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Positronium Formation in Positron-Hydrogen Collisions*

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The Harris–Nesbet algebraic close-coupling method is used to calculate the S-wave phase shift and positronium-formation cross section for various types of close-coupling expansions of the total wave function. The positronium channels are included explicitly, and polarization effects, in both the hydrogen and positronium atoms, are incorporated by pseudostates that give the correct static polarizabilities.

I. INTRODUCTION

This paper presents the results of a study of low-energy positron-hydrogen collisions by the close-coupling scheme for energies up to the second-excitation threshold of hydrogen. The main purpose of this work was to include explicitly the positronium channels as well as polarization effects. Only the zero-total-angular-momentum states of the system are considered.

Positronium formation by positron-hydrogen impact is a model three-body rearrangement-collision problem. Because of the unavailability of a low-energy positron source as well as an atomic hydrogen gas, there are as yet no experimental data available. However, various theories have been applied to this problem giving an amazingly inconsistent set of results.

The Born approximation was first applied to this problem by Massey and Mohr[1] yielding a peak of $4.5\pi a_0^2$ for the formation cross section at ~ 14 eV. This maximum is ten times smaller than that calculated later by Cheshire[2] using the impulse approximation. However, these approximations are known to be poorly defined for rearrangement collisions. Also it is well established that the Born approximation breaks down for low energies since one cannot assume a plane-wave form for the scattered-particle wave function.

Two major works have appeared that dealt with the low-energy aspect of this problem. Chen and Mittleman[3] have shown that a geometric rearrangement of the coordinates normally chosen leads to an approximate set of coupled ordinary differential equations for which solutions are relatively easy to calculate. The geometric rearrangement corresponds basically to labeling specifically the coordinate of the outgoing positron in the positronium channel rather than the center of mass of the positronium atom as is usually done. Fels and Mittleman[4] applied the above approximation using trial phenomenological potentials to describe polarization in both the hydrogen and positronium atoms. They obtained a positronium-formation cross section which is 40 times below that of the Born approximation. Bransden and Jundi[5] did a nonvariational calculation using a projection-operator formalism. The method of polarized orbitals was employed to incorporate the polarization effects. Their positronium-formation results are drastically different from those of Fels and Mittleman; however, both of the above works have particularly emphasized the dominance of the polarization forces on the cross section.

More recently, Majumdar and Rajagopal[6] solved the problem using equations of three-particle scattering which in principle leads to Faddeev equations. Their cross section showed a peak which is 25% higher than that of given by the Born approximation but drops below the Born results at high energies.

In a very recent pair of articles,[7,8] Dirks and Hahn have carried on what seems to be the first fairly rigorous work on the positron-hydrogen problem for low energies. The generalized variational-bounds method of Hahn,[9] which correctly treats the nonorthogonality problem of the rearrangement channels, was applied in a two-channel approximation for energies between the positronium-formation threshold and the $n = 2$ threshold of hydrogen. Their positronium-formation cross section is about a factor of π less than that of Fels and Mittleman[4] while both are considerably smaller than that found by Bransden and Jundi.[5]

For the elastic-scattering case (i.e., incident energies below the 1s threshold of positronium) Schwartz[10] and more recently Bhatia *et al.*[11] have done the most rigorous calculations to date. Schwartz used an elaborate Hylleraas trial wave function while Bhatia *et al.* employed a similar trial wave function with added flexibility in the nonlinear parameters. The resulting calculations were very tedious and yielded phase shifts which are generally assumed to be exact.

The most workable method to date for low-energy inelastic processes is the close-coupling method advanced by Burke and his followers.[12] The calculations reported in this paper have been done within the framework of this method using the recent algebraic techniques advanced by Harris[13] and Nesbet[14] to solve the resulting equations. The details of the close-coupling method and algebraic solutions are sketched in Sec. II. Section III discusses the various approximations used to represent the effects of virtual transitions to closed channels not explicitly included in the trial wave function. In Sec. IV the elastic phase shifts and inelastic cross sections are presented.

II. THEORY

A direct application of the close-coupling method to positron-hydrogen scattering with the inclusion of the positronium channels leads to a system of coupled integrodifferential equations. The integral terms contain nonanalytical kernels times the undetermined scattered functions.[15] Since it is very hard if not impossible to solve these equations by the usual iterative methods for more than two channels, we have resorted to the algebraic close-coupling method of Callaway *et al.*,[16] a derivative of the Harris–Nesbet variational principle.[14] Consider the reaction

$$e^+ + \mathrm{H} \to (e^+, e^-) + \mathrm{H}^+ \,. \tag{2.1}$$

The Hamiltonian operator for the Schrödinger equation has two equivalent forms: before collision,

$$\hat{H} = -\frac{\hbar^2}{2m}\nabla_{\vec{r}_1}{}^2 - \frac{\hbar^2}{2m}\nabla_{\vec{r}_2}{}^2 - \frac{e^2}{r_1} + \frac{e^2}{r_2} - \frac{e^2}{|\vec{r}_1 - \vec{r}_2|}\,; \tag{2.2}$$

and after collision,

$$\hat{H} = -\frac{\hbar^2}{m}\nabla_{\vec{\rho}}{}^2 - \frac{\hbar^2}{4m}\nabla_{\vec{R}}{}^2 - \frac{2e^2}{\rho} - \frac{e^2}{|\vec{R} - \frac{1}{2}\vec{\rho}|} + \frac{e^2}{|\vec{R} + \frac{1}{2}\vec{\rho}|}\,, \tag{2.3}$$

where $\vec{r}_1$ is the coordinate of the orbital electron, $\vec{r}_2$ that of the incident positron, and

$$\rho = |\vec{r}_1 - r_2|\;;\quad \vec{R} = \tfrac{1}{2}(\vec{r}_1 + \vec{r}_2)\,. \tag{2.4}$$

The wave function for the above reaction is written in the standard close-coupling expansion form as

$$\Psi^L(1,2) = \sum_{nl_1l_2} u_{nl_1}(r_1) F_{nl_1l_2}(r_2) Y^{M_L}_{Ll_1l_2}(\hat{r}_1\cdot\hat{r}_2) + \sum_{\mu q_1 q_2} \phi_{\mu q_1}(\rho) G_{\mu q_1 q_2}(R) Y^{M_L}_{Lq_1q_2}(\hat{\rho}\cdot\hat{R})\,, \tag{2.5}$$

where n, μ are the principal quantum numbers of the hydrogen and positronium atoms, respectively; l_1, q_1 specify the orbital angular momentum of the two respective atoms; l_2, q_2 are the respective orbital momentum of the scattered positron and the center of mass of the positronium; $u_{nl_1}(r_1)$ are the radial hydrogenic eigenstates and the $\phi_{\mu q_1}(\rho)$ are their corresponding positronium eigenstates; the F's and G's are the scattered-particles amplitudes of the respective positron and the positronium center of mass; the Y's are the angular-momentum coupling functions and are given by

$$Y^{M_L}_{Ll_1l_2}(\hat{r}_1\cdot\hat{r}_2) = \sum_{m_1m_2} c(l_1, l_2, L, m_1, m_2M_L) \times Y_{l_1m_1}(\hat{r}_1) Y_{l_2m_2}(\hat{r}_2)\,, \tag{2.6a}$$

$$Y^{M_L}_{Lq_1q_2}(\hat{\rho}\cdot\hat{R}) = \sum_{m_1'm_2'} c(q_1, q_2, L, m_1', m_2', M_L) \times Y_{q_1m_1'}(\hat{\rho}) Y_{q_2m_2'}(\hat{R})\,, \tag{2.6b}$$

in which c is a Clebsch–Gordan coefficient.

