

Positronium scattering by helium

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Coupled-state calculations are presented for $\text{Ps}(1s) + \text{He}(1^1S)$ scattering in the energy range 0–40 eV. Up to 22 Ps states are employed but only one He state is retained. Pseudostates are used to represent the Ps continuum. First Born estimates of cross sections in which the He is excited or ionized are found to be negligible in the chosen energy range. Calculation shows that ionization of the Ps is the main process at the higher energies. Comparison is made with available experimental measurements of the total cross section and with other theories. At low energies there is not only serious conflict between different experiments but also between the different theoretical approximations. In particular, the calculations of Biswas and Adhikari [Phys. Rev. A **59**, 363 (1999)] and Peach (unpublished) predict a much smaller elastic cross section at low energies than that obtained in the present work. The relative merits of the different approximations are discussed. [S1050-2947(99)04212-2]

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I. INTRODUCTION

With the advent of monoenergetic energy tunable positronium (Ps) beams [1–13] a whole new area of atomic collision physics has been opened up. Positronium is special in that it is a *light* neutral projectile. The states of Ps fall into two classes, ortho (*o*) and para (*p*), depending upon whether the electron and positron are in a spin triplet or spin singlet state, respectively. The significance of this classification lies in the different lifetimes of these spin states against annihilation of the electron and positron into photons. Thus, in its electronic ground level, $\text{Ps}(1s)$, *o*-Ps has a lifetime of 142 ns and decays predominantly into three photons, while *p*-Ps has a lifetime of 0.125 ns and decays predominantly into two photons [14,15]. Similar to a hydrogen atom (H), positronium can be created in any electronic state $\text{Ps}(nlm)$. It is therefore necessary that the electronic condition of the beam be defined. In the present state of the art, Ps beams consist of essentially *o*-Ps in the ground $1s$ state [13], *p*-Ps($1s$) is too short lived to be transportable as a beam. Experimental capability is presently at an early stage and, except for a very limited amount of rough data on differential scattering [13], is confined to total cross section measurements. So far, such measurements have been made for Ps scattering by He, Ar, H_2 , and O_2 [9–13]. In addition to the beam measurements there are also some cross section data at very low energies deduced from observations of the annihilation rate of *o*-Ps($1s$) in various gases [4,16–19].

From a theoretical viewpoint, Ps scattering is a very difficult problem. Unlike electron and positron scattering, the projectile, Ps, now has internal degrees of freedom which must be taken into account as well as those of the target, this is a significant complication [20]. Because the center of charge of the Ps coincides with its center of mass, the direct Coulomb interaction between the Ps and the atomic or molecular target is very much weakened compared with that arising from electron exchange. However, the exchange process is very difficult to calculate since it involves electron swapping between two different centers, the target, and the

Ps. Because of these difficulties, progress in the theoretical treatment of Ps-atom collisions has been slow [4]. The archetypical system is $\text{Ps} + \text{H}$, which is also a classic example of the Coulomb four-body problem. This system has a history going back to the pioneering work of Massey and Mohr [21]. The first realistic calculation of electron exchange in $\text{Ps} + \text{H}$ scattering was made by Fraser [22,23] in the static-exchange approximation. In the 1970s Drachman and Houston [24,25] published some results on S-wave scattering, using the variational method, and Drachman [26] predicted the existence of resonances in which the positron orbits the H^- ion. In more recent times the static-exchange approximation has been revisited by Ray and Ghosh [27,28] and coupled-state calculations have started to appear in the literature [29–33]. The largest of these has been performed by Campbell *et al.* [33]. These authors have used a coupled-pseudostate approximation employing 22 Ps states to produce a picture of $\text{Ps} + \text{H}$ scattering over the energy range 0–40 eV. Resonances were found in the electronic spin singlet partial waves up to H wave, consistent with the suggestion of Drachman [26], and the fate of the Ps, whether to be elastically scattered, or excited, or ionized (the main process at higher energies), was described. One important restriction on this coupled-state approximation was the assumption that the H atom remained in its ground state. Allowance for real (but not virtual) excitation and ionization of the H atom was made by using the first Born approximation [20].

