0.97	0.97
1	0.67	0.71

B. Nonlinearity

The simplicity of the theoretical treatment of enhancement in an electron gas of high density derives mainly from the application of the first-order Born approximation. As opposed to the situation for low densities typical, say, for conduction electrons in a metal, a first-order approximation is expected to be quite accurate for the high densities corresponding to atomic cores. Still it is desirable to be able to assess the accuracy from simple estimates of deviations from linearity.

Such an estimate can fairly easily be obtained for the average density enhancement $\bar{F}$ at a positive particle of infinite mass. As discussed in Sec. IV, for $M \to \infty$ the total electron density can be obtained as a sum of independent single-particle contributions. Therefore, if the one-particle Schrödinger equation corresponding to the scattering potential around the positive particle is solved exactly for all electron momenta a value of $\bar{F}$ is obtained, which is exact in the sense that scattering in the average screened potential is included to all orders. Exact analytical solutions are available, not only for the pure Coulomb field but also for the following screened Coulomb potential introduced by Hulthén,[14]

$$V(r) = -\frac{e^2}{a_H}(e^{r/a_H}-1)^{-1} \quad . \tag{29}$$

The index H has been introduced to distinguish the screening length in this expession from the one given in Eq. (23), which belongs to the Yukawa potential (22). The relation between the two lengths is discussed below.

For an electron of momentum $\hbar\vec{k}$ at large distances from the center of the scattering potential (29), the density-enhancement factor $\chi(k)$, defined as the ratio between the densities at $r=0$ and $r=\infty$, is given by the expression[15]

$$\chi(k) = \frac{2\pi}{ka_0}\frac{\sinh(2\pi ka_H)}{\cosh(2\pi ka_H)-\cos(2\pi(2a_H/a_0-(ka_H)^2)^{1/2})} \quad . \tag{30}$$

In the limit $a_H \to \infty$ this expression reduces to the exact formula for the enhancement for Coulomb scattering,

$$\chi(k) = \frac{2\pi}{ka_0}(1-e^{-2\pi/ka_0})^{-1}, \quad a_H \to \infty \quad , \tag{31}$$

which to first order in $(ka_0)^{-1}$ gives the formula (13). The corresponding Born result for the Hulthén potential is obtained from Eq. (30) in the limit $a_0 \to \infty$,

$$\chi(k) = 1 + \frac{\pi}{ka_0}[\coth(2\pi ka_H) - (2\pi ka_H)^{-1}] \quad . \tag{32}$$

In order to use these expressions to estimate the importance of nonlinear effects for the density enhancement at the position of a heavy positive particle in an electron gas, we must first determine the screening length a_H as a function of gas density. It turns out that in the Born approximation the enhancements $\chi(k)$ obtained with the two potentials (22) and (29) are virtually identical for all momenta $k < k_F$ if we choose the value of a_H to be $a_H = 0.6a$, where a is the screening length for the Yukawa potential, given by Eq. (23). With this value of a_H the average enhancement for an electron gas has been calculated from the expression

$$\bar{F} = \frac{3}{k_F^3}\int_0^{k_F} dk\, k^2\chi(k) \quad . \tag{33}$$

According to the discussion in Sec. IV, this procedure is correct for an infinitely heavy positive particle. Results obtained with different approximations for $\chi(k)$ are shown in Fig. 3(a). Since the effects of screening and nonlinearity partly cancel, the total correction to the first-order result for a pure Coulomb interaction is not very large in the density region of interest, $r_s < 1$.

Although these estimates only apply in the limit $M \to \infty$ we might expect the situation to be similar for positrons, i.e., for $M = m$. If we make the plausible assumption that for fixed magnitude of the first-order density correction the additional correction due to nonlinear effects is similar for a positron and for a heavy particle, we may use the curves in Fig. 3(a) to derive an estimate of nonlinear effects for a positron, as shown in Fig. 3(b). In this case the cancellation between screening and nonlinearity effects is even more pronounced than that observed in Fig. 3(a), and we may conclude that for gas densities corresponding to $r_s < 1$ the density enhancement for a positron in a gas is obtained quite accurately from a first-order calculation with pure Coulomb interaction [Eq. (18)]. The high degree of cancellation is perhaps a little surprising since it is known that in the limit of high densities the leading correction to pure Coulomb scattering with small momentum transfer is due to screening.[16] On the other hand, the density enhancement at the position of a positive particle is dominated by scattering with fairly large transfer of momentum, and our conclusion therefore does not contradict this result.