The essence of the algebraic close-coupling method is an expansion of the functions $F_{nl_1l_2}(r_2)$ and $G_{\mu q_1 q_2}(R)$ in terms of a bound part and a free part (see Refs. 14 and 16 for a complete treatment):

$$F_p(r_2) = \alpha_{0p} A_{0p}(r_2) + \alpha_{1p} A_{1p}(r_2) + \chi_p(r_2), \tag{2.7a}$$

$p \equiv nl_1l_2$ denotes a hydrogenic channel;

$$G_q(R) = \alpha'_{0q} A'_{0q}(R) + \alpha'_{1q} A'_{1q}(R) + \chi'_q(R)\,, \tag{2.7b}$$

$q \equiv \mu q_1 q_2$ denotes a positronium channel; where the free parts are given by $A_{ip}(r_2)$ and $A'_{iq}(R)$, $i = (0, 1)$,

$$\begin{aligned} A_{0p}(r_2) &= k_p j_{l_2}(k_p r_2), \\ A_{1p}(r_2) &= k_p(1 - e^{-\beta r_2})^{2l_2+1} n_{l_2}(k_p r_2)\,, \end{aligned} \tag{2.8a}$$

$$\begin{aligned} A'_{0q}(R) &= \sqrt{2}\, k_q j_{l_2}(k_q R)\,, \\ A'_{1q}(R) &= \sqrt{2}\, k_q (1 - e^{-\gamma R})^{2q_2+1} n_{q_2}(k_q R)\,, \end{aligned} \tag{2.8b}$$

and are the asymptotic solutions of the Schrödinger equation. The j_l and n_l are spherical Bessel and Neumann functions and β, γ are arbitrary parameters introduced so that the shielding factors $(1 - e^{-\beta r_2})^{2l_2+1}$ and $(1 - e^{-\gamma R})^{2q_2+1}$ make the Neumann functions $n_{l_2}(k_p r_2)$ and $n_{q_2}(k_q R)$ behave as $r_2^{l_2}$ and R^{q_2}, respectively, at the origin. Also $E = E_n + k_p^2 = E_\mu + \frac{1}{2}k_q^2$.

The bound parts are to be expanded over any complete set of square-integral basis functions. It has been found convenient to use a Slater-orbital basis set which is given by

$$\chi_p(r_2) = \textstyle\sum_i c_{pl_2,i}\,\eta_{\;2,i}(r_2)\,, \tag{2.9a}$$

$$\chi'_q(R) = \textstyle\sum_b c'_{qq_2,b}\,\eta_{q_1,b}(R)\,, \tag{2.9b}$$

where

$$\eta_{l_2,a}(r_2) = \left(\frac{(2z_a)^{2l_2+3}}{\Gamma(2l_2+3)}\right)^{1/2} r_2^{l_2} e^{-z_a r_2}\,, \tag{2.10a}$$

$$\eta_{q_2,b}(R) = \left(\frac{(2z_b)^{2q_2+3}}{\Gamma(2q_2+3)}\right)^{1/2} R^{q_2} e^{-z_b R}\,. \tag{2.10b}$$

The set of z_a's and z_b's are chosen over a wide range and their number is determined by the convergence of the scattering parameters calculated. The computational problem involved proceeds as follows.

The Hamiltonian H is diagonalized on the short-range bound functions given by Eqs. (2.10a) and

(2. 10b) leading to a set of eigenvectors ψ_α and corresponding eigenvalues E_α.

The set of bound-free integrals is then defined as follows:

$$B_{i\alpha}^{\nu} = \begin{cases} \sum_{\text{all } p}\langle\langle c_{i\nu}|H-E|\,\psi_\alpha^p\rangle\rangle + \sum_{\text{all } q}\langle\langle c_{i\nu}|H-E|\,\psi_\alpha^q\rangle\rangle & \text{if } \nu \text{ is a hydrogenic channel,} \quad (2.\,11\text{a}) \\ \sum_{\text{all } p}\langle\langle c'_{i\nu}|H-E|\,\psi_\alpha^p\rangle\rangle + \sum_{\text{all } q}\langle\langle c'_{i\nu}|H-E|\psi_\alpha^q\rangle\rangle & \text{if } \nu \text{ is a positronium channel,} \quad (2.\,11\text{b}) \end{cases}$$

where

$$c_{i\nu}=u_\nu(r_1)A_{i\nu}(r_2)\,Y_{Ll_1l_2}^{M_L}(\hat{r}_1\cdot\hat{r}_2)\,, \qquad (2.\,12\text{a})$$

$$c'_{i\nu} = \Phi_\nu(\rho)A'_{i\nu}(R)\,Y_{Lq_1q_2}^{M_L}(\hat{\rho}\cdot\hat{R})\,, \qquad (2.\,12\text{b})$$

and the double ket implies a double space integration. The free-free integrals are given by

$$N_{ij}^{\nu\nu'} = \begin{cases} \langle\langle c_{i\nu}|\,H-E\,|c_{j\nu'}\rangle\rangle & \text{if } \nu,\,\nu'=p, \quad (2.\,13\text{a}) \\ \langle\langle c'_{i\nu}|H-E|\,c'_{j\nu'}\rangle\rangle & \text{if } \nu,\,\nu'=q, \quad (2.\,13\text{b}) \\ \langle\langle c'_{i\nu}|H-E|\,c_{j\nu'}\rangle\rangle & \text{if } \nu=q \text{ and } \nu'=p, \quad (2.\,13\text{c}) \\ \langle\langle c_{i\nu}|H-E|\,c'_{j\nu'}\rangle\rangle & \text{if } \nu=p \text{ and } \nu'=q, \quad (2.\,13\text{d}) \end{cases}$$

where p, q are hydrogenic and positronium channels, respectively. The explicit means by which these matrix elements were calculated is given in the Appendix. If one defines

$$M_{ij}^{\nu\nu'} = N_{ij}^{\nu\nu'} + \sum\nolimits_\alpha B_{i\alpha}^{\nu}(E-E_\alpha)^{-1}B_{\alpha j}^{\nu'}\,, \qquad (2.\,14)$$

then it follows that the R matrix is given by[14]

$$R_{\nu\nu'} = -(k_\nu k_{\nu'})^{-1/2}\,(M_{00}^{\nu\nu'} + \sum\nolimits_s\gamma_{\nu s}M_{10}^{s\nu'})\,, \qquad (2.\,15)$$

where $\gamma_{\nu s}$ is a solution of the inhomogeneous linear system:

$$\sum\nolimits_s M_{11}^{\nu' s}\,\gamma_{\nu s} = -M_{10}^{\nu'\nu}. \qquad (2.\,16)$$

