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# Ps-He scattering below the first target excitation threshold

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Scattering of a Ps atom off a He target has been investigated in the framework of the close-coupling approximation using two basis sets: (a) $\mathrm{Ps}(1s)+\mathrm{He}(1s^2,1s2^1s,1s2^1p)$ and (b) $\mathrm{Ps}(1s,2p)+\mathrm{He}(1s^2,1s2^1s,1s2^1p)$. Target inelastic channels reduce the elastic cross sections appreciably near zero energy. The present results are in good agreement with the theoretical prediction of Drachman and Houston and the measured data of Canter, McNutt, and Roellig and Coleman *et al.* and are also in good agreement with the measured data of the UCL group from 15–20 eV.

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With the advent of monoenergetic energy tunable ortho positronium (O-Ps) beam, it is now possible to measure positronium atom-molecule scattering parameters. Measurements have already been carried out for total cross sections on Ps scattering off He, Ar, $O_2$, and $H_2$ targets using beam techniques [1–5]. In addition to these beam measurements, some cross-section data have been deduced from observations of the annihilation rate of O-Ps in various gases at very low energies [6–9]. At the very low energies, annihilation measurements correspond to momentum-transfer cross-section (MTC), which is given by,

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

where, $d\sigma_{\mathrm{el}}/d\Omega$ is the elastic differential cross section. The MTC at very low energy may be considered to be the total cross section since *S*-wave cross section is rather essentially the sole contributor to the total cross section at these energies. The zero (or near zero) energy cross-section data obtained so far by different groups on Ps-He scattering differs dramatically among themselves. The largest cross section is obtained by Nagashima *et al.* [6] as $13(\pm4)\pi a_0^2$, whereas Skalsey *et al.* [7] give the lowest value as $(2.6\pm0.5)\pi a_0^2$. Values of cross section due to Coleman *et al.* [9] and Canter, McNutt and Roellig [8] are $9\pi a_0^2$ and $(8.4\pm0.9)\pi a_0^2$ respectively. No error estimates have been provided by Coleman *et al.* [9]. The last two measured data are very close to each other. The direct value measurement of the UCL [1] group at 10 eV, the lowest energy they considered, is around $3.3\pi a_0^2$. Present situations warrant further measurements on the Ps-He scattering system to settle the behavior of cross section near zero energy.

Here we consider Ps-He scattering up to the energy below the first excitation threshold (up to 20 eV) of the He atom. Our earlier predicted results (Sarkar, Chaudhuri, and Ghosh [10]), are in excellent agreement with the measured data of the UCL group [1] in the energy region 20–30 eV. We are in particular more interested about the zero (or near zero) energy cross section due to anomaly in the experimental values. Theoretically, Ps-He scattering has been initiated by Fraser [11,12] and Fraser and Kraidy [13] using the static exchange model. The static exchange model has also been used by Barker and Bransden [14,15] and they have also included van der Waals' interaction between Ps and He atoms adiabatically in their calculations. Fraser predicted a MTC of $12\pi a_0^2$ and Bransden predicted the same as $9.38\pi a_0^2$ at 0.272 eV. Recently, Sarkar and Ghosh [16] have also employed the static exchange model for a wider range of energies. Sarkar *et al.* [10] have also applied a three-state $[\mathrm{Ps}(1s,2s,2p)+\mathrm{He}(1s^2)]$ target elastic close-coupling approximation and predicted the results up to 200 eV giving the near zero energy cross section at $14.584\pi a_0^2$. Most recently Blackwood *et al.* [17] (Belfast group) have investigated Ps-He scattering using a target elastic coupled pseudostate (22 states) calculation in the energy range 0–40 eV predicting $13.193\pi a_0^2$ as the zero energy cross section. This is the most elaborate coupled channel target elastic calculation. The zero energy cross section of both groups are close to each other and also very close to that of Nagashima *et al.* [6]. Drachman and Houston [18] have investigated Ps-He scattering and obtained the value of $Z_{\mathrm{eff}}$ and scattering length. The exchange of electrons between the atoms has been taken into account by using a local model potential. They included the effect of correlation by taking close channel wave functions having eighty-four independent terms. Ultimately the problem is solved by the Kohn variational principle in the framework of adiabatic approximation. They predicted a zero energy cross section of $7.73\pi a_0^2$. In a very recent calculation Biswas and Adhikari [19] have investigated Ps-He scattering using a different version of the close-coupling method where the exchange of electrons between two atoms has been incorporated by using a nonlocal model potential. Their results are in good agreement with the UCL group and the zero energy cross section is close to the measurement of Skalsey *et al.* [7]. However their results differ appreciably from all other theoretical values predicted so far. We would like to add that Peach [20], as reported by the Belfast group [1], has included the effect of inelastic chan-

