

Nonradiative formation of the positron-helium triplet bound state

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We have previously calculated the cross section for radiative formation of the interesting bound state consisting of a positron bound to helium, where the atomic electrons are in the triplet spin state. That process uses the metastable triplet helium system as target, and, as expected, it has a very small cross section. In this paper we examine a more probable process in which the state of interest is produced in an exchange rearrangement collision between a positronium atom and the singlet helium ground state: $\text{Ps} + \text{He}(^1S^e) \rightarrow \text{PsHe}^+(^3S^e) + e^-$. The present calculation is done in the plane-wave Born approximation, using simple initial and final wave functions and compares post and prior forms.

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I. INTRODUCTION

In our previous paper [1] about the weakly bound system consisting of a positron and a helium atom in the triplet spin state we briefly reviewed the history of this problem. It took many years between the first unsuccessful attempt [2] to establish binding and the first rigorous variational demonstration [3] that the system is nonrelativistically stable against breakup. In addition, if the total spin (including the positron) $S=3/2$ the annihilation must be into at least three photons and therefore relatively slow. In Ref. [1] we estimated the cross section for the simplest way of forming the system—radiative capture of a positron in collision with the lowest-lying triplet state of helium. As expected, this cross section was very small.

Another obvious process capable of producing the bound system is the exchange rearrangement collision $\text{Ps} + \text{He}(^1S^e) \rightarrow \text{PsHe}^+(^3S^e) + e^-$, where the electron of the positronium atom replaces one of the atomic electrons to form the triplet spin state. In fact, as conjectured in Ref. [2] and shown in Ref. [3], the bound state is best described not as a positron bound to the triplet helium atom but as a positronium atom bound loosely to a helium ion with the two electrons appropriately symmetrized. (For this reason we use the symbol shown above to represent the bound state, and we suggest the chemical name “Positronium Helide ion” for it.) In the present calculation we use the Born approximation with simple initial and final wave functions that simulate the exact wave functions to obtain a first estimate of this rearrangement cross section.

II. FORMULATION

The total Hamiltonian for the system consisting of three electrons $[r_i]$, one positron $[x]$, and a helium nucleus fixed at the origin is (in Rydberg atomic units)

$$H = T - \sum_{i=1}^3 \frac{4}{r_i} + \frac{4}{x} - \sum_{i=1}^3 \frac{2}{\rho_i} + \sum_{i<j=2}^3 \frac{2}{r_{ij}}, \quad (1)$$

where the kinetic energy operator is $T = -\sum_{i=1}^3 \nabla_i^2 - \nabla_x^2$, where $\rho_i = |\vec{x} - \vec{r}_i|$, and where $r_{ij} = |\vec{r}_i - \vec{r}_j|$. Since we are doing the

plane-wave Born approximation the initial wave function has the form

$$\Psi_I = \frac{1}{\sqrt{3}} \left[e^{i\vec{k} \cdot \vec{R}_1} \phi_{\text{Ps}}(\rho_1) \psi_{\text{He}}(\vec{r}_2, \vec{r}_3) \left(\frac{\alpha_2 \beta_3 - \beta_2 \alpha_3}{\sqrt{2}} \right) \alpha_1 \alpha_4 \right. \\ \left. + \text{cyclic permutation of (1), (2), (3)} \right], \quad (2)$$

where $\phi_{\text{Ps}}(\rho) = \exp(-\rho/2) / \sqrt{8\pi}$ and the final wave function has the form

$$\Psi_F = \frac{1}{\sqrt{3}} \{ e^{i\vec{k}' \cdot \vec{R}_3} \psi_{\text{PsHe}^+}(\vec{r}_1, \vec{r}_2, \vec{x}) \alpha_1 \alpha_2 \beta_3 \alpha_4 \\ + [\text{cyclic permutation of (1), (2), (3)}] \}. \quad (3)$$

The spin functions α and β represent up and down spins, respectively, and we have assumed that the initial positronium atom is itself in the triplet long-lived state with total spin projection $M=+1$. The relationship between the final momentum k' and the incident momentum k is derived from the energy equation:

$$E_{\text{Ps}} + E_{\text{He}} + \frac{k^2}{2} = E_{\text{PsHe}^+} + k'^2 = E_{\text{Ps}} + E_{\text{He}^+} - \mathcal{E}_B + k'^2.$$

Using the known value for the energy of the helium ground state $E_{\text{He}} = -5.807\,448$ and Frolov's value [4] of the binding energy $\mathcal{E}_B = 0.001\,187\,4$ we obtain the expression $k' = \sqrt{k^2/2 - 1.806\,261}$. The threshold momentum of the incident Ps atom is $k = 1.900\,663$, corresponding to an energy $E_{\text{Th}} = 24.5756$ eV.