Hence the partial cross section for transition from channel ν' to ν is calculated from[14]

$$Q_{\nu\nu'} = \frac{4}{k_{\nu'}^2}\left|\left(\frac{R}{1-iR}\right)_{\nu\nu'}\right|^2. \qquad (2.\,17)$$

In the case of elastic scattering, the tangent of the phase shift is given (Kohn method) by[14]

$$t_k = -(M_{10}/M_{11}) - \det(M)/kM_{11}, \qquad (2.\,18)$$

and the cotangent of the phase shift (inverse Kohn's method) is[14]

$$c_k = -(M_{01}/M_{00}) + \det(M)/kM_{00}, \qquad (2.\,19)$$

where

$$\det(M) = M_{00}M_{11} - M_{10}M_{01}. \qquad (2.\,20)$$

The inverse Kohn cross sections are calculated from the R^{-1} matrix. Details for calculating the Kohn and inverse Kohn parameters are given in Eq. (26), page 62, of Ref. 14. The matrix-inversion technique is found necessary for energies close to threshold where a cluster of eigenvalues E_α around the total energy E would cause numerical inaccuracy in the matrix elements given by Eq. (2. 14) because of the extremely small energy denominators $(E-E_\alpha)$. In this case, Eq. (2. 14) is replaced by

$$M_{ij}^{\nu\nu'} = N_{ij}^{\nu\nu'} - \sum_{rs}\sum_{ab} M_{ia}^{\nu r}(M^{-1})_{ab}^{rs}M_{bj}^{s\nu'}\,, \qquad (2.\,21)$$

where

$$M_{ab}^{pq} = (\Theta_a^p|H-E|\Theta_b^q)\,, \qquad (2.\,22)$$

$$M_{ai}^{pq} = (\Theta_a^p|H-E|A_{iq} \text{ or } A'_{iq})\,, \qquad (2.\,23)$$

a, b being basis indices. p, q stand for channel indices and

$$\Theta_a^\nu = u_\nu(r_1)\eta_a^\nu(r_2)Y_{Ll_1l_2}^{M_L}(\hat{r}_1,\ \hat{r}_2) \qquad (2.\,24)$$

or

$$\Theta_a^\nu = \phi_\nu(\rho)\eta_a^\nu(R)Y_{Lq_1q_2}^{M_L}(\hat{\rho},\ \hat{R}), \qquad (2.\,25)$$

depending, respectively, on whether ν is a hydrogenic- or a positronium-channel index.

For the inelastic case, the eigenphases and coupling parameters are calculated by diagonalizing the reactance matrix given by Eq. (2. 15). The eigenvalues of this matrix are $\tan\delta_1$ and $\tan\delta_2$, where δ_1, δ_2 are the eigenphases. The coupling parameter ϵ is given in terms of the elements of the orthogonal matrix U which diagonalizes the R matrix as

$$U = \begin{pmatrix} \cos\epsilon & \sin\epsilon \\ -\sin\epsilon & \cos\epsilon \end{pmatrix}\,.$$

III. SUMMARY OF APPROXIMATION USED FOR TRIAL WAVE FUNCTION

The major objective of the present work is to investigate the relative importance of different contributions to the scattering parameters, namely, those of positronium formation and polarization effects. To this end, the following approximations to the trial wave function (2. 5) are studied.

(a) Positronium formation is completely ignored. The total wave function is expanded in terms of 1*s*, 2*s*, 2*p* hydrogenic states. To avoid lengthy expressions we write the resulting wave function (2.5) symbolically as

$$\psi^L(1,\ 2) = 1s(\mathrm{H}) + 2s(\mathrm{H}) + 2p(\mathrm{H}) \tag{3.1}$$

to denote a 1*s*, 2*s*, 2*p* hydrogenic expansion.

(b) The 1*s* positronium (Ps) channel is now included and the total wave function is expanded in terms of only 1*s* hydrogenic and 1*s* positronium channels. This is called the coupled static approximation,

$$\psi^L(1,\ 2) = 1s(\mathrm{H}) + 1s(\mathrm{Ps})\,. \tag{3.2}$$

(c) Since the 2*p* hydrogenic state includes 68% of the atomic polarizability of hydrogen, the following expansion is tried which incorporates a significant amount of hydrogenic polarization together with explicit positronium formation:

$$\psi^L(1,\ 2) = 1s(\mathrm{H}) + 2s(\mathrm{H}) + 2p(\mathrm{H}) + 1s(\mathrm{Ps})\,. \tag{3.3}$$

(d) To include a significant portion of the polarization of both the hydrogen and positronium atoms and also explicit positronium formation, the following six-channel expansion is used:

$$\psi^L(1,\ 2) = 1s(\mathrm{H}) + 2s(\mathrm{H}) + 2p(\mathrm{H}) + 1s(\mathrm{Ps}) + 2p(\mathrm{Ps}) + 2p(\mathrm{Ps})\,. \tag{3.4}$$

(e) In order to bypass non-necessary complex expansions and to include the full ground-state polarizabilities of both the hydrogen and positronium atoms, it is very convenient to use pseudostates. These pseudostates were constructed by Damburg and Karule[17] for e^--H scattering and were later used by Burke, Gallaher, and Geltman.[18] They are fictitious states; they are normalized and orthogonalized to the other states included in the close-coupling expansion and are essentially the long-range part of the multipole components of the perturbed orbital which is a solution of the perturbation equation for a hydrogen atom perturbed by an incident electron. In essence, they reproduce the full ground-state polarizabilities of the hydrogen atom. The pseudostates used in this work are equivalent to the dipole $2\bar{p}$ state given by Damburg and Karule.[17] For the case of a positron incident on a hydrogen atom, the pseudostate used is the negative of that given by Ref. 17:

$$u_{2\bar{p}}(r_1) = -\,(32/129)^{1/2}(r_1 + \tfrac{1}{2}r_1^2)e^{-r_1}\,, \tag{3.5}$$

while in a similar fashion, we have constructed the pseudostate for a positronium as perturbed by an incident proton:

$$\phi_{2\bar{p}}(\rho) = -(1/129)^{1/2}(\rho + \tfrac{1}{4}\rho^2)e^{-\rho/2}\,. \tag{3.6}$$

Hence, the approximation used for Eq. (2.5) is

$$\psi^L(1,\ 2) = 1s(\mathrm{H}) + 2\bar{p}(\mathrm{H}) + 1s(\mathrm{Ps}) + 2\bar{p}(\mathrm{Ps})\,. \tag{3.7}$$

All the above approximations were solved for the elastic-scattering region. However, only approximations (b) and (e) were calculated in the inelastic region.

IV. RESULTS

There does not exist a rigorous criterion for choosing either the coefficients of the Slater-orbitals basis or the number of these orbitals. The procedure followed here is to calculate the scattering parameters versus an increasing number of Slater orbitals as well as a wide range of their coefficients. Adequate convergence to at least three significant figures was obtained with a maximum of 25 Slater orbitals per channel in the most difficult case [approximation (e)].