In this paper we announce the extension of the approximation of Campbell *et al.* [33] to Ps scattering by $\text{He}(1^1S)$. The motivation for this work is provided by the existence of experimental data [10,13,16–19] which can be used to test the model, an opportunity so far denied to the $\text{Ps} + \text{H}$ system. For $\text{Ps} + \text{He}$ scattering there are already static-exchange calculations by Fraser [34,35], Fraser and Kraidy [36], Barker and Bransden [37,38], and Sarkar and Ghosh [39]. Barker and Bransden [37,38] have also investigated the importance of the van der Waals interaction between the Ps and the He atom. A model potential calculation has been made by Drachman and Houston [40]. More recently, Biswas and

Adhikari [41] and Sarkar *et al.* [42] have made three-state [Ps(1s,2s,2p) + He] close-coupling calculations. These have been augmented in various ways (to be described later) to also take account of ionization of the Ps and excitation of the Ps to states with principal quantum number $n \geq 3$. The present work is a much larger coupled-pseudostate approximation (22 states) which uses the same Ps states as Campbell *et al.* [33] and as an earlier nonexchange calculation of McAlinden *et al.* [20]. This approximation includes, in a self-consistent way, both ionization and excitation of the Ps. Finally, we note the presence in the literature [10,13] of unpublished theoretical results by Peach.

II. THEORY

The approximation we use may be described as follows [43]. We expand the collision wave function Ψ for the Ps+He system in Ps states ϕ_a and He states ψ_b according to

$$\Psi = A \sum_{a,b} G_{ab}(\mathbf{R}_1) \phi_a(\mathbf{t}_1) \psi_b(\mathbf{r}_2, \mathbf{r}_3) \chi(s_1) \times \frac{1}{\sqrt{2}} [\alpha(s_2) \beta(s_3) - \alpha(s_3) \beta(s_2)], \quad (1)$$

where $\mathbf{R}_i \equiv (\mathbf{r}_p + \mathbf{r}_i)/2$ is the position vector of the Ps center of mass, $\mathbf{t}_i \equiv \mathbf{r}_p - \mathbf{r}_i$ is the Ps internal coordinate, $\mathbf{r}_p(\mathbf{r}_i)$ is the position vector of the positron (*i*th electron), all position vectors are referred to the atomic nucleus as origin, A is the antisymmetrization operator, α and β are the usual spin- $\frac{1}{2}$ functions, χ ($=\alpha$ or β) is the spin function for the electron in the positronium, and we need not make explicit mention of the positron spin which, under the Hamiltonian (6), is conserved in the collision. In writing Eq. (1) we have restricted the expansion to spin singlet states ψ_b of the atom. A consequence of this is that an *o*-Ps projectile cannot be converted into *p*-Ps or vice versa and so the collision cross sections for *o*-Ps and *p*-Ps are the same. In general the sets of states ϕ_a and ψ_b will consist of both pseudostates and eigenstates satisfying

$$\langle \phi_a(\mathbf{t}) | H_{\text{Ps}}(\mathbf{t}) | \phi_{a'}(\mathbf{t}) \rangle = E_a \delta_{aa'}, \quad \langle \phi_a(\mathbf{t}) | \phi_{a'}(\mathbf{t}) \rangle = \delta_{aa'}, \quad (2)$$

$$\langle \psi_b(\mathbf{r}_2, \mathbf{r}_3) | H_A(\mathbf{r}_2, \mathbf{r}_3) | \psi_{b'}(\mathbf{r}_2, \mathbf{r}_3) \rangle = \epsilon_b \delta_{bb'}, \quad \langle \psi_b(\mathbf{r}_2, \mathbf{r}_3) | \psi_{b'}(\mathbf{r}_2, \mathbf{r}_3) \rangle = \delta_{bb'}, \quad (3)$$

where H_{Ps} is the Ps Hamiltonian

$$H_{\text{Ps}}(\mathbf{t}) \equiv -\nabla_t^2 - \frac{1}{t} \quad (4)$$

and H_A is the atomic Hamiltonian

$$H_A(\mathbf{r}_2, \mathbf{r}_3) \equiv -\frac{1}{2} \nabla_2^2 - \frac{1}{2} \nabla_3^2 - \frac{2}{r_2} - \frac{2}{r_3} + \frac{1}{|\mathbf{r}_2 - \mathbf{r}_3|}. \quad (5)$$

