Theory of Positron Annihilation in Real Metals*

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A theory of positron annihilation applicable to real metals is developed. It is based on a band model for a solid and the ladder approximation for the electron-positron Green's function. The Block character of the positron as well as the conduction-band single-particle wave functions are included. The core electrons are treated within the tight-binding approximation. Throughout, the effect of the direct Coulomb coupling between the annihilating pair is stressed. The general formulas are then used to derive a theory of core annihilation. In the course of the derivation it was necessary to make a number of simplifying assumptions which restrict the theory to simple metals. We find that the contribution to the partial annihilation rate $R[\mathbf{p}]$ coming from a core electron is proportional to the square of the sum of two terms: the usual $\mathbf{p}$th Fourier component of the product of the positron and core function plus another term accounting for the polarization of the ion core by the positron. After studying core annihilation in detail using an idealized model for the unoccupied electron Bloch states in sodium, we conclude that the second term is just as important as the first, although it has never been included in past treatments of this problem. Unfortunately our model is too crude to give quantitative results. An accurate calculation of core annihilation is very much more difficult than the corresponding computation of annihilation in a conduction-electron gas.

1. INTRODUCTION

IT has been known for sometime now[1] that to even begin understanding the observed lifetimes of positrons annihilating in simple metals it is essential to take into account very carefully the Coulomb force between the annihilating electron-positron pair. This coupling leads to a large enhancement of the electronic density at the positron which is the quantity that essentially determines the total annihilation rate. On the other hand, for a number of simple metals, the main features of the two-photon angular-correlation curves can be understood reasonably well on the basis of a Sommerfeld model. This arises because the annihilation cross sections, although considerably increased by the positron force, are not very sensitive to the velocity of incidence of the electron partner. However, even for sodium, long and rather broad tails still remain, extending considerably beyond the natural Fermi momentum cutoff which necessarily enters an electron-gas theory.[2] These tails must come entirely from the existence of the crystal lattice and it is the purpose of this paper to develop a theory which includes lattice effects.

To understand the general viewpoint on which our whole approach rests, it is necessary to give a brief account of our present understanding of positron annihilation in an interacting electron gas. The work of K-II was based on the ladder approximation for the electron-positron propagator as well as a static limit for the dynamic effective potential in the random-phase approximation. No attempt was made to include further correlations. This left the analysis open to criticism since the question of possible corrections to the ladder graphs was left unanswered.[3] The choice of a static limit is also a nontrivial matter because the total rates are quite sensitive to the form of the screened potential.[4] These problems were recently studied in Ref. 2.

By making an estimate of all the lower order graphs in the complete perturbation expansion for the electron-positron Green's function, it was concluded that the ladder approximation is indeed much more exact than might have been expected. This occurs not only because the remaining Feynman graphs involving electron-positron interaction lines lead to small corrections, but also because cancellations arise between them.

This work further served to clarify both the use of the static approximation to the dynamic potential, and the way in which self-energy processes are to be incorporated in the general theory. Provided one introduces a plasmon correction, it was shown that retaining only the zeroth frequency component in the effective potential is quite appropriate since this has much the same effect on the two photon counting rate as including self-energy corrections.[5] These results are of practical value to us in the present discussion since they indicate clearly that the ladder approximation with static potential can be used with confidence in generalizing the theory to include lattice corrections.

Another result (which to some extent is a question of principle) to come out of the analysis of CK is perhaps even more important. It was shown that the positron can introduce quite subtle distortions in the electronic configuration. For instance, the angular correlation curve arrived at in CK bears little resemblance in detail

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[1] S. Kahana, Phys. Rev. **129**, 1662 (1963). Referred to from here on as K-II.
[2] This was recently shown to be the case by S. Kahana and the present author; J. P. Carbotte and S. Kahana, Phys. Rev. **139**, A213 (1965). Referred to from here on as CK.
[3] These difficulties with the ladder approximation were emphasized particularly by B. Bergersen in a Brandeis University Ph.D. dissertation, 1964 (unpublished).
[4] S. Kahana, Phys. Rev. **117**, 123 (1960) and Ref. (1).
[5] Strictly speaking this result was established only within the Born approximation. The arguments presented there, however, are expected to go through in much the same way for higher order contributions, although these are smaller and less important.

to that determined on the basis of the momentum distribution of the quasiparticles in an interacting electron gas. This result casts doubt on the usual interpretation of the data for the counting rate using a simplified model where one ignores the positron polarization of the surroundings. While this point of view has undoubtedly a good deal of validity and has been useful in the past in understanding these measurements[6-9] we cannot expect it to be correct in detail. A fundamental interpretation of the data requires treating the positron Coulomb field as an essential feature of the problem.

In this paper an attempt is made to include the lattice within the framework of the ladder approximation. This involves, in some way, two distinct generalizations of the usual formalism. First, the ion lattice potential introduces higher momentum components in the conduction-electron single-particle wave function. Second, core annihilation is now a possibility. Both these effects introduce tails in the counting rate. However, for a metal like sodium we expect the latter to be by far the more important and for this reason we soon specialize to the case of core annihilation although our formulas initially refer to both conduction and core electrons.

In Sec. 2 we define the zeroth-order propagators from which the general perturbation series for the electron-positron correlation function can be constructed. Our basic approximation is then specified. Sec. 3 contains mostly formal algebraic manipulations. We show how the Green's-function expression for the partial annihilation rate $R[\mathbf{p}]$ can be rewritten as the square of a generalized Bethe-Goldstone-type amplitude which must, however, first be weighted by an appropriate overlap integral of an electron and a positron single-particle Bloch state. In this form the expressions are still quite unmanageable if one is interested in making a practical calculation. In this sense the work so far has been purely formal.

In Sec. 4 we use our general formula to derive a theory of core annihilation which is the main concern of this paper. To make any progress, a number of approximations are necessary, but these are of little consequence. They restrict us to systems with small cores and for which the conduction single-particle Bloch functions do not differ very much from plane waves. In this way we find that the contribution to $R[\mathbf{p}]$ from a core electron in a state ϕ_{core} can be written as the square of the sum of two distinct terms. The first is the $\mathbf{p}$th Fourier component of the familiar core electron-positron product wave function. The second involves matrix elements which describe virtual transitions of the core electrons to unoccupied conduction states. The evaluation of these matrix elements is difficult and a complete numerical calculation is not attempted. Instead, a simplified model is studied in the hope of getting some understanding of the physics of the problem. This is the subject of Sec. 5. The computations are presented for sodium since it is for this metal that the theory is expected to apply best. Because the model used for the conduction states is quite crude even in this simple case, the calculation is only preliminary. It is nevertheless useful since the simple physical picture that evolves is certainly qualitatively correct. In Sec. 6 we present a discussion of the results obtained and draw conclusions.

2. FORMAL PRELIMINARIES

We begin with the expression for the partial annihilation rate $R[\mathbf{p}]$ as the $\mathbf{p}$th Fourier component of an appropriate contraction of the electron-positron Green's function

$$R[\mathbf{p}]=\frac{(-i)^2\lambda}{V}\int d^3x d^3y e^{-i\mathbf{p}\cdot(\mathbf{x}-\mathbf{y})}G_{ep}(x,x;y^+,y^+). \quad (2.1)$$

The notation is as in CK. This is a perfectly general expression for $R[\mathbf{p}]$ provided the particles involved are of low energy, i.e. well within the nonrelativistic regime. It is important to realize that the complete contraction $(-i)^2G_{ep}(x,x;x^+,x^+)$ which enters the total rate $R=\sum_p R[\mathbf{p}]$ has a simple physical meaning. It is just the ground-state expectation value of the product of the second quantized density operator for the electron and the positron field. Implied is the assumption that the electron system is at zero temperature and that the positron is thermalized before annihilating.

Once an approximation to $G_{ep}(x,x';y,y')$ is chosen the problem is completely determined. It was pointed out in the Introduction that physically the ladder graphs are expected to give by far the dominant contribution to $R[\mathbf{p}]$. We should perhaps be a little more specific. For the conduction electrons all the remaining lower order Feynman graphs were essentially evaluated in CK. Admittedly a plane-wave approximation was used and the Bloch character of the single-particle states must certainly modify each contribution somewhat; however, this will not change the fact that any given term is either small or almost cancels against another. The core electrons are more problematical since some of the matrix elements involved in the various perturbation terms will not resemble at all plane-wave matrix elements. Also the energy denominators will be significantly modified. Thus, in this case, the ladder approximation has not really been justified by a detailed numerical calculation although the only first-order term contributing is the first ladder. Nevertheless, this is certainly a physically reasonable assumption even for core electrons, since it describes the modifications in the annihilating electron-positron-pair wave function due to the direct Coulomb coupling between them. Thus, in the present discussion, self-energy effects and plasmon corrections will not be treated.