For approximation (b), numerical calculations by Dirks and Hahn are available for direct comparison. In this case, our calculations converged with 15 Slater orbitals per channel. The 15 z parameters [Eqs. (2.10)] used in the coupled static case were z_a, z_b = 0.001, 0.005, 0.008, 0.01, 0.02, 0.05, 0.08, 0.15, 0.4, 0.5, 0.7, 1.1, 1.5, 2, and 3. The additional ten parameters used in approximation (e) were z_a, z_b = 0.0001, 0.0005, 0.0002, 0.003, 0.006, 0.009, 0.2, 0.9, 2.5, and 5.

A. Elastic Scattering below the Positronium Threshold

The Kohn and inverse Kohn variational procedures as described in Ref. 14 were used to calculate the elastic phase shifts for the five approximations discussed in Sec. III. Phase shifts calculated by both procedures agree to at least four significant figures. Table I lists the results corresponding to the five approximations, and columns (a′) and (b′) list results of approximations (a) and (b) as calculated by different methods.[19] There is no previous work done via approximations (c)–(e) to use for comparison. Figure 1 displays the corresponding phase-shift curves in comparison with results of Schwartz.[10]

Our results for approximation (a) agree quite well with those of Burke and Smith[12] who used the ordinary close-coupling method. For approximation (b), Cody *et al.*[19] used four different methods to solve the resulting integrodifferential coupled equations. Their first three methods utilized a Green's-function approach and their corresponding results, although being in disagreement, seemed to converge from above to the results of their fourth method [listed in column (b′)] in which they expanded the potentials and the positronium's wave function in terms of Legendre's polynomials. Our results listed under column (b) are about 2% lower than those of their fourth method. In all elastic phase-shift calculations, the results were found to be essen-

TABLE I. S-wave elastic phase shifts in radians calculated by the five approximations (a), (b), (c), (d), (e), discussed in Sec. III. (a′) represents results of approximation (a) in the ordinary close-coupling method (Ref. 12). (b′) corresponds to phase shifts of approximation (b) (from Ref. 19). (f) represents the results of Schwartz (Ref. 10).

k	E(Ry)	(a)	(a′)	(b)	(b′)	(c)	(d)	(e)	(f)
0.1	−0.99	−0.0050	−0.0054	−0.0191	−0.0188	+0.0324	+0.0491	+0.0646	+0.151
0.2	−0.96	−0.0426	−0.0426	−0.0472	−0.0465	+0.0204	+0.0321	+0.0597	+0.188
0.3	−0.91	−0.0935	−0.0931	−0.0874	−0.0858	+0.0189	+0.0055	+0.0198	+0.168
0.4	−0.84	−0.1476	−0.1472	−0.1365	−0.1339	−0.0696	−0.0500	−0.0352	+0.120
0.5	−0.75	−0.1997	−0.1990	−0.1894	−0.1861	−0.1259	−0.1150	−0.0943	+0.062
0.6	−0.64	−0.2469	−0.2461	−0.2415	−0.2379	−0.1831	−0.1773	−0.1517	+0.007
0.7	−0.51	−0.2919	···	−0.2901	−0.2864	−0.2362	−0.2260	−0.2048	−0.054

tially independent of the parameter β [Eq. (2.8a)] so long as the 15 or more Slater orbitals were used per channel. A convenient choice of $\beta = 2$ was used in all calculations reported here.

Taking into consideration the bound property on the phase shifts, the results of approximations (c), (d), and (e) show the improvement on the phase shift due to inclusion of polarization and virtual positronium formation. It also illustrates that positronium polarization is not as important as the hydrogen polarization.

The Nesbet procedure is a resonance formalism. The set of negative eigenvalues obtained by diagonalizing the Hamiltonian on the short-range bound functions may represent bound states for the system. An eigenvalue whose position does not change by varying the internal basis set and which is not an eigenvalue of the unperturbed system but close to it, is likely to be a resonance.[13] No such eigenvalues are observed below the positronium threshold. This is in disagreement with Bransden and Jundi[5] who reported on the existence of such a resonance using a nonvariational polarized-orbital method. However, our observation is consistent with that of Dirks and Hahn[7] and Bhatia *et al.*[11]

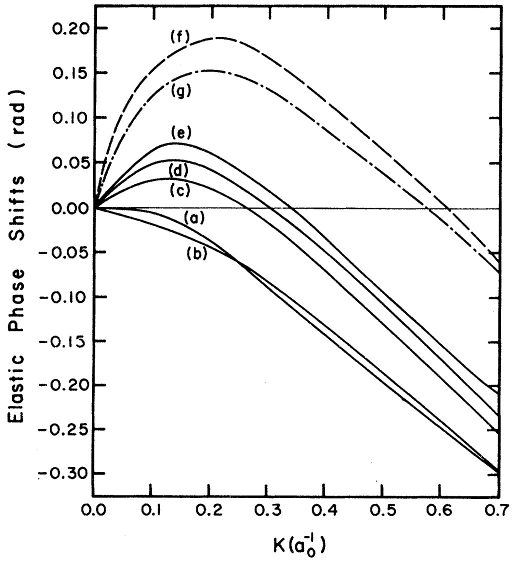

FIG. 1. S-wave elastic phase shifts for the five approximations (a)–(e) discussed Sec. III. (f): Schwartz: (g): Drachman.

Also, for the five approximations discussed above and for as many as 27 Slater orbitals per channel, none of the eigenvalues were less than − 1 Ry, the ground-state energy of hydrogen. This supports the contention that there does not exist a positron-hydrogen bound state.[20]

B. Inelastic Scattering below $n=2$ Threshold of Hydrogen

In this case, only approximations (b), Eq. (3.2), and (e), Eq. (3.7) are calculated. Results of approximation b serve as a good comparison with previous work done on the same approximation, namely, that of Bransden and Jundi,[5] and Dirks and Hahn.[7] Close agreement for the cross sections is obtained between present calculations and both Refs. 5 and 7. However, our reactance matrix shows more symmetry, and Table II lists its elements versus those of Dirks and Hahn. The best values of β and γ [Eqs. (2.8a) and (2.8b)] that are used are those that would give the best possible short-range representation of the scattered functions, namely, $\beta = k_p$, $\gamma = k_q$.[16]

Tables III and IV list correspondingly the R-matrix elements, eigenphases, coupling parameters and inelastic cross sections for approximation (e) which incorporates polarization. Figures 2 and 3 display the elastic- and positronium-formation cross sections, respectively. Substantial changes from the coupled static case are observed for all cross sections. As many as 25 Slater orbitals per channel were needed to span adequately the bound part of the wave function. The values for β, γ used are the same for approximation (b), namely, $\beta = k_p$, $\gamma = k_q$.

