Formation of positronium in $e^+ + H^-$ collisions

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Cross sections for positronium formation by capture from the negative hydrogen ion are given. Orthogonalization corrections to the Coulomb (first-order) Born approximation (CBA) differential and total cross sections are calculated using approximate H^- wave functions of both Löwdin [Phys. Rev. **90**, 123 (1953)] and Chandrasekhar [Astrophys. J. **100**, 176 (1944)]. The present calculation of the CBA cross sections using the post interaction for Löwdin's wave function (LCBAPS) disagrees with the calculation of Choudhury, Mukherjee, and Sural (CMS) [Phys. Rev. A **33**, 2358 (1986)], whereas our results using the prior interaction agree. Thus, where CMS found an order of magnitude post-prior discrepancy in the differential cross sections except at forward angles, and a markedly different shape to the minima, the present post and prior results differ by 1–10 % at 100 eV, and the minima have the same shape and occur within one degree of each other. Chandrasekhar's "open-shell" wave function, which is superior to Löwdin's in bound-state problems since it gives a negative binding energy, gives post and prior cross sections that are almost indistinguishable at this energy and are $\frac{1}{2}$ to $\frac{2}{3}$ as large as the LCBA. Various methods of orthogonalizing the unbound projectile to the possible bound states are considered. It is found that treating the atomic nuclei as if they were isotopic spin projections [Straton and Girardeau, Phys. Rev. A **40**, 2991 (1989)] of a single type of "nucleon" gives cross sections that are an improvement over the CBA.

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I. INTRODUCTION

Reliable cross sections for the various positronium (Ps) formation processes are essential for an accurate calculation of the width of the 0.511-MeV annihilation line that has been observed in the region of the galactic center [1], in solar flares [2], and in planetary nebulae [3]. In the transition regions of planetary nebulae the concentration of the negative hydrogen ion [4] should be large enough for the reaction

$$e^+ + H^- \rightarrow Ps(n\ell) + H(1s) \tag{1}$$

to make an important contribution to the linewidth [5]. Furthermore, because this reaction is exothermic, it appears to be the dominant mechanism for positronium formation at energies below the 6.8-eV positron kinetic-energy threshold for electron capture from neutral hydrogen even in regions where the H^- density is low.

The present calculation relies on the exact treatment of the three species of bound states inherent in Fock-Tani representation. Also included is the further presumption [6] of treating the proton and positron as isospinlike projections (of different mass) of a single species of "nucleon," that produced remarkable agreement between the orthogonalized first-order calculation [7] of charge transfer from hydrogen and the (presumably exact) variational result [8].

II. ORTHOGONALIZATION

In scattering processes involving bound states, one must subtract the projection of the translational states of free particles onto the corresponding bound states if the contribution of these particles to the amplitude is not to be counted twice. Fock-Tani representation [9] has been a powerful tool for generating these orthogonalization corrections. In this representation the reactants, intermediate states, and products are treated symmetrically, and composites are treated exactly within a single second-quantized Hamiltonian. Unbound particles are *exactly* orthogonal to bound states, and all interactions contain the proper orthogonalization subractions so that free particles do not have sufficient energy to bind (this binding energy is accounted for in the asymptotic Hamiltonian), and assuring that there is no double counting.

Because the Lippmann-Schwinger series for the Fock-Tani T matrix contains higher-order contributions at each order than does the standard Born series, one has the hope of improved results at each order. Ojha *et al.* [10] have calculated the first-order Fock-Tani cross sections for the reaction

$$H^+ + H \rightarrow H + H^+ \tag{2}$$

and have obtained good agreement with experiment [11] for differential angles within 1 mrad of the forward direction at 25, 60, and 125 keV and for total cross sections at energies greater than 10 keV. They noted that the or-

thogonalization correction substantially cancels the internuclear potential. Straton [12] has shown that excluding these p-p terms yields Fock-Tani cross sections that are 18% smaller than when these terms are included. In contrast, the Brinkman-Kramers result [13], which excludes the p-p term, is 1000% larger than the first-order Born total cross section that includes this term [14]. Thus the Fock-Tani Hamiltonian produces substantial agreement *at first order* between experiment and Wick's observation [14] that the internuclear potential should play a negligible role in *exact* calculations of this process.

Finally, it may be seen that the *first-order* Fock-Tani differential cross section is virtually identical to that of the *second-order* boundary-corrected Born approximation [15] (B2B) at 125 keV. This correspondence both affirms the appropriateness of testing the lowest-order Fock-Tani theory in problems for which generic first-order theories would not be expected to be reliable, and points to the need for a deeper study of the question of why it should do so well.

III. ISO-ORTHOGONALIZATION

The obvious region in which a first-order theory might not be expected to be reliable is at low energies. Straton [12] calculated the Fock-Tani total cross section for the reaction

$$e^+ + \mathrm{H} \rightarrow \mathrm{Ps}(1s) + \mathrm{H}(1s) \tag{3}$$

and obtained a result that was larger than the first-order Born approximation (FBA), whereas the (presumably exact) variational result of Brown and Humberston [8] was smaller than the FBA.