The Hamiltonian for the collision system we take to be

$$H = -\frac{1}{4} \nabla_{\mathbf{R}_1}^2 + H_{\text{Ps}}(\mathbf{t}_1) + H_A(\mathbf{r}_2, \mathbf{r}_3) + V(\mathbf{r}_p; \mathbf{r}_1, \mathbf{r}_2, \mathbf{r}_3), \quad (6)$$

where

$$V(\mathbf{r}_p; \mathbf{r}_1, \mathbf{r}_2, \mathbf{r}_3) = \left(\frac{1}{|\mathbf{r}_1 - \mathbf{r}_2|} + \frac{1}{|\mathbf{r}_1 - \mathbf{r}_3|} - \frac{2}{r_1} \right) - \left(\frac{1}{|\mathbf{r}_p - \mathbf{r}_2|} + \frac{1}{|\mathbf{r}_p - \mathbf{r}_3|} - \frac{2}{r_p} \right) \quad (7)$$

gives the interaction between the Ps and the atom.

Substituting Eq. (1) into the Schrödinger equation with the Hamiltonian (6), projecting with $\phi_a(\mathbf{t}_1) \psi_b(\mathbf{r}_2, \mathbf{r}_3)$, and using Eqs. (2) and (3), leads to the coupled equations

$$(\nabla_{\mathbf{R}}^2 + p_{ab}^2) G_{ab}(\mathbf{R}) = 4 \sum_{a',b'} \left[V_{ab,a'b'}(\mathbf{R}) G_{a'b'}(\mathbf{R}) - \int L_{ab,a'b'}(\mathbf{R}, \mathbf{R}') G_{a'b'}(\mathbf{R}') d\mathbf{R}' \right], \quad (8)$$

where p_{ab} is the momentum of the Ps in the “*ab*” channel and

$$V_{ab,a'b'}(\mathbf{R}) \equiv \langle \phi_a(\mathbf{t}_1) \psi_b(\mathbf{r}_2, \mathbf{r}_3) | V(\mathbf{r}_p; \mathbf{r}_1, \mathbf{r}_2, \mathbf{r}_3) | \phi_{a'}(\mathbf{t}_1) \psi_{b'}(\mathbf{r}_2, \mathbf{r}_3) \rangle. \quad (9)$$

The local potentials $V_{ab,a'b'}(\mathbf{R})$ give the direct Coulombic interaction between the Ps and the atom. The nonlocal couplings $L_{ab,a'b'}(\mathbf{R}, \mathbf{R}')$, which we do not quote explicitly here, arise from electron exchange between the Ps and the atom and describe how the state $\phi_{a'} \psi_{b'}$ is converted into $\phi_a \psi_b$ by this process. It is not difficult to show that $V_{ab,a'b'} = 0$ if the Ps states ϕ_a and $\phi_{a'}$ have the same parity. In particular this implies that $V_{ab,ab} = 0$ so that the direct Coulomb interaction is nondiagonal. This property has the consequence that the direct term is weakened relative to the exchange interaction which has nonzero diagonal elements $L_{ab,ab}(\mathbf{R}, \mathbf{R}')$, hence the pronounced importance of exchange in Ps-atom scattering. Equations (8) are solved in partial wave form. For the solution of the partial wave equations we have adopted the *R*-matrix technique [44].

From Eq. (1) it is clear that the scale of the calculation grows rapidly as the product of the number of Ps states ϕ_a times the number of He states ψ_b . In order to contain the size of the calculation we follow Campbell *et al.* [33] and keep only the He ground state in the expansion (1). For the He ground state wave function we have used the Hartree-Fock representation of Clementi and Roetti [45] which gives a ground state energy of -2.8617 a.u., the exact energy being -2.9037 a.u. [46]. We report results in three levels of approximation. (i) The static-exchange (SE) approximation in which only the Ps(1s) and He(1¹S) states are retained in the expansion (1)—this approximation is driven solely by the exchange interaction since, see above, $V_{ab,ab} = 0$. (ii) A nine [47] state approximation (9ST) consisting of the 1s, 2s, and 2p eigenstates of Ps together with 3s, 4s, 3p, 4p, 3d, and 4d pseudostates [48], these pseudostates are the Ps counterparts [49] of the H states used by Fon *et al.* [50] for electron-H scattering. (iii) A 22-state approximation (22ST)