[6] S. Berko and J. S. Plaskett, Phys. Rev. **112**, 1877 (1958).
[7] E. Daniel, J. Phys. Chem. Solids **6**, 205 (1958).
[8] P. R. Wallace, in *Solid State Physics*, edited by F. Seitz and D. Turnbull (Academic Press Inc., New York, 1960), Vol. 10, p. 1.
[9] K. L. Rose and S. De Benedetti, Phys. Rev. **138**, A927 (1965).

The integral equation for the sum of the ladders is

$$G_{ep}(x,x';y,y') = G_e^0(x;y)G_p^0(x';y') - i\int d^4z d^4z' u(z;z')G_e^0(x;z) \times G_p^0(x';z')G_{ep}(z,z';y,y'), \quad (2.2)$$

with $u(z;z')=u_s(\mathbf{z};\mathbf{z}')\delta(t_z-t_{z'})$, $u_s(\mathbf{z};\mathbf{z}')$ being the usual screened Coulomb force of an electron-gas theory[1]; i.e. only the conduction electrons are assumed to take part significantly in the screening, and in computing their effect a plane-wave model is used. The functions G_e^0 and G_p^0 are, respectively, the zeroth-order electron and positron propagators which we will now define. To construct $G_e^0(x;x')$ we can use the best possible self-consistent Hartree-Fock Bloch states. They are denoted by $\Psi_{[\mathbf{m}]}(\mathbf{x})$ where for a core electron in the (nl) shell with magnetic quantum number m and crystal momentum $\mathbf{s}$ (restricted to the first Brillouin zone) the Bloch label $[\mathbf{m}]$ stands for $[nlm\mathbf{s}]$. For a conduction or higher exicted state the label $[\mathbf{m}]$ is to represent a restricted momentum plus a band index in a reduced zone scheme, or alternatively an unrestricted momentum label in an extended zone scheme. It should be noted at this point that, although for a large part of the analysis it is not a necessary assumption, we will always have in mind metals with small relatively stiff cores so that in constructing the corresponding tight-binding states it is reasonable to use the Hartree-Fock solutions for the free ion. In other words any distortion of the cores due to their solid-state surroundings is neglected.

The positron Bloch states denoted by $\phi_{[\mathbf{m}]}(\mathbf{x})$ are to be solved for, using in each Wigner-Seitz cell as crystal potential the Hartree field of the rigid ion core, plus the field of a conduction electron smeared throughout the volume. The positron propagator is then

$$G_p^0(x;x') = \sum_{[\mathbf{m}]} \phi_{[\mathbf{m}]}(\mathbf{x})\phi_{[\mathbf{m}]}^*(\mathbf{x}') \times \int \frac{d\omega}{2\pi} e^{-i\omega(t_x-t_{x'})} G_p^0([\mathbf{m}];\omega) \quad (2.3)$$

with

$$G_p^0([\mathbf{m}];\omega) = \frac{\theta_p^{\text{u.o.}}([\mathbf{m}])}{E_{[\mathbf{m}]}^p-\omega-i0^+} + \frac{\theta_p^{\text{o.}}([\mathbf{m}])}{E_{[\mathbf{m}]}^p-\omega+i0^+}. \quad (2.4)$$

In (2.4), $E_{[\mathbf{m}]}^p$ is the eigenvalue corresponding to the state $\phi_{[\mathbf{m}]}(\mathbf{x})$ while $\theta_p^{\text{u.o.}}([\mathbf{m}])$ is a theta function equal to 1 for all unoccupied states and zero otherwise. The function $\theta_p^{\text{o.}}([\mathbf{m}])=1-\theta_p^{\text{u.o.}}([\mathbf{m}])$. Since the positron is assumed thermalized on annihilation $\theta_p^{\text{o.}}([\mathbf{m}])$ is in fact a delta function $\delta_{[\mathbf{m}],0}$. Finally, we will not write down $G_e^0(x;x')$ explicitly since it can essentially be put in the form (2.3) and (2.4) with $\phi_{[\mathbf{m}]}\to\Psi_{[\mathbf{m}]}$, $E_{[\mathbf{m}]}^p\to/E_{[\mathbf{m}]}^e$ and $\theta_p^{\text{o.}}([\mathbf{m}])\to\theta_e^{\text{o.}}([\mathbf{m}])$ where, for instance, $\theta_e^{\text{o.}}([\mathbf{m}])$ is 1 for all the core and occupied conduction single-particle Bloch states and zero beyond.

3. ALGEBRAIC DEVELOPMENT

We are concerned here with reducing expression (2.1) and Eq. (2.2) to more tractable forms. First notice that in Eq. (2.2) y and y' are inert variables and that since the two-body potential is static we need to know the electron-positron Green's function $G_{ep}(z,z';y,y')$ only for $t_z=t_{z'}$. Throughout this section for any pair of variables x and x' it is always understood that $t_x=t_{x'}$. Introduce an amplitude $\Omega(x,x';y,y')$ according to the prescription

$$G_{ep}(x,x';y,y') = \int d^4z d^3z' \Omega(x,x';z,z') \times G_e^0(z;y)G_p^0(z';y'). \quad (3.1)$$

This definition is consistent with the two-body propagator given by (2.2) and, by inspection, we immediately get that $\Omega(x,x';y,y')$ must satisfy the equation

$$\Omega(x,x';y,y') = \delta^4(x-y)\delta^3(\mathbf{x}'-\mathbf{y}') - i\int d^4z d^3z' u_s(\mathbf{z};\mathbf{z}') \times G_e^0(x;z)G_p^0(x';z')\Omega(z,z';y,y'). \quad (3.2)$$

Because of translational invariance in time, $\Omega(x,x';y,y')$ can depend only on the time difference t_x-t_y. Thus, we can introduce for Ω a "generalized Fourier transform,"

$$\Omega(x,x';y,y') = \sum_{[\mathbf{m}],[\mathbf{n}];[\mathbf{m}'],[\mathbf{n}']} \Psi_{[\mathbf{m}]}(\mathbf{x})\phi_{[\mathbf{n}]}(\mathbf{x}') \int \frac{d\omega}{2\pi} e^{-i\omega(t_x-t_y)} \times [\Omega_{[\mathbf{m}],[\mathbf{n}];[\mathbf{m}'],[\mathbf{n}']}(\omega)]\Psi_{[\mathbf{m}']}^*(\mathbf{y})\phi_{[\mathbf{n}']}^*(\mathbf{y}'), \quad (3.3)$$

which when substituted into (3.2) yields an integral equation for $\Omega_{[\mathbf{m}],[\mathbf{n}];[\mathbf{m}'],[\mathbf{n}']}(\omega)$ of the form,

$$\Omega_{[\mathbf{m}],[\mathbf{n}];[\mathbf{m}'],[\mathbf{n}']}(\omega) = \delta_{[\mathbf{m}],[\mathbf{m}']}\delta_{[\mathbf{n}],[\mathbf{n}']} - i\sum_{[\mathbf{k}],[\mathbf{k}']} H_{[\mathbf{m}],[\mathbf{n}];[\mathbf{k}],[\mathbf{k}']} \int \frac{d\epsilon}{2\pi} \Omega_{[\mathbf{k}],[\mathbf{k}'];[\mathbf{m}'],[\mathbf{n}']}(\omega) \times G_e^0([\mathbf{m}];\epsilon)G_p^0([\mathbf{n}];\omega-\epsilon). \quad (3.4)$$