The formation cross section as can be seen from Fig. 3 is about four orders of magnitude lower than that of the Born[1] approximation and Bransden and Jundi,[5] while it is about one order of magnitude

TABLE II. Elements of the reactance matrix R_{ij} for approximation (b). Row *a* is present results and *b* represents results of Dirk and Hahn (Ref. 7).

k	E_p(Ry)		R_{11}	R_{21}	R_{12}	R_{22}
0.7154	−0.488 15	*a*	−0.3062	−0.0009	−0.0009	−0.4735
0.725	−0.474 375	*a*	−0.3109	−0.0017	−0.0016	−0.7501
		b	−0.310	−0.002	−0.002	−0.750
0.750	−0.437 5	*a*	−0.3231	−0.0052	−0.0052	−1.4860
		b	−0.322	−0.005	−0.006	−1.485
0.775	−0.399 375	*a*	−0.3349	−0.0130	−0.0130	−2.6459
		b	−0.335	−0.013	−0.014	−2.643
0.800	−0.360 0	*a*	−0.3466	−0.0356	−0.0356	−5.4896
		b	−0.346	−0.035	−0.036	−5.475
0.825	−0.319 375	*a*	−0.3600	−0.2716	−0.2716	−33.101
		b	−0.360	−0.266	−0.270	−32.434
0.835	−0.302 775	*a*	−0.3586	+0.3854	+0.3854	+42.953
		b	−0.359	+0.397	+0.402	+44.314
0.850	−0.277 5	*a*	−0.3674	+0.1036	+0.1036	+10.192
		b	−0.367	+0.104	+0.106	+10.290

lower than Fells–Mittleman[4] and Dirks–Hahn.[8] The off-diagonal R-matrix elements undergo a change in sign between $k = 0.725$ and 0.750 (Table III). In between, they must pass through zero with a resulting zero in the formation (and destruction) cross section (σ_{21} and σ_{12}). No such behavior has been predicted by any other calculations and this may be an artifact of our method. In any event, since we have only calculated the S-wave contribution to the total cross section, higher partial-wave components of the formation cross section would most likely not vanish at the same energy (if at all) and combine to give a nonzero result.

V. CONCLUSIONS

For the elastic-scattering case, the difference between the present phase shifts and the results of Schwartz–Bhatia *et al.* could probably be one or two of the following reasons.

In this work, the short-range correlation that represents virtual excitations into the closed channels is largely ignored. Schwartz–Bhatia *et al.* implicitly incorporated close-range correlation by including terms in their trial wave function.

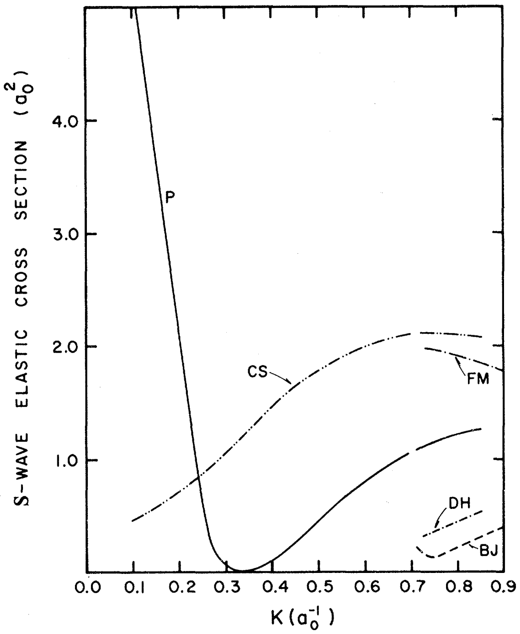

FIG. 2. S-wave elastic cross section in units of a_0^2 as calculated by approximation (e). FM: Fels and Mittleman: BJ: Bransden and Jundi; DH: Dirks and Hahn; CS: coupled static result of approximation (b); P: present calculation approximation (e).

Second, the pseudostates used here are essentially the long-range part of the dipole component of the perturbed orbital. To include polarization fully, one might in principle use higher multipoles or the complete form of the perturbed orbital as in the case of Drachman's[21] work which gave good results. Unfortunately, none of the above two shortcomings could be taken care of within the present framework owing to computational complexities.

As for the inelastic-scattering case, the positronium-formation cross section is smaller than that of Bransden and Jundi[5] by a factor of 10^4. Although Bransden and Jundi incorporated polarization in essentially the same way, the reason for

TABLE III. Elements of the reactance matrix R_{ij}, eigenphases, and coupling parameters for approximation (e) as calculated by the Kohn method for 25 bases.

k	E(Ry)	R_{11}	$R_{12} = R_{21}$	R_{22}	δ_1	δ_2	ϵ
0.7154	−0.488 15	−0.215	+0.0006	+0.119	−0.212	+0.118	0.0019
0.725	−0.474 375	−0.220	+0.0005	−0.121	−0.217	−0.121	0.0041
0.750	−0.437 5	−0.233	−0.0007	−0.586	−0.229	−0.530	0.0020
0.775	−0.399 375	−0.245	−0.0021	−1.050	−0.240	−0.810	0.0026
0.80	−0.36	−0.257	−0.0051	−1.642	−0.251	−1.024	0.0037
0.825	−0.319 375	−0.268	−0.0111	−2.574	−0.262	−1.200	0.0048
0.835	−0.302 775	−0.273	−0.0153	−3.152	−0.266	−1.264	0.0053
0.850	−0.277 5	−0.280	−0.0256	−4.489	−0.272	−1.352	0.0061

TABLE IV. Cross sections in units of a_0^2 for approximation (e).

k	E (Ry)	σ_{11}	σ_{21}	σ_{12}	σ_{22}
0.7154	−0.48815	1.089	0.00001	0.0002	7.407
0.725	−0.474375	1.109	0.000004	0.00004	3.555
0.750	−0.4375	1.150	0.000008	0.00003	25.68
0.775	−0.399375	1.187	0.00004	0.0001	32.74
0.80	−0.36	1.215	0.00012	0.0003	32.73
0.825	−0.319375	1.240	0.00027	0.0005	30.22
0.835	−0.302775	1.248	0.00036	0.0006	28.94
0.85	−0.2775	1.259	0.00050	0.0008	26.90

their high cross section is probably due to their nonvariational approach.

The Harris–Nesbet variational method seems promising for treating such rearrangement collision problems. It avoids the computational difficulties of evaluating complex kernels and iterating coupled integrodifferential equations. However, its only drawback is the numerical evaluation of matrix elements. The number of these matrix elements (except for the free-free) depends upon the number of short-range Slater orbitals used. There is no criterion we know of for choosing these orbitals except the convergence of the cross sections. Other experience (Ref. 16 and our calculations via approximation (a) of Sec. III and Ref. 22) has shown that when the calculations by the Harris–Nesbet method converge, they converge to the same results as an exact (numerical) solution of the same set of equations. We thus consider our results reported here as accurate to the significant figures quoted.

In regard to the application of the Harris–Nesbet method to e^--H inelastic scattering, problems were previously noted due to the long-range coupling between degenerate channels.[16] This was taken care of by including energy-dependent trigonometric functions in the short-range basis set. There is a possibility that this coupling is removed by the inclusion of the positronium channels in which case one might avoid evaluating and diagonalizing the bound-bound matrices for every energy. Such a situation would enable us to solve the positronium problem for energies up to the $n=3$ threshold of hydrogen.

