Self-consistent solution of the Kahana equation for a positron in an electron gas

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A self-consistent development of the Kahana formalism is presented. The merits of this approach in comparison with the traditional one consist of including the effect of electron-electron correlations and achieving full self-consistency between the potential used in the Bethe-Goldstone equation and the screening charge distribution around the positron, obtained from its solutions. In this way the well-known low-density divergence of the annihilation rate λ is removed. At low electron densities the latter approaches the averaged free-positronium value. The annihilation parameters obtained in this work are in reasonable agreement with experimental results.

I. INTRODUCTION

The application of positron annihilation to investigations of the one-electron structure of metallic systems is based on the belief that the positron gives information about one-electron states of the material. Experiments confirm, rather than contradict, this way of understanding of the behavior of the positron in metals.[1]

On the other hand, the density of particular electronic states "as seen" by the positron is strongly enhanced from its initial value. Therefore, the momentum-dependent enhancement factor $\varepsilon(p)$, usually defined as a ratio of perturbed to unperturbed densities of electrons with momentum p on the positron is one of the most important parameters necessary in the interpretation of positron annihilation data. However, the theoretical determination of $\varepsilon(p)$ is only a partially solved many-body problem, even for such a simple model as the electron gas.[2-5]

The theory of Arponen and Pajanne[3] is a many-body one based on the bosonization scheme. The positron interaction with an electron gas is described as a set of collective excitations of Sawada bosons[6] from the random-phase-approximation (RPA) ground state. An outline of the approach of Refs. 3 has been presented by one of the authors of this paper in Ref. 7. Note that the approach of Refs. 3 to electron-positron interaction does not conform to the belief that the positron gives information about one-electron states. According to Arponen and Pajanne "... the problem of a light impurity in an electron gas cannot ultimately be reduced to a two-body problem, whatever effective interaction is used." For low electron densities this formalism leads to momentum-dependent enhancement factors which are difficult to adjust with experiment.[8]

Alternative two-body approaches enabling us to calculate $\varepsilon(p)$ were proposed by Lowy[5] (based on the theory of Lowy and Jackson[9]) and Kahana.[2] The differences between them are investigated in details in Sec. II.

Of the approaches enabling us to calculate $\varepsilon(p)$ the Kahana theory[2] (developed in many papers[10-14]) seems to be the most popular. Its results are quoted most often in experimental as well as in theoretical papers. However, for a long time the unphysical divergence of the total annihilation rate λ occuring for low ($r_s > 4$) electron densities was a major deficiency of the Kahana formalism. This feature was attributed to several reasons,[3,9] e.g., lack of normalization of the electron-positron pair wave function or incorrect application of the Pauli exclusion principle.

Recently[12] it has been shown (by using in the Kahana equation an improved effective electron-positron interaction potential) that the lack of self-consistency was the main reason of this divergence (such a suggestion was made earlier by Boroński *et al.*[11] after determining the total screening charge around a positron).

Although the self-consistency of the Kahana approach has been improved in Refs. 12 appreciably, nevertheless full self-consistency was not achieved and, as a consequence, for $r_s \geq 6$ the value of the total annihilation rate λ fell below the free-positronium value $\lambda_{pos} \simeq 2 \times 10^9\ s^{-1}$. It should be pointed out that because of the strong dependence of the resulting annihilation parameters on the potential used in the Bethe-Goldstone equation, definitive and reliable conclusions about the partial (and therefore total) annihilation rates can be drawn only after reaching full self-consistency in the Kahana theory (electron-electron correlations should also be included). Therefore, there is a real need for performing self-consistent calculations within the Kahana theory.

In this work an iterative method of self-consistent determination of the effective electron-positron interaction potential as well as of the density of the screening electronic charge around a positron is presented. The effect of taking into account electron-electron correlations is computed. Including electron-electron correlations and reaching self-consistency in the calculations we got the proper behavior of the annihilation rate at low electron densities ($\lambda \geq \lambda_{pos}$).

II. THEORY

The Kahana[2] approach is based on the Bethe-Goldstone-type equation:

$$\chi(\mathbf{p},\mathbf{k})=\frac{Av(|\mathbf{k}-\mathbf{p}|)}{k^2+(\mathbf{k}-\mathbf{p})^2-p^2}+\frac{A}{k^2+(\mathbf{k}-\mathbf{p})^2-p^2}\int_{q>1} v(|\mathbf{k}-\mathbf{q}|)\chi(\mathbf{p},\mathbf{q})d^3q \tag{2.1}$$

for the Fourier coefficients of the electron-positron pair wave function assumed in the form

$$\psi_{\mathbf{p}}(\mathbf{x}_e,\mathbf{x}_p)=\frac{1}{\Omega}e^{i\mathbf{p}\cdot\mathbf{x}_e}+\frac{1}{\Omega}\sum_{k>1}\chi(\mathbf{p},\mathbf{k})e^{i\mathbf{k}\cdot\mathbf{x}_e}e^{i(\mathbf{p}-\mathbf{k})\cdot\mathbf{x}_p}, \tag{2.2}$$

where $\mathbf{x}_e$ and $\mathbf{x}_p$ indicate electron and positron coordinates, respectively, $v(q)$ is the Fourier transform of the effective electron-positron interaction potential and $v(|\mathbf{x}_e-\mathbf{x}_p|)$, $\mathbf{p}$ is the initial momentum of the electron, and Ω is the volume of the sample $A=(4\pi^3k_Fa_0)^{-1}\simeq 0.33r_s/(8\pi^2)$, where k_F is the Fermi momentum and all momenta are expressed in units of k_F.

The form (2.2) of the pair wave function, namely, the Pauli projection operator applied in it, was the reason of the objection of Lowy and Jackson[9] to the Kahana formalism.

In order to explain these doubts as well as to compare the Kahana formalism with other ones, a new approach to the Kahana theory is presented in this section.

Generally, the wave function describing the behavior of a particular electronic state $\mathbf{p}$ scattered on the positron in its lowest momentum state has the form

$$\begin{aligned}\psi_{\mathbf{p}}(\mathbf{x}_e,\mathbf{x}_p)&=\frac{1}{\Omega}e^{i\mathbf{p}\cdot\mathbf{x}_e}+\frac{1}{\Omega}\sum_{\mathbf{k}}\chi(\mathbf{p},\mathbf{k})e^{i\mathbf{k}\cdot\mathbf{x}_e}e^{i(\mathbf{p}-\mathbf{k})\cdot\mathbf{x}_p}\\&=\frac{1}{\sqrt{\Omega}}e^{i\mathbf{p}\cdot\mathbf{x}_p}\left[\frac{1}{\sqrt{\Omega}}e^{i\mathbf{p}\cdot\mathbf{r}}+\sum_{\mathbf{k}}\chi(\mathbf{p},\mathbf{k})e^{i\mathbf{k}\cdot\mathbf{r}}\right]\\&=\frac{1}{\sqrt{\Omega}}e^{i\mathbf{p}\cdot\mathbf{x}_p}\phi_{\mathbf{p}}(\mathbf{r}),\end{aligned} \tag{2.3}$$

where $\mathbf{r}=\mathbf{x}_e-\mathbf{x}_p$ and the function $\psi_{\mathbf{p}}(\mathbf{x}_e,\mathbf{x}_p)$ obeys the Schrödinger equation:

$$[-\tfrac{1}{2}\nabla_e^2-\tfrac{1}{2}\nabla_p^2+v(\mathbf{x}_e-\mathbf{x}_p)]\psi_{\mathbf{p}}(\mathbf{x}_e,\mathbf{x}_p)=\frac{p^2}{2}\psi_{\mathbf{p}}(\mathbf{x}_e,\mathbf{x}_p). \tag{2.4}$$