In going from (3.2) to (3.4) we have made use of definition (2.3). The quantity H in (3.4) is

$$H_{[\mathbf{m}],[\mathbf{n}];[\mathbf{k}],[\mathbf{k}']} = (1/V)\textstyle\sum_{\mathbf{q}} u_s(\mathbf{q})[\mathbf{m}|\mathbf{q}|\mathbf{k}]^e \times [\mathbf{n}|-\mathbf{q}|\mathbf{k}']^p, \quad (3.5)$$

where $\mathbf{q}$ is an ordinary momentum variable as opposed to a Bloch-state label and $u_s(\mathbf{q})$ is the usual Fourier transform of the static effective potential $u_s(\mathbf{x};\mathbf{x}')$. The matrix elements $[\mathbf{m}|\mathbf{q}|\mathbf{k}]^e$ and $[\mathbf{n}|-\mathbf{q}|\mathbf{k}']^p$ are, respectively, equal to

$$\int \Psi_{[\mathbf{m}]}(\mathbf{x})e^{i\mathbf{q}\cdot\mathbf{x}}\Psi_{[\mathbf{k}]}^*(\mathbf{x})d^3x \quad (3.6a)$$

and

$$\int \phi_{[n]}(\mathbf{x})e^{-i\mathbf{q}\cdot\mathbf{x}}\phi_{[k']}{}^*(\mathbf{x})d^3x. \tag{3.6b}$$

We next want to introduce expression (3.1) into Eq. (2.1) for the partial annihilation rate $R[\mathbf{p}]$ and carry out the necessary Fourier analysis. This gives

$$R[\mathbf{p}]=\frac{(-i)^2\lambda}{V}\sum_{[m],[n];[m'],[n']} I_{[m],[n]}(\mathbf{p})I_{[m'],[n']}{}^*(\mathbf{p}) \times\int\frac{d\omega d\epsilon}{(2\pi)^2}e^{i\omega 0^+}[\Omega_{[m],[n];[m'],[n']}(\omega)] \times G_e{}^0([\mathbf{m}'];\epsilon)G_p{}^0([\mathbf{n}'];\omega-\epsilon), \tag{3.7}$$

where I is the overlap integral

$$I_{[m],[n]}(\mathbf{p})=\int\Psi_{[m]}(\mathbf{x})e^{-i\mathbf{p}\cdot\mathbf{x}}\phi_{[n]}(\mathbf{x})d^3x. \tag{3.8}$$

Taking note of the definition (2.4) of $G_{(p/e)}{}^0([\mathbf{m}];\omega)$, the ϵ integration in both (3.4) and (3.7) can be carried out by contour integration. Thus

$$\Omega_{[m],[n];[m'],[n']}(\omega) =\delta_{[m],[n']}\delta_{[n],[n']}+\{P_{[m],[n]}{}^+(\omega)+P_{[m],[n]}{}^-(\omega)\} \times\sum_{[k],[k']}H_{[m],[n];[k],[k']}\Omega_{[k],[k'];[m'],[n']}(\omega), \tag{3.9}$$

and

$$R[\mathbf{p}]=\frac{-i\lambda}{V}\sum_{[m],[n];[m'],[n']} I_{[m],[n]}(\mathbf{p})I_{[m'],[n']}{}^*(\mathbf{p}) \times\int\frac{d\omega}{2\pi}\Omega_{[m],[n];[m'],[n']}(\omega) \times e^{i\omega 0^+}[P_{[m'],[n']}{}^+(\omega)+P_{[m'],[n']}{}^-(\omega)], \tag{3.10}$$

with

$$P_{[m],[n]}{}^+(\omega)=\frac{\theta_e{}^{\text{u.o.}}([\mathbf{m}])\theta_p{}^{\text{u.o.}}([\mathbf{n}])}{E_{[n]}{}^p+E_{[m]}{}^e-\omega-i0^+} \tag{3.11a}$$

and

$$P_{[m],[n]}{}^-(\omega)=-\frac{\theta_e{}^{\text{o.}}([\mathbf{m}])\theta_p{}^{\text{o.}}([\mathbf{n}])}{E_{[n]}{}^p+E_{[m]}{}^e-\omega+i0^+}. \tag{3.11b}$$

Equations (3.9) and (3.10) can be reduced further. However, the analysis is quite tedious and, since all the quantities necessary to write down the final answer have now been defined, we leave the details to the Appendix. It is shown there that (3.9) can be replaced by the formula

$$R[\mathbf{p}]=\frac{\lambda}{V}\sum_{[m'],[n']}\theta_e{}^{\text{o.}}([\mathbf{m}'])\theta_p{}^{\text{o.}}([\mathbf{n}'])\Big|\sum_{[m],[n]}I_{[m],[n]}(\mathbf{p}) \times\Omega^0{}_{[m],[n];[m'],[n']}(E_{[n']}{}^p+E_{[m']}{}^e)\Big|^2 \tag{3.12}$$

where $\Omega^0{}_{[m],[n];[m'],[n']}(\omega)$ satisfies an equation identical to (3.9) except that the $P_{[m],[n]}{}^-(\omega)$ term does not appear. The $[\mathbf{n}']$ sum in (3.12) reduces to a single term $[\mathbf{n}']=[0]$ which is a consequence of the assumption that the positron is thermalized on annihilating. This leaves a single sum over the occupied single-particle electron states. We see that each electron can be treated separately. A final step is useful. Write

$$\Omega^0{}_{[m],[n];[m'],[0]}=\delta_{[m],[m']}\delta_{[n],[0]}+X^0{}_{[m],[n];[m'],[0]};$$

then X^0 satisfies the integral equation

$$X^0{}_{[m],[n];[m'],[0]}(\omega)=P_{[m],[n]}{}^+(\omega)[H_{[m],[n];[m'],[0]} +\sum_{[k],[k']}(H_{[m],[n];[k],[k']})X^0{}_{[k],[k'];[m'],[0]}(\omega)] \tag{3.13}$$

and

$$R[\mathbf{p}]=\frac{\lambda}{V}\sum_{[m']}\theta_e{}^{\text{o.}}([\mathbf{m}'])\Big|I_{[m'],[0]}(\mathbf{p})+\sum_{[m],[n]}I_{[m],[n]}(\mathbf{p}) \times(X^0{}_{[m],[n];[m'],[0]}(E_{[0]}{}^p+E_{[m']}{}^e))\Big|^2. \tag{3.14}$$

Equations (3.13) and (3.14) are the basic relations entering our formulation of the theory of positron annihilation in real metals. They are exact within the ladder approximation. In principle, they can be applied to a discussion of core annihilation or used to investigate lattice effects within the conduction-electron gas. An important question that needs to be settled in this regard is what value of enhancement factors must one use for the Fourier coefficients in the conduction-electron wave functions associated with nonzero inverse lattice vectors. From the rather complicated structure of Eq. (3.14) it appears that this problem can probably be resolved satisfactorily only by making a numerical calculation. Such considerations, however, should be only of secondary importance in the case of metallic sodium where most of the tails must come from core annihilation. For this reason we limit ourselves in the remainder of this paper to the exposition of a theory of core annihilation.

Consider for a moment expression (3.14) in the case where the Bloch label $[\mathbf{m}']$ refers to a core electron and the direct Coulomb force between the electron-positron pair is ignored. Only the first term remains and the expression for the partial annihilation rate reduces to the prescription of Berko and Plaskett.[6] Our general expression for $R[\mathbf{p}]$ goes beyond the independent-particle formulation of the problem and includes a correction term which has never been discussed in past treatments. In the next two sections we will try to better understand its physical meaning and get an idea of its relative importance. As we shall see it is numerically just as large as the conventional term although more difficult to handle.

4. CORE ANNIHILATION

We want to evaluate expression (3.14) when the Bloch label $[\mathbf{m}']$ refers to a core electron in the (nlm) band with crystal momentum $\mathbf{s}$ restricted to the first Brillouin zone. In the tight-binding approximation the wave function for such an electron is

$$\Psi_{[\mathbf{m}']}(\mathbf{x})=(1/\sqrt{N})\sum_{\mathbf{R}_\nu}e^{i\mathbf{s}\cdot\mathbf{R}_\nu}u_{nlm}(\mathbf{x}-\mathbf{R}_\nu), \quad (4.1)$$

where N is the number of primitive cells in the crystal and the $\mathbf{R}_\nu$'s are vectors giving the various lattice sites. The function $u_{nlm}(\mathbf{y})=(P_{nl}(y)/y)Y_{lm}(\hat{\mathbf{y}}/y)$ is the atomic Hartree-Fock wave function for the (nlm) shell of the corresponding free ion. The notation is as in the Hartree papers.