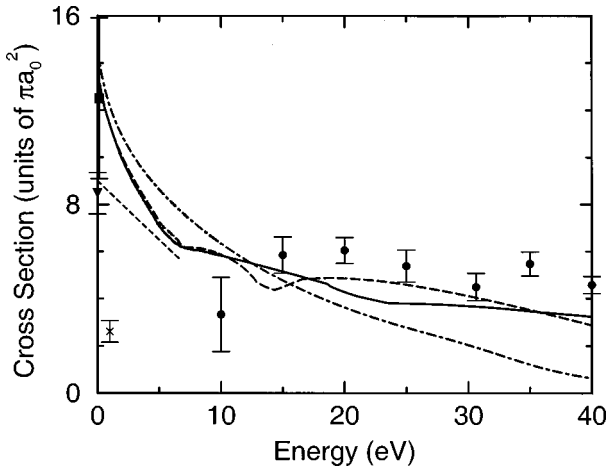


FIG. 1. Total cross section for o -Ps($1s$) + He(1^1S) scattering. Theoretical results: solid curve, 22ST; long-dashed curve, 9ST; dash-dot curve, SE. Experimental data: solid circles, Garner *et al.* [10,13]; solid square, Nagashima *et al.* [18]; solid triangle down, Canter *et al.* [16]; cross, Skalsey *et al.* [19]; short-dashed curve, Coleman *et al.* [17] (no error estimates are given by these authors).

involving the $1s$, $2s$, and $2p$ eigenstates of Ps as well as $3s-7s$, $3p-7p$, $3d-7d$, and $4f-7f$ pseudostates [20].

III. RESULTS

Our results are shown in Fig. 1–3. Although the captions refer to scattering of o -Ps by He, in the approximations adopted here, the cross sections for o -Ps and p -Ps scattering are identical (see above). The experimental data in the figures correspond to o -Ps. Figure 1 compares the total cross section σ_T calculated in our three approximations, 22ST, 9ST, and SE, over the energy range 0–40 eV. Since these approximations do not allow the He atom to be excited or ionized, in the terminology of McAlinden *et al.* [20], this is, strictly speaking, the “target elastic” total cross section σ_T^{TE} . Using the first Born approximation, McAlinden *et al.* [20] have estimated the “target inelastic” total cross section

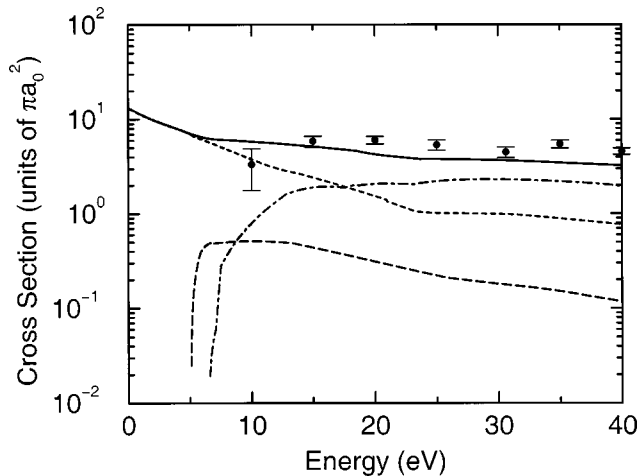


FIG. 2. Cross sections in the 22ST approximation: solid curve, total cross section; short-dashed curve, elastic scattering; dash-dot curve, Ps ionization; long-dashed curve, Ps($n=2$) excitation; solid circles, total cross section measurements of Garner *et al.* [10,13].