If the wave function of the system is a Slater determinant built out of $\psi_{\mathbf{p}}$ functions, then taking into account the fact that $\exp[i(\sum_p \mathbf{p})\cdot\mathbf{x}_p]=1$ leads to the conclusion that the wave function $\Psi(\mathbf{x}_1,\mathbf{x}_2,\ldots,\mathbf{x}_N,\mathbf{x}_p)$ of the system consisting of N electrons plus one positron being independent of the positron coordinates $\mathbf{x}_p$ because of thermalization can be expressed in the form

$$\Psi(\mathbf{x}_1,\mathbf{x}_2,\ldots,\mathbf{x}_N,\mathbf{x}_p)=\frac{1}{\sqrt{\Omega}}\Phi(\mathbf{r}_1,\mathbf{r}_2,\ldots,\mathbf{r}_N),$$

where $\mathbf{r}_i=\mathbf{x}_i-\mathbf{x}_p$ and $\mathbf{x}_i$ are coordinates of the ith electron.

The N-particle wave function $\Phi(\mathbf{r}_i,\mathbf{r},\ldots,\mathbf{r}_N)$ has the form of a Slater determinant built out of the functions $\phi_{\mathbf{p}}(\mathbf{r})$ describing the unbounded electronic state $\mathbf{p}$ scattered on the positron at rest, defined by the formulas (2.3) and (2.4).

If the electron-positron interaction is small the scattering term $\chi(\mathbf{p},\mathbf{k})$ in (2.3) can be represented as a series according to powers of the small parameter α, characterizing the potential of interaction. For weak interaction we can retain only terms linear in α (RPA or Born approximation).

As shown in Appendix A for momenta $k<k_F$, $\chi(\mathbf{p},\mathbf{k})$ in (2.3) gives in $\Psi(\mathbf{x}_1,\mathbf{x}_2,\ldots,\mathbf{x}_N,\mathbf{x}_p)$ a contribution of second order only and can be neglected if we use a linear-response-type approximation; otherwise it should be taken into account. The Kahana approach neglects these terms altogether and therefore the pair wave function in Ref. 2 has the form (2.2) instead of (2.3).

An essential step of the theory consists of the computation of the electronic distribution around the positron. This last step is obtained from the general formula

$$\begin{aligned}\rho(r_i)&=N\frac{\int|\Psi(\mathbf{x}_1,\mathbf{x}_2,\ldots,\mathbf{x}_N,\mathbf{x}_p)|^2d\mathbf{x}_2\cdots d\mathbf{x}_N\,d\mathbf{x}_p}{\int|\Psi(\mathbf{x}_1,\mathbf{x}_2\ldots,\mathbf{x}_N,\mathbf{x}_p)|^2d\mathbf{x}_1\cdots d\mathbf{x}_N\,d\mathbf{x}_p}\\&=N\frac{\int|\Phi(\mathbf{r}_1,\mathbf{r}_2,\ldots,\mathbf{r}_N)|^2d\mathbf{r}_2\cdots d\mathbf{r}_N}{\int|\Phi(\mathbf{r}_1,\mathbf{r}_2,\ldots,\mathbf{r}_N)|^2d\mathbf{r}_2\cdots d\mathbf{r}_N},\end{aligned} \tag{2.5}$$

where N is the number of electrons in the system. Formally we can write

$$|\Phi(\mathbf{r}_1,\ldots,\mathbf{r}_N)|^2=\frac{1}{N!}\sum\sum(-1)^{p_1+p_2}\prod_{j=1}^{n}\phi^*_{k_j}(\mathbf{r}_j)\phi_{m_j}(\mathbf{r}_j), \tag{2.6}$$

where summation is over all the permutations of indices k_j and m_j, p_1 and p_2 are the parities of these permutations, and $k_j(m_j)$ correspond to the states $\phi_{\mathbf{k}_j}(\phi_{\mathbf{m}_j})$.

When the functions $\phi_{\mathbf{k}}$ are orthonormal the only terms in (2.6) giving a contribution to ρ are these with $\mathbf{k}_j=\mathbf{m}_j$. This leads to the well-known formula for the electron density around the positron:

$$\rho(r_1)=2\sum_{\mathbf{p}\ \text{occupied}}|\phi_{\mathbf{p}}(\mathbf{r}_1)|^2. \tag{2.7}$$

This formula is exactly true for $\phi_{\mathbf{p}}(\mathbf{r})$ being solutions of the Schrödinger equation for one electron in the screened Coulomb field of the proton. However, the functions $\phi_{\mathbf{p}}(\mathbf{r})$ in (2.3) are not solutions of any one particle Schrödinger-like equation, so they are not orthogonal, and the electron distribution cannot be expressed in the form of the formula (2.7).

Introducing (after Lowy and Jackson[9] or Stachowiak[15]) the reduced coordinates $\mathbf{R}=\frac{1}{2}(\mathbf{x}_e+\mathbf{x}_p)$ and $\mathbf{r}=\mathbf{x}_e-\mathbf{x}_p$ we can rewrite the functions ψ_p of form (2.3) in the following way:

$$\begin{aligned}\psi_{\mathbf{p}}(\mathbf{x}_e,\mathbf{x}_p)&=\frac{1}{\Omega}e^{i\mathbf{p}\cdot\mathbf{R}}\left[e^{i\mathbf{p}\cdot\mathbf{r}/2}+\sum_{\mathbf{k}}\chi(\mathbf{p},\mathbf{k})e^{i(\mathbf{k}-\mathbf{p}/2)\cdot\mathbf{r}}\right]\\&=\frac{1}{\sqrt{\Omega}}e^{i\mathbf{p}\cdot\mathbf{R}}\psi_{\mathbf{p}}^{LJ}(\mathbf{r}).\end{aligned}$$

The one-particle functions $\psi_{\mathbf{p}}^{\mathrm{LJ}}$ are not orthogonal either, because they violate the periodicity condition in $\mathbf{r}$ space. This shows that the approach of Lowy and Jackson [Eq. (33) of Ref. 9] suffers from nonorthogonality as well as the Kahana formalism, though this problem needs further studies.

If the Pauli exclusion operator is applied to $\phi_{\mathbf{p}}(\mathbf{r})$ and the Slater determinant is built out of the functions of type (2.2) instead of (2.3) then the Kahana-type functions $\phi_{\mathbf{p}}(\mathbf{r})$ are orthogonal at least in linear approximation (see Appendix B). So, in this case (i.e., in linear-response approximation) formula (2.7) is at least partially true.