The first electron-positron overlap integral I appearing in (3.14) is well known and can be worked out to be

$$I_{[\mathbf{m}'];[0]}(\mathbf{p})=(N/V)^{1/2}\delta_{\mathbf{s}-\mathbf{p},\boldsymbol{\kappa}} \times[4\pi(2l+1)]^{1/2}i^l\delta_{m,0}J_{nl}{}^{+}(\mathbf{p}), \quad (4.2)$$

with

$$J_{nl}{}^{+}(p)=\int_0^\infty dr R_0{}^{+}(r)j_l(pr)P_{nl}(r). \quad (4.3)$$

In (4.2) $\boldsymbol{\kappa}$ is a reciprocal lattice vector, $j_l(pr)$ is the lth order spherical Bessel function and $R_0{}^{+}(r)/r$ is the lowest energy positron Bloch state.

To evaluate the second term in (3.14) we require the solution of Eq. (3.13) for the amplitude $X^0{}_{[\mathbf{m}],[\mathbf{n}];[\mathbf{m}'],[0]}$ which, at first sight, would seem to be a formidable if not hopeless task. Before discussing how it is nevertheless possible to get a very good approximate solution, it is necessary to make quite clear an important distinction between a core state and a conduction electron or positron single-particle Bloch function. Within each Wigner-Seitz cell a core state is highly localized about the center while a conduction state extends substantially throughout the cell volume. It follows that the value of a matrix element $[\mathbf{m}|\mathbf{q}|\mathbf{k}]$, where $[\mathbf{k}]$ is a core state and $[\mathbf{m}]$ is a conduction electron or positron wave function, is quite sensitive to the deviations of $[\mathbf{m}]$ from a plane wave. That is, band effects in $[\mathbf{m}]$ are essential in computing such overlap integrals. If however $[\mathbf{k}]$ is not a core state, band effects in both $[\mathbf{m}]$ and $[\mathbf{k}]$ are not so important, at least for the simpler metals, and it is then quite reasonable to set $[\mathbf{m}|\mathbf{q}|\mathbf{k}]$ equal to a delta function $\delta_{\mathbf{m}+\mathbf{q}-\mathbf{k},0}$.[10] We will return to these points in Sec. 5. For the moment we simply keep them in mind and proceed to evaluate X^0 given by (3.13).

First from (3.5) we have that

$$H_{[\mathbf{m}],[\mathbf{n}];[nlm\mathbf{s}],[0]}\cong(1/V)u_s(\mathbf{n})[\mathbf{m}|\mathbf{n}|nlm\mathbf{s}]^e \quad (4.4a)$$

and

$$H_{[\mathbf{m}],[\mathbf{n}];[\mathbf{k}],[\mathbf{k}']}\cong(1/V)u_s(\mathbf{n}-\mathbf{k}')\delta_{\mathbf{m}+\mathbf{n},\mathbf{k}+\mathbf{k}'}, \quad (4.4b)$$

where the labels $\mathbf{n}$, $\mathbf{m}$, $\mathbf{k}$, and $\mathbf{k}'$ on the right-hand side are ordinary momenta since we are using an extended-zone scheme. Thus (3.13) becomes,

$$X^0{}_{\mathbf{m},\mathbf{n};[nlm\mathbf{s}],0}(\omega)=P_{\mathbf{m},\mathbf{n}}{}^{+}(\omega)(1/V)u_s(\mathbf{n})[\mathbf{m}|\mathbf{n}|nlm\mathbf{s}]^e + P_{\mathbf{m},\mathbf{n}}{}^{+}(\omega)\sum_{\mathbf{k}}\frac{1}{V}u_s(\mathbf{k}-\mathbf{m})X^0{}_{\mathbf{k},\mathbf{n}+\mathbf{m}-\mathbf{k};[nlm\mathbf{s}],0}(\omega). \quad (4.5)$$

In $P_{\mathbf{m},\mathbf{n}}{}^{+}(\omega)$ the $\mathbf{m}$ and $\mathbf{n}$ index refer to excited states. We can then approximate the energies $E_{\mathbf{m}}{}^{e}$ and $E_{\mathbf{n}}{}^{p}$ appearing in its denominator by $(\mathbf{m})^2$ and $(\mathbf{n})^2$, respectively. Implied is our choice to measure electronic energies from the bottom of the $3s$ band and positron energies from the $1s$ band. Further $I_{[\mathbf{m}],[\mathbf{n}]}(\mathbf{p})$ in Eq. (3.14) can be safely replaced by a delta function $\delta_{\mathbf{m}+\mathbf{n},\mathbf{p}}$. Hence we need to know (4.5) only for $\mathbf{n}=\mathbf{p}-\mathbf{m}$. In this case we have

$$X^0{}_{\mathbf{m},\mathbf{p}-\mathbf{m};[nlm\mathbf{s}],0}(\omega)=J_{\mathbf{m},\mathbf{p}-\mathbf{m}}{}^{(1)}(\omega)[\mathbf{m}|\mathbf{p}-\mathbf{m}|nlm\mathbf{s}]^e + \sum_{\mathbf{k}}J_{\mathbf{m},\mathbf{p}-\mathbf{m};\mathbf{k}}{}^{(2)}(\omega)X^0{}_{\mathbf{k},\mathbf{p}-\mathbf{k};[nlm\mathbf{s}],0}(\omega) \quad (4.6)$$

with

$$J_{\mathbf{m},\mathbf{p}-\mathbf{m}}{}^{(1)}(\omega)=(1/V)P_{\mathbf{m},\mathbf{p}-\mathbf{m}}{}^{+}(\omega)u_s(\mathbf{p}-\mathbf{m}), \quad (4.7a)$$

$$J_{\mathbf{m},\mathbf{p}-\mathbf{m};\mathbf{k}}{}^{(2)}(\omega)=(1/V)P_{\mathbf{m},\mathbf{p}-\mathbf{m}}{}^{+}(\omega)u_s(\mathbf{k}-\mathbf{m}). \quad (4.7b)$$

To solve (4.6) we make the ansatz

$$X^0{}_{\mathbf{m},\mathbf{p}-\mathbf{m};[nlm\mathbf{s}],0}(\omega)=\sum_{\mathbf{k}}\Phi_{\mathbf{m},\mathbf{p}-\mathbf{m};\mathbf{k}}(\omega)J_{\mathbf{k},\mathbf{p}-\mathbf{k}}{}^{(1)}(\omega) \times[\mathbf{k}|\mathbf{p}-\mathbf{k}|nlm\mathbf{s}]^e. \quad (4.8)$$

Thus, $\Phi_{\mathbf{m},\mathbf{p}-\mathbf{m};\mathbf{k}}(\omega)$ must be given by

$$\Phi_{\mathbf{m},\mathbf{p}-\mathbf{m};\mathbf{k}}(\omega)=\delta_{\mathbf{m},\mathbf{k}}+\sum_{\mathbf{k}_1}(J_{\mathbf{m},\mathbf{p}-\mathbf{m};\mathbf{k}_1}{}^{(2)}(\omega))\Phi_{\mathbf{k}_1,\mathbf{p}-\mathbf{k}_1;\mathbf{k}}(\omega). \quad (4.9)$$

The quantity that enters (3.14) is

$$\sum_{\mathbf{m}}X^0{}_{\mathbf{m},\mathbf{p}-\mathbf{m};[nlm\mathbf{s}],[0]}(E_0{}^{p}+E_{[nlm\mathbf{s}]}{}^{e}),$$

which from (4.8) is equal to

$$\sum_{\mathbf{k}}\Big[\sum_{\mathbf{m}}\Phi_{\mathbf{m},\mathbf{p}-\mathbf{m};\mathbf{k}}(E_0{}^{p}+E_{[nlm\mathbf{s}]}{}^{e})\Big] \times J_{\mathbf{k},\mathbf{p}-\mathbf{k}}{}^{(1)}(E_0{}^{p}+E_{[nlm\mathbf{s}]}{}^{e})[\mathbf{k}|\mathbf{p}-\mathbf{k}|nlm\mathbf{s}]^e. \quad (4.10)$$

Because of our choice of zeros for measuring electron and positron energies $E_0{}^{p}=0$ and $E_{[nlm\mathbf{s}]}{}^{e}=-\Delta_{nl}$ where Δ_{nl} is the band gap between the core level $[nlm\mathbf{s}]$ and the bottom of the $3s$ band.