TABLE I. Scattering length for Ps-He in different approximations (in a.u.).

| | |
|---|---|
| Fraser | 1.72 |
| Drachman and Houston | 1.389 |
| Model (a) | 1.394 |
| Model (b) | 1.360 |

nels of the He atom through a model potential adiabatically and predicted a total cross section of about $3.3\pi a_0^2$ at zero energy. Thus we see that the theoretical predictions run from $2.7\pi a_0^2$ to $14.584\pi a_0^2$. Therefore, zero energy cross section is still a complete open question. Further theoretical investigations are required to determine the exact behavior of the cross section at very low energies.

Here we consider Ps-He scattering at low energies. As the theoretical as well as experimental predictions for the total cross section at zero energy differ dramatically among themselves, we focus our attention on such a low-energy region. Literature reveals that above 5.1 eV, the dominant contribution to the total cross section in the Ps-atom scattering is due to the inelastic channels of Ps [17]. The extensive calculations of Blackwood *et al.* [17] show that (Table I in Ref. [17]) the zero energy cross-section changes very marginally from 14.584 in the static exchange approximation to 13.193 in their 22-state target elastic calculation, a change of 9.5%. It is worth mentioning that the 22-state target elastic calculation incorporates, via pseudostates, the effects of higher excitations and continuum of the projectile atom. It is evident from the above discussion that the zero (or near zero) energy elastic cross section does not depend much on the inelastic channels of the Ps atom. On the other hand, the calculations of Ray and Ghosh [21], Sinha, Basu, and Ghosh [22] and Basu, Sinha, and Ghosh [23] on Ps-H scattering show that the low-energy elastic cross section reduce drastically due to the inclusion of target inelastic channels. Keeping this in mind, we include the $n=2$ singlet excitation channels of the target He atom in our present calculations. All the He wave functions used are taken from Winter and Lin [24]. Further, the van der Waals' interaction is supposed to play a vital role in determining the scattering parameters in Ps-atom scattering [22,25]. Hence, we investigate Ps-He scattering using two basis sets,

$$(\mathrm{a})\quad \mathrm{Ps}(1s)+\mathrm{He}(1s^2,1s2\,^1s,1s2\,^1p)$$

$$(\mathrm{b})\quad \mathrm{Ps}(1s,2p)+\mathrm{He}(1s^2,1s2\,^1s,1s2\,^1p).$$

Our experience on Ps-H [22,23] and on Ps-He [16] scattering shows that the Ps($2s$) does not contribute significantly to the low-energy elastic cross sections. Guided by this and also to save computer time, we do not include the Ps($2s$) excitation channel in our model (b).

The present calculation takes two extra effects for the system under consideration, which have not been considered earlier: effect of higher excited states of target atom and the van der Waals' interaction. The van der Waals' interaction is included dynamically through the inclusion of $p$ states of both the atoms in the expansion scheme.

We use the close-coupling approximation (CCA) to solve the problem using our numerical code. In actual calculation one has to solve the one-dimensional coupled integral equation,

$$T^{J\pm}(\tau'k';\tau k)=B^{J\pm}(\tau'k';\tau k)-\frac{1}{2\pi^2}\sum_{\tau''}\int dk''k'' \times\frac{B^{J\pm}(\tau'k';\tau''k'')T^{J\pm}(\tau''k'';\tau k)}{k^2_{\eta''\nu''}-k''^2+i\varepsilon},$$

where $\tau\equiv(n_p,l_p,n_a,l_a,J_1,L)$. The details of the theory are given in Refs. [22,25]. These equations are converted into simultaneous equations and are solved by a matrix inversion technique for each partial wave.

Table I compares the values of the scattering lengths using our present models with the other available theoretical predictions. Using a static exchange model, Fraser predicted a high scattering length while the other three quoted results are much lower and close to each other. The value of Drachman and Houston lies in between our present results, the value predicted by model (b) being the lowest one.