The angular correlation of annihilation quanta provides a method of measuring the contribution of different momentum states to the screening cloud density. As it has been already remarked in linear-response approximation the terms $\chi(\mathbf{p},\mathbf{k})$ for $k<k_F$ give no contribution to the wave function of the system, $\Psi(\mathbf{x}_1,\mathbf{x}_2,\ldots,\mathbf{x}_N,\mathbf{x}_p)$ [or $\Phi(\mathbf{r}_1,\ldots,\mathbf{r}_N)$]. Thus, using them in electron wave functions cannot lead to observable effects. This remark is also valid when determining the momentum-dependent enhancement factors, according to Kahana,[2] from the formula

$$\varepsilon(p)=\frac{|\psi_{\mathbf{p}}(\mathbf{x}_p,\mathbf{x}_p)|^2}{|\psi_{\mathbf{p}}^0(\mathbf{x}_p,\mathbf{x}_p)|^2}=\left|1+\sum_{k>1}\chi(\mathbf{p},\mathbf{k})\right|^2, \tag{2.8}$$

where $\psi_{\mathbf{p}}^0(\mathbf{x}_e,\mathbf{x}_p)=(1/\sqrt{\Omega})e^{i\mathbf{p}\cdot\mathbf{x}_e}$ and $\psi_{\mathbf{p}}(\mathbf{x}_e,\mathbf{x}_p)$ is of the form (2.2).

Electrons in order to scatter on the positron have to overcome an energy gap between their energy state and the Fermi energy. This leads to enhancement of the annihilation probability for electrons close to the Fermi surface in comparison with electrons deep in the Fermi sea. Experimentally this is a well-established fact, though with some noticeable exceptions.[16] In the case of multiple scattering (beyond the Born approximation) one can ask the question when should the Pauli projection operator be applied: to solutions of the Schrödinger equation (2.4) or when using an iterative approach to each step of iteration (this last case would lead to a Bethe-Goldstone equation). The difference consists in considering electrons scattered to occupied states inside the Fermi sphere—can they be effective as concerns subsequent scattering outside the Fermi surface. According to the Bethe-Goldstone equation they cannot and there is no reason to contest that. Note that Lowy and Jackson allow for scattering to intermediate states inside the Fermi sea when computing the t matrix [Eq. (3) in Ref. 9]. As concerns Ref. 5, it is difficult to conclude how far the Pauli exclusion operator has been applied in the misprinted Eq. (5). From the author's comments it follows that "the electron wave functions are approximately antisymmetrized using the analogy of a recoilless impurity. The recoil is neglected insofar as antisymmetrization is concerned." In the present work the recoil of the positron is included in the effective electron-positron interaction in the energy denominators.

The approach described above is approximate, of course, as far as it assumes exact features occuring to that extent only in linear-response approximation [such as Pauli exclusion principle (2.2) and orthogonality of Kahana wave functions]. We give to this approximation the name of the Kahana approach, though it could differ from the original Kahana assumptions. Let us summarize these features as follows.

(1) Two-body approach to electron-positron interaction. This feature is common with Lowy and Jackson[5,9] but different from a few other approaches, in particular from the theory of Arponen and Pajanne.[3]

(2) The wave function of the system consisting of electrons and one positron has the form of a Slater determinant built out of one electron wave functions $\phi_{\mathbf{p}}(\mathbf{r})$ describing a free electron which scatters on the positron at rest (a good approximation if the positron is thermalized).

(3) The electron-positron pair wave functions $\psi_{\mathbf{p}}(\mathbf{x}_e,\mathbf{x}_p)$ [and therefore one-particle functions $\phi_{\mathbf{p}}(\mathbf{r})$] are of the form (2.2) [instead of (2.3)], i.e., the influence of higher-order terms softening the Pauli exclusion principle is neglected.

(4) The terms following from nonorthogonality of ϕ functions are omitted while determining the screening charge distribution around a positron.

(5) The Bethe-Goldstone equation (2.1) is applied for calculating $\psi_{\mathbf{p}}(\mathbf{x}_e,\mathbf{x}_p)$ or $\phi_{\mathbf{p}}(\mathbf{r})$.

(6) It is assumed that no bound state exists. The purpose of this paper is to draw all the conclusions following from this approach, in particular, by adding a Poisson-like equation to the theory as well as taking into account electron-electron correlations (in the Kohn-Sham meaning of the word).

In the next two sections a method of achieving full self-consistency in the Kahana approach is presented and the annihilation characteristics based on it are found.

III. SELF-CONSISTENT SOLUTION OF THE KAHANA EQUATION

The Kahana formalism[2] does not include self-consistency between the Coulomb potential assumed in the Bethe-Goldstone equation (2.1) and the screening charge distribution $\rho(r)$ [formula (2.7)] following from its solutions. Bergersen[10] was the first who pointed out (in his Ph.D. thesis) that the charge sum rule was violated in the Kahana calculation. On the other hand, the annihilation parameters resulting from the Kahana approach are strongly dependent on the effective electron-positron interaction potential used in its basic equation (2.1).[11,12,14] Therefore, in order to draw reliable conclusions from the Kahana formalism, there is a real need for determining this potential self-consistently. It should be noted here that the positron's correlated screening charge was first treated self-consistently by Lowy and Jackson.[9]

As concerns the Kahana approach, practically this is equivalent to adding to the theory, apart from Eq. (2.1), the Poisson equation:

$$q^2v(q)=-4\pi[1-\Delta\rho(q)], \tag{3.1}$$

where $\Delta\rho(q)$ is the Fourier transform of the screening charge distribution $\Delta\rho(r)=\rho(r)-\rho_0$, $\rho_0=3/4\pi r_s^3$ is the density of the unperturbed system, and $\rho(r)$ is the electron distribution around the positron calculated according to (2.7) on the basis of exact solutions of the Kahana equation (2.1) with potential $v(q)$.

The screening charge distribution $\Delta\rho(q)$ is determined from the formula[14]

$$\Delta\rho(q)=\frac{8\pi}{q}\sum_n a_n\int_0^1 p\,dp\int_{\max\{1,|q-p|\}}^{q+p} dz\,\chi_n(p,z)P_n((p^2-q^2+z^2)/2pz)$$
$$+\frac{8\pi^2}{q}\sum_n a_n\int_0^1 p^2\,dp\int_1^\infty dk\,\chi_n(p,k)\int_{\max\{1,|k-q|\}}^{k+q} dz\,\chi_n(p,z)P_n((k^2-q^2+z^2)/2kz)\,, \tag{3.2}$$

where $a_n=(2n+1)/2$ and $\chi_n(p,k)$ are the coefficients of the expansion

$$\chi(\mathbf{p},\mathbf{k})=\frac{1}{k}\sum_{n=0}^{\infty} a_n\chi_n(p,k)P_n(\cos\vartheta)\,, \tag{3.3}$$

P_n being Legendre polynomials of order n and ϑ the angle between the vectors $\mathbf{p}$ and $\mathbf{k}$. In this work Eq. (2.1) was solved in the way proposed by Boroński *et al.*[11] while six partial waves in expansion (3.3) were taken into account.

It should be pointed out that if one applies an iterative scheme in order to determine the potential $v(q)$ then the self-consistency requirement (3.1) cannot be used directly. This follows from the fact that for momenta $\mathbf{q}$ close to zero the values of $v(q)$, calculated according to (3.1), diverge to infinity if only the total electronic charge around a positron, $\Delta\rho(q=0)$ [obtained from the exact solutions of the Kahana equation—Eqs. (2.1), (3.2), and (3.3)], is not exactly equal to the charge of one electron.[17] In this work, in order to avoid the low momentum divergence of $v(q)$, formula (3.1) was modified according to the method used in the work of Manninen *et al.*[18] and replaced by

$$(q^2+\beta^2)v(q)=-4\pi[1-\Delta\rho(q)]+\beta^2 v(q)\,, \tag{3.4}$$

where $\beta^2\geq 0$. It should be remarked here that Manninen *et al.* applied the above modification to quite a different problem and used a coordinate representation. The conversion to momentum space, applied in the present work, proved to be very convenient.