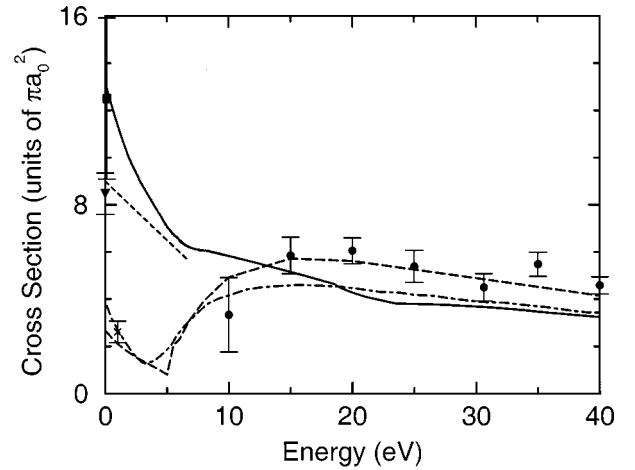


FIG. 3. Total cross section for o -Ps($1s$) + He(1^1S) scattering. Theoretical results: solid curve, 22ST; long-dashed curve, Biswas and Adhikari [41]; dash-dot curve, Peach [55]. Experimental data: solid circles, Garner *et al.* [10,13]; solid square, Nagashima *et al.* [18]; solid triangle down, Canter *et al.* [16]; cross, Skalsey *et al.* [19]; short-dashed curve, Coleman *et al.* [17] (no error estimates are given by these authors).

σ_T^{TI} , i.e., the sum of cross sections in which the target is excited or ionized. This estimate turns out to be negligible compared with the cross sections shown in Fig. 1, although at higher impact energies target inelastic scattering does become very important [20]. We therefore regard the theoretical curves in Fig. 1 as giving the full total cross section $\sigma_T = \sigma_T^{\text{TE}} + \sigma_T^{\text{TI}}$, in the energy range 0–40 eV. It should also be noted that the SE total cross section is the same as the SE elastic cross section since this is the only process that is represented in this approximation.

Figure 1 shows excellent agreement between the two pseudostate calculations, 9ST and 22ST, in the energy range up to 10 eV. To the extent that our approximation of retaining only the He ground state in Eq. (1) is valid, this inspires considerable confidence in the 22ST results. In the same energy range, it is also seen that there is not a great difference between the pseudostate calculations and the SE approximation. This suggests that the exchange interaction is dominant and that coupling to states of Ps other than $1s$ is not so significant at these impact energies. We think that this is yet another example of the Pauli exclusion mechanism discussed by Walters [51] and manifested at low impact energies in triplet S-wave $e^- + \text{H}(1s)$ and $\text{Ps}(1s) + \text{H}(1s)$ elastic scattering and in S-wave $e^- + \text{He}(1^1S)$ elastic scattering, this mechanism leads to insensitivity at low energies to the form of the approximation beyond the static-exchange level [52]. Above 10 eV differences between the two pseudostate approximations, 22ST [53] and 9ST, become apparent. However, it is seen that the 9ST cross section curls around the 22ST result and is “on average,” in agreement with the latter. This is a pattern of behavior that has already been noted in e^+ -atom scattering [54,55] where a lesser pseudostate approximation averages to the result of a better calculation. In this sense the 9ST calculation continues to support the 22ST cross section. Above 15 eV the SE cross section begins to fall well below the pseudostate curves. Two factors contribute to this decline. First, as noted above, the

SE approximation can only describe elastic scattering. As we shall see from Fig. 2, inelastic effects, principally ionization of the Ps, become dominant with increasing energy. Secondly, the SE approximation is driven exclusively by electron exchange, with increasing impact energy this will fade away in comparison with the direct couplings $V_{ab,a'b'}$ which are active in the pseudostate approximations. Unlike the case of $\text{Ps}(1s) + \text{H}(1s)$ scattering [33] there is a noteworthy absence of resonances in Fig. 1. On the basis of the model for the $\text{Ps} + \text{H}$ resonances [26], i.e., a positron orbiting the H^- ion, we would not expect resonances in the $\text{Ps}(1s) + \text{He}(1^1\text{S})$ system since He does not support a stable or metastable negative ion with total electronic spin $= \frac{1}{2}$. But it does have a metastable negative ion with total electronic spin $= \frac{3}{2}$ [56] and so we would expect resonances if the Ps were scattered off $\text{He}(2^3\text{S})$, say.