Note added in proof. In the course of checking the calculations in this work two additional approximations were examined which help to elucidate the results. Using the convention of Sec. III, the two additional approximations for the trial wave function may be represented symbolically as

$$\psi^L(1,2) = 1s(\mathrm{H}) + 1s(\mathrm{Ps}) + 2\bar{p}(\mathrm{H}) \qquad \text{(A)}$$

and

$$\psi^L(1,2) = 1s(\mathrm{H}) + 1s(\mathrm{Ps}) + 2\bar{p}(\mathrm{Ps}). \qquad \text{(B)}$$

They thus correspond to first [(A)] adding the hydrogen pseudo p state to the ground hydrogen and positronium states and second [(B)] adding just the positronium pseudo p state. The most extensive calculation in Sec. III included both pseudo states together [approximation (e)]. In all cases, only S-wave scattering ($L=0$) has been considered.

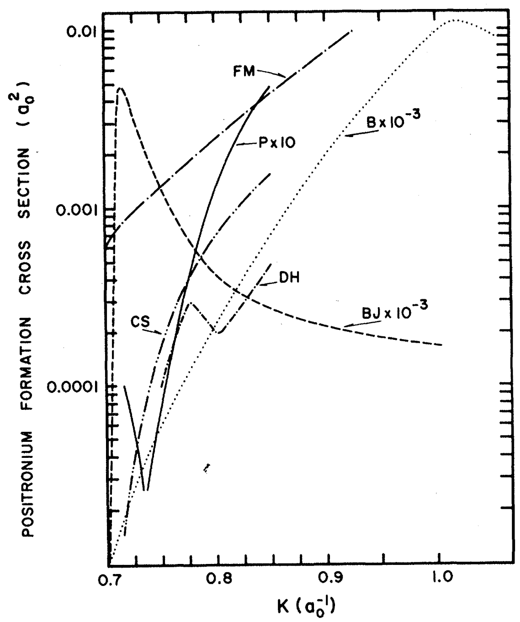

FIG. 3. Positronium-formation cross section in units of a_0^2. FM: Fels and Mittlemen; BJ: Bransden and Jundi; DH: Dirks and Hahn; CS: coupled static result of approximation (b); P: present calculation of approximation (e).

The results of the current approximations, (A) and (B), are given in Table V for the elastic phase shifts, in Table VI for the R-matrix elements, eigenphase shifts, and coupling parameters, and in Figs. 4 and 5 for the elastic- and positronium-formation cross sections, respectively. Also plotted in Figs. 4 and 5 are our coupled static (CS) and approximation $e(P)$ calculations and the generalized variational-bounds (GVB) calculations of Dirks and Hahn.[8] The CS approximation corresponds to just coupling to ground hydrogen and positronium states [i.e., $1s(\mathrm{H}) + 1s(\mathrm{Ps})$].

TABLE V. Elastic s-wave phase shifts in radians for the present approximations (A) and (B).

k	(A)	(B)
0.1	0.0556	0.0015
0.2	0.0457	−0.0131
0.3	0.0037	−0.0459
0.4	−0.0516	−0.0903
0.5	−0.1102	−0.1396
0.6	−0.1667	−0.1890
0.7	−0.2185	−0.2361

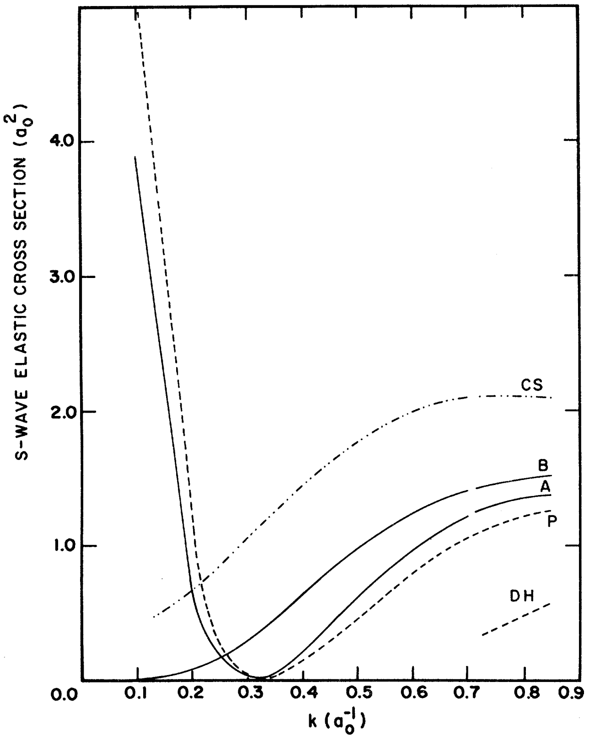

FIG. 4. S-wave elastic cross sections for positron scattering by hydrogen. CS and P are the coupled static and approximation (e) results, respectively. DH are the results of Dirks and Hahn (Ref. 8). A and B are the results of approximations (A) and (B) of the present work.

Observation of Fig. 4 shows that the hydrogen pseudo *p* state has considerably more influence on the cross section below threshold, as should be expected. In addition, it also has a somewhat greater influence on the elastic cross section above threshold. Observation of Fig. 5 shows the opposite effect in that the positronium pseudo *p* states has a significantly greater effect on the (formation) cross section than the hydrogen pseudo *p* state.

Comparison of the eigenphase shifts of the test calculations [(A) and (B) in Table VI] with those of the CS approximation,[7] approximation (e), and the GVB calculation of Dirks and Hahn[8] (DH) yields

$$\delta_1^{CS} < \delta_1^{B} < \delta_1^{A} < \delta_1^{e} < \delta_1^{DH}\,, \quad \delta_2^{CS} < \delta_2^{A} < \delta_2^{DH} < \delta_2^{B} < \delta_2^{e}\,,$$

under the premise that if the algebraic variational method converges, it converges to the exact solution of the corresponding equations and by virtue of the bounding principles on the eigenphase shifts ($\tan\delta$, actually), these relations show that the Dirks and Hahn GVB calculations are superior in the hydrogen channel while our approximations *B* and *e* are superior in the positronium channel. On the other hand, if one uses the criteria proposed by Geltman and Burke[23] of comparing the sums of

TABLE VI. *R*-matrix elements, eigenphase shifts, and coupling parameters for the present approximations, (A) and (B).