After using the orthonormal properties of the spin functions and the antisymmetry of the spatial wave function ψ_{PsHe^+} we can write two forms of the Born approximation as follows:

$$M_I = \frac{1}{\sqrt{2}} \int d\tau [e^{-i\vec{k}' \cdot \vec{r}_3} \psi_{\text{PsHe}^+}(\vec{r}_1, \vec{r}_2, \vec{x}) \\ + e^{-i\vec{k}' \cdot \vec{r}_2} \psi_{\text{PsHe}^+}(\vec{r}_1, \vec{r}_3, \vec{x})] V_I e^{i\vec{k} \cdot \vec{R}_1} \phi(\rho_1) \psi_{\text{He}}(\vec{r}_2, \vec{r}_3), \quad (4a)$$

$$M_F = \frac{1}{\sqrt{2}} \int d\tau e^{-i\vec{k}\cdot\vec{r}_3} \psi_{\text{PsHe}^+}(\vec{r}_1, \vec{r}_2, \vec{x}) V_F [e^{i\vec{k}\cdot\vec{r}_1} \phi(\rho_1) \psi_{\text{He}}(\vec{r}_2, \vec{r}_3) + e^{i\vec{k}\cdot\vec{r}_2} \phi(\rho_2) \psi_{\text{He}}(\vec{r}_1, \vec{r}_3)]. \quad (4b)$$

(The factor of 3 is canceled by the three identical terms that appear.) We denote the volume element by $d\tau$, but it is actually the 12-dimensional volume over the three electronic coordinates and one positronic coordinate. The two forms of the perturbation $V_{I,F}$ refer to the partial Hamiltonians whose eigenfunctions are the initial and final wave functions, respectively. That is, $V_{I,F} = H - H_{I,F}$, where

$$H_I = T - \frac{4}{r_2} - \frac{4}{r_3} + \frac{2}{r_{23}} - \frac{2}{\rho_1} \quad \text{and} \quad (5a)$$

$$H_F = T - \frac{4}{r_1} - \frac{4}{r_2} + \frac{4}{x} - \frac{2}{\rho_1} - \frac{2}{\rho_2} + \frac{2}{r_{12}}. \quad (5b)$$

(Note that because of the symmetry of both forms of the potential it is clear that the two terms in brackets in Eqs. (4) give identical results. We will keep only one term in each case and double the result.) At this point we will introduce three fairly severe simplifications, designed to make the integrals in the matrix element tractable.

(i) First, we use the open-shell approximation for the ground-state helium atom:

$$\psi_{\text{He}}(r_2, r_3) = N_I [e^{-(ar_2+br_3)} + e^{-(br_2+ar_3)}], \quad (6)$$

where $a=2.183\,170\,865$, $b=1.188\,530\,838$, and $N_I=0.708\,930\,737$. This wave function gives a value of the helium energy within about 1% of the exact value, and it has the form of two hydrogenic s -wave electrons, one seeing the full nuclear charge ($Z \approx 2$) and the other shielded ($Z \approx 1$).