In Fig. 1 we also compare our calculations with the available experimental data. These consist of some cross sections at very low energies from Canter *et al.* [16], Coleman *et al.* [17], Nagashima *et al.* [18], and Skalsey *et al.* [19], deduced from observations of the annihilation rate of *o*- $\text{Ps}(1s)$ in He, and of beam measurements at higher energies by Garner *et al.* [10,13]. While, technically speaking, the very low energy annihilation measurements may correspond to the momentum transfer cross section, see Ref. [18] and [19],

$$\sigma_m = \int (1 - \cos \theta) \frac{d\sigma_{el}}{d\Omega} d\Omega, \quad (10)$$

where $d\sigma_{el}/d\Omega$ is the elastic differential cross section and θ is the scattering angle, in effect, at such low impact energies, we may treat the cross section as being the total elastic cross section ($= \sigma_T$ at these energies), since the scattering is almost entirely *S* wave. The measurements of Garner *et al.* [10,13] are straight measurements of the total cross section. From Fig. 1 we see that there is considerable disagreement between the low energy measurements, with the most recent of these, by Skalsey *et al.* [19], being by far the smallest. The largest cross section, that of Nagashima *et al.* [18] is $(13 \pm 4)\pi a_0^2$ and agrees very well with our pseudostate calculations. Above 15 eV the pseudostate cross sections generally lie below the measurements of Garner *et al.* [10,13] but are close. An intriguing situation is presented by the point of Garner *et al.* at 10 eV. This suggests a down turn in the cross section at lower energies, perhaps towards the measurement of Skalsey *et al.*, a trend that would be totally at variance with our calculations.

Figure 2 shows the total cross section for the 22ST approximation dissected into its principal components, i.e., the elastic cross section, the Ps ionization cross section σ_I , and the $\text{Ps}(n=2)$ excitation cross section. The ionization cross section has been extracted in the usual way [54,55] by taking

$$\sigma_1 = \sum_a f_a \sigma_a, \quad (11)$$

where σ_a is the cross section for exciting the Ps state ϕ_a and f_a is the fraction of this state overlapping the Ps continuum. The pattern of Fig. 2 is the same as that obtained by Camp-

bell *et al.* [33] in $\text{Ps}(1s) + \text{H}(1s)$ scattering. At high energies ionization is dominant, while at any energy $\text{Ps}(n=2)$ excitation is unimportant.

Figure 3 compares our 22ST total cross section with the theoretical calculations of Biswas and Adhikari [41] and of Peach [57], and again with the experimental data. Unlike the present work, these two theories predict a down turn in the total cross section at low energies and both are in agreement with the 10 eV measurement of Garner *et al.* [10,13] and with the point of Skalsey *et al.* [19]. At higher energies the cross section of Biswas and Adhikari is in particularly good agreement with the measurements of Garner *et al.* while the result of Peach lies close to the 22ST curve. It is therefore important to understand the difference between these calculations and the present work.

As in the present work, the approximation of Biswas and Adhikari does not take account of excitation/ionization, either real or virtual, of the He atom. The approximation of Peach [58] does not allow for real excitation or ionization of the He atom either but does include virtual excitations, in elastic scattering, through the use of model potentials (see below). For excitation and ionization of the Ps Peach uses a version of the first Born approximation and so do Biswas and Adhikari except that they calculate the $\text{Ps}(n=2)$ excitations in their three-state close coupling approximation. By contrast our approach is completely nonperturbative but relies on the Ps pseudostates in the expansion (1) to carry these processes. At the higher energies, where ionization of the Ps dominates the total cross section, see Fig. 2, all three approximations give similar results. Where the 22ST approximation is most different from the other two theories is in the estimate of the elastic cross section. In the other two approximations this is very much smaller than the 22ST prediction, this is clear from Fig. 3 where, below 5.1 eV, the total cross section is just the elastic cross section. When the inelastic channels switch on at 5.1 eV the extra addition to the comparatively small elastic cross section of the other two approximations causes a sudden rise in their total cross sections, this is the origin of the down turn in these theories on going below 10 eV. In the 22ST approximation, on the other hand, the inelastic contribution adds to an already large, but rapidly decreasing, elastic cross section and so results only in a shoulder in the total cross section near 5 eV. The primary difference between the 22ST approximation and the other two theories therefore rests upon the elastic cross section.