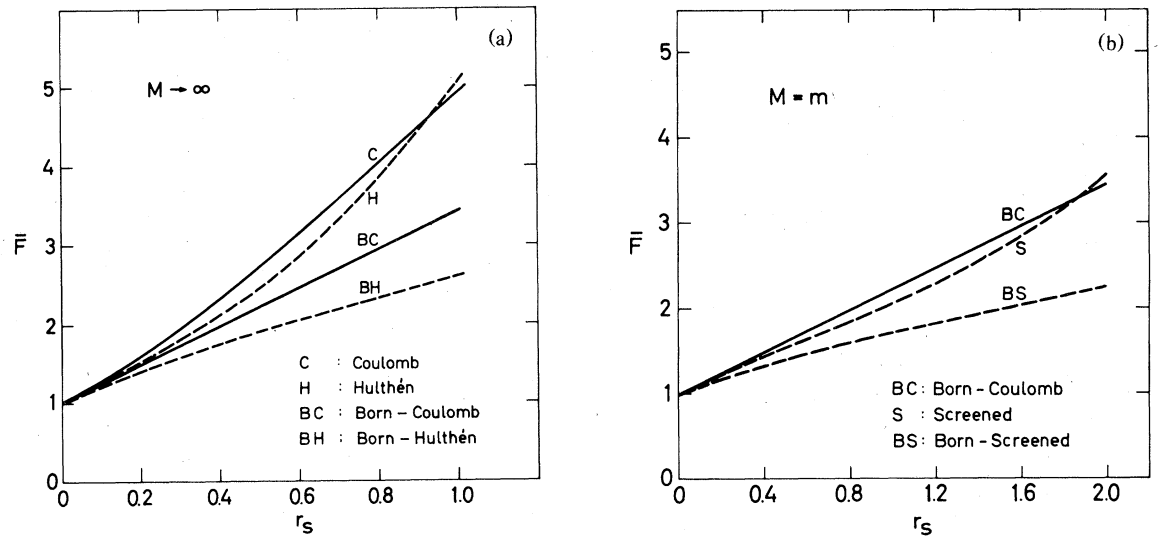

FIG. 3. (a) Average enhancement $\bar{F}$ as a function of the density parameter r_s, in the limit $M \to \infty$. The evaluation of $\bar{F}$ is based on Eq. (33), with functions $\chi(k)$ given in the Eqs. (31), (30), (13), and (32), respectively, for the curves labeled *C*, *H*, *BC*, and *BH*. For $\bar{F} \lesssim 2$ nonlinear effects and the correction for screening nearly cancel, i.e., the curves labeled *H* and *BC* nearly coincide. (b) Average enhancement $\bar{F}$ for positron, as a function of density parameter r_s. The evaluation of the curves labeled *BC* and *BS* is based on Eq. (18) and on Eq. (16) with the replacement (25), respectively. The curve labeled *S* includes an estimated correction for both screening and nonlinear effects and it is constructed from the curve labeled *BS* in the following manner: A Born value $(\bar{F}_{BS}-1)$ in Fig. 3(b) is multiplied by the ratio $(\bar{F}_H-1)/(\bar{F}_{BH}-1)$ taken from Fig. 3(a), the relation between the r_s values in the two figures being such that $\bar{F}_{BH}$ in Fig. 3(a) is equal to $\bar{F}_{BS}$ in Fig. 3(b). For all values of $r_s < 2$, the combined correction for screening and nonlinear effects is small, i.e., the curves labeled *S* and *BC* nearly coincide.

VI. ATOMIC CALCULATION OF CORE ANNIHILATION

In Secs. IV–V we have analyzed positron annihilation in a uniform electron gas of high density with the aim of applying the results to core annihilation in solids through a Thomas-Fermi-type local gas approximation. We now complement this approach with calculations of the enhancement of positron annihilation with a single electron closely bound to an atomic nucleus. This quantity is important for estimating the core contribution to the total annihilation rate in a solid, since in the independent-particle model the contributions from different orbitals are calculated separately. In the local gas picture no distinction is made between shells, and the enhancement of annihilation with individual electrons is not easily obtained.

In addition to complementing the Thomas-Fermi-type treatment in this way, atomic calculations with realistic positron and electron wave functions may serve as a check on the applicability of the simple electron-gas picture, in which the independent-particle wave functions are assumed to be plane waves. Finally, in the calculations to be presented below, we use the same type of procedure as that employed by Carbotte and Salvadori in a series of publications,[3,10,11] and subsequently by other authors using their expressions.[17] As noted earlier, Carbotte and Salvadori arrived at much larger enhancement factors than those obtained in this paper. We shall show that this discrepancy results from errors in their evaluation of certain matrix elements.

According to the previous discussion, a first-order perturbation treatment suffices for the evaluation of core enhancement factors. We consider a positron with unperturbed wave function ϕ_0 and energy ϵ_0 interacting with an atomic electron described by the orbital $\psi_0^{(i)}$ and with energy $-\Delta^{(i)}$. To first order in the electron-positron interaction potential $U(r)$ the wave function $\psi^{(i)}(\vec{x},\vec{y})$ for the interacting pair is given by

$$\psi^{(i)}(\vec{x},\vec{y}) = \psi_0^{(i)}(\vec{x},\vec{y}) + \delta\psi^{(i)}(\vec{x},\vec{y})$$

$$= \psi_0^{(i)}(\vec{x})\phi_0(\vec{y}) - \sum_{\alpha,\beta} \frac{\psi_\alpha(\vec{x})\phi_\beta(\vec{y})\,\langle\psi_\alpha\phi_\beta|\,U\,|\psi_0^{(i)}\phi_0\rangle}{E_\alpha + \epsilon_\beta + \Delta^{(i)} - \epsilon_o} \,. \tag{34}$$

The summation extends over all excited positron states ϕ_β with energy ϵ_β and over all excited electron states ψ_α with positive energy E_α. According to the electron-gas results, the exclusion of excited bound states accounts for the main effect of the correlation with other bound atomic electrons. The contribution of electron orbital i to the momentum-dependent annihilation rate is given by

$$\Gamma^{(i)}(\vec{q}) = \frac{r_0^2 \cdot c}{8\pi^2} \left| \int d^3\vec{r}\, e^{-i\vec{q}\cdot\vec{r}} \psi^{(i)}(\vec{r},\vec{r}) \right|^2$$

$$\simeq \frac{r_0^2 \cdot c}{8\pi^2} \left[\left| \int d^3\vec{r}\, e^{-i\vec{q}\cdot\vec{r}} \psi_0^{(i)}(\vec{r},\vec{r}) \right|^2 + 2\,\mathrm{Re}\left(\int d^3\vec{r}\, e^{-i\vec{q}\cdot\vec{r}} \delta\psi^{(i)}(\vec{r},\vec{r}) \int d^3\vec{r}\, e^{i\vec{q}\cdot\vec{r}} \psi_o^{(i)*}(\vec{r},\vec{r}) \right) \right] . \tag{35}$$