This failure was due to an anomaly of the product form of the Fock-Tani transformation, which does not produce orthogonalizations with respect to all species of bound states. This was immaterial in the reaction (2) since the initial and final bound-state species were identical.

Straton and Girardeau [6] were able to generalize the Fock-Tani transformation on the two-nucleon, one-electron Hilbert space to produce a T matrix for either (2) or (3) that was post-prior symmetrical. This was accomplished by thinking of the two atomic nuclei as isospinlike projections of a single species of "nucleon," just as in nuclear physics it is useful to think of the proton and the neutron as isospin projections of a single species of nucleon. The consequence of this way of viewing the system is an up-leveling of the nucleon-exchange term in the scattering (elastic and inelastic) amplitude, as in Fig. 1 (with diagram correspondences given in Figs. 2–4), to a reactive amplitude. Since exchange essentially amounts to a reactive process, it is not surprising that Fig. 1 may be promoted to a reactive matrix element by promoting an "effective" difference between incoming and outgoing free particles to a true difference through the use of an isotopic spin formalism.

Lo and Girardeau [7] applied this iso-orthogonalized matrix element to reaction (3) with superb agreement with the variational result of Brown and Humberston [8], reproduced in Fig. 5.

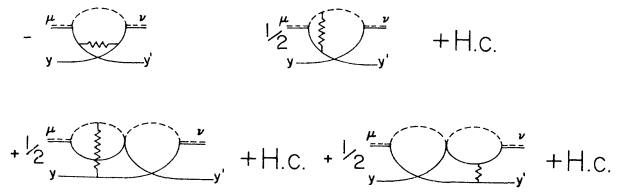

FIG. 1. Proton exchange terms in the Coulomb and orthogonalization interactions for proton-hydrogen scattering. The solid lines are proton propagators, the dashed line is the electron propagator, and the doubled line is the hydrogen atom (composite elementary particle) propagator. Time flows right to left so that the first term represents breakup of a bound state with quantum numbers ν followed by formation of bound state μ due to interaction with the exchanged proton. The last two terms contain the post and prior orthogonalization projectors $\mathcal{X} \Leftrightarrow \sum_b |b\rangle\langle b|$.

IV. THE FOCK-TANI AMPLITUDES

Straton has developed [16] a Fock-Tani Hamiltonian for a system that contains two "nucleons" and two electrons using the product form of transformations that each orthogonalize to one of the three bound species in (1). By working in a coordinate system in which one atomic nucleus is fixed at the origin, and therefore ceases to be a dynamic particle [12], the unitary operator that transforms the Fock Hamiltonian into the subspace in which the three bound states may be treated as elementary particles may be compounded by the product

$$\hat{U} = \hat{U}_A \hat{U}_B \hat{U}_E \ , \tag{4}$$

where A =Ps, B is the state with two electrons bound to the origin, and E is the state with one electron bound to the origin.

In Straton's diagrammatic notation [16], the correspondences between annihilation operators and propagator lines is given by Fig. 2, with an implied integral or sum over the argument and crossed fermionic lines giving a factor of -1. The bound-state wave functions are represented by Fig. 3, and the Schrödinger operators are given by Fig. 4, where the W's are the inertial potentials (mass-polarization terms) arising from the accelerated frame of reference in which the target nucleus

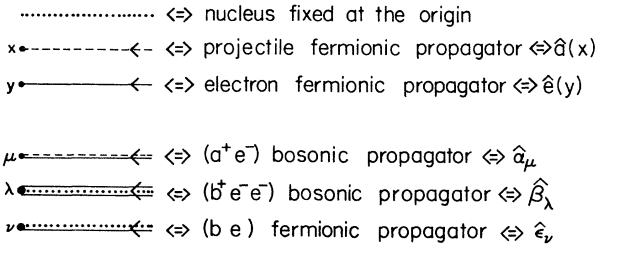

FIG. 2. Diagram correspondences for propagators and annihilation operators.

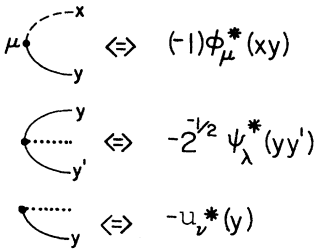

FIG. 3. Diagram correspondences for bound-state wave functions.

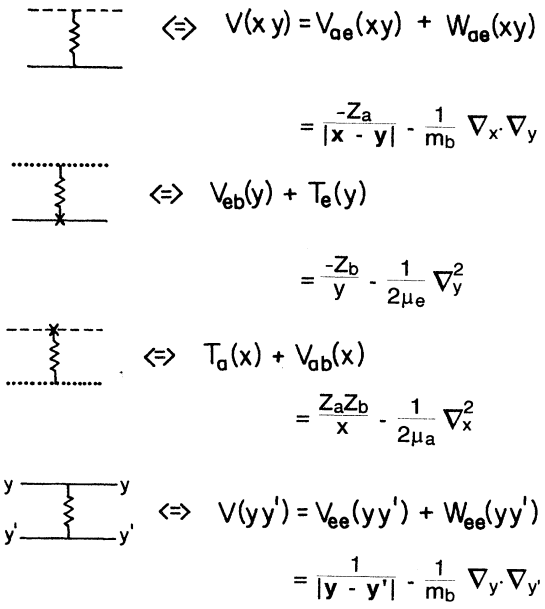

FIG. 4. Diagram correspondence for Schrödinger operators.

is fixed at the origin [17].