By first iterating (4.9) and then summing over $\mathbf{m}$ one can easily verify that if we define

$$X_{\mathbf{p}}(\mathbf{k};\omega)=\sum_{\mathbf{m}}\Phi_{\mathbf{m},\mathbf{p}-\mathbf{m};\mathbf{k}}(\omega),$$

then $X_{\mathbf{p}}(\mathbf{k};\omega)$ is given by

$$X_{\mathbf{p}}(\mathbf{k};\omega)=1+\frac{1}{V}\sum_{\mathbf{k}_1}X_{\mathbf{p}}(\mathbf{k}_1;\omega)P_{\mathbf{k}_1,\mathbf{p}-\mathbf{k}_1}{}^{+}(\omega)u_s(\mathbf{k}-\mathbf{k}_1). \quad (4.11)$$

[10] Notice that at this point we are explicitly making use of an extended zone scheme to specify the conduction and higher excited electron as well as positron states.

Thus the second term in 3.14 becomes

$$(1/V)\sum_{\mathbf{k}} \epsilon_{\mathbf{p}}{}^{nl}(\mathbf{k})[\mathbf{k}|\mathbf{p}-\mathbf{k}|nlms]^e \qquad (4.12)$$

with

$$\epsilon_{\mathbf{p}}{}^{nl}(\mathbf{k})=X_{\mathbf{p}}(\mathbf{k};-\Delta_{nl})[P_{\mathbf{k},\mathbf{p}-\mathbf{k}}{}^{+}(-\Delta_{nl})]u_s(\mathbf{p}-\mathbf{k}).$$

Perhaps the most important quantities that enter the theory of core annihilation are the matrix elements $[\mathbf{k}|\mathbf{p}-\mathbf{k}|nlms]^e$. These enter when one wants to account for the possible virtual transitions of core electrons to unoccupied electron states induced by the positron Coulomb field.

All the approximations made so far are quite reasonable. Also the amplitude $X_{\mathbf{p}}(\mathbf{k};-\Delta_{nl})$ can be reliably calculated on an electronic computer. The overlap integral $[\mathbf{k}|\mathbf{p}-\mathbf{k}|nlms]^e$ however presents some difficulty and our ability to make an accurate estimate of core annihilation depends very much on how well such matrix elements can be computed. To see more clearly what this involves we rewrite $[\mathbf{k}|\mathbf{p}-\mathbf{k}|nlms]^e$ in the form

$$\left(\frac{N}{V}\right)^{1/2}\delta_{\mathbf{p}-\mathbf{s},\kappa}\int e^{i\mathbf{p}\cdot\mathbf{x}}u_{\mathbf{k}}(\mathbf{x})\frac{P_{nl}(r)}{r}Y_{lm}{}^{*}(\hat{x}/x)d^3x. \qquad (4.13)$$

Again we point out that since $P_{nl}(r)$ peaks strongly somewhere inside the ion core, the precise deviations of $u_{\mathbf{k}}(\mathbf{x})$ from 1 in this region will dominate the value of (4.13). There is in addition a strong directional dependence implied by the spherical harmonic $Y_{lm}(\hat{x}/x)$ for $l\neq 0$. Because of this angular factor only the l part of the product $e^{i\mathbf{p}\cdot\mathbf{x}}u_{\mathbf{k}}(\mathbf{x})$ contributes to this integral. We will not emphasize these points further here except to note that such quantities are well known in the theory of lattice dynamics. The matrix elements that are important there are between an occupied and an unoccupied conduction state. When one or more orthogonalized plane waves are used to describe the conduction states, matrix elements of the type (4.13) enter.

For a simple metal like sodium it may be argued that a single orthogonalized plane wave (O.P.W.) should give reasonable results. This is a particularly attractive suggestion since for the present problem we do not need to know $[\mathbf{k}|\mathbf{p}-\mathbf{k}|nlms]^e$ for all $\mathbf{k}$'s but only the angular average of the product of $[\mathbf{k}|\mathbf{p}-\mathbf{k}|nlms]^e$ with the weighting function $\epsilon_{\mathbf{p}}{}^{nl}(\mathbf{k})$. However, such a calculation requires heavy numerical computations which inevitably obscure the basic underlying physics. In this paper we set ourselves a rather more modest goal. We will study core annihilation using a simple although admittedly crude model for the conduction-electron Bloch states in sodium. We hope in this way to arrive at a qualitative understanding of the important physical features entering a more refined calculation. The choice of the model was to a large extent motivated by the practical reason that the computations should be simple. We have not made a critical analysis of the errors introduced in this way although we shall see in Sec. 5 that the model does not lead to agreement with experiment. It is nevertheless relevant since there can be little doubt that the important ingredients of a more complete calculation are ncluded.

Before specifying the model, we would like to collect in a single formula the two contributions (4.2) and (4.12) to $R[\mathbf{p}]$ coming from a core electron in the state $[nlms]$. Using an obvious notation,

$$R^{nlms}[\mathbf{p}]=(\lambda/V)(N/V)\delta_{\mathbf{p}-\mathbf{s},\kappa}4\pi(2l+1)\times|i^l\delta_{m,0}J_{nl}{}^{+}(\mathbf{p})+\mathcal{J}_{nl}{}^{m}(\mathbf{p})|^2, \qquad (4.14)$$

where

$$\mathcal{J}_{nl}{}^{m}(\mathbf{p})=\int e^{i\mathbf{p}\cdot\mathbf{x}}M_{\mathbf{p}}(\mathbf{x})P_{nl}(r)rdr\frac{d\Omega_{\mathbf{x}}}{[4\pi(2l+1)]^{1/2}}Y_{lm}{}^{*}(\hat{x}/x) \qquad (4.15)$$

with

$$M_{\mathbf{p}}(\mathbf{x})=1/V\sum_{\mathbf{k}}\epsilon_{\mathbf{p}}{}^{nl}(\mathbf{k})u_{\mathbf{k}}(\mathbf{x}). \qquad (4.16)$$

Finally, to get the contribution from the entire shell (nl) we must sum (4.14) over the magnetic quantum number m and all $\mathbf{s}$'s in the first Brillouin zone. For fixed $\mathbf{p}$ as $\mathbf{s}$ ranges over this zone the delta function $\delta_{\mathbf{p}-\mathbf{s},\kappa}$ clicks for a unique $\boldsymbol{\kappa}$. Thus

$$R^{nl}[\mathbf{p}]=2(2l+1)R^0(4\pi/V)\times\sum_m|i^l\delta_{m,0}J_{nl}{}^{+}(\mathbf{p})+\mathcal{J}_{nl}{}^{m}(\mathbf{p})|^2, \qquad (4.17)$$

where a factor of 2 was introduced for spin degeneracy and R^0 is the Sommerfeld total annihilation rate.

Formula (4.17) is still an almost exact expression for core annihilation, We now make the most serious approximation of the present discussion. Assume that the unoccupied conduction states as well as all higher excited Bloch states can be approximated by $(1/\sqrt{V})e^{i\mathbf{k}\cdot\mathbf{x}}u_0(\mathbf{x})$ where $u_0(\mathbf{x})$ is the state at the bottom of the conduction band. Then (4.16) reduces to $X^{nl}(\mathbf{p})u_0(\mathbf{x})$ where $X^{nl}(\mathbf{p})=1/V\sum_{\mathbf{k}}\epsilon_{\mathbf{p}}{}^{nl}(\mathbf{k})$. Hence (4.17) becomes

$$R^{nl}[\mathbf{p}]=2(2l+1)R^0(4\pi/V)\times|J_{nl}{}^{+}(\mathbf{p})+X^{nl}(\mathbf{p})J_{nl}{}^{-}(\mathbf{p})|^2, \qquad (4.18)$$

where $J_{nl}{}^{-}$ is defined by (4.3) except that instead of the positron function $R_0{}^{+}(r)$ the electron function $R_0{}^{-}(r)=ru_0(x)$ is to appear. This is a relatively simple formula. The "effective enhancement factor" $X^{nl}(p)$ can be written as $\sum^0_{\mathbf{m}}\Phi_{\mathbf{m},\mathbf{p}-\mathbf{m}}(-\Delta_{nl})$ with $\Phi_{\mathbf{m},\mathbf{p}-\mathbf{m}}{}^0(-\Delta_{nl})$ satisfying an integral equation very similar to that discussed in CK,[11] namely

$$\Phi_{\mathbf{m},\mathbf{p}-\mathbf{m}}{}^0(-\Delta_{nl})=[\theta(m-P_F)/(m^2+(\mathbf{p}-\mathbf{m})^2+\Delta_{nl})]u_s(\mathbf{p}-\mathbf{m})+[\theta(m-P_F)/m^2+(\mathbf{p}-\mathbf{m})^2+\Delta_{nl}](1/V)\times\sum_{\mathbf{q}}u_s(\mathbf{q})\Phi_{\mathbf{q}+\mathbf{m},\mathbf{p}-\mathbf{q}-\mathbf{m}}{}^0(-\Delta_{nl}). \qquad (4.19)$$