If the electron-positron interaction is represented by a Yukawa potential $U(r) = -e^2 \exp(-r/a)/r$, the expression for $\Gamma^{(i)}(\vec{q})$ can be transformed into a convenient form through a straightforward calculation. With the electron i in a state of angular momentum l_0 in the spherically symmetric atomic potential, and with an s state for the positron ground state, we obtain for the annihilation rate, averaged over the values of the magnetic quantum number m_0 corresponding to l_0,

$$\Gamma^{(i)}(q) = \Gamma_0^{(i)}(q) + \delta\Gamma^{(i)}(q)$$

$$= \frac{r_0^2 \cdot c}{8\pi^2} \left| \int_0^\infty dr\, r^2 j_{l_0}(qr) R_0^-(r) R_0^+(r) \right|^2$$

$$+ \frac{r_0^2 \cdot c}{8\pi^2} \frac{4}{a_0} \sum_l (2l+1) \sum_{l'} |C(l0l_00|l'0)|^2 \int_0^\infty dk \int_0^\infty dk' \left[k'^2 + k^2 + \frac{2m}{\hbar^2}(\Delta - \epsilon_0) \right]^{-1}$$

$$\times \left(\int_0^\infty dr\, r^2 G_a^l(k,r) R_{k'l'}^+(r) R_0^+(r) \right) \left(\int_0^\infty dr\, r^2 j_{l_0}(qr) R_{kl}^-(r) R_{k'l'}^+(r) \right) \left(\int_0^\infty dr\, r^2 j_{l_0}(qr) R_0^-(r) R_0^+(r) \right) , \tag{36}$$

where the function $G_a^l(k,R)$ is given by

$$G_a^l(k,R) = -\frac{1}{a} h_l^{(1)}\left(\frac{iR}{a}\right) \int_0^R dr\, r^2 j_l\left(\frac{ir}{a}\right) R_{kl}^-(r) R_0^-(r) - \frac{1}{a} j_l\left(\frac{iR}{a}\right) \int_R^\infty dr\, r^2 h_l^{(1)}\left(\frac{ir}{a}\right) R_{kl}^-(r) R_0^-(r) . \tag{37}$$

In these expressions R_{kl}^+ and R_{kl}^- are the positron and electron radial wave functions corresponding to wave number k and angular momentum l, and j_l and $h_l^{(1)}$ are spherical Bessel functions and spherical Hankel functions of the first kind. The ground states are described by the radial functions R_0^+ and R_0^-. The quantities $C(lml'm'|LM)$ are Clebsch-Gordan coefficients, and as usual a_0 denotes the Bohr radius $a_0 = \hbar^2/me^2$. The function $G_a^l(k,R)$ only depends on electron wave functions. It also appears in the description of processes like proton-induced inner shell ionization, and in the Coulomb limit, $a \to \infty$, our numerical values agree with published curves.[18]

The numerical evaluation of the momentum-dependent annihilation rate and of the corresponding enhancement factor is hampered by the second last factor in Eq. (36). At large values of r the integrand is proportional to r^{-1} times a product of sine functions and the integral is only slowly converging. The integral is essentially a Fourier component of one of the excited electron-positron states in terms of which the perturbation $\delta\psi^{(i)}(\vec{x},\vec{y})$ is expanded. The perturbation of a localized function $\psi_0(\vec{x},\vec{y})$ must again be fairly localized, but since the perturbation is expanded in extended continuum states, the localization is only obtained after the final summation over the quantum numbers (k,k',l).

A similar difficulty is avoided for the total rate of annihilation with electron i and the corresponding average enhancement factor $\bar{F}_i$. Utilizing the property of the j_l functions,

$$\int_0^\infty dq\, q^2 j_l(qr) j_l(qr') = \tfrac{1}{2}\pi \frac{1}{r^2} \delta(r - r') , \tag{38}$$

we obtain an expression for the quantity $\bar{F}_i$ in which all of the integrals contain the localized product function $R_0^+ R_0^-$,

$$\bar{F}_i - 1 = \int_0^\infty dq\, q^2 \delta\Gamma^{(i)}(q) \Big/ \int_0^\infty dq\, q^2 \Gamma_0^{(i)}(q)$$

$$= \int_0^\infty \int_0^\infty dk\, dk' \frac{4}{a_0} \sum_l (2l+1) \sum_{l'} |C(l0l_00|l'0)|^2 \left[k'^2 + k^2 + \frac{2m}{\hbar^2}(\Delta - \epsilon_0) \right]^{-1} \left(\int_0^\infty dr\, r^2 G_a^l(k,r) R_{k'l'}^+(r) R_0^+(r) \right)$$

$$\times \left(\int_0^\infty dr\, r^2 R_{kl}^-(r) R_0^-(r) R_{k'l'}^+(r) R_0^+(r) \right) \Big/ \left(\int_0^\infty dr\, r^2 (R_0^-(r) R_0^+(r))^2 \right) . \tag{39}$$

A numerical evaluation of this expression has been performed with Coulomb wave functions, which are solutions of the Schrödinger equation with potential $\pm Ze^2/r$. The integrand of the double integral in Eq. (39) is shown in Figs. 4(a) and 4(b) in the form of contour curves in the (k,k') plane. It is seen that the integral receives appreciable contributions from a fairly localized region around the line $k=k'$. To obtain convergence in the l summation in Eq. (39) it was necessary to include 10–20 partial waves. Owing to the scaling properties of the model the figures describe the results for all values of Z.