(ii) Bearing in mind the fact that the positronium helide ion wave function looks like a Ps atom weakly bound to a helium ion, we approximate it as follows:

$$\psi_{\text{PsHe}^+}(\vec{r}_1, \vec{r}_2, \vec{x}) = N_F [F(R_1) \phi_{\text{Ps}}(\rho_1) \psi_{\text{He}^+}(r_2) - (1 \leftrightarrow 2)], \quad (7)$$

where the Ps center-of-mass coordinate is $\vec{R}_i = (\vec{x} + \vec{r}_i)/2$ and $\psi_{\text{He}^+}(r) = \exp(-2r)\sqrt{8/\pi}$. In our previous work [1] we took the form $F(R) = (e^{-\gamma R} - e^{-\beta R})/R$ to describe the motion of the center of mass and fixed the two parameters at $\gamma = 0.048\,733$ and $\beta = 0.248\,145$. The resulting wave function gives the asymptotic form of F and the expectation value of x in agreement with the results of the well-converged calculation of Frolov [4] and also gives quite reasonable values for other expectation values, as shown in Ref. [1]. With these values of the parameters the normalization constant is $N_F = 0.085\,053$.

(iii) Finally, we restrict the calculation to S waves. This involves replacing the plane waves in the initial and final wave functions by the spherical Bessel functions $j_0(kR_1)$ and $j_0(k'r_3)$, respectively. The S -wave cross section will be a lower bound to the complete Born cross section.

III. CALCULATION OF THE MATRIX ELEMENT

(i) With the approximations described above the Born matrix elements take the following forms. First, $M_I(k)$

$= M_I^{\text{Dir}}(k) + M_I^{\text{Exch}}(k)$, where the two terms come from the two terms in our form of the PsHe⁺ wave function:

$$M_I^{\text{Dir}}(k) = \frac{2N_F}{\sqrt{2}} \iint d\vec{r}_2 d\vec{r}_3 j_0(k'r_3) \psi_{\text{He}}(r_2, r_3) \psi_{\text{He}^+}(r_2) \times \iint d\vec{r}_1 d\vec{x} F(R_1) \phi_{\text{Ps}}^2(\rho_1) j_0(kR_1) \times \left[\left(\frac{4}{x} - \frac{4}{r_1} \right) + \left(\frac{2}{r_{12}} - \frac{2}{\rho_2} \right) + \left(\frac{2}{r_{13}} - \frac{2}{\rho_3} \right) \right], \quad (8a)$$

$$M_I^{\text{Exch}}(k) = \frac{-2N_F}{\sqrt{2}} \int \int \int d\vec{r}_1 d\vec{r}_2 d\vec{x} F(R_2) \phi_{\text{Ps}}(\rho_2) \psi_{\text{He}^+}(r_1) \times j_0(kR_1) \phi_{\text{Ps}}(\rho_1) \int d\vec{r}_3 j_0(k'r_3) \psi_{\text{He}}(r_2, r_3) \times \left[\left(\frac{4}{x} - \frac{4}{r_1} + \frac{2}{r_{12}} - \frac{2}{\rho_2} \right) + \left(\frac{2}{r_{13}} - \frac{2}{\rho_3} \right) \right]. \quad (8b)$$

Several things should be noted about these expressions. First, the factor $1/\sqrt{2}$ appearing in Eqs. (8) comes from the spin parts of the wave functions, and the extra factor of 2 is from the two identical terms in Eqs. (4). Then we have arranged the terms in the potential in Eq. (8a) to make it obvious that the direct matrix element vanishes identically since its integrand is antisymmetric under interchange of \vec{r}_1 and \vec{x} . We have isolated the \vec{r}_3 integral in Eq. (8b) since that integral is particularly easy to carry out. The remaining integrals take the form

$$M_I^{\text{Exch}}(k) = \frac{128\pi^2 b N_I N_F}{\sqrt{2}(k^2 + b^2)^2} \int_0^\infty dx x^2 \int d\vec{r}_2 \phi_{\text{Ps}}(\rho_2) F(R_2) e^{-ar_2} \times \int d\vec{r}_1 \psi_{\text{He}^+}(r_1) j_0(kR_1) \phi_{\text{Ps}}(\rho_1) \left[\frac{1}{\rho_2} + g(b, x) - \frac{2}{x} - g(b, r_1) + \frac{2}{r_1} - \frac{1}{r_{12}} \right] + \{a \leftrightarrow b\}, \quad (9)$$

$$\int d\vec{r} j_0(k'r) \frac{e^{-cr}}{|\vec{z} - \vec{r}|} = \frac{8\pi c}{(k'^2 + c^2)^2} g(c, z) \quad \text{and} \quad g(c, z) = \frac{1}{z} \left[1 - e^{-cz} \left(\cos k'z + \frac{c^2 - k'^2}{2k'c} \sin k'z \right) \right]. \quad (10)$$

In Eq. (9) the \vec{r}_2 and \vec{r}_1 integrals depend on r_i , x , and $\hat{r}_i \cdot \hat{x}$ only, so they are two-dimensional integrals leading to functions of x , for the first three terms in the square bracket. We integrated them numerically, after which the integral over x could also be readily evaluated. The last term in the bracket is of a different form, and its evaluation is discussed in the Appendix.