Table II displays the different predictions for the zero (or near zero) energy cross sections. This table also carries the

TABLE II. Zero energy total cross section for Ps-He in units of $\pi a_0^2$.

| Theory | | Experiment | |
|---|---|---|---|
| References | Cross sections | References | Cross sections |
| Sarkar *et al.* | 14.584 | Nagashima *et al.*[a] | 13(±4) |
| Blackwood *et al.* | 13.193 | Coleman *et al.* | 9.0 |
| Fraser[a] | 12.0 | Canter, McNutt, and Roellig | 8.4(±0.9) |
| Barker and Bransden[a] | 9.38 | Skalsey *et al.*[a] | 2.6(±0.5) |
| Drachman and Houston | 7.73 | | |
| Model (a) | 7.78 | | |
| Model (b) | 7.40 | | |
| Peach | 3.30 | | |
| Biswas and Adhikari | 2.70 | | |

[a] Near zero energy.

outcomes of different annihilation measurements. The lowest theoretical value has been predicted by Biswas and Adhikari [19] and is in excellent agreement with the finding of Skalsey *et al.* [7]. The estimate of Peach is also very close to that of Biswas and Adhikari. But their results are far away from other corresponding theoretical predictions. The results of Blackwood *et al.* and those of Sarkar, Chaudhuri, and Ghosh corroborate well with the measured data of Nagashima *et al.* [6]. There are other two nearby [8,9] measured data for zero energy cross section. Our results, using both the present models, are close to the findings of Canter, McNutt, and Roellig and Coleman *et al.* Our extrapolated zero energy cross-sections are 7.78 [using model (a)] and 7.4 [using model (b)]. It is evident that the inclusion of $n=2$ target states decrease the near zero energy elastic cross section by a huge amount when compared with other *ab initio* calculations. On allowing the target atom to be virtually excited, the low-energy impinging Ps atom, for small separation between the atoms, feels a wider charge distribution of the target atom, which gives rise to a more attractive potential compared to the situation where the target is tightly bound to its ground state. This drops the zero energy cross section approximately by 50% [model (a)]. The results are lowered further on inclusion of a virtual excitation of the Ps atom in the expansion basis [model (b)]. The van der Waals' interaction, which we have talked about earlier, arises due to the interaction of induced dipole moments of the colliding atoms. The effect of induced polarizability is well accounted by the *p* states. Thus our second model takes into account, at least partially, the van der Waals' interaction dynamically through the inclusion of *p* states of both the atoms. The attractive van der Waals' interaction reduces the zero energy cross section further from that obtained in model (a). In this connection, it is worth mentioning that the Drachman and Houston [18] prediction is in fair agreement with ours. In our calculation on Ps-H [22], we avoided the calculation of $\mathrm{Ps}(1/2s)-\mathrm{H}(1/2s)\rightarrow\mathrm{Ps}(2p)+\mathrm{H}(2p)$ exchange elements on the ground that the exchange is a short-range interaction while the van der Waals' interaction is a long-range one. Here we have performed the calculation [model (b)] with and without $\mathrm{Ps}(1s)+\mathrm{He}(1s^2/1s2\,^1s)\rightarrow\mathrm{Ps}(2p)+\mathrm{He}(1s2\,^1p)$ exchange elements and found no significant change in the zero energy cross-section, which confirms our earlier assumption. We also included in our calculation, not quoted, the higher $(n>2)$ excited states of the He atom in a calculation similar to model (a) and found a marginal change in the zero energy cross section. This encouraged us to restrict ourselves to include only up to $n=2$ target states in both the models.