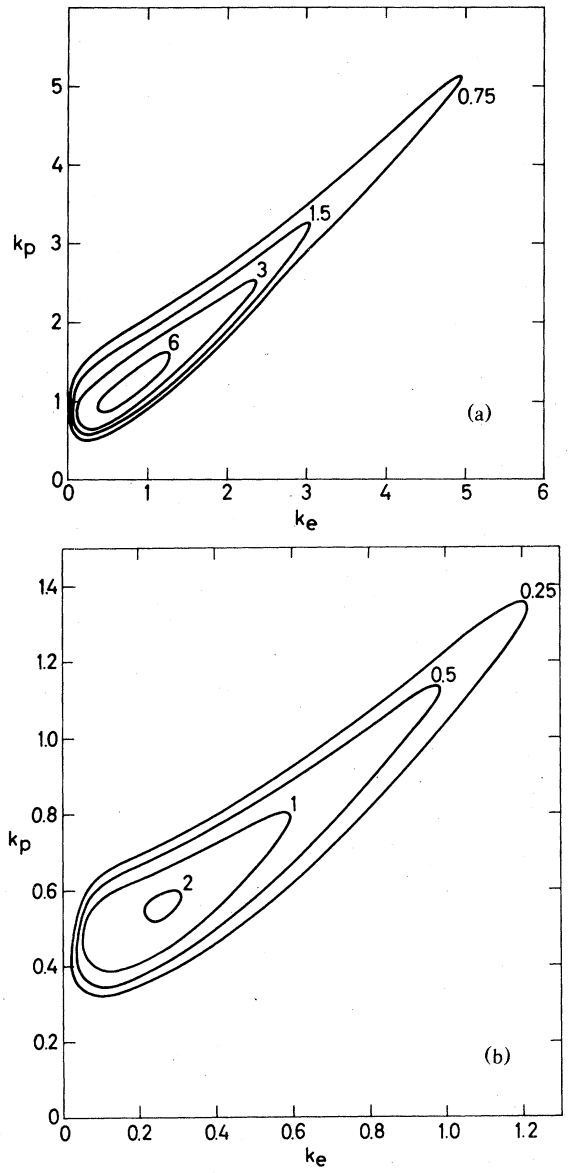

FIG. 4. (a) Contour plot of the integrand in the double integral in Eq. (39), for a $1s$ electron in a hydrogenic system of atomic number Z. Electron and positron wave numbers k_e and k_p are in units of Z/a_0, and the integrand is in units of a_0^2/Z^3. The integrand has been evaluated with pure Coulomb interaction between the electron and the positron. (b) Similar to Fig. 4(a), but for a $3s$ electron.

The quantities $\bar{F}_i-1$ are proportional to Z^{-1}, i.e., as a function of Z they are inversely proportional to electron velocity. Moreover, the values of $\bar{F}_i-1$ for different orbitals are found to be inversely proportional to the characteristic velocity for the i th orbital, $v_i=\langle v^2\rangle_i^{1/2}$. This is seen from Table III, which gives the enhancement factors for the orbitals $1s$, $2s$, $2p$, and $3s$ in the case of an unscreened electron-positron interaction. The result

$$\bar{F}_i-1\simeq\frac{v_0}{v_i},\quad v_0=\frac{e^2}{\hbar} \tag{40}$$

is analogous to the electron gas formula (18). Not only have we retrieved the proportionality to the inverse of a characteristic electron velocity, but also the factor of proportionality $\frac{1}{2}\pi$ in Eq. (18) between $\bar{F}-1$ and the quantity $v_0\langle v^{-1}\rangle=\frac{3}{2}v_0v_F^{-1}$ compares very well with the factor ~ 1 in Eq. (40). It is also instructive to relate the results to the density enhancement at the center of the atom, when an extra proton is added to the nucleus. The relative density increase $(Z+1)^3/Z^3-1\simeq 3/Z$ is of the same order as that obtained from Eq. (40) with a value of v_i corresponding to a $1s$ electron, $v_i=Zv_0$. The agreement becomes even closer when we allow for the usual factor of 2 between electron densities induced by protons and positrons.

As for the electron gas the effect of screening turns out to be small. To estimate the effect we introduced a Yukawa potential with a screening length determined from the total electron density around the maximum of the radial density for the orbital. For Al the decrease in $\bar{F}_i-1$ due to screening was found to be $\lesssim 10\%$ for the $1s$ and $\lesssim 20\%$ for the $3s$

TABLE III. Enhancement factors corresponding to unscreened electron-positron interaction in hydrogenic atom with atomic number Z. The evaluation is based on Eq. (39) with Coulomb wave functions for electron and positron excited states. The velocities v_0 and v_i are the Bohr velocity $v_0=e^2/\hbar$ and the characteristic orbital velocity, $v_i=\langle v^2\rangle_i^{1/2}$. The accuracy of the calculated values of $\bar{F}-1$ is about 10%.

	$1s$	$2s$	$2p$	$3s$
$Z(\bar{F}-1)$	1.1	2.2	2.0	3.0
Zv_0/v_i	1	2	2	3

electrons. For heavier materials screening will be even less significant. Since the electron-positron interaction is not completely local, and the positron wave function decreases strongly towards the atomic center these calculations probably overestimate the effect of screening. Furthermore, according to the results of Sec. V, the small screening effects are expected to be largely compensated for by nonlinear terms.