To see how this comes about it is perhaps simplest to recall the definition of $X^{nl}(\mathbf{p})$ and $X_{\mathbf{p}}(\mathbf{k};-\Delta_{nl})$. By

[11] See Sec. 6 of Ref. 2.

definition

$$X^{nl}(\mathbf{p}) = (1/V)\sum_{\mathbf{k}} X_{\mathbf{p}}(\mathbf{k}; -\Delta_{nl}) P_{\mathbf{k},\mathbf{p}-\mathbf{k}}{}^{+}(-\Delta_{nl}) u_s(\mathbf{p}-\mathbf{k})$$
$$= (1/V)\sum_{\mathbf{k}} [\sum_{\mathbf{m}} \Phi_{\mathbf{m},\mathbf{p}-\mathbf{m};\mathbf{k}}(-\Delta_{nl})] \times [P_{\mathbf{k},\mathbf{p}-\mathbf{k}}{}^{+}(-\Delta_{nl})] u_s(\mathbf{p}-\mathbf{k})$$
$$= (1/V)\sum_{\mathbf{m}} [\sum_{\mathbf{k}} \Phi_{\mathbf{m},\mathbf{p}-\mathbf{m};\mathbf{k}}(-\Delta_{nl}) \times \{P_{\mathbf{k},\mathbf{p}-\mathbf{k}}{}^{+}(-\Delta_{nl})\} u_s(\mathbf{p}-\mathbf{k})]$$
$$= (1/V)\sum_{\mathbf{m}} \Phi_{\mathbf{m},\mathbf{p}-\mathbf{m}}{}^{0}(-\Delta_{nl}),$$

where the last equality defines $\Phi_{\mathbf{m},\mathbf{p}-\mathbf{m}}{}^{0}(-\Delta_{nl})$. From (4.7b) and Eq. (4.9) we see immediately that $\Phi_{\mathbf{m},\mathbf{p}-\mathbf{m}}{}^{0}(-\Delta_{nl})$ satisfies Eq. (4.18). This completes the algebraic part of the paper and we turn now to a numerical calculation of core annihilation based on the approximate formula (4.18).

5. NUMERICAL RESULTS

Our starting point is the approximate expression (4.18). Since this expression for $R^{nl}[\mathbf{p}]$ is based on a simplified model for the conduction Bloch states the results obtained will not be as important as the physical picture which emerges.[12] The necessary ingredients are the overlap integrals $J^{\pm}(\mathbf{p})$ and the "effective enhancement factors" $X^{nl}(\mathbf{p})$. In computing $J_{nl}{}^{-}(\mathbf{p})$ we used the conduction Bloch state $u_0(\mathbf{x})$ as tabulated by Callaway,[13] and the core functions for Na^{+} were taken from a paper by Hartree and Hartree.[14]

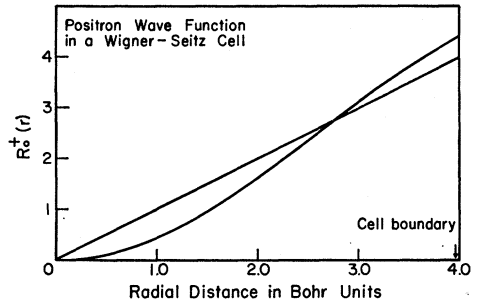

FIG. 1. Normalized positron wave function in a Wigner-Seitz cell as a function of distance from the center. The straight line of slope one corresponds to a plane wave.

To determine the positron Bloch state $v_0(\mathbf{x})$ at the bottom of the 1s band, a cellular method was used. In each Wigner-Seitz cell the average Hartree field acting on the positron was taken to be the potential from the rigid ion core plus that of a single valence electron smeared uniformly throughout the cell. The results for $R_0{}^{+}(r) = rv_0(r)$ are shown in Fig. 1. Over the entire cell we can state that deviations from a straight line are small although inside the core they can amount to much more than 50%. For comparison we have also plotted the electron function $R_0{}^{-}(r) = ru_0(r)$ in Fig. 2. Notice that the main difference between $R_0{}^{+}(r)$ and $R_0{}^{-}(r)$ is inside the core. This is a consequence of the Pauli exclusion principle requiring $R_0{}^{-}(r)$ to have two nodes. We stress this here, since as we shall see next $J^{+}(\mathbf{p})$ and $J^{-}(\mathbf{p})$ are quite distinct functions of momentum $\mathbf{p}$ although they differ only through the appearance of $R_0{}^{+}(r)$ rather than $R_0{}^{-}(r)$ in the defining overlap integral. This is, of course, because the core function in these quadratures effectively emphasizes only a relatively small part of the $R_0(r)$'s near the origin. In passing we point out again that this is in contrast to the case when both functions under consideration extend throughout the cell with maximum weight at the cell boundary. Deviations from plane waves now amount to only small corrections to the main contribution.

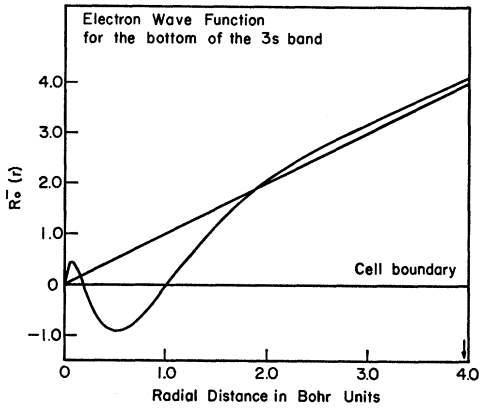

FIG. 2. Normalized electron wave function $R_0{}^{-}(r) = ru_0(r)$ as given by Callaway (Ref. 13)

The overlap integrals $J_{nl}{}^{\pm}(\mathbf{p})$ for the 2s and 2p electrons are shown in Figs. 3 and 4, respectively. The 1s integrals are negligibly small. We see explicitly now that for any given shell (nl) the two curves $J^{+}(\mathbf{p})$ and $J^{-}(\mathbf{p})$ are really considerably different and do not carry the same sign for all p's. Thus, when these are added and the

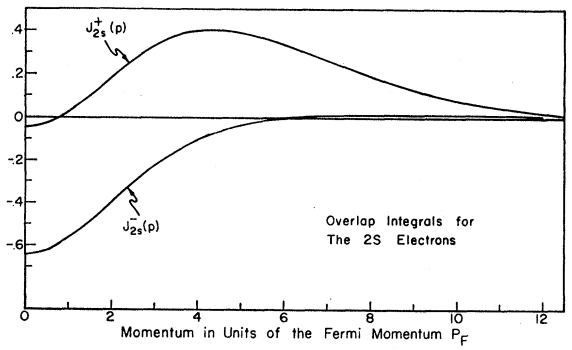

FIG. 3. The overlap integrals $J^{+}(p)J^{-}(p)$ and or the 2s electrons.

[12] Note: The results of this section were presented at The Wayne State University Positron Annihilation Conference, 1965 (unpublished).

[13] J. Callaway, Phys. Rev. **123**, 1255 (1961).

[14] D. R. Hartree and W. Hartree, Proc. Roy. Soc. (London) **A193**, 299 (1948).

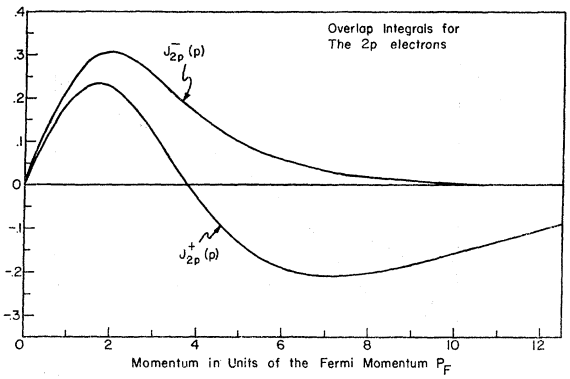

FIG. 4. The overlap integrals $J^+(p)$ and $J^-(p)$ for the $2p$ electrons.

sum squared as prescribed by Eq. (4.18), destructive interference between the two terms takes place. This is certainly a feature that will remain in a more exact calculation. It should be quite apparent also that our model is only qualitatively correct and that to get reliable results we need to treat with much more care the conduction-core matrix elements $[\mathbf{k}|\mathbf{p}-\mathbf{k}|nlms]^e$.