		(A)						(B)					
k	E (Ry)	R_{11}	$R_{12}=R_{21}$	R_{22}	δ_1	δ_2	ϵ	R_{11}	$R_{12}=R_{21}$	R_{22}	δ_1	δ_2	ϵ
0.7154	−0.48815	−0.230	−0.0194	−0.403	−0.224	−0.385	0.110	−0.248	+0.0049	+0.0711	−0.243	+0.071	+0.015
0.725	−0.474374	−0.235	−0.0257	−0.629	−0.229	−0.562	0.065	−0.252	+0.0047	−0.171	−0.248	−0.169	+0.058
0.750	−0.04375	−0.248	−0.0418	−1.181	−0.241	−0.869	0.045	−0.264	+0.0045	−0.655	−0.258	−0.580	−0.011
0.775	−0.399375	−0.261	−0.0651	−1.905	−0.253	−1.088	0.039	−0.276	+0.0047	−1.161	−0.269	−0.860	−0.0050
0.80	−0.36	−0.274	−0.108	−3.148	−0.264	−1.264	0.038	−0.287	+0.0036	−1.843	−0.279	−1.074	−0.0023
0.825	−0.319375	−0.290	−0.217	−6.216	−0.275	−1.411	0.036	−0.298	+0.0008	−3.001	−0.290	−1.249	−0.0003
0.835	−0.302775	−0.298	−0.332	−9.374	−0.279	−1.464	0.036	−0.302	−0.0014	−3.778	−0.294	−1.312	+0.0004
0.850	−0.2775	−0.341	−1.136	−31.49	−0.285	−1.539	0.036	−0.308	−0.0074	−5.775	−1.299	−1.399	+0.0014

the eigenphase shifts, which here is simply,

$$\sum\delta = \delta_1 + \delta_2\ ,$$

then one obtains

$$\sum\delta^{\mathrm{CS}} < \sum\delta^{\mathrm{A}} < \sum\delta^{\mathrm{B}} < \sum\delta^{\mathrm{DH}} < \sum\delta^{e}$$

for $k < 0.80$ with $\sum\delta^{\mathrm{B}}$ and $\sum\delta^{\mathrm{DH}}$ interchanged for $k > 0.80$. According to this comparison, our approximation (e) is better over-all than the GVB calculations of Dirks and Hahn and approximation (B) is slightly better than DH at higher energies. However, as noted by Dirks and Hahn,[8] their GVB calculations were only preliminary tests of their method and further effort could undoubtedly extend their results to be superior over-all. Extension of our calculations would entail inclusion of more states in the eigenstate expansion which is straightforward in principle but exceedingly trying on computing resources.

APPENDIX: MATRIX ELEMENTS

The matrix elements required in Sec. II are of three kinds: bound-bound, bound-free, and free-free. In any of these it is fairly simple to evaluate analytical expressions for the matrix elements of the Hamiltonian between two respective hydrogenic states or two respective positronium states. In the former, one uses the "before collision" form of the Hamiltonian operator (2.2), while in the latter, the "after collision" Hamiltonian (2.3) is used. However, the major difficulty in this work comes about in evaluating the matrix elements between a hydrogenic and a positronium state as in the case, for example, in the second term of (2.11a) and the first terms of (2.11b), (2.13c), and (2.13d). These integrals can be written in the following three basic forms:

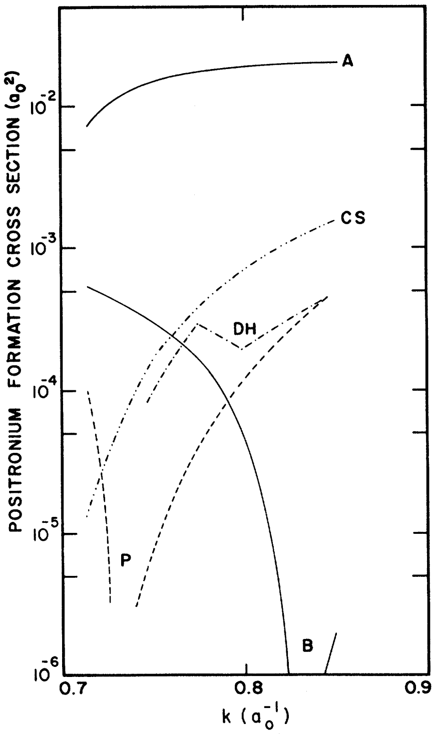

FIG. 5. *S*-wave positronium formation cross sections. Labeling of the curves has the same meaning as in Fig. 4.

(i) bound-bound,

$$\langle\langle u_{nl_1}(r_1) r_2^{\,l_2} e^{-z_i r_2} Y^{M_L}_{Ll_1l_2}(\hat{r}_1\cdot\hat{r}_2)\,|\hat{H}|\,\phi_{\mu q_1}(\rho) R^{q_2} e^{-z_j R} Y^{M_L}_{Lq_1q_2}(\hat{\rho}\cdot\hat{R})\rangle\rangle\ ; \tag{A1}$$

(ii) bound-free,

$$\langle\langle u_{nl_1}(r_1) r_2^{\,l_2} e^{-z_i r_2} Y^{M_L}_{Ll_1l_2}(\hat{r}_1\cdot\hat{r}_2)\,|\hat{H}-E|\,\phi_{\mu q_1}(\rho) R^{q_2} \begin{bmatrix} k_q j_{q_2}(k_q R) & \\ k_q(1-e^{-\gamma R})^{2q_2+1} & n_{q_2}(k_q R) \end{bmatrix} Y^{M_L}_{Lq_1q_2}(\hat{\rho}\cdot\hat{R})\rangle\rangle \tag{A2}$$

or

$$\left\langle\!\!\left\langle \phi_{\mu q_1}(\rho) R^{q_2} e^{-z_i R} Y^{M_L}_{Lq_1q_2}(\hat{\rho}\cdot\hat{R})\,|\hat{H}-E|\,u_{nl_1}(r_1) r_2^{\,l_2} \begin{bmatrix} k_p j_{l_2}(k_p r_2) & \\ k_p(1-e^{-\beta r_2})^{2l_2+1} & n_{l_2}(k_p r_2) \end{bmatrix} Y^{M_L}_{Ll_1l_2}(\hat{r}_1\cdot r_2) \right\rangle\!\!\right\rangle ; \tag{A3}$$

(iii) free-free,

$$\left\langle\!\!\left\langle \phi_{\mu q_1}(\rho) R^{q_2} Y^{M_L}_{Lq_1q_2}(\hat{\rho}\cdot\hat{R}) \begin{bmatrix} k_q j_{q_2}(k_q R) & \\ k_q(1-e^{-\gamma R})^{2q_2+1} & n_{q_2}(k_q R) \end{bmatrix} \right.\right.$$

$$\left.\left. \times\,|\hat{H}-E|\,u_{nl_1}(r_1) r_2^{\,l_2} Y^{M_L}_{Ll_1l_2}(\hat{r}_1\cdot\hat{r}_2) \begin{bmatrix} k_p j_{l_2}(k_p r_2) & \\ k_p(1-e^{-\beta r_2})^{2l_2+1} & n_{l_2}(k_p r_2) \end{bmatrix} \right\rangle\!\!\right\rangle\ . \tag{A4}$$

To calculate these matrix elements, it is convenient to use the following transformation: Referring to Fig. 6, for a fixed distance r_2 between the positron and the proton define the spheroidal coordinates

$$\xi = (r_1 + \rho)/r_2 \,;\, \eta = (r_1 - \rho)/r_2 \,;$$

$\phi \equiv$ the angle between the plane containing e^+, e^-, P, and some arbitrary plane through e^+P. These form an orthogonal system with volume element

$$d\tau = \tfrac{1}{8} r_2^3 (\xi^2 - \eta^2)\, d\xi\, d\eta\, d\phi \,. \tag{A5}$$