The results obtained in this section may be applied in the shell-by-shell subtraction of core events needed in studies of annihilation with outer electrons. We shall postpone discussion of this to Sec. VII and turn to a discussion of how the atomic calculations clear up an apparent difficulty in applying the Thomas-Fermi picture to estimate enhancements.

Within the Thomas-Fermi treatment both electrons and positrons are represented by plane waves. Although it was shown in Sec. III that such a procedure gives a satisfactory distribution of electron momenta, serious problems might seem to arise in the description of the positron. Low-lying positron states must penetrate high potential barriers and are strongly reduced in intensity when they reach the core region. Consequently, matrix elements involving such states are vastly overestimated if the positron is represented by a plane wave as in the Thomas-Fermi calculation. In spite of the fact that free positron states are inapplicable in the calculation of core annihilation rates, they can still be used to evaluate the corresponding enhancement factors. This may be understood from the expression in Eq. (39). The positron ground state appears twice in the numerator and twice in the denominator, and thus an overall depletion of intensity in the core region does not affect the ratio. On the other hand, low-lying excited states with a similar barrier penetration are only present in the numerator. We obtained a quantitative check on these effects by repeating the evaluation of enhancement for the $1s$ electron in the absence of a positron barrier. The resulting enhancement factor changed by less than 10%. The main reason for this is that the contribution to the integral (39) from small k' values is insignificant even when the density of excited positron states is not reduced by barrier penetration.

In the papers by Carbotte and Salvadori positron states were also effectively replaced by plane waves, but only in the expression $\delta\Gamma^{(i)}(q)$ for the increase in annihilation rate due to correlation and *not* in the corresponding independent-particle value $\Gamma_0^{(i)}(q)$. This amounts to applying plane waves in the numerator but not in the denominator of the expression (39) for the enhancement factor. Since the IPM overlap is reduced by orders of magnitude due to barrier penetration, this clearly leads to gross overestimates of the enhancement. The manner in which this error was introduced is discussed in detail in the Appendix.

VII. CORE ANNIHILATION IN SOLIDS

In this final section we discuss positron annihilation with core electrons in a solid, on the basis of the results obtained in Secs. IV–VI. The quantity of interest is the enhancement of the annihilation rate relative to that calculated in the independent-particle model, and we shall consider partly the total enhancement of annihilation with individual tightly bound atomic electrons, and partly the momentum-dependent annihilation rate in the high momentum region, where the core contribution dominates. First we try to draw some general conclusions concerning the order of magnitude of the enhancement, and then we shall derive more precise estimates, which may be directly applied in the analysis of experiments.

The starting point of the discussion has been the simple result obtained for the scattering of a particle in a Coulomb field or equivalently, for the mutual scattering of two charged particles. The probability for finding two free particles with charges $\pm e$ at the same point in space is enhanced by the factor $\sim(1+\pi v_0/v)$, where v is the relative velocity of the particles, assumed large compared to the Bohr velocity $v_0=e^2/\hbar$. For core electrons the velocity is generally much higher than v_0, and on the basis of this simple estimate the enhancement of core annihilation is expected to be small. Our analysis of enhancement of positron annihilation in an electron gas and annihilation with inner electrons in an isolated atom may be seen as an investigation of the applicability of the simple free-particle result to more complicated systems of many interacting electrons moving in the attractive Coulomb field of an atomic nucleus. The result of the investigation is that the simple free-particle enhancement provides a good qualitative estimate, and that in fact the enhancement of core annihilation is small. This is in contrast to the finding in earlier treatments, in particular that of Carbotte and Salvadori,[3] of large enhancement factors for positron annihilation with strongly bound electrons. In Sec. VI we have identified the inadmissible approximation which is the main source of error in their treatment (see also the Appendix).

Although the perturbation result for free particles provides an excellent guide for order-of-magnitude estimates, the modifications for many-particle systems of bound electrons are important for more accurate calculations. It was found both for the electron gas and for an electron in an inner atomic orbital that the enhancement is reduced relative to the free-particle result by a factor of the order of 2 to 3. For both cases the reduction may qualitatively be explained as an effect of the Pauli principle, which only allows virtual excitations to states above the Fermi level and to continuum states of positive energy, respectively. For the purpose of obtaining realistic

estimates of core annihilation in solids, the two models complement each other. The atomic calculation provides the total enhancement for annihilation with specific atomic shells, which is needed for subtraction of the core contribution to the total annihilation rate. On the other hand, the Thomas-Fermi picture, which does not group electrons into shells, is particularly valuable for estimating the momentum-dependent enhancement in the high momentum tail of the annihilation rate.

A. Average enhancement for core annihilation

The results from the atomic calculation are remarkably simple. Apart from a reduction to ~ 1 of the factor π in the single-particle formula (13), this result applies with a value of v corresponding to the average kinetic energy of the bound electron. The model is of course greatly simplified compared to the case of an atom embedded in a solid, and it is appropriate to discuss the possible modifications we might expect for this case.

First, wave functions and binding energies for a hydrogenic atom have been applied. It would be straightforward to introduce more realistic values but only minor modifications of the results would be expected. Thus, the rather drastic changes in binding energies turn out to be fairly unimportant, since these energies are added to larger energies of excited states. The main effect of screening is a replacement of Z by an effective atomic number $Z-\sigma$, where $\sigma \simeq 4$ for L electrons.