In Fig. 1 we compare the integrated elastic cross section for O-Ps-He scattering up to incident energy 20 eV using different theoretical predictions. The three-state target elastic results of Sarkar, Chaudhuri, and Ghosh [10] lie always near those of static exchange [16,17] predictions. The 22-state target elastic calculation [17] predicts appreciably lower cross sections compared to those of the static exchange model. With increase in energy, the difference between the eigenstate predictions [16,10] and the corresponding pseudostate [17] predictions increase gradually. Evidently, the inclusion of projectile inelastic channels, mainly the effect of ionization, lowers the elastic cross sections appreciably, the effect increases with increasing energy in the energy range considered. The elastic cross sections using our present two models give much lower values compared to target elastic cases at very low energies. The rate of fall of elastic cross section, using present models, are much slower than that of the 22-state calculation. Beyond the Ps incident energy of 5 eV, our present models predict higher values for integrated elastic cross section than those of the 22-state calculation. With the increase in energy the effect of $n=2$ target singlet excitation channels decreases and the results of model (a) and model (b) approach, respectively, to the predictions of static exchange and three-state target elastic approximations. Obviously, near zero incident energies, it is the target inelastic channels, mainly $n=2$ excitation channels, which is the main factor for the reduction in the elastic cross section, but at relatively higher energies, the projectile inelastic channels influence the elastic cross sections. We infer that near zero energy, the effect of virtual loosening of the target is very important, while at higher energies, the effect of Ps ionization is dominant.

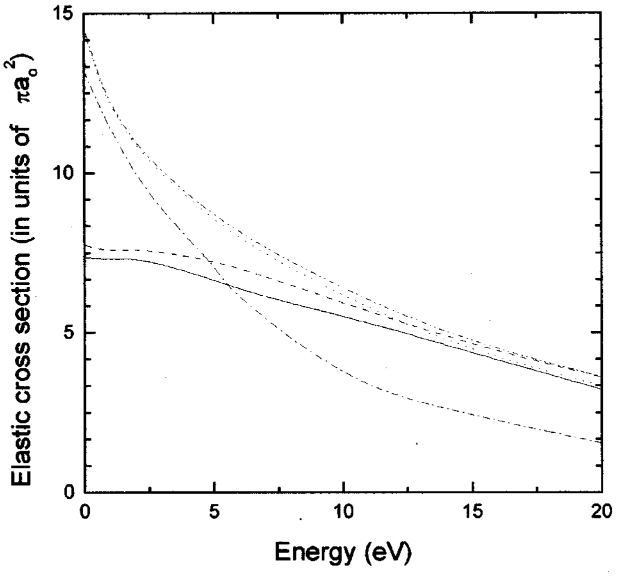

FIG. 1. Integrated elastic cross sections. Curves: dash-double dot, static exchange, Ref. [16]; dot, three-state target elastic CCA, Ref. [10]; dash dot, 22-state target elastic CCA, Ref. [17]; dash, three-state projectile elastic CCA [model (a)]; solid, full CCA [model (b)].

In Fig. 2, we compare the integrated total cross sections using our present full CCA model [model (b)] along with the corresponding predictions of Sarkar, Chaudhuri, and Ghosh and those of Blackwood *et al.* This figure also carries the measured data of the UCL [1] group in the same energy range as in figure 1. We define the total cross section as

$$\sigma_T=\sigma_{\mathrm{el}}^{\mathrm{CCA}}+\sigma_{\mathrm{ex(Ps:}n=2)}^{\mathrm{CCA}}+\sigma_{\mathrm{ex(Ps:}2<n\leq 4)}^{\mathrm{B\text{-}O}}+\sigma_{\mathrm{ion(Ps)}}^{\mathrm{FBA}},$$

where $\sigma_{\mathrm{el}}^{\mathrm{CCA}}$ is the elastic cross section using model (b), $\sigma_{\mathrm{ex(Ps:}n=2)}^{\mathrm{CCA}}$ is the $\mathrm{Ps}(n=2)$ excitation cross sections, $\sigma_{\mathrm{ex(Ps:}2<n\leq 4)}^{\mathrm{B\text{-}O}}$ is the Ps excitation cross sections (for $n=3$ and