The relevent term for (3) in the product-form Fock-Tani Hamiltonian is given by Fig. 6, where the second oval is given by Fig. 7. The first oval in Fig. 6 is given by the first four terms of Fig. 7 with the y' propagator replaced by the dotted line representing the nucleon fixed at the origin.

Thus the algebraic translation of Fig. 7 in the second term of Fig. 6, after the asymptotic states select the bound state quantum numbers from the sums, is [6, 18]

$$\int dx\,dy\,dy'dy''u_\lambda(y'')\Big(\delta(y'-y'')[V(yy')+V(y'x)]\phi_\mu(xy)$$
$$-\delta(y'-y'')\int dx'dy_1\phi^*_\mu(x'y_1)[V(y'x')+V(y'y_1)]$$
$$\times\Delta(x'y_1,xy)+\int dx'\phi^*_\mu(y'x')[H(y'x')\Delta(x'y'',xy)+\tfrac{1}{2}\Delta(x'y'',xy)H(xy)]$$
$$+\int dx'\phi^*_\mu(x'y')[\tfrac{1}{2}V(xy')+V(y'y'')+\tfrac{1}{2}V(yy')+V(y''x')]\Delta(x'y'',xy)\Big)\psi_\nu(yy'). \quad (5)$$

V. ISOSPIN SYMMETRY

Because (1) is similar to, and more complicated than, (3), one would expect that the problems associated with a Fock-Tani Hamiltonian derived using a product transformation for the one-electron case would also arise in using a product transformation for the two-electron case. Indeed, the cancellation of the even-parity orthogonalization terms appears in both cases, and if the positron is replaced by a proton the internuclear Coulomb term is canceled by the corresponding orthogonalization term. It is hoped that the ideas behind the correction of these problems in (3), which lead to excellent agreement with the variational result, will likewise give a reliable result for (1).

Girardeau and Straton [19] have been able to formally generalize the Fock-Tani transformation to include any number of nucleons, electrons, and bound-state species, but the exacting process of applying Wick's theorem to produce the Hamiltonian on the two-nucleon–two-electron Hilbert space has not been completed. Until this process is completed one must use physical ideas to extract the correct form.

One might look at the amplitude, Fig. 1, for reac-

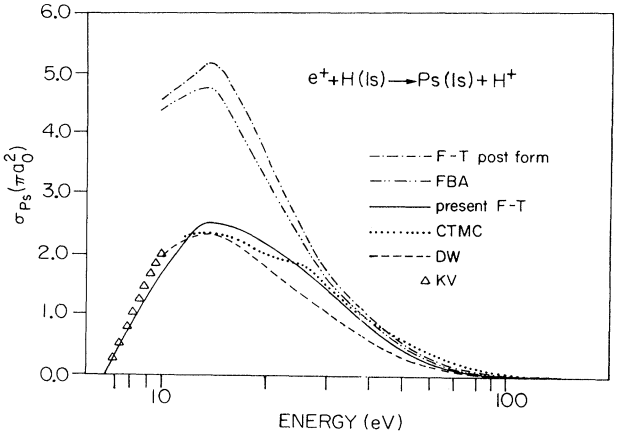

FIG. 5. Total cross section for positronium formation in the ground state. The dashed-dotted line is the Fock-Tani post form, the dashed-double-dotted line is the FBA, the dotted line is the classical trajectory Monte Carlo (CTMC) result, the dashed line is the polarized-orbital distorted wave (POM) result, and the solid line is the Fock-Tani result from Lo and Girardeau [7]. △ are the Kohn variational (KV) principle results [8].

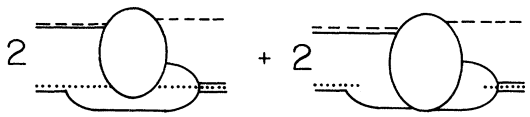

FIG. 6. The term in the Fock-Tani interaction Hamiltonian yielding reaction (3).

tion (3) and postulate that the desired amplitude for (1) should be the average of the amplitudes derived by the post and prior product transformations. Indeed the prior product form corresponding to (4),

$$\hat{U} = \hat{U}_B \hat{U}_A \hat{U}_E, \tag{6}$$

is also allowed (though E before A or B is not because its constutuents are a proper subset of the constituents of both A and B) [20]. The amplitude for this transition is particularly simple because all of the electron-electron interaction energy is included in the bound states and the internuclear potential does not appear (or one might say that the Coulomb term is exactly canceled by the orthogonalization term for all masses). This amplitude is given in Fig. 8. Its evaluation follows that of the Coulomb (first-order) Born approximation (CBA) closely.