Next we must compute the effective enhancement factors $X^{nl}(\mathbf{p})$. Because of the rather large energy parameters[15] $\Delta_{nl}(\Delta_{2s}\cong 60$ eV, $\Delta_{2p}\cong 27$ eV) entering the denominator of (4.19), one might argue that the Born approximation is sufficient to calculate the necessary amplitude. This turns out not to be the case. The results from the solution of the integral Eq. (4.19) are compared with those from the Born approximation in Fig. 5. Clearly, to get reasonable enhancement factors for small p's we cannot use first-order perturbation theory. This is another important feature of the problem which will have to be kept in mind in any further work. As a consistency check, notice that as p increases, the difference between the $2p$ and $2s$ enhancement factors becomes less pronounced and both tend towards the Born-approximation result. This is precisely what we expect intuitively.

The answer for the two-photon counting rate,

$$R_{p_z}=R^0\sum_{nl}(2l+1)\int_{p_z}^{\infty}\frac{2udu}{\pi}|J_{nl}^+(u)+X^{nl}(u)J_{nl}^-(u)|^2,$$

is shown in Fig. 6, where we also compare our results with those of the usual simple theory. Although the two curves are similar the areas under them are quite different. Without enhancement we get a total annihilation rate of $R^{\text{core}}=1.02R^0$ while including polarization corrections we find $R^{\text{core}}=2.23R^0$.

Finally we compare our results with experiment. In CK the best theoretical value for the total rate coming from the conduction electrons is $R^{\text{cond}}=14.03R^0$. Thus we arrive at a composite result $R^{\text{total}}=R^{\text{core}}+R^{\text{cond}}=3.12\times10^9$ sec^{-1} which agrees well with the experimental value given by Bell and Jørgensen.[16] However, the agreement with the two photon counting rate as recently measured by Stewart[17] is not good. For momentum p just above the Fermi surface, core annihilation accounts for only half the experimental tails while our simple model seems to introduce too many events around $2p_F$ and further out. A better calculation of core annihilation is necessary. Also, even for sodium, a small part of the tails is certainly due to lattice effects within the conduction-electron gas—a question which needs further investigation.

6. DISCUSSION AND CONCLUSION

On the basis of the ladder approximation to the electron-positron correlation function we have managed to derive an expression for the partial annihilation rate which is applicable to real metals, i.e. a crystal-lattice potential is included. When our general formula is specialized to the case of conduction electrons we find that, without carrying out an actual numerical calculation, it is difficult to make specific quantitative statements about lattice corrections to an electron gas theory. In particular, the expression obtained does not break up into the independent-particle-model result multiplied by a slowly varying enhancement factor as one may have naively expected. Our main concern in this paper, however, was to develop a theory of core annihilation. To reduce the general expression to a more tractable form it was necessary to make a plane-wave approximation when computing intermediate matrix elements involving only conduction electron or positron states. This enables us to write the contribution to the partial annihilation rate $R[\mathbf{p}]$ from any given core electron as the square of the sum of two terms. The first is the usual single particle result, while the second is more complicated. It involves an effective enhancement factor $\epsilon_{\mathbf{p}}(\mathbf{k})$ depending on $\mathbf{p}$ and some extra index $\mathbf{k}$ which is to be multiplied with an overlap integral of the appropriate core function and an unoccupied conduction state $[\mathbf{k}]$ modulated by a plane wave of momentum $\mathbf{p}-\mathbf{k}$. The entire expression is then to be summed over

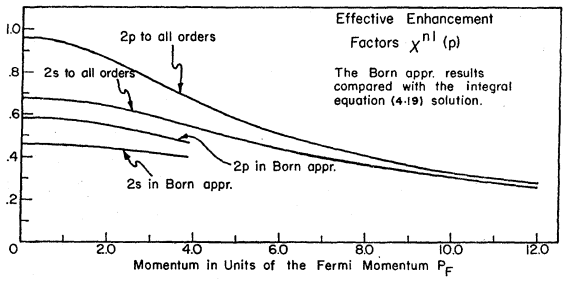

FIG. 5. Comparison of the effective enhancement factors $X^{nl}(p)$ with the Born approximation.

[15] These parameters were supplied to the author by Dr. T. Watanabe from x-ray-emission data.

[16] R. E. Bell and M. H. Jørgensen, Can. J. Phys. 38, 652 (1960).

[17] A. T. Stewart (private communication).

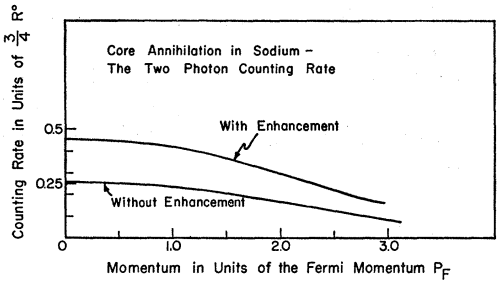

FIG. 6. The contribution of the core electrons to the two-photon counting rate as given by formula (4.18). The lower curve gives the results of the usual independent-particle theory.

all unoccupied states. This term accounts for the polarization of the ion core by the incident positron.

By studying a model, we conclude that the enhancement factors $\epsilon_p(\mathbf{k})$ cannot be calculated in Born approximation despite the appearance of relatively large energy-gap parameters in the denominator of the defining integral Eq. (4.19). Further the core-conduction overlap integrals $[\mathbf{k}|\mathbf{p}-\mathbf{k}|nlm\mathbf{s}]^e$ are sensitive to the precise deviations of the $[\mathbf{k}]$'s from plane waves inside the core and must be evaluated with some care. This difficulty is further emphasized in the present context because delicate destructive interference occurs between the single-particle term and the core-polarization corrections which do not necessarily carry the same sign for each momentum p.

The calculation does not give good agreement with experiment. This is no surprise as the discrepancy is without doubt a result of the limitations of our model. There is no reason, at least at present, to assign it to a breakdown, for instance, of the ladder approximation for core electrons. A careful calculation based on the nearly exact expression (4.17) rather than on the simpler, but quite approximate relation (4.18) should lead to a considerable improvement in the final results, although we expect no important change in the general qualitative features of the problem to come from such a refinement. An accurate computation of core annihilation is then more involved than calculating lifetimes in a conduction electron gas. Not only must we solve a rather complicated integral equation of the form (4.11) for a number of $\mathbf{p}$'s and all $\mathbf{k}$'s above the Fermi surface, but we also need to know the conduction-core overlap integrals. We plan to carry out such a calculation in the near future.

In concluding we would like to stress again that the positron Coulomb field plays a dominant role in the annihilation process.[18] Thus, the positron is in some ways a poor probe since it distorts significantly the electronic configuration of which we would like information. This is certainly a serious limitation on the method, but it can be overcome if we learn how to calculate accurately this distortion—an undeniably hard, but not impossible problem. For the near future, however, it seems likely that the aim of theoretical calculations will be to reproduce the experimental angular correlation curves and total rates simultaneously, rather than attempt to extract from the counting rates alone detailed information of a fundamental nature about the momentum distributions in real metals. On the other hand, there is substantial evidence, both experimental and theoretical that the method can be used to map out quite directly the Fermi surface in momentum space. On the theoretical side there is a paper by Majumdar[19] in which a proof is given that the positron force does not disturb the Fermi surface in the sense that there should be a sharp discontinuity in slope in the two-photon counting rate at the true Fermi momentum p_F in any given z direction. This result is further supported by the numerical work of Ref. 2. Experimentally, as instrument resolution has been improved over the years the discontinuity at p_F has become sharper and in a number of metals, variations of p_F with direction have been observed. A good example of this is beryllium.[20] It should be stated, however, that such measurements do not detect directly the difference between p_F in two distinct directions, but rather determine the total p_F in each direction separately, so that instrument resolution is an important factor.