For the feasibility of the calculation the most important simplification is the representation of excited electron and positron states by Coulomb wave functions. It is difficult to estimate quantitatively the influence of this approximation on the results, but it could hardly be expected to be very large. As seen from Figs. 4(a) and 4(b), the enhancement receives contributions from a broad range of excited electron and positron momenta, and a restructuring of the continuum into the bands characteristic of the solid should to a large extent be averaged out.

Finally, since the enhancement $\bar{F}-1$ is so small, only limited accuracy is needed to improve on the methods for subtraction of the core contribution from total annihilation rates.

B. Momentum-dependent enhancement

In measurements of the momentum dependence of positron annihilation rates in a solid, the velocity of the annihilating electron (or at least one component) is apparently specified and it would be tempting to apply the corresponding free-particle enhancement. However, in our analysis of the momentum-dependent annihilation rate in an electron gas we found an important qualitative modification of this picture. The momentum dependence of the enhancement is strongly reduced by the Pauli principle, in particular when screening effects are included, and the enhancement may be approximated by a constant value determined by the gas density. This result suggests a Thomas-Fermi-type estimate of the momentum-dependent annihilation rate

$$\Gamma(q)=\frac{r_0^2\cdot c}{4\pi^2}\int_0^{R(q)} dr\, r^2 R_+^2(r)\bar{F}(r) \quad , \tag{41}$$

with

$$k_F(R(q))=q \quad .$$

This formula is an extension of the IPM result (10) based on the local gas approximation, which in Sec. III was shown to give results in good agreement with those obtained from an IPM calculation with atomic orbitals. The contribution from distance r is increased by the average enhancement factor for an electron gas with the local density. An even better result should be obtained by calculating the IPM annihilation rate with realistic atomic orbitals, according to Eq. (3), and applying the local gas approximation only to calculate the (small) enhancement,

$$F(q)=\frac{\int_0^{R(q)} dr\, r^2 R_+^2(r)\bar{F}(r)}{\int_0^{R(q)} dr\, r^2 R_+^2(r)} \quad , \tag{42}$$

with

$$k_F(R(q))=q \quad .$$

In this formula we have neglected the momentum dependence of F for fixed density, illustrated in Fig. 2. As it turns out, the inclusion of this relatively weak dependence in the expression (42) has a negligible effect on the resulting function $F(q)$. It might also be questionable to introduce such details of the gas results in the description of an atomic system, for which the local density in the core region is dominated by a few energy levels well below the Fermi level. As was illustrated in Fig. 3(b), the reduction in enhancement from screening is nearly cancelled by nonlinear terms, and the simple formula (18) has therefore been applied in the evaluation of the expression (42). The major contributions come from distances close to $R(q)$, and therefore the value of $[F(q)-1]$ is expected to be of the order of $1.228 r_s(q)$, where $r_s(q)$ is the density parameter for a gas with Fermi momentum $\hbar q$. With $r_s(q)=1.92/(qa_0)$, this estimate may be written as $[F(q)-1]\simeq 2.36/(qa_0)$. For both Al and Cu we obtain by numerical evaluation the result

$$F(q)-1=\frac{2.0}{(qa_0)}, \quad qa_0>2 \quad , \tag{43}$$

which agrees closely with the simple estimate.

C. Comparison with experiment

For an annihilating electron-positron pair with finite momentum the angle between the two emitted γ rays differs slightly from π, and the energies of the photons are Doppler shifted in opposite directions. Either of these two effects may be used to measure one component of the momentum of the annihilating pair, and a one-dimensional probability distribution in a single component of the momentum $\hbar\vec{q}$ is obtained. Let $P_i(q_1)dq_1$ denote the probability that a given positron will annihilate with an electron in state i and that the annihilating pair will have a momentum component in the direction of interest with absolute value lying between $\hbar q_1$ and $\hbar(q_1+dq_1)$. Theoretically it is given by the expression

$$P_i(q_1)=\tau\int_{q_1}^{\infty}dq\,q\int d\Omega_{\vec{q}}\Gamma_i(\vec{q}) \quad , \tag{44}$$

where

$$\tau=\left[\sum_i\int d^3\,\vec{q}\,\Gamma_i(\vec{q})\right]^{-1} \tag{45}$$

is the total lifetime of the positron in the material. This quantity is determined mainly by annihilation with outer electrons. Any inaccuracy in the calculation of this constant of proportionality would lead to additional and unnecessary uncertainties in the comparison between experimental values of $P_i(q_1)$ for core electrons and the corresponding theoretical distribution. Therefore, as noted in Ref. 4, the experimentally obtained total lifetime should be applied in the formula (44) to obtain a probability distribution from the calculated (absolute) core-annihilation rate.