But the fundamental idea that leads to the excellent results for (3) was not post-prior averaging. That was the consequence. The fundamental idea was the treatment of particles of different mass and same charge as if they were isospin projections of a single species of "nucleon."

If one draws the electron-nucleon interaction diagrams corresponding to the direct and nucleon-exchange processes (in a coordinate system in which all four particles are dynamical), Fig. 9, it can be seen that the latter may be transformed into the former by a vertical stretching procedure (multiplying by -1 for each fermion line that is crossed or uncrossed in this procedure), so that they represent the same physical process. The corresponding direct and exchange orthogonalization projectors onto the prior bound states are also equivalent, Fig. 10. Thus, *isospin symmetry does not imply post-prior symmetry* in reaction (1).

The corresponding direct and nucleon-exchange orthogonalization projectors onto the upper post bound state are shown in Fig. 11. These are topologically different and must be treated as two distinct physical processes. Deforming the latter diagram so that the post bound-state propagators interchange positions reveals the interpretation of this diagram as the direct orthogonalization projector onto the lower post bound state. Thus the prescription for promoting the exchange amplitude to a reactive amplitude, by promoting the "effective" difference between upper and lower "nucleons" to a true difference through use of an isotopic spin formalism, leads to an amplitude in which the projectile is orthogonalized using the average of the direct projectors onto the two post bound states.

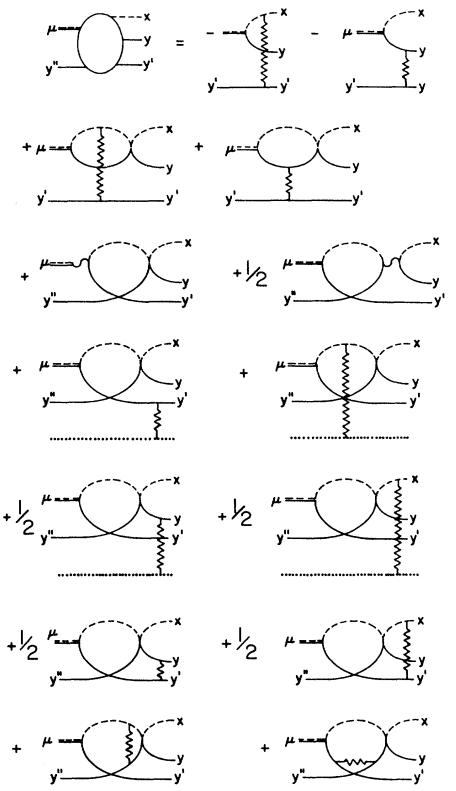

FIG. 7. The second oval in Fig. 6 in more detail.

VI. THE ANALYTICAL REDUCTION

The post Coulomb-Born approximation (CBPS), the first two terms of Fig. 7 inserted in the second term of Fig. 6 and the corresponding internuclear terms inserted in the first term of Fig. 6, has algebraic translation [for asymptotic states dictated by (1)]

$$T^{\mathrm{CBPS}} = \sqrt{2}\int d\mathbf{x}\, d\mathbf{y}\, d\mathbf{y}'\, \phi^{\mu *}_{n\ell}(\mathbf{x}\mathbf{y}')\, u^{\lambda *}_{1s}(\mathbf{y}) \left(\frac{1}{\mathbf{x}} - \frac{1}{\mathbf{y}} - \frac{1}{|\mathbf{x}-\mathbf{y}|} + \frac{1}{|\mathbf{y}-\mathbf{y}'|}\right) \psi_B(\mathbf{y}'\mathbf{y}) \frac{\chi^+_c(\mathbf{k}_i,\mathbf{x})}{(2\pi)^{3/2}}$$
$$= T^{\mathrm{CBA}}_{12} + T^{\mathrm{CBA}}_{34}, \tag{7}$$

where we have neglected the inertial potentials in Fig. 4 and where

$$\phi^{\mu *}_{n\ell}(\mathbf{x}\mathbf{y}) = \frac{1}{(2\pi)^{3/2}}\, e^{i\mathbf{k}\cdot\mathbf{R}}\, u^{\mu}_{1s}(\mathbf{r}), \tag{8}$$

$$\mathbf{R} = \zeta\mathbf{x} + \eta\mathbf{y}, \quad \mathbf{r} = \mathbf{y} - \mathbf{x}, \tag{9}$$

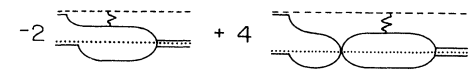

FIG. 8. The prior amplitude for (1).

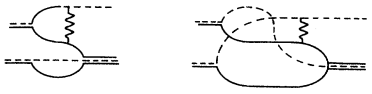

FIG. 9. Direct and (nucleon) exchange Coulomb terms for the electron-nucleon transition amplitude for reaction (1).