In the work of Biswas and Adhikari the elastic cross section is calculated in a three state $\text{Ps}(1s, 2s, 2p) + \text{He}$ close-coupling approximation. This, as the paper of Sarkar *et al.* [42] clearly shows, should result in an elastic cross section not very different from the SE approximation given in Fig. 1. However, Biswas and Adhikari [32,41] argue that there is an ‘‘orthogonality’’ problem with the exchange term in the coupled-state approach. They therefore modify the $\text{Ps}(1s, 2s, 2p) + \text{He}$ approximation to remove this ‘‘orthogonality problem,’’ the result is a very different approximation with a very much smaller elastic cross section. We do not subscribe to the view that there is an ‘‘orthogonality problem’’ and we regard the modification of the coupled-state approximation as unfounded.

In the approximation of Peach [58] the $\text{Ps} + \text{He}$ system is modelled as a three-body problem, i.e., e^+, e^- and a He core.

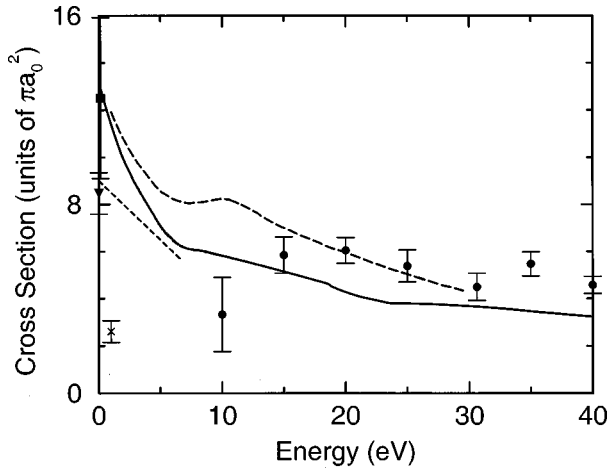


FIG. 4. Total cross section for o -Ps($1s$) + He(1^1S) scattering. Theoretical results: solid curve, 22ST; long-dashed curve, Sarkar *et al.* [42]. Experimental data: solid circles, Garner *et al.* [10,13]; solid square, Nagashima *et al.* [18]; solid triangle down, Canter *et al.* [16]; cross, Skalsey *et al.* [19]; short-dashed curve, Coleman *et al.* [17] (no error estimates are given by these authors).

Model potentials, which include “polarization” terms up to $1/r^6$ are constructed for the interaction of the e^+ and e^- with the He core, this is achieved by matching as closely as possible known $e^- + \text{He}$ and $e^+ + \text{He}$ scattering data [59,60]. In addition, three-body terms that depend upon the He “polarization” are added to the interaction. An adiabatic potential curve for the Ps($1s$) in the field of the He core is then generated by diagonalizing the model Hamiltonian for the system in a basis consisting of Ps states as well as the unphysical He($1s^3$) state which is supported by the model potential. Phase shifts are then calculated for Ps scattering in the adiabatic potential.

This approach to the elastic Ps($1s$) + He(1^1S) cross section differs in two substantive ways from the present work. First, the approximation of Peach allows for virtual excitation/ionization of the He by employing model potentials that replicate the full interaction between the e^+/e^- and the He; in our approximation neither real nor virtual excitation/ionization of the He is permitted. Secondly, Peach treats the scattering problem from an adiabatic viewpoint, whereas our approximation to the scattering is fully dynamic. At the present time it is hard to assess the merits and disadvantages of these differences between the two theories.

In Fig. 4 we compare our 22ST total cross section with the total cross section of Sarkar *et al.* [42] and with the experimental data. Sarkar *et al.* use a three-state close-coupling approximation [Ps($1s, 2s, 2p$) + He(1^1S)] to calculate the elastic and Ps($n=2$) cross sections. To obtain the total cross section they add on the ionization cross section of McAlinden *et al.* [20] which was calculated in the same 22ST approximation as here but neglecting exchange. Although the general trend of the two approximations of Fig. 4 is roughly similar, particularly at low energies, there are noticeable differences in detail.

Finally, we remark upon the model potential calculation of Drachman and Houston [40]. This gives a zero energy cross section of $7.73\pi a_0^2$ which is almost half of our 22ST result of $13.19\pi a_0^2$. In this approximation a local model po-

TABLE I. Cross sections (in units of πa_0^2) in the SE and 22ST approximations.