As we have seen, the independent-particle model may, to a good approximation, be applied to calculate the annihilation yield from inner-shell electrons. This is the quantity needed for core subtraction. As an example we consider the case of Al. With a measured lifetime $\tau=175$ psec[4] we obtain by integrating $P_i(q_1)$ in Eq. (44) or, alternatively, by a three-dimensional integration of the curves in Fig. 1(a), an independent particle value of $3.7\pm0.7\%$ for the total probability for annihilation with the ten core electrons. The shell-by-shell calculations in Fig. 1(a) are identical to the ones presented in Ref. 4.[19] As explained there, the quoted uncertainty of the IPM value is associated with the difficulty of normalizing the positron wave function. Inclusion of the average enhancement factors found in Sec. VI leads to a value of $4.3\pm0.8\%$ for the total probability for annihilation with core electrons. Clearly the uncertainty of the enhancements is insignificant for this estimate. The result is much lower than the value $\sim15\%$ obtained from an empirical fitting procedure.[2,20]

For convenience in comparing the results from the electron-gas picture with high momentum spectra we finally present a plot of the function

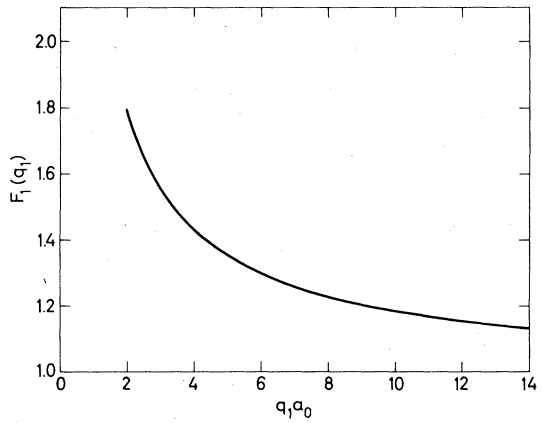

FIG. 5. $F_1(q_1)$ from Eq. (46). The IPM-annihilation rate, $\Gamma^{\rm IPM}$, is given in Eq. (10), while $\Gamma(q)$ is obtained from the formula (41). The enhancement $\bar{F}(r)$ in this formula is obtained from Eq. (18) with a value of r_s determined by the local electron density at distance r. Virtually identical results were obtained for Al and Cu, and hence the curve applies for both materials.

$$F_1(q_1)=\frac{\int_{q_1}^{\infty}dq\,q\int d\Omega_{\vec{q}}\Gamma(\vec{q})}{\int_{q_1}^{\infty}dq\,q\int d\Omega_{\vec{q}}\Gamma^{\rm IPM}(\vec{q})} \quad , \tag{46}$$

where the annihilation rates $\Gamma(q)$ and $\Gamma^{\rm IPM}(q)$ are obtained from Eqs. (41) and (10), respectively. Again the results for Al and Cu are indistinguishable, and a common curve may be drawn as shown in Fig. 5. The numerical results are still represented fairly well (with $\sim10\%$) by a formula similar to Eq. (43),

$$F_1(q_1)-1\simeq\frac{1.8}{(q_1a_0)} \quad . \tag{47}$$

Due to the averaging over two momentum components the constant in Eq. (47) is slightly lower than that in Eq. (43), and the proportionality to the inverse momentum is not quite as accurate.

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APPENDIX

In this Appendix we shall show explicitly at which point Carbotte and Salvadori introduced the error leading to their large overestimates of core-enhancement factors. We refer to Ref. 11, where the correlated wave function for a positron and a core electron, interacting through a Coulomb potential, is presented in the following form

$$\psi_{ep}(\vec{x}_e,\vec{x}_p)=\psi_c(\vec{x}_e)\chi_0(\vec{x}_p)+\phi_{ep}(\vec{x}_e,\vec{x}_p)\ . \quad \text{(A1)}$$

The correction term ϕ_{ep} is calculated to first order

$$\phi_{ep}(\vec{x}_e,\vec{x}_p)=\sum_{\vec{k},\vec{k}'}\frac{\psi_{\vec{k}}(\vec{x}_e)\chi_{\vec{k}'}(\vec{x}_p)}{E_c^e+E_0^p-E_{\vec{k}}^e-E_{\vec{k}'}^p}\times\int\psi_{\vec{k}}^*(\vec{x}_e')\chi_{\vec{k}'}^*(\vec{x}_p')\frac{-2}{|\vec{x}_e'-\vec{x}_p'|}\times\psi_c(\vec{x}_e')\chi_0(\vec{x}_p')\,d\vec{x}_e'\,d\vec{x}_p'\ . \quad \text{(A2)}$$

The Eqs. (A2)–(A6) are numbered as in Ref. 11, and the notation and units (atomic) of this reference are used. Orbitals ψ and χ refer to electrons and positrons respectively, the ground states of which are denoted by indices c and 0. The excited states, compatible with the Pauli principle, are all in the continuum, and they are identified through an index $\vec{k}$. The above expression is analogous to Eq. (34) of the present paper.

The matrix element of the Coulomb potential is expressed in Fourier components and the correction term $\phi_{ep}(\vec{x}_e,\vec{x}_p)$ takes the form

$$\phi_{ep}(\vec{x}_e,\vec{x}_p)=\sum_{\vec{k},\vec{k}'}\frac{\psi_{\vec{k}}(\vec{x}_e)\chi_{\vec{k}'}(\vec{x}_p)}{k^2+k'^2+\Delta_c}\frac{1}{\Omega}\times\sum_{\vec{q}}\frac{8\pi}{q^2}\langle\vec{k}\,|\,\vec{q}\,|c\rangle^e\langle\vec{k}'|-\vec{q}\,|0\rangle^p\ , \quad \text{(A3)}$$

where Ω is the quantization volume. The integration over electron and positron coordinates is now performed in separate matrix elements,

$$\langle\vec{k}\,|\,\vec{q}\,|c\rangle^e\equiv\int d\vec{x}_e'\,\psi_{\vec{k}}^*(\vec{x}_e')e^{i\vec{q}\cdot\vec{x}_e'}\psi_c(\vec{x}_e') \quad \text{(A4a)}$$

and

$$\langle\vec{k}'|-\vec{q}\,|0\rangle^p\equiv\int d\vec{x}_p'\,\chi_{\vec{k}'}^*(\vec{x}_p')e^{-i\vec{q}\cdot\vec{x}_p'}\chi_0(\vec{x}_p')\ . \quad \text{(A4b)}$$

The binding energy Δ_c of the core electron has been introduced together with the values $E_0^p\simeq 0$, $E_{\vec{k}}^e\simeq k^2$, and $E_{\vec{k}'}^p\simeq k'^2$.