The Poisson equation in form (3.4) enables us to apply an iterative scheme

$$v_{n+1}(q)=\frac{-4\pi[1-\Delta\rho_n(q)]+\beta^2 v_n(q)}{q^2+\beta^2}\,, \tag{3.5}$$

where $v_n(q)$ is the potential calculated in the nth iterative step and $\Delta\rho_n(q)$ is the screening charge distribution obtained from the exact solutions of the Kahana equation [Eqs. (2.1), (3.2), and (3.3)] with potential v_n. It should be stressed here that the potential $v_{n+1}(q)$, determined according to Eq. (3.5) with the constant $\beta^2>0$ is well defined for momenta q close to zero as well. This follows from the fact that the denominator of the expression on the right-hand side of (3.5) never vanishes and therefore this expression is finite, even when $\Delta\rho(q=0)\neq 1$. The value β^2 was initially chosen (following the suggestion in Ref. 18) equal to $(0.5\pi k_F a_0)^{-1}\simeq 0.33 r_s$. With increasing convergence of the procedure, the value of β^2 was diminished.

As the first iterative step $v_1(q)$ in the procedure (3.5) the quadratic response potential[12] was applied. The calculations performed for $r_s=2$, 4, and 6 were pursued until the condition

$$\max_q\left\{\left|\frac{v_{n+1}(q)-v_n(q)}{v_n(q)}\right|\right\}\leq 1\%$$

was satisfied. For higher values of q the agreement between *a priori* (v_n) and *a posteriori* (v_{n+1}) potentials was 1 order of magnitude better.

The resulting total screening charge around the positron was obtained equal to one electronic charge within an error of about 0.5%. The total annihilation rates λ resulting from these calculations are shown in Fig. 1 by the solid line.

It should be pointed out that neglecting electron-electron correlations is the main deficiency of the approach presented in this section. This reflects on the resulting values of λ: although the low-density divergence of the total annihilation rate does not occur, nevertheless for $r_s\geq 6$ it falls below the free-positronium value $\lambda_{pos}\simeq 2\times 10^9\ s^{-1}$. On the other hand, the values of λ obtained in this work agree with those calculated self-consistently by Gondzik and Stachowiak,[19] based on the theory of liquids, when the electron-electron correlations were neglected (dashed curve in Fig. 1).

Taking into account electron-electron correlations and exchange led to an increase of the total annihilation rate[19–21] and in Ref. 19 to its correct behavior at low electron densities. The results of Gondzik and Stachowiak encourage us to include electron-electron correlations to the self-consistent Kahana approach. Section IV is devoted to self-consistent calculations of the screening charge distribution and annihilation parameters while including the effect of electron-electron exchange and correlations.

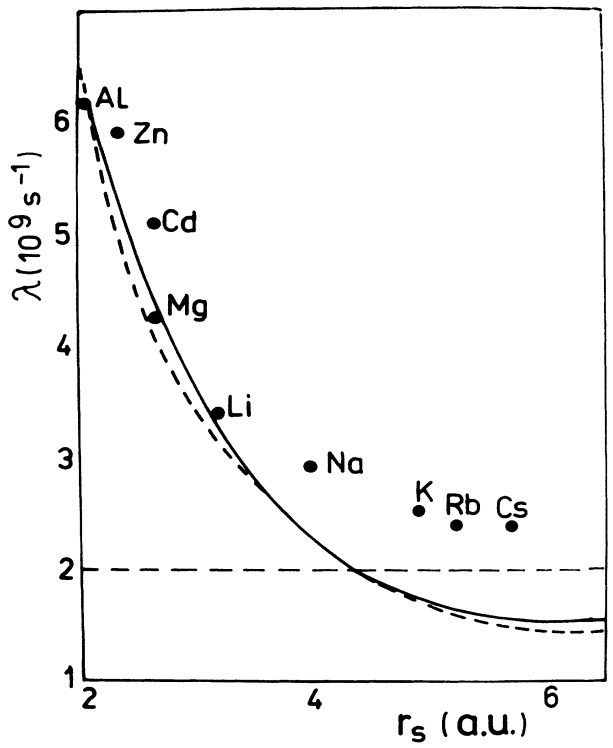

FIG. 1. The total annihilation rate λ calculated while electron-electron correlations are neglected. The corresponding result of Gondzik and Stachowiak (Ref. 19) is denoted by a dashed curve.

IV. TAKING ACCOUNT OF ELECTRON-ELECTRON CORRELATIONS

In this section the electron-electron correlations will be included into the Kahana formalism. In a few previous calculations (cf., e.g., Refs. 3, 15, and 19–21) it has been shown that they play an important role in this problem (however with one noticeable exception[5]). For this reason the effective electron-positron interaction potential used in the Kahana equation (2.1) should be composed not only of the screened Coulomb part but also of the electron-electron correlations and exchange correction v^{exc}.

The Poisson equation (3.1) should be replaced by a Hartree-Fock–type one:

$$q^2[v(q)-v^{\mathrm{exc}}(q)]=-4\pi[1-\Delta\rho(q)] \tag{4.1}$$

and, analogically, the iterative equation (3.7) by

$$v_{n+1}(q)=\frac{-4\pi[1-\Delta\rho_n(q)]+\beta^2 v_n(q)+q^2 v_n^{\mathrm{exc}}(q)}{q^2+\beta^2} . \tag{4.2}$$

Here v_n^{exc} denotes the electron-electron exchange and correlation potential calculated in the nth iterative step based on the values of $\Delta\rho_n(r)$. This potential was introduced by many authors in different ways. In this work (following the Almbladh *et al.*[22] self-consistent calculations for a proton or those of Gondzik and Stachowiak[19] for a positron) the Hedin and Lundqvist[23] exchange and correlation potential v^{exc} was used.

When determining v_n^{exc} the average electron density ρ_0 was replaced in the Hedin and Lundqvist formula for v^{exc} by its local value

$$\rho_n(r)=\rho_0+\Delta\rho_n(r)=[\tfrac{4}{3}\pi r_s^{(n)}(r)]^{-1/3} \tag{4.3}$$

and the values $\Delta\rho_n(r)$ were calculated (based on the exact solutions of the Kahana equation with potential v_n) in the way proposed by Boroński *et al.*[11] [formulas (4.2)–(4.3) of Ref. 11]. This modified Hedin and Lundqvist potential was taken in the form

$$v_n^{\mathrm{exc}}(r)=-\frac{e^2}{\pi\alpha r_s^{(n)}(r)}\left[1+Br_s^{(n)}(r)\ln\left[1+\frac{C}{r_s^{(n)}(r)}\right]\right]-v_\infty , \tag{4.4a}$$

where

$$v_\infty=-\frac{e^2}{\pi\alpha r_s}\left[1+Br_s\ln\left[1+\frac{C}{r_s}\right]\right]$$

$$\alpha=\left[\frac{4}{9\pi}\right]^{1/3}\simeq 0.521\,06,\quad B=0.0368 , \tag{4.4b}$$

and $C=21.0$.