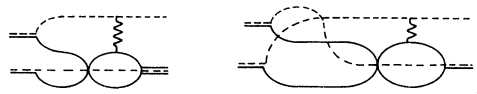

FIG. 10. Direct and (nucleon) exchange prior orthogonalization corrections for the electron-nucleon transition amplitude for reaction (1).

$$\zeta = \frac{m_p}{m_p + m_e}, \quad \eta = 1 - \zeta, \tag{10}$$

$$\mu = \zeta m_e, , \quad \lambda = \frac{m_t m_e}{m_t + m_e}, \tag{11}$$

$$\chi_c^+(\mathbf{k}_i\mathbf{x}) = e^{i\mathbf{k}_i\cdot\mathbf{x}}\, e^{-(1/2)\pi\nu_i}\, \Gamma(1+\nu_i) \times {}_1F_1(-i\nu_i, 1, i(k_i x - \mathbf{k}_i\cdot\mathbf{x})), \tag{12}$$

$$\nu_i = -\frac{Z}{k_i}, \tag{13}$$

and $u_\sigma^\tau(\mathbf{x})$ is the hydrogenic wave function in the quantum state σ with $\tau = Z/a_0$. Defining

$$\psi_{A'AB'B}^{\alpha'\alpha\beta'\beta}(\mathbf{y}',\mathbf{y}) = \frac{1}{4\pi}(AA' e^{-\alpha' y' - \alpha y} + BB' e^{-\beta' y' - \beta y} + A'B e^{-\alpha' y' - \beta y} + AB' e^{-\beta' y' - \alpha y}), \tag{14}$$

Löwdin's H^- wave function [21] is $\psi_B(y'y) = \psi_{AABB}^{\alpha\alpha\beta\beta}(y'y)$ with $\alpha = 0.4228$, $A = 0.300\,25$, $\beta = 0.9794$, and $B = 1.0001$. Chandrasekhar's wave function [22] is $\psi_B(y'y) = \psi_{A'AB'B}^{\alpha\alpha\beta\beta}(y'y)$ with the products $AA' = BB' = 0$ and $AB' = A'B = C = 0.395\,13$ and with $\alpha = 0.283\,09$ and $\beta = 1.039\,25$.

The post positronium direct orthogonalization terms, the third and fourth terms of Fig. 7 inserted in the second term of Fig. 6 and the corresponding internuclear interaction terms inserted in the first term of Fig. 6, have algebraic translation

$$T^{\mathrm{DOPS}} = -\sqrt{2}\int d\mathbf{x}\, d\mathbf{y}\, d\mathbf{y}\, d\mathbf{y}_2 d\mathbf{x}_2\, \phi_{n\ell}^{\mu*}(\mathbf{x}_2\mathbf{y}_2)\, u_{1s}^{\lambda*}(\mathbf{y}) \left(\frac{1}{x_2} - \frac{1}{y_2} - \frac{1}{|\mathbf{x}_2 - \mathbf{y}|} + \frac{1}{|\mathbf{y}_2 - \mathbf{y}|}\right) \times \Delta^\mu(\mathbf{x}_2\mathbf{y}_2;\mathbf{x}\mathbf{y}')\, \psi_B(\mathbf{y}'\mathbf{y}) \frac{\chi_c^+(\mathbf{k}_i,\mathbf{x})}{(2\pi)^{3/2}}, \tag{15}$$

where

$$\Delta^\mu(xy, x'y') = \delta(\mathbf{R} - \mathbf{R}') \sum_\gamma u_\gamma^\mu(\mathbf{r})\, u_\gamma^{\mu*}(\mathbf{r}'). \tag{16}$$

The remaining terms of Fig. 8 have algebraic translation given in Ref. [18]. They involve a mixing of coordinates that prevent their analytic reduction to a number of integral dimensions less than five. They will be neglected because they are the exchange corrections to the direct-orthogonalization corrections and are expected to be small.

The post hydrogen direct-orthogonalization term (DOE) is

$$T^{\mathrm{DOE}} = -\sqrt{2}\int dx\, dy\, dy'\, dy_1\, \phi_{n\ell}^{\mu*}(\mathbf{x}\mathbf{y})\, u_{1s}^{\lambda*}(y_1) \left(\frac{1}{x} - \frac{1}{y} - \frac{1}{|\mathbf{x} - \mathbf{y}_1|} + \frac{1}{|\mathbf{y} - \mathbf{y}_1|}\right) \Delta^\lambda(y_1, y')\, \psi_B(yy') \frac{\chi_c^+(\mathbf{k}_i,\mathbf{x})}{2\pi^{3/2}} = T_{12}^{\mathrm{DOE}} + T_{34}^{\mathrm{DOE}}, \tag{17}$$

where in the last expression the subscript 12 refers to the first and second terms in the large parentheses, and likewise for subscript 34, and where

$$\Delta^\lambda(y, y') = \sum_\gamma u_\gamma^\lambda(y_1)\, u_\gamma^{\lambda*}(y'). \tag{18}$$

Noting that

$$\left(\frac{1}{x} - \frac{1}{y}\right) \int d^3y,\, u_{1s}^{\lambda*}(\mathbf{y}_1) \sum_\gamma u_\gamma^\lambda(\mathbf{y}_1)\, u_\gamma^{\lambda*}(y') = \left(\frac{1}{x} - \frac{1}{y}\right) u_{1s}^{\lambda*}(y'), \tag{19}$$

the first two terms of (17), T_{12}^{DOE}, are just the negative of the first two terms of (7), T_{12}^{CBPS}.