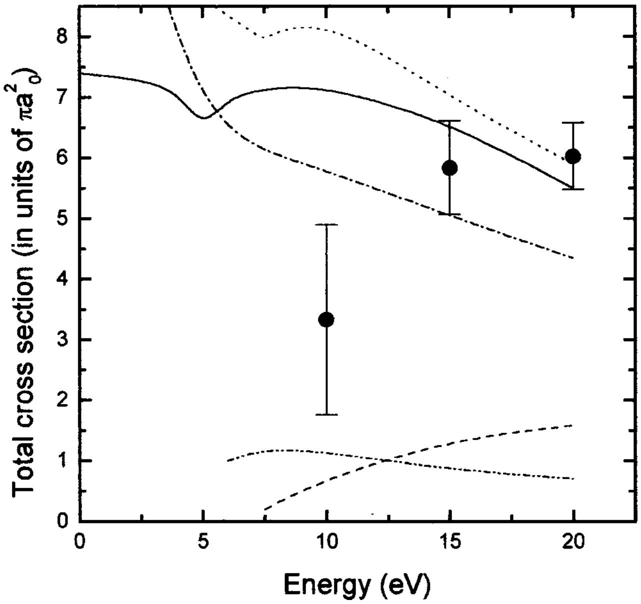

FIG. 2. Total cross sections. Curves: dot, three-state target elastic CCA, Ref. [10]; dash dot, 22-state-target elastic CCA, Ref. [17]; dash, Ps ionization; dash-double dot, Ps ($n=3$ and 4) excitation cross sections; solid, full CCA [model (b)]; solid circles, measured data of the UCL group, Ref. [1].

4), using the Born-Oppenheimer approximation, and $\sigma_{\text{ion(Ps)}}^{\text{FBA}}$ is the Ps ionization cross section evaluated using the first Born approximation. For Ps$(2s)$ excitation cross sections we use the results of Sarkar, Chaudhuri, and Ghosh [10] and, as in our present models, the Ps$(2s)$ state is not included. However, except the $\sigma_{\text{el}}^{\text{CCA}}$, the other partial cross sections are added to $\sigma_T$ when they are energetically accessible. Our predictions for the total cross sections [Sarkar, Chaudhuri, and Ghosh and model (b)] show a minimum but this is not present in the results of Blackwood *et al.* This is also in the calculations of Biswas and Adhikari and Peach. In our models the minima are in the vicinity of the Ps $n=2$ excitation threshold. Below 5.1 eV, the total cross section is nothing but the elastic cross section. With increase in energy, the elastic cross section decreases and 5.1 eV onwards, Ps inelastic contributions to the total cross section give a raising trend. Thus, a minimum is well expected. The present results are in fair agreement with the measured data of the UCL group [1] beyond 15 eV. We would like to add that Sarkar, Chaudhuri, and Ghosh had an excellent agreement with UCL data in the energy range 20–30 eV. The difference between the two sets of results of our group is due to the fact that our earlier work included the Ps ionization cross section as extracted by McAlinden, McDonald, and Walters from their 22-state nonexchange calculation [26]. On the other hand, predicted value of the Belfast group are in fair agreement at 15 eV only. All the theoretical predictions, including Biswas and Adhikari, are at variance with the measured data at 10 eV. Our present results are expected to be modified by two reasons, first the effects of higher excitations and ionization of Ps atoms, which will reduce the elastic cross section and second, proper evaluation of the ionization cross section. Proper estimates for Ps ionization is expected to yield a larger value than the present one (as cited in Refs. [17], [26]) obtained by using the first Born approximation. Effect of ionization of the He target is also expected to reduce the very low-energy elastic cross section. Our investigation [23] on Ps-H shows that the continuum of the target reduces the *s*-wave elastic cross section. These two effects are expected to more or less compensate each other and the total cross section, as given by us, may be modified at best by 10%. Thus, the present paper reports a good estimate to the total cross section near zero energy as well as beyond 10 eV when compared to measured data. In this connection we like to add that a paper containing the detailed results of the present models has already been communicated.

We have investigated Ps-He scattering using two models: a projectile elastic CCA model (a), and a more realistic approach in which both the atoms are allowed to be excited simultaneously, model (b). We have obtained a dramatic change in the near zero energy elastic cross section by allowing the virtual excitations of the target. Moreover, the present results are in good agreement with the UCL group beyond 10 eV. Near the zero energy, the total cross section has a fair agreement with measured data of Canter, McNutt, and Roellig and Coleman *et al.* and the theoretical prediction of Drachman and Houston. Near zero energy the cross section obtained by us may be modified if one takes into account the effect of the continuum of the He atom. However, we have verified, by inclusion of $n=3$ target (singlet) states, that the elastic cross section changes marginally. We expect that near zero energy cross section may be reduced further by 10% if all the effects, stated earlier, are considered. Here we have introduced two effects, the effect of target excitations and the van der Waals' interaction for the Ps-He system. For a most meaningful calculation, we advocate for the full CCA, which includes the effects of inelastic channels of both the atoms.

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