The positron matrix element in Eq. (A4b) is now replaced by a δ function

$$\langle\vec{k}'|-\vec{q}\,|0\rangle^p\simeq\delta_{\vec{k}',\vec{q},\vec{0}} \quad \text{(A5)}$$

and this leads to

$$\phi_{ep}(\vec{x}_e,\vec{x}_p)=\frac{1}{\Omega}\sum_{\vec{k},\vec{k}'}\frac{\psi_{\vec{k}}(\vec{x}_e)\chi_{\vec{k}'}(\vec{x}_p)}{k^2+k'^2+\Delta_c}\times\frac{8\pi}{|\vec{k}'|^2}\langle\vec{k}\,|-\vec{k}'|c\rangle^e\ . \quad \text{(A6)}$$

The approximation (A5) is based on the observation that positron wave functions are farly well approximated by plane waves outside the small core regions. The approximation is, however, completely inadequate in the summation over $\vec{q}$ in Eq. (A3), since the many small contributions from $\vec{q}$ values in the vicinity of $\vec{q}=-\vec{k}'$ add up to a term which almost cancels the contribution from the δ function. To see this, we note that the core wave function ψ_c is strongly localized, and hence the matrix element $\langle\vec{k}\,|\,\vec{q}\,|c\rangle^e$ depends only weakly on $\vec{q}$ within the range of $\vec{q}$ values for which the matrix element (A4b) is appreciably different from zero. Therefore, instead of Eq. (A6) we obtain as an order of magnitude estimate

$$\phi_{ep}(\vec{x}_e,\vec{x}_p)\simeq\sum_{\vec{k},\vec{k}'}\frac{\psi_{\vec{k}}(\vec{x}_e)\chi_{\vec{k}'}(\vec{x}_p)}{k^2+k'^2+\Delta_c}\frac{1}{\Omega}\frac{8\pi}{|k'|^2}\langle\vec{k}\,|-\vec{k}'|c\rangle^e\int d\vec{x}_p'\,\chi_{\vec{k}'}^*(\vec{x}_p')\sum_{\vec{q}}e^{-i\vec{q}\cdot\vec{x}_p'}\chi_0(\vec{x}_p')\ . \quad \text{(A7)}$$

The last factor in this expression gives

$$\int d\vec{x}_p'\,\chi_{\vec{k}'}^*(\vec{x}_p')\sum_{\vec{q}}e^{-i\vec{q}\cdot\vec{x}_p'}\chi_0(\vec{x}_p')=\int d\vec{x}_p'\chi_{\vec{k}'}^*(\vec{x}_p')\,\Omega\,\delta(\vec{x}_p')\chi_0(\vec{x}_p')=\Omega\chi_{\vec{k}'}^*(\vec{0})\chi_0(\vec{0})\ . \quad \text{(A8)}$$

Because of the high potential barriers for positrons close to nuclei the factor $\Omega\chi_{\vec{k}'}^*(\vec{0})\chi_0(\vec{0})$ is much smaller than the corresponding factor of $\Omega(\Omega)^{-1/2}(\Omega)^{-1/2}=1$ in Eq. (A6).

By way of a simple analytical example in one dimension we may illustrate in a little more detail, how the integral over the delta function is almost cancelled by the integral over the correction terms. The one-dimensional analogue of the $\vec{q}$ summation in Eq. (A3) is of the type

$$\int_{-\infty}^{\infty}dq\,f(q)g(q)\ . \quad \text{(A9)}$$

The function $g(q)$ is the Fourier transform of a function $g(x)$, which increases from small values in the vicinity of $x=0$ to a much larger constant absolute value in the limits $x\to\pm\infty$. As an example of

such a function we may take

$$g(x) = e^{ik_0 x}\left(\frac{1}{L} - \frac{A}{x^2 + A^2}\right), \quad A \simeq L \ , \qquad \text{(A10)}$$

where the lengths k_0^{-1}, L, and A are constants.

The integrand in the expression (A9) is the product of the Fourier transform

$$g(q) = \frac{1}{2\pi}\int_{-\infty}^{\infty} dx\, e^{-iqx} g(x)$$
$$= \frac{1}{L}\delta(q - k_0) - \tfrac{1}{2}\, e^{-A|q-k_0|} \qquad \text{(A11)}$$

and the Fourier transform $f(q)$ of a function which is localized within a distance short compared to A.

We therefore obtain

$$\int_{-\infty}^{\infty} dq\, f(q) g(q) \simeq f(k_0)\left(\frac{1}{L} - \frac{1}{A}\right)$$
$$= f(k_0) g(x = 0) \ . \qquad \text{(A12)}$$

With the approximation introduced by Carbotte and Salvadori, only the δ-function part of $g(q)$ is retained. This leads to an overestimate of the integral (A9) by a factor of the order of $|g(x \to \infty)/g(x = 0)|$, in analogy to the difference between the Carbotte-Salvadori expression (A6) and the estimate (A7) and (A8).

Finally we may mention that in Ref. 10 the same error is introduced, when the expression in Ref. 10, Eq. (3.5) is replaced by the quantities in Eqs. (4.4a) and (4.4b) of that reference.

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