Consider the y' integral in the last two terms of (17), T_{34}^{DOE}, with $\gamma = 1s$,

$$u_{1s}^{\lambda}(\mathbf{y}_1)\int d^3y'\, u_{1s}^{\lambda}(\mathbf{y}')\,\psi_{AABB}^{\alpha\alpha\beta\beta}(y'y)=\frac{\lambda^3}{4\pi}\,8\left(AA\frac{e^{-\lambda y_1-\alpha y}}{(\alpha+\lambda)^3}+BB\frac{e^{-\lambda y_1-\beta y}}{(\beta+\lambda)^3}+AB\frac{e^{-\lambda y_1-\beta y}}{(\alpha+\lambda)^3}+AB\frac{e^{-\lambda y_1-\alpha y}}{(\beta+\lambda)^3}\right)$$
$$=\psi_{A_1AB_1B}^{\lambda\alpha\lambda\beta}(\mathbf{y}_1\mathbf{y}), \tag{20}$$

where

$$A_1=\frac{8A}{(\alpha/\lambda+1)^3},\quad B_1=\frac{8B}{(\beta/\lambda+1)^3}. \tag{21}$$

Thus $T_{34,\gamma=1s}^{\mathrm{DOE}}$ has an identical form to T_{34}^{CBPS}, but with altered constants, so that the integration scheme for $T_{12}^{\mathrm{DOE}}+T_{34,\gamma=1s}^{\mathrm{DOE}}$ follows that of Choudhury, Mukherjee, and Sural (CMS). From (20) it is readily apparant that $\gamma=2P$ gives zero contribution to T_{34}^{DOE}, but $T_{34,\gamma=2s}^{\mathrm{DOE}}$ contributes since $\lambda\neq\alpha,\beta$. The integration scheme for the latter closely follows the technique of CMS. $T_{34,\gamma=3s}^{\mathrm{DOE}}$ was not included since similar terms for (3) were found to be negligible.

The reduction of the positronium direct-orthogonalization terms, the third and fourth terms in Fig. 7, is much more difficult because of the extra three-dimensional integral. The y' integral may be done directly giving four terms in the pairings of $V\nu V'\nu'$ (permutations of $\{A,\alpha,B,\beta\}$)

$$T_{V\nu V'\nu'}=\sum_{\gamma}[T_{V\nu V'\nu'}^{a1\gamma}-(-1)^{\ell_\gamma}T_{V\nu V'\nu'}^{1a\gamma}], \tag{22}$$

where a is the ratio of the nucleon to electron masses in the final bound state, and the sum is over all possible final bound states. In positronium this ratio is one so that only the odd-parity terms in the sum are nonzero, as was found [12] for the orthogonalization corrections in reaction (3). In the results below, only the $2p$ contributions are included since the $3p$ contributions for the similar terms in (3) were negligible. The T's are

$$T_{V\nu V'\nu'}^{ab\gamma}=-\frac{2\sqrt{2}VV'(a+b)^3\lambda^{3/2}}{(2\pi)^3\sqrt{\pi}(\lambda+\nu)^3}\int d\mathbf{x}\,d\mathbf{r}\,ds\,e^{-i\mathbf{k}_f\cdot[\mathbf{s}+(\eta+\zeta)\mathbf{x}]}u_{1s}^{\mu*}(\mathbf{r})$$
$$\times\exp\left(-\frac{\lambda+\nu}{\eta(a+b)}\mid\mathbf{s}+(\eta+\zeta)\mathbf{x}-\eta b\mathbf{r}\mid\right)\left(\frac{\eta(a+b)}{\mid\mathbf{s}+(\eta+\zeta)\mathbf{x}-\eta b\mathbf{r}\mid}+\frac{\nu+\lambda}{2}\right)$$
$$\times u_{\gamma}^{\mu}(\mathbf{r})u_{\gamma}^{\mu*}(\mathbf{s}/\eta)e^{-\nu'|\mathbf{s}/\eta+\mathbf{x}|}\chi_c^{+}(\mathbf{k}_i,\mathbf{x}). \tag{23}$$

Introducing the Fourier (three-dimensional integral) representation of the exponential function and the Yukawa potential allows the $\mathbf{r}$ integral to be evaluated [23]. One may then introduce a (one-dimensional integral) Gaussian transform [24] to evaluate the $\mathbf{s}$ and $\mathbf{x}$ integrals, leaving a final expression requiring numerical evaluation of a four-dimensional integral. At low energies and small angles the (momentum) radial, θ, ϕ, and (Gaussian) ρ integrals required 32, 16, 24, and 16 Gaussian points, respectively, which used 11 hours of CPU time per energy data point on a VAX 750.