The local treatment of v^{exc} was the reason of some deficiency. For higher values of momentum q an unphysical result was found:

$$q^2 v_n^{\mathrm{exc}}(q)+4\pi\Delta\rho_n(q)<0 , \tag{4.5}$$

where $v_n^{\mathrm{exc}}(q)$ is the Fourier transform of the potential $v_n^{\mathrm{exc}}(r)$, given by formulas (4.4). Of course, the expression on the left-hand side of (4.5) must always be positive. [Because in the opposite case Eq. (4.2), with parameter $\beta^2=0$ leads to the potential $v_{n+1}(q)<-4\pi/q^2$, i.e., less than the bare Coulomb potential.] The authors of this work have found that the substitution for $r\simeq 0$ of the local density $\Delta\rho_n(r)$ in formula (4.4) by its value averaged over the exchange hole leads to a decrease of absolute values of $q^2 v^{\mathrm{exc}}(q)$. Thus, the result (4.5) can be attributed to the local treatment of the exchange and correlation effects. Therefore, in the iterative scheme (4.2), for all momenta $\mathbf{q}$ for which (4.5) occurs, the potential v_n^{exc} given by (4.4) should be replaced by the one calculated according to the formula

$$q^2 v_n^{\mathrm{exc}}(q)=-4\pi\Delta\rho_n(q) . \tag{4.6}$$

Similar conclusions concerning the correctness of the local-density approximation while determining v^{exc} were drawn by other authors (Ref. 24 and the papers quoted therein). Gunnarson *et al.*[24] noted that nonlocal effects play an important role in this case (cf. also Ref. 15) and neglecting this fact leads to the overestimation of the absolute values of $v^{\mathrm{exc}}(r)$ for small distances r [and therefore $q^2 v^{\mathrm{exc}}(q)$ for higher values of momenta $\mathbf{q}$—this last value corresponds to the result (4.5)]. The method of avoiding this overestimation, applied in this work [Eq. (4.6)] is very crude. Nevertheless, it coincides with the approach

of Almbladh *et al.*[22] to this problem. It should be stressed here that in the paper by Gondzik and Stachowiak,[19] where the Hedin and Lundqvist correlations corrections are also used, the problem of nonlocal effects is completely neglected.

The calculations within the iterative scheme (4.2) were performed for $r_s=2$, 4, 6, and 8 in the way described in the previous section. The speed of the convergence of this procedure depends on the electron gas density (e.g., for $r_s=2$ six iterations were sufficient, while for $r_s=6$ ten iterations were needed).

The effective electron-positron interaction potential $v(q)$ is presented in Fig. 2 for $r_s=2$, 4, and 6 by solid lines. For comparison the starting quadratic response theory potential[12] for $r_s=4$ is shown in Fig. 2 by the dashed curve.

The screening charge distribution $\Delta\rho(q)$ (in momentum space), is presented in Fig. 3. $\Delta\rho(q)$ has been calculated for $r_s=2$, 4, 6, and 8 from Eqs. (3.2)–(3.4) based on the exact solutions of the Kahana equation (2.1) with the potential $v(q)$. It satisfies the Hartree-Fock–type equation (4.2) according to the potential $v(q)$ as well. For $r_s\geq 4$ one observes an overscreening near the positron. This fact will be discussed below. The charge distribution calculated in coordinate space $\Delta\rho(r)$ is shown in Fig. 4 (r is expressed in atomic units). Its radial density $4\pi r^2\Delta\rho(r)$ is given in Fig. 5 (r is expressed in units of $k_F\simeq 0.52r_s$). The Friedel oscillations of the radial density are seen in Fig. 5.

The screening charge around the positron contained in the sphere of radius r,

$$\Delta Q(r)=\int_0^r 4\pi r_1^2\Delta\rho(r_1)dr_1 \tag{4.7}$$

is presented in Fig. 6 for $r_s=2$ (solid line), 4 (dashed curve), $r_s=6$ (dotted curve), and $r_s=8$ (dash-dotted curve). It is visible that the total screening charge $\Delta Q(\infty)$ is almost equal to unity (within 0.5%). Here a remark should be made. Theoretically the condition

$$\lim_{r\to\infty}\Delta Q(r)=\lim_{q\to 0}\Delta\rho(q)$$

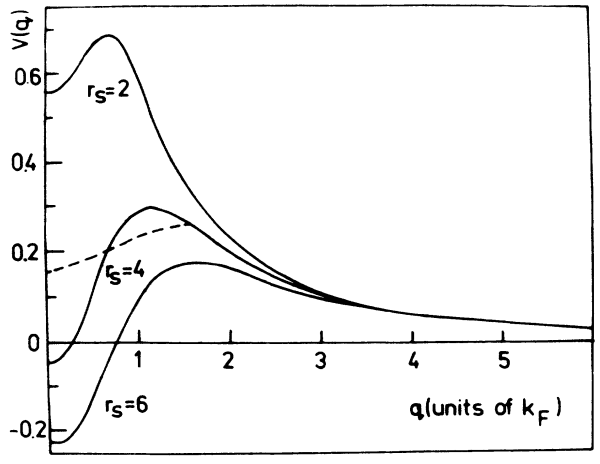

FIG. 2. The effective electron-positron interaction potential $v(q)$ for $r_s=2$, 4, and 6. $v(q)$ is expressed in units of $-4\pi/q^2$.

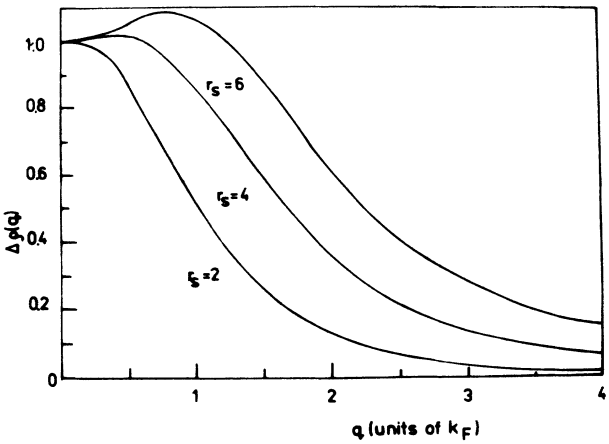

FIG. 3. The screening charge distribution $\Delta\rho(q)$ calculated self-consistently in the momentum space. Momenta are expressed in units of k_F.

should be satisfied. On the other hand, although the values $\Delta Q(\infty)$ and $\Delta\rho(0)$ were both obtained based on the exact solutions of the self-consistent Kahana equation, nevertheless in two numerically different ways: $\Delta Q(\infty)$ according to the formulas (4.2) and (4.3) of Ref. 11 and $\Delta\rho(0)$—from Eqs. (3.2)–(3.4) of this work. The agreement of the results for $\Delta Q(\infty)$ and $\Delta\rho(0)$ is a good test of the exactitude and correctness of the performed computations.

In the neighborhood of the positron overscreening is observed for $r_s\geq 4$ (cf. also Figs. 3 and 6). The results for $\max_r\Delta Q(r)$ obtained in this work are similar to those of Arponen and Pajanne[3] (cf. Table I). It should be stressed here that in Ref. 3 the Ps^- ion was obtained in the low-density limit ($r_s\to\infty$). Comparison of the values of $\Delta Q(r)$ calculated within the present formalism with the ones of Ref. 3 allows us to conclude that the fully self-consistent Kahana theory also leads for low electron densities to the Ps^- electron density distribution. This is certainly an advantage of the approach. It should be noted here that up to $r_S=8$ this overscreening is less than one electronic charge (and therefore no bound state

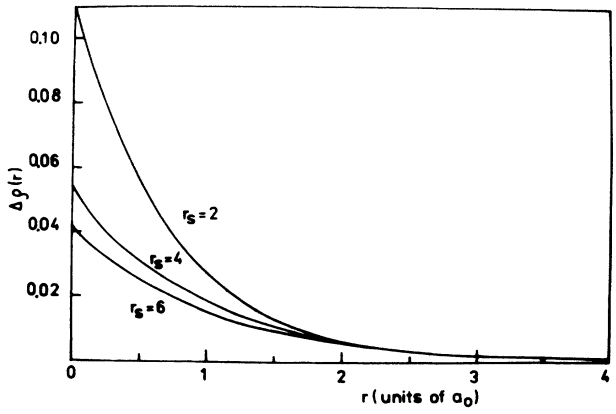

FIG. 4. The charge distribution calculated in coordinate space. r is expressed in atomic units.