The variables that now appear in the above matrix elements are written in terms of these coordinates and r_2 where

$$\begin{aligned} &\rho = \tfrac{1}{2} r_2(\xi - \eta)\,; \quad r_1 = \tfrac{1}{2} r_2(\xi + \eta)\,; \\ &R = \tfrac{1}{4} r_2(\xi^2 + \eta^2 + 6\xi\eta + 8)^{1/2} \,. \end{aligned} \tag{A6}$$

The angular terms, i.e., $Y^{M_L}_{L l_1 l_2}(\hat{r}_1 \cdot \hat{r}_2)$ and $Y^{M_L}_{L a_1 a_2}(\hat{\rho} \cdot \hat{R})$, have to be written in terms of their corresponding angles which in turn can be evaluated using analytical geometry, as functions of ξ, η, ϕ. Once this is done, the integration over $d^3 r_2$ and $d\phi$ can be carried out. As an example, consider the simplest case where we are interested in evaluating a bound-bound matrix element for S-wave scattering between a 1s hydrogenic and a 1s positronium state: Equation (3.8) reduces to, in atomic units,

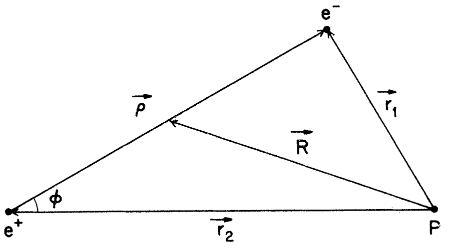

FIG. 6. Coordinates relations used in the calculations.

$$\begin{aligned} &\frac{1}{(4\pi)^2} \left\langle\!\left\langle 2e^{-r_1} e^{-z_i r_2} \right| - \frac{1}{r_2} \frac{d^2}{dr_2^2} r_2 + \frac{2}{r_2} + H_A - \frac{2}{|\vec{r}_1 - \vec{r}_2|} \left| \frac{1}{\sqrt{2}} e^{-\rho/2} e^{-z_j R} \right\rangle\!\right\rangle \\ &\qquad = \frac{1}{8\sqrt{2}} \int_0^\infty dr_2 \int_1^\infty d\xi \int_{-1}^{+1} d\eta \left[\left(2z_i + 2 - \frac{4}{(\xi - \eta)} \right) r_2^{\,4} - (z_i^2 + 1) r_2^{\,5} \right] (\xi^2 - \eta^2) e^{-y(\xi,\eta) r_2} \\ &\qquad = \frac{1}{8\sqrt{2}} \int_1^\infty d\xi \int_{-1}^{+1} d\eta\, (\xi^2 - \eta^2) \left[\left(2z_i + 2 - \frac{4}{(\xi - \eta)} \right) \frac{4!}{y^5} - \frac{(z_i^2 + 1) 5!}{y^6} \right] , \end{aligned} \tag{A7}$$

where

$$y(\xi,\, \eta) = \tfrac{1}{2}(\xi + \eta) + \tfrac{1}{4}(\xi - \eta) + \tfrac{1}{4} z_j (\xi^2 + \eta^2 + 6\xi\eta + 8)^{1/2} \,.$$

Now the integrals over ξ are all of the form of a basic integral

$$\int_1^\infty \frac{\xi^n d\xi}{[a_1\xi + a_2 + (a_3 + a_4\xi + a_5\xi^2)^{1/2}]^m} \,, \tag{A8}$$

n, m being integers. This can be reduced to quadrature by using the transformation

$$(a_3 + a_4 + a_5\xi^2)^{1/2} = t + \xi a_5^{1/2} \tag{A9}$$

which, using the binomial theorem, leads to a set of integrals of the form

$$\int_{(a_3 + a_4 + a_5)^{1/2} - a_5^{1/2}}^{a_4/2a_5^{1/2}} \frac{t^{n'} dt}{R^m} \,,$$

where R is a second-degree polynomial in t; $R = a + bt + ct^2$. This in turn could be evaluated using the recursion relation

$$\begin{aligned} \int \frac{t^{n'} dt}{R^m} = &- \frac{t^{n'-1}}{(2m - n' - 1)cR^{m-1}} \\ &- \frac{(m - n')b}{(2m - n' - 1)c} \int \frac{t^{n'-1}}{R^m} dt \\ &+ \frac{(n' - 1)a}{(2m - n' - 1)c} \int \frac{t^{n'-2}}{R^m} dt \,, \end{aligned} \tag{A10}$$

which reduces to integrals of the form $\int (t/R^m)\, dt$ and $\int dt/R^m$ that can be done analytically.

We were not able to carry out the integration in such a manner in the free-free matrix element Eq. (A4), and the double integration instead was done numerically using a 96-point Gaussian quadrature.

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Screening Effects in Atomic Pair Production below 5 MeV*

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Quantitative predictions for atomic-electron screening effects in low-energy pair production follow from the knowledge that the small-distance shape of screened-electron and positron continuum wave functions is close to that of point-Coulomb wave functions of shifted energy. These predictions are verified by making exact numerical calculations in representative cases. The energy-shift normalization theory is then used in conjunction with the point-Coulomb results of Øverbø to obtain predictions for atomic-pair-production energy distributions and total cross sections for photon energies from threshold to 5 MeV. Atomic-electron screening effects cause appreciable modifications of the total cross sections for photon energies below 1.5 MeV and continue to have a major effect on some portions of the energy distribution at higher photon energies. Results are also compared with Bethe–Heitler predictions and with experiments.

With the continuing improvements in computers it is becoming feasible to make fairly accurate theoretical calculations of atomic-pair-production cross sections in the low-energy region where the Bethe–Maximon[1] high-energy results and Born approximation[2] (the well-known Bethe–Heitler formula) need not be valid. Relativistic calculations of pair production in a point-Coulomb-potential model have now been reported by Øverbø, Mork, and Olsen (ØMO); more extensive results have been given by Øverbø.[3] This use of a point-Coulomb model relies on the expectation, based on form-factor estimates,[4] that the effects of atomic-electron screening would be unimportant in this energy region. Such an estimate is obtained because the maximum impact parameter $r_{\max}$ discussed by Heitler,[5] equal to $q_{\min}^{-1}$ with $q_{\min} = k - p_+ - p_-$, is of the order of the electron Compton wavelength and is quite small compared to the radius of the atom. However, we subsequently performed the lengthy relativistic calculations[6] of pair-production cross sections in screened potentials and found that, near threshold, atomic-electron screening effects are important. At electron-Compton-wavelength distances an electron sees a point-Coulomb potential corresponding to the nuclear charge Z. The electron wave function has a hydrogenlike shape; the only effect of atomic-electron screening, as described by a central potential V deviating from the point-Coulomb form, is to modify the normalization. For a very-low-energy continuum wave function (but not for higher energies) this normalization is indeed sensitive to the screening. We showed in fact that we could roughly obtain screened pair-production cross sections from point-Coulomb cross sections simply by using a multiplicative normalization factor.

We have recently examined[7] in greater detail the