VII. RESULTS

In the following discussion, abbreviations for cross sections will have a prefix of L if they use Löwdin's wave function and C if they use Chandrasekhar's wave function. Prior cross sections will have PR suffixed and post cross sections have PS suffixed. Of the intervening letters, CBS refers to the Coulomb Born approximation, DO refers to the positronium direct orthorgonlization result, and DIO refers to the direct iso-orthogonlization

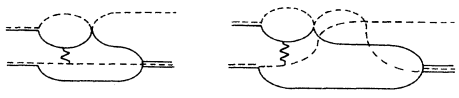

FIG. 11. Direct and (nucleon) exchange corrections orthogonalizing the free nucleon with respect to the upper post bound state, for the electron-nucleon transition amplitude for reaction (1).

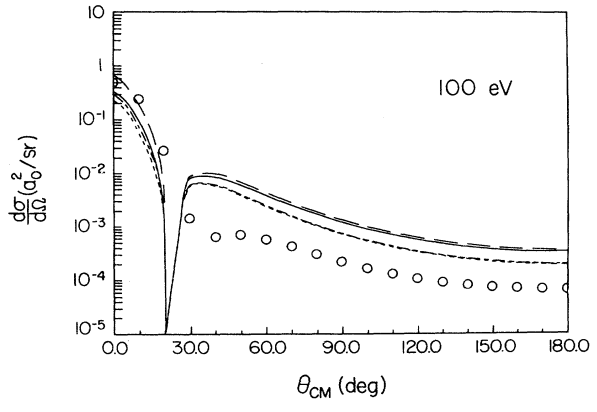

FIG. 12. Differential cross section, of center-of-mass angle θ_{CM}, for electron capture from H^- into the ground state of positronium. The solid line is the present calculation of the post CBA using Löwdin's wave function (LCBAPS), the open circles are the LCBAPS of CMS [25], the dashed lines are, in order of decreasing length, the prior LCBA (LCBAPR), the CBAPR using Chandrasekhar's wave function (CCBAPR), and the CCBAPS.

result. The differential cross section for reaction (1) is given in Fig. 12 for a positron energy of 100 eV. Although the present prior CBA using Löwdin's wave function (LCBAPR) and the calculation of Choudhury, Mukherjee, and Sural [25] agree, the present calculation of the post CBA cross sections using the post interaction for Löwdin's wave function [21] (LCBAPS) disagree with the calculation of CMS. Where they found an order of magnitude post-prior discrepancy in the differential cross sections except at forward angles, and a markedly different shape to the minima, the present post and prior results differ by 1–10% at 100 eV, and the minima have the same shape and occur within one degree of each other.

A cross-check of the present analytic result and their result (which they kindly sent) produced agreement at this stage, so the disagreement is in the computer codes. Four independent reprogrammings, two using alternate reductions of the integrals giving a different but equivalent analytical result, have reproduced the present results. Additionally, there is a "phase-space" argument in favor of the present result: that it is less likely that an error would produce nearly identical post and prior curves if they were truly dissimilar than that an error would produce dissimilar curves if they were truly nearly identical.

Chandrasekhar's "open-shell" wave function [22] gives a binding energy of $-0.522\,592$ atomic units for H^-, which is within 0.4% of the correct value, but Löwdin's wave function does not give a negative binding energy. One would suspect that the former would also yield better results in a scattering problem. It may be seen in Fig. 12 that the post and prior results are almost indistinguishable for the former. Also the magnitude of the CCBA results are $\frac{1}{2}$ to $\frac{2}{3}$ as large as the LCBA results, which is expected to exceed the exact result.

The iso-orthogonalized differential cross sections

$$\frac{d\sigma}{d\Omega} = (2\pi)^4 \frac{k_f}{k_i} M_f M_i |T^{\mathrm{CBPS}} + \tfrac{1}{2}\left(T^{\mathrm{DOPS}} + T^{\mathrm{DOE}}\right)|^2 \tag{24}$$

at energies 0.1, 0.5, and 1 eV are given in Fig. 13 and the total cross sections are given in Table I. The total cross section was obtained by a simple extended Simpson's rule from the differential cross sections so the error may be of order 10%, as seen by comparing LCBAPR at 100 eV to the result, 0.255×10^{-1}, of CMS. This is certainly smaller than the error due to the approximate H^- wave function, which may be estimated by taking the difference between the LDIOPS and CDIOPS results.