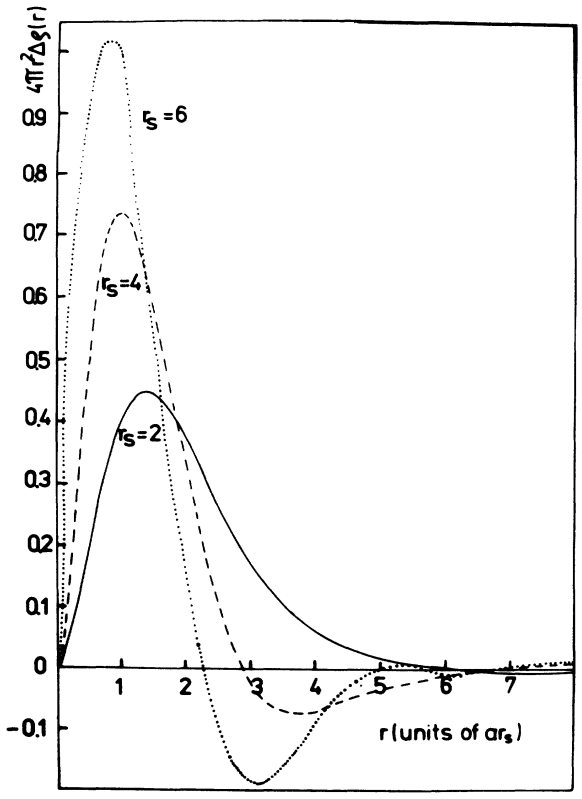

FIG. 5. The radial density of screening charge around a positron. r is expressed in units of $1/k_F$.

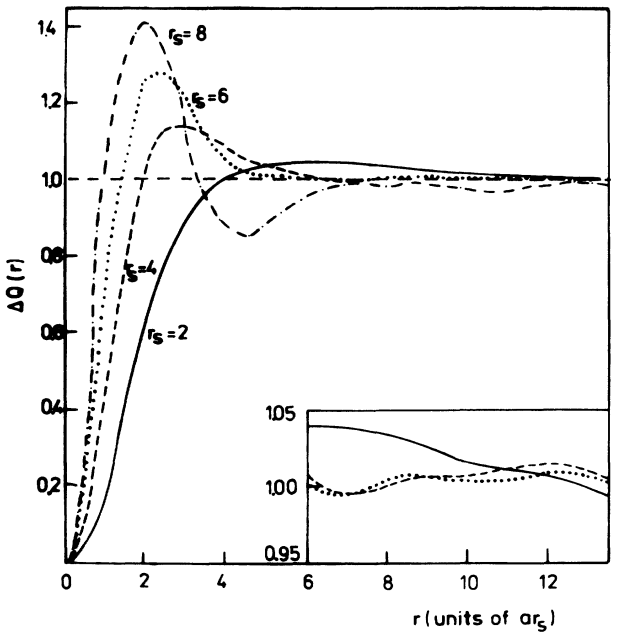

FIG. 6. The screening charge around a positron contained in a sphere of radius r: $\Delta Q(r)$ for $r_s=2$ (solid line), 4 (dashed line), 6 (dotted line), and 8 (dot-dashed line). r is expressed in units of $1/k_F$.

TABLE I. Overscreening nearby the positron in terms of $\max_r\{\Delta Q(r)\}$.

r_s	This work	Arponen and Pajanne[a]
4	0.13	0.02
6	0.27	0.12
8	0.41	0.26

[a]Reference 3.

comes out).

The existence of bound states for low electron densities needs some discussion. In Sec. II the assumption that no bound state exists was included in the features of the Kahana theory considered in this work. We would like to explain this point of view. Formally, knowing an effective electron-positron interaction potential $v(q)$ we are able (following Lowy and Jackson[9]) to determine the poles of the t matrix and therefore to state the existence of bound states. On the other hand, in the case of formation of positronium the interaction potential is different from $v(q)$ (which was calculated for free electronic states). Therefore, this approach cannot be treated literally. Arponen and Pajanne[8] debate the problem whether the poles of t matrix should be interpreted as signifying the existence of a true bound positronium (Ps) atom in the system. According to the remarks of Ref. 8, "the appearance of isolated poles clearly indicates the existence of a closely correlated positron-electron structure in the many-body system. However, from this it does not necessarily follow that real positronium could exist even in dilute electron gas." The criteria for the existence of positronium "demand that there should exist essentially no interaction and no spin exchange between the electron-positron pair and the electron gas surrounding it. In our opinion these criteria cannot be met in the density region close to metallic densities. . .it should be no sharp transition at a definite density signifying sudden appearance of bound Ps, although undoubtedly the correlations of the positron with the surrounding electrons become more and more positroniumlike as r_s increases."

The annihilation rates λ calculated within the presented formalism are compared with experimental data[25] in Fig. 7. In Fig. 7 the results obtained when neglecting electron-electron correlations (cf. Sec. III and Fig. 1) are quoted for comparison by a dashed curve. It is seen that taking these correlations into account causes an increase of the calculated values of λ. Our result coincides with those of Refs. 19 and 20. Neither the low-density divergence of total annihilation rate nor its falling below the positronium value $\lambda_{pos}\simeq 2\times 10^9$ s^{-1} occurs (in contradistinction to results of Refs. 12 and 21).

For the densities characterized by $r_s>2$ the agreement between the theoretical and experimental values of λ is reasonable. Including the lattice effect[26] still improves this agreement. For $r_s\to\infty$ the proper behavior of λ is observed. For $r_s=2$ we obtain a value of λ equal to 7.03, i.e., appreciably greater than the experimental result $\lambda_{expt}=6.21$.[27] A similar overestimation of annihilation rates results from other electron gas theories: in Ref. 9

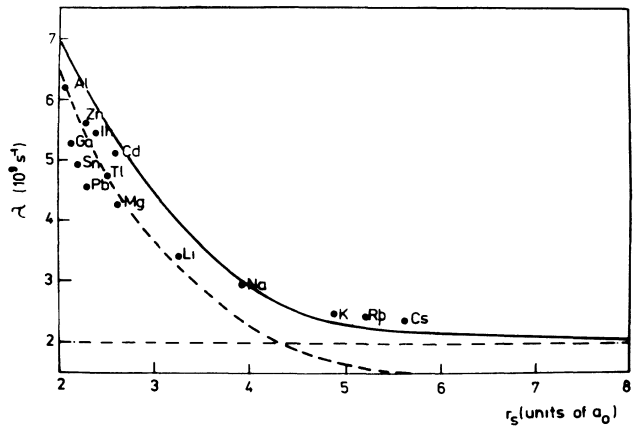

FIG. 7. Annihilation rate λ as a function of r_s (solid line) compared with the results obtained when the electron-electron correlations are neglected (dashed curve). The experimental data are quoted in Refs. 12.