ACKNOWLEDGMENTS

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APPENDIX

In this Appendix we wish to start from Eq. (3.9) and (3.10) and show that the partial annihilation rate can be rewritten in the form (3.12). In order not to obscure the basic but quite simple idea which is central to the development that follows, it is convenient to introduce a formal matrix notation. This allows us to suppress the explicit Bloch state labels in (3.9) and (3.10) and deal with operator quantities rather than matrix elements. Symbolically we rewrite (3.9) as

$$\Omega(\omega)=1+(P^+(\omega)+P^-(\omega))H\Omega(\omega)\,, \tag{A1}$$

where for instance

$$\langle\mathbf{m},\mathbf{n}|P^{\pm}(\omega)|\mathbf{m}',\mathbf{n}'\rangle=[P_{[\mathbf{m}],[\mathbf{n}]}{}^{\pm}(\omega)]\delta_{[\mathbf{m}],[\mathbf{m}']}\delta_{[\mathbf{n}],[\mathbf{n}']}\,, \tag{A2a}$$

and

$$\langle\mathbf{m},\mathbf{n}|H|\mathbf{m}',\mathbf{n}'\rangle=H_{[\mathbf{m}],[\mathbf{n}];[\mathbf{m}'],[\mathbf{n}']}\,. \tag{A2b}$$

Whenever a set of intermediate Bloch labels is introduced a summation is always implied. Our notation

[18] A relevant reference here is the recent work on solid argon by E. J. Woll, Jr., and K. L. Rose, Phys. Rev. (to be published).

[19] C. K. Majumdar, Phys. Rev. **140**, A227 (1965).

[20] S. Berko, Phys. Rev. **128**, 2166 (1962).

should now be clear. Further, the partial annihilation rate is

$$R[\mathbf{p}]=-(i\lambda/V)\sum_{[\mathbf{m}],[\mathbf{n}];[\mathbf{m}'],[\mathbf{n}']} I_{[\mathbf{m}],[\mathbf{n}]}(\mathbf{p})I_{[\mathbf{m}'],[\mathbf{n}']}{}^{*}(\mathbf{p})$$
$$\times\int\frac{d\omega}{2\pi}e^{i\omega 0^{+}}\langle\mathbf{m},\mathbf{n}|\,\Omega(\omega)(P^{+}(\omega)+P^{-}(\omega))\,|\mathbf{m}',\mathbf{n}'\rangle. \quad \text{(A3)}$$

We fix our attention on the integrand $\Omega(\omega)(P^{+}(\omega)+P^{-}(\omega))$. Consider iterating (A1) for the amplitude $\Omega(\omega)$ before attempting the ω integration. This leads to an infinite number of terms, the integrand for the nth contribution being

$$e^{i\omega 0^{+}}(P^{+}+P^{-})H(P^{+}+P^{-})\cdots H(P^{+}+P^{-}), \quad \text{(A4)}$$

where $(n-1)$ H's are to appear. The first term must be treated separately. In this case the integral of interest is

$$\int\frac{d\omega}{2\pi}e^{i\omega 0^{+}}(P_{[\mathbf{m}],[\mathbf{n}]}{}^{+}(\omega)+P_{[\mathbf{m}],[\mathbf{n}]}{}^{-}(\omega))\delta_{[\mathbf{m}],[\mathbf{m}']}\delta_{[\mathbf{n}],[\mathbf{n}']} \quad \text{(A5)}$$

which, recalling the definition (3.11), can be evaluated trivially by contour integration in the upper half plane. Only P^{-} contributes. The result is

$$i\theta_{e}{}^{0}\cdot([\mathbf{m}])\theta_{p}{}^{0}\cdot([\mathbf{n}])\delta_{[\mathbf{m}],[\mathbf{m}']}\delta_{[\mathbf{n}],[\mathbf{n}']}. \quad \text{(A6)}$$

For $n\geq 2$ the quantity (A4) can be expressed further as the sum of 2^{n} products, a possible member being

$$P^{+}HP^{+}H\cdots HP^{+}, \quad \text{(A7)}$$

where the exponential factor has now been dropped since it is irrelevant for $n\neq 1$. As a function of a complex variable ω, expression (A7) is analytic in the upper-half-plane and therefore contributes nothing to $R[\mathbf{p}]$. Another possible product occurring is (A7) with one of the P^{+}'s replaced by a P^{-}. There are, in fact, n such products

$$\begin{aligned}&P^{-}HP^{+}HP^{+}\cdots P^{+}HP^{+},\\ &P^{+}HP^{-}HP^{+}\cdots P^{+}HP^{+},\\ &P^{+}HP^{+}HP^{+}\cdots P^{+}HP^{-}.\end{aligned} \quad \text{(A8)}$$

If an intermediate amplitude Ω^{0} and its conjugate $\Omega^{0\dagger}$ are introduced by the equations

$$\Omega^{0}=1+P^{+}H\Omega^{0}, \quad \text{(A9a)}$$

$$\Omega^{0\dagger}=1+\Omega^{0\dagger}HP^{+}, \quad \text{(A9b)}$$

then clearly the nth term in the perturbation expansion of $\Omega^{0}P^{-}\Omega^{0}$ is just (A8).

Provided the only nth order terms in the expansion of $\Omega(P^{+}+P^{-})$ contributing to $R[\mathbf{p}]$ are the (n) products of (A8), we can write the partial annihilation rate (A3) in the form

$$R[\mathbf{p}]=-\frac{i\lambda}{V}\sum_{[\mathbf{m}],[\mathbf{n}];[\mathbf{m}'],[\mathbf{n}']} I_{[\mathbf{m}],[\mathbf{n}]}(\mathbf{p})I_{[\mathbf{m}'],[\mathbf{n}']}{}^{*}(\mathbf{p})$$
$$\times\int\frac{d\omega}{2\pi}e^{i\omega 0^{+}}\langle\mathbf{m},\mathbf{n}|\,\Omega^{0}(\omega)P^{-}(\omega)\Omega^{0\dagger}(\omega)\,|\mathbf{m}',\mathbf{n}'\rangle, \quad \text{(A10)}$$

where the first-order term is also included. But as a function of a complex ω all the singularities of $\Omega^{0}(\omega)$ and $\Omega^{0\dagger}(\omega)$ are in the lower half-plane. Closing the contour above and introducing a set of intermediate states we get immediately

$$R[\mathbf{p}]=\frac{\lambda}{V}\sum_{[\mathbf{m}''],[\mathbf{n}'']}\theta_{e}{}^{0}\cdot([\mathbf{m}''])\theta_{p}{}^{0}\cdot([\mathbf{n}''])$$
$$\times[\sum_{[\mathbf{m}],[\mathbf{n}]}I_{[\mathbf{m}],[\mathbf{n}]}(\mathbf{p})\Omega_{[\mathbf{m}],[\mathbf{n}];[\mathbf{m}''],[\mathbf{n}'']}{}^{0}(E_{[\mathbf{m}'']}{}^{e}+E_{[\mathbf{n}'']}{}^{p})]$$
$$\times[\sum_{[\mathbf{m}'],[\mathbf{n}']}I_{[\mathbf{m}'],[\mathbf{n}']}{}^{*}(\mathbf{p})\Omega_{[\mathbf{m}''],[\mathbf{n}''];[\mathbf{m}'],[\mathbf{n}']}{}^{0\dagger}$$
$$\times(E_{[\mathbf{m}'']}{}^{e}+E_{[\mathbf{n}'']}{}^{p})]. \quad \text{(A11)}$$

In this last equation the expression in the second square bracket is just the complex conjugate of that occurring in the first bracket. After a trivial redefinition of the Bloch labels Eq. (3.12) follows. To complete the proof we need only convince ourselves that terms of the form (A7) with at least two P^{+}'s replaced by P^{-}'s make no contribution to $R[\mathbf{p}]$. This can be seen quite easily. Notice that each $P^{-}(\omega)$ factor contains a positron theta function $\theta_{p}{}^{0}\cdot([\mathbf{n}])$ i.e. a delta function which can be used to eliminate one of the intermediate Bloch state summations leaving a factor one over the volume (V) in front of this term with no corresponding summation. This clearly leads to a contribution of the order $1/V$ as compared to those from the (A8) terms. Since as we shall see these latter terms are finite, all further terms must vanish in the limit of infinite volume. Or, stated in a more physical way, such contributions must be proportional to at least the first power of the positron density in the system, which is negligibly small.