It may be seen that all orthogonalization corrections tend to remove the minimum that appears in the CBA results, a minimum that was shown to be spurious in reaction (2). However, the CDOPR and CDOPS cross sections (and the result obtained by averaging these amplitudes) are larger than both the CCBAPR and CCBAPS cross sections. Since the Coulomb Born approximation for the exact H^- wave function appears to be larger than the unitarity limit near zero incident energy, one would want cross sections less than the CBA result in this re-

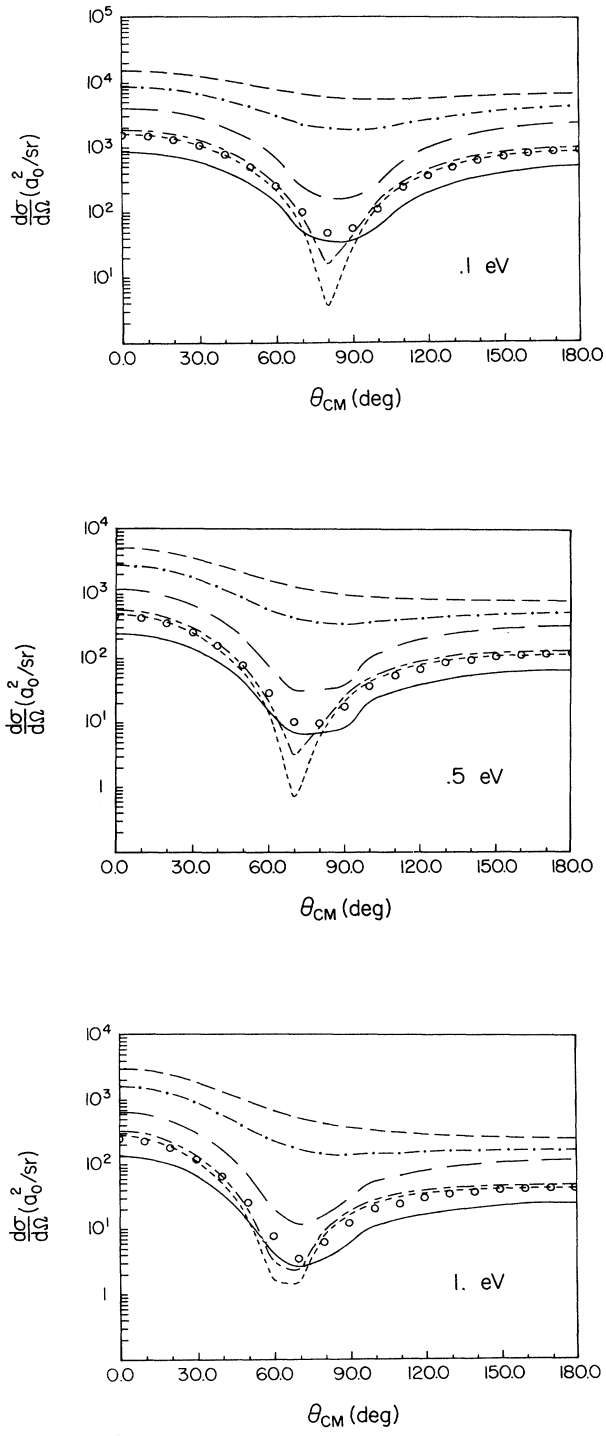

FIG. 13. Electron capture from H^- into the ground state of positronium using the "open-shell" wave function. The solid line is the present calculation including the (post direct) iso-orthogonalization (CDIOPS) [the open circles are the same result using Löwdin's wave function (LDIOPS)], the dashed lines are, in order of decreasing length, the post direct-orthogonalization result (CDOPS), the prior direct-orthogonalization result (CDOPR), the CCBAPR, and the CCBAPS.

TABLE I. Total cross sections for electron capture from H^- into the ground state of positronium, in units of πa_0^2. Numbers in square brackets denote powers of 10.

E (eV)	LCBAPR	LCBAPS	CCBAPR	CCBAPR	CDOPR	CDOPS	LDIOPS	CDIOPS
0.1	0.167[4]	0.237[4]	0.201[4]	0.170[4]	0.304[5]	0.458[4]	0.904[3]	0.947[3]
0.5	0.634[3]	0.456[3]	0.384[3]	0.327[3]	0.576[4]	0.865[3]	0.321[3]	0.178[3]
1.0	0.303[3]	0.217[3]	0.181[3]	0.155[3]	0.269[4]	0.402[3]	0.149[3]	0.825[2]
100.0	0.232[−1]	0.151[−1]	0.112[−1]	0.986[−2]	0.791[−1]			

gion. The iso-orthogonalization correction gives a result that is less than the CBA in this region.

VIII. CONCLUSION

Cross sections for positronium formation by electron capture from the negative hydrogen ion have been calculated in the energy region below the 6.8-eV threshold for capture from hydrogen. The lowest-order Born approximation has been augmented by orthogonalization corrections. The present treatment has utilized the perspective of treating the atomic nuclei (of like charge and vastly different mass) as if they were isospin projections of a single species of "nucleon," and has examined the consequences of this perspective. In capture from hydrogen this iso-orthogonalized Fock-Tani result yielded excellent agreement with the variational result. To date there is no variational result for capture from H^-, due to difficult integrals involving Coulomb waves, but the iso-orthogonalized result shows promise of yielding a reliable result.

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