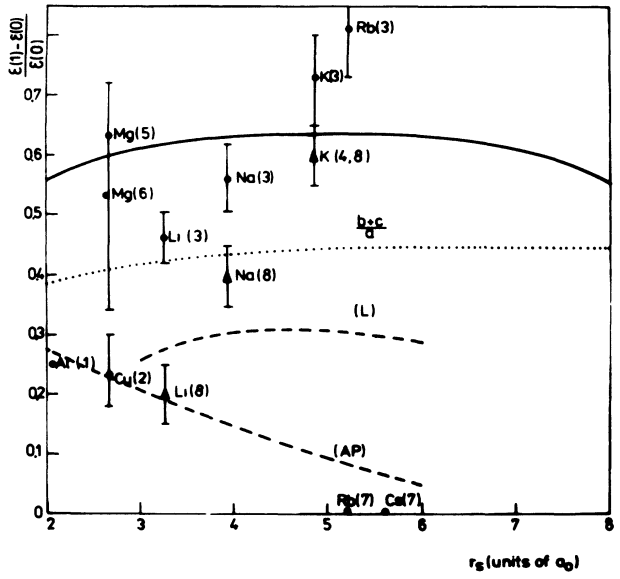

FIG. 8. Relative enhancement factors on a Fermi surface (solid line) compared with their biparabolic analogue $(b+c)/a$. The dashed curve denoted (AP) corresponds to the results of Refs. 3 for $(b+c)/a$ and the one denoted (L) to the values extracted from Ref. 5 for γ. The experimental data are quoted in Ref. 13.

$\lambda_{\text{theor}}=7.0$, in Ref. 3—6.8, in Ref. 19—7.55, in Ref. 22—7.6, and only in Ref. 28—6.45.

This difference between the theoretical and experimental values of λ should be attributed not only to using the electron gas model in calculations but also to the local way of introducing the electron-electron correlation and exchange correction v^{exc}. For $r_s=2$ it was found that as early as for $q \geq 2.9k_F$ the inequality (4.5) occurs and v^{exc} was calculated according to (4.6). For these momenta an effective electron-positron potential $v(q)$ was equal to the bare Coulomb potential. In the coordinate space this means that in some area around the positron the potential $v(r)$ is unscreened. This causes an overaccumulation of electronic charge on the positron and therefore an overestimation of λ. Similar conclusions, concerning the local approximation to the electron-electron correlations and exchange, were drawn in the case of a heavy impurity by Gunnarson *et al.*[24] These authors remarked that in the local approximation the size of the exchange and correlation hole is overestimated for small distances r from the impurity. The same result is obtained by us for a positron. For this reason the electron-electron correlations and exchange should be treated very carefully and nonlocal effects should be taken into account.

Finally it should be mentioned here that together with the progress in the experimental technique the experimental value λ_{expt} for Al ($r_s=2.07$) increased from $\lambda_{\text{expt}}=4.97$ (Ref. 29) to $\lambda_{\text{expt}}=6.21$ (Refs. 27). The relative enhancement factor on a Fermi surface $\gamma=[\varepsilon(1)-\varepsilon(0)]/\varepsilon(0)$ as a function of r_s is presented in Fig. 8 by the solid line (the choice of this parameter was justified in Refs. 12 and 13). If the biparabolic approximation of Kahana is used [according to this approximation[30] $\varepsilon(p)\simeq a+bp^2+cp^4$], γ takes the value $(b+c)/a$. $(b+c)/a$ are shown in Fig. 8 by a dotted line. The dashed curve denoted (AP) corresponds to the results of Ref. 3 for $(b+c)/a$ and the one denoted (L)—to the values extracted from Ref. 5 for γ. The experimental values quoted in Fig. 8 are in our opinion intermediate between γ and $(b+c)/a$.[13]

For $r_s=2$ the theoretical value of γ obtained in this work is appreciably greater than the experimental one. This overestimation of γ can be attributed to the same reasons as corresponding overestimation of annihilation rate λ. It should be noted here that the Kahana approach is based by itself on some approximations (cf. Sec. II) which become inexact for higher electron densities.

For $r_s>2$ the agreement between the theoretical and experimental relative enhancement factors is reasonable. This enhancement factor is up to $r_s=6$ an increasing function of r_s (just the opposite as follows from the approach of Arponen and Pajanne[3] but in agreement with the majority of the experimental results). Also the comparison with Lowy's[5] results allow for more confidence in the self-consistent Kahana approach, at least for low electron densities.

V. CONCLUSIONS

We consider our results as definitive as concerns conclusions following from the Kahana formalism and only including the electron-electron correlations in a nonlocal way could slightly change the annihilation characteristics.

It is worthwhile to point out that the self-consistent Kahana theory, in spite of its simplicity, leads to the proper behavior of the total and partial annihilation rates in the range of metallic and low densities. The annihilation rate λ exhibits no low density falling below the positronium value in contradistinction to our previous results.

There is a disparity between different theories as concerns the momentum-dependent enhancement factors.

The most sophisticated approach of Arponen and Pajanne leads to better enhancement factors for higher electron densities ($r_s \simeq 2$). For low densities (especially for alkalis) the enhancement factors following from the self-consistent Kahana theory seem to be the most reliable. It is encouraging that for low electron densities ($r_s \to \infty$) the annihilation rate λ calculated within the present formalism is converging to this corresponding to positronium.

It should be remembered, however, that the Kahana formalism relies on some assumptions which are true only approximately and have been contested. Among problems which remain to be solved let us mention the proper treatment of the wave function of the whole system and its relation to the electron density distribution, including terms following from the nonorthogonality of the one electron wave functions.

There is still the problem of the influence of explicit three-body correlations on the annihilation characteristics. Arponen and Pajanne in 1979 found a many-body tail in the momentum distribution of annihilation photons corresponding to momenta beyond the Fermi sphere. This prediction has hardly been confirmed experimentally by anybody. Carbotte and Kahana[31] found reasons why the many-body tail should be deenhanced. We suspect that they were right. Anyway the formalism used in the present paper neglects the many-body tail *a priori*. As it was shown by Boroński[32] replacing the rectangular momentum distribution of the electron gas used in the Kahana approach by the RPA distribution of the Daniel and Vosko[33] type with diminished discontinuity on the Fermi surface would lead to the results of Arponen and Pajanne even within the formalism applied in this paper.