E(eV)	SE	22ST			
		Elastic	Ps($n=2$)	Ionization	Total
0.0	14.584	13.193			13.193
0.5	13.114	12.256			12.256
1.0	12.175	11.394			11.394
2.0	10.912	9.920			9.920
3.0	10.003	8.849			8.849
4.0	9.268	7.953			7.953
5.0	8.640	7.089			7.089
5.5	8.355	6.493	0.239		6.732
6.0	8.085	6.124	0.416		6.540
7.0	7.587	5.435	0.486	0.055	6.157
7.5	7.355	5.116	0.494	0.278	6.087
8.0	7.134	4.814	0.500	0.366	6.053
9.0	6.717	4.260	0.509	0.565	5.946
10.0	6.332	3.773	0.512	0.795	5.818
11.0	5.975	3.353	0.510	1.056	5.687
12.5	5.483	2.912	0.497	1.505	5.487
15.0	4.764	2.415	0.437	1.895	5.141
20.0	3.622	1.534	0.311	2.067	4.269
25.0	2.776	1.016	0.221	2.210	3.794
30.0	2.038	0.992	0.181	2.310	3.685
35.0	1.214	0.888	0.151	2.197	3.467
40.0	0.636	0.757	0.117	1.950	3.239

tential was constructed to represent electron exchange between the Ps and the atom. This potential was arranged so that the [corrected (see Ref. [40])] static-exchange results of Fraser and Kraidy [36] were reproduced in the static-exchange limit. This approximation does not allow for distortion of the atom and in physical content is therefore exactly the same as 22ST. However, unlike the model potential calculation, 22ST does not resort to a local approximation to exchange but treats it properly in its correct nonlocal form. For this reason the 22ST approximation is to be preferred. For future reference, we give in Table I a sample of our SE and 22ST results. The SE cross sections are in excellent agreement with those reported by Sarkar and Ghosh [39] also using a Hartree-Fock wave function for the ground state of He.

IV. CONCLUSIONS

The comparisons made in this paper highlight some very serious problems in our understanding of Ps-He collisions. While above 15 eV the theoretical calculations and the only available experiment, that of Garner *et al.* [10,13], might be described as being more or less mutually compatible (see Fig. 3 and 4), below this energy there is total discord both on the experimental side and on the theoretical front. As far as the present work is concerned, it is the contrast with the theories of Biswas and Adhikari [41] and of Peach [58] which is the most disquieting. The latter disagree markedly with the present work at low energies by predicting a much smaller elastic cross section. At very low energies the mea-

sured cross sections vary by a factor of 5, ranging from $(13 \pm 4)\pi a_0^2$ (Nagashima *et al.* [18]), which is in excellent agreement with our 22ST calculation, to $(2.6 \pm 0.5)\pi a_0^2$ (Skalsey *et al.* [19]), which is in very good agreement with the work of Biswas and Adhikari and of Peach. A tantalizing question is how the higher energy beam measurements of Garner *et al.* will connect up with the low energy data (which are based on observation of the annihilation process). The datum point of Garner *et al.* at 10 eV suggests a down turn in the total cross section at low energies which could then well continue towards the point of Skalsey *et al.* Clearly, what happens in the energy range below 15 eV is critical and it is here where future experiments should be concentrated.

In Sec. III we discussed the relative merits of the theories compared in Fig. 3. To summarize, our opinion was that the approximation of Biswas and Adhikari [32,41] was based upon an unfounded modification of the three-state $\text{Ps}(1s,2s,2p) + \text{He}(1^1S)$ close-coupling approximation. The work of Sarkar *et al.* [42] shows clearly that it is this modification which accounts for the substantial discrepancy between the Biswas-Adhikari approximation and our 22ST calculation at low energies. In comparison with the

approximation of Peach [58], there are two points of contrast. The first is her adiabatic treatment versus the fully dynamic approach adopted here. The second is the restriction of the present approximation to one undistorted atom state compared with Peach's allowance for distortion of the atom through the use of model potentials. At the present time we do not know the importance of either of these factors. The main criticism of the present work undoubtedly lies in the restriction of the expansion (1) to the He ground state. Yet, we find it hard to believe that allowance for all He states, both singlet and triplet, in Eq. (1) would lead to so substantial a change in the 22ST cross section as to give agreement with the lowest of the measurements shown in Fig. 3, that of Skalsey *et al.* [19], however, only a fully fledged calculation can substantiate this prejudice.

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