ACKNOWLEDGMENT

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APPENDIX A

The function $\Phi(\mathbf{r}_1, \ldots, \mathbf{r}_N)$ is assumed in the form of a Slater determinant built out of one-electron functions $\phi_j(r_i)$ of the form (2.3), where j denotes the state $\mathbf{p}_j$. Taking into account (2.3) for some m we have

$$\Phi(\mathbf{r}_1, \ldots, \mathbf{r}_N) = \frac{1}{\sqrt{N}} \det[\phi_j(\mathbf{r}_i)] = \frac{1}{\sqrt{N!}} \frac{1}{\sqrt{\Omega}} \left| \begin{vmatrix} \phi_1(\mathbf{r}_1) & \cdots & \phi_N(\mathbf{r}_i) \\ & \cdots & \\ e^{i\mathbf{p}_m \cdot \mathbf{r}_1} & \cdots & e^{i\mathbf{p}_m \cdot \mathbf{r}_N} \\ & \cdots & \\ \phi_N(\mathbf{r}_1) & \cdots & \phi_N(\mathbf{r}_N) \end{vmatrix} + \sum_{\mathbf{q}} \chi(\mathbf{p}_m, \mathbf{q}) \begin{vmatrix} \phi_1(\mathbf{r}_1) & \cdots & \phi_1(\mathbf{r}_N) \\ & \cdots & \\ e^{i\mathbf{q} \cdot \mathbf{r}_1} & \cdots & e^{i\mathbf{q} \cdot \mathbf{r}_N} \\ & \cdots & \\ \phi_N(\mathbf{r}_1) & \cdots & \phi_N(\mathbf{r}_N) \end{vmatrix} \right| . \tag{A1}$$

For every $q < k_F$ there exists some momentum $\mathbf{p}_n$ within the Fermi sphere such that $\mathbf{q} = \mathbf{p}_n$ and

$$\phi_n(\mathbf{r}) = \frac{1}{\sqrt{\Omega}} \left[e^{i\mathbf{p}_n \cdot \mathbf{r}} + \sum_{\mathbf{k}} \chi(\mathbf{p}_n, \mathbf{k}) \cdot e^{i\mathbf{k} \cdot \mathbf{r}} \right]$$
$$= \frac{1}{\sqrt{\Omega}} \left[e^{i\mathbf{q} \cdot \mathbf{r}} + \sum_{\mathbf{k}} \chi(\mathbf{q}, \mathbf{k}) \cdot e^{i\mathbf{k} \cdot \mathbf{r}} \right] .$$

Then

$$\begin{vmatrix} \phi_1(\mathbf{r}_1) & \cdots & \phi_1(\mathbf{r}_N) \\ & \cdots & \\ e^{i\mathbf{q} \cdot \mathbf{r}_1} & \cdots & e^{i\mathbf{q} \cdot \mathbf{r}_N} \\ & \cdots & \\ \phi_n(\mathbf{r}_1) & \cdots & \phi_n(\mathbf{r}_N) \\ & \cdots & \\ \phi_N(\mathbf{r}_1) & \cdots & \phi_N(\mathbf{r}_N) \end{vmatrix} = \frac{1}{\sqrt{\Omega}} \begin{vmatrix} \phi_1(\mathbf{r}_1) & \cdots & \phi_1(\mathbf{r}_N) \\ & \cdots & \\ e^{i\mathbf{q} \cdot \mathbf{r}_1} & \cdots & e^{i\mathbf{q} \cdot \mathbf{r}_N} \\ & \cdots & \\ e^{i\mathbf{q} \cdot \mathbf{r}_1} & \cdots & e^{i\mathbf{q} \cdot \mathbf{r}_N} \\ & \cdots & \\ \phi_N(\mathbf{r}_1) & \cdots & \phi_N(\mathbf{r}_N) \end{vmatrix} + \frac{1}{\sqrt{\Omega}} \sum_{\mathbf{k}} \chi(\mathbf{q}, \mathbf{k}) \begin{vmatrix} \phi_1(\mathbf{r}_1) & \cdots & \phi_1(\mathbf{r}_N) \\ & \cdots & \\ e^{i\mathbf{q} \cdot \mathbf{r}_1} & \cdots & e^{i\mathbf{q} \cdot \mathbf{r}_N} \\ & \cdots & \\ e^{i\mathbf{k} \cdot \mathbf{r}_1} & \cdots & e^{i\mathbf{k} \cdot \mathbf{r}_N} \\ & \cdots & \\ \phi_N(\mathbf{r}_1) & \cdots & \phi_N(\mathbf{r}_N) \end{vmatrix} . \tag{A2}$$

The first term on the right-hand side of (A2) vanishes. Therefore, the terms $\chi(\mathbf{p}, \mathbf{q})$ with $q < k_F$ give in $\Phi(\mathbf{r}_1, \ldots, \mathbf{r}_N)$ [or $\Psi(\mathbf{x}_1, \ldots, \mathbf{x}_N, \mathbf{x}_p)$] a contribution of second order in the interaction parameter and can be neglected in linear-response approximation.

APPENDIX B

For two electronic states $\mathbf{p}$ and $\mathbf{q}$ scattered out of the Fermi sphere we have, according to (2.2),

$$\langle \phi_{\mathbf{p}} | \phi_{\mathbf{q}} \rangle = \int d\mathbf{r}\, \phi_{\mathbf{p}}^{*}(\mathbf{r})\phi_{\mathbf{q}}(\mathbf{r}) = \frac{1}{\Omega}\int d\mathbf{r} \left[e^{-i\mathbf{p}\cdot\mathbf{r}} + \sum_{k>k_F} \chi^{*}(\mathbf{p},\mathbf{k}) e^{-i\mathbf{k}\cdot\mathbf{r}} \right] \left[e^{i\mathbf{q}\cdot\mathbf{r}} + \sum_{s>k_F} \chi(\mathbf{q},\mathbf{s}) e^{i\mathbf{s}\cdot\mathbf{r}} \right]$$

$$= \frac{1}{\Omega}\int d\mathbf{r}\, e^{i(\mathbf{q}-\mathbf{p})\cdot\mathbf{r}} + \frac{1}{\Omega}\sum_{k>k_F}\int d\mathbf{r} \left[\chi^{*}(\mathbf{p},\mathbf{k}) e^{i(\mathbf{q}-\mathbf{k})\cdot\mathbf{r}} + \chi(\mathbf{q},\mathbf{k}) e^{i(\mathbf{k}-\mathbf{p})\cdot\mathbf{r}} \right]$$

$$+ \frac{1}{\Omega}\sum_{k>k_F}\sum_{s>k_F} \chi^{*}(\mathbf{p},\mathbf{k})\chi(\mathbf{q},\mathbf{s}) \int dr\, e^{i(\mathbf{s}-\mathbf{k})\cdot\mathbf{r}} . \tag{B1}$$

Therefore

$$\langle \phi_{\mathbf{p}} | \phi_{\mathbf{q}} \rangle = \delta_{\mathbf{p},\mathbf{q}} + \sum_{k>k_F} [\chi^{*}(\mathbf{p},\mathbf{k})\delta_{\mathbf{k},\mathbf{q}} + \chi(\mathbf{q},\mathbf{k})\delta_{\mathbf{k},\mathbf{p}}] + \sum_{k>k_F} \chi^{*}(\mathbf{p},\mathbf{k})\chi(\mathbf{q},\mathbf{k}) . \tag{B2}$$

The third term on the right-hand side of (B2) can be neglected in the linear-response approximation. For momenta $p,q < k_F$ the second term vanishes as a consequence of applying the Pauli operator to the form of the functions $\phi_{\mathbf{p}}(\mathbf{r})$. This leads to the approximate orthogonality of these functions.

It should be stressed here that in the case of functions $\phi_p(r)$ of the form (2.3), where the Pauli operator is neglected, the second term on the right-hand side of Eq. (B2) has a nonzero value, $\chi^{*}(\mathbf{p},\mathbf{q}) + \chi(\mathbf{q},\mathbf{p})$, and therefore the functions $\phi_{\mathbf{p}}$ and $\phi_{\mathbf{q}}$ are not orthogonal. Thus, in this case the application of the Pauli projection operator makes possible the orthogonality of functions $\phi_{\mathbf{p}}$.

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