(ii) In the same way $M_F(k) = M_F^{\text{Dir}}(k) + M_F^{\text{Exch}}(k)$ and the two terms this time are

TABLE I. Nonradiative formation cross sections in units of 10^{-3} \AA^2 .

$k (1/a_0)$	σ_I	σ_F
1.91	2.12	1.63
2.0	3.42	3.48
2.2	1.26	2.36
2.4	0.344	1.20
2.6	0.0874	0.564
2.8	0.0214	0.254
3.0	0.0050	0.113

$$M_F^{Dir}(k) = \frac{2N_F}{\sqrt{2}} \iint d\vec{r}_2 d\vec{r}_3 j_0(k'r_3) \psi_{He}(r_2, r_3) \psi_{He^+}(r_2) \times \iint d\vec{r}_1 d\vec{x} F(R_1) \phi_{Ps}^2(\rho_1) j_0(kR_1) \times \left[\left(\frac{2}{r_{23}} - \frac{4}{r_3} \right) + \left(\frac{2}{r_{13}} - \frac{2}{\rho_3} \right) \right], \quad (11a)$$

$$M_F^{Exch}(k) = \frac{-2N_F}{\sqrt{2}} \iiint d\vec{r}_1 d\vec{r}_2 d\vec{x} F(R_2) \times \phi_{Ps}(\rho_2) \psi_{He^+}(r_1) j_0(kR_1) \phi_{Ps}(\rho_1) \times \int d\vec{r}_3 j_0(k'r_3) \psi_{He}(r_2, r_3) \left[\frac{2}{r_{23}} - \frac{4}{r_3} + \frac{2}{r_{13}} - \frac{2}{\rho_3} \right]. \quad (11b)$$

Again the last two terms in the bracket in Eq. (11a) vanish by symmetry, but the other two terms remain. After making a change of variables the second double integral simplifies:

$$\int d\vec{R}_1 F(R_1) j_0(kR_1) \int d\vec{\rho}_1 \phi_{Ps}^2(\rho_1) = \frac{4\pi}{k} \int_0^\infty dR (e^{-\gamma R} - e^{-\beta R}) \sin kR = \frac{4\pi(\beta^2 - \gamma^2)}{(k^2 + \gamma^2)(k^2 + \beta^2)}, \quad (12)$$

where we have made use of the fact that the Ps wave func-

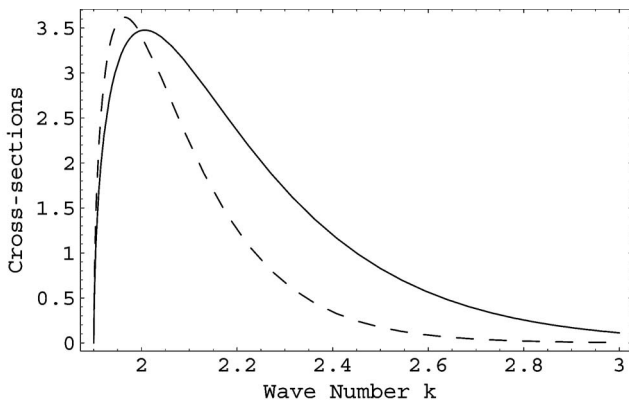


FIG. 1. Nonradiative formation cross sections in units of 10^{-3} \AA^2 : σ_F is solid and σ_I is dashed.

tion is normalized. The \vec{r}_3 integral can also be carried out analytically; it gives rise to a function similar to $g(c, r_2)$ that appears in Eq. (9). Finally, the last integral over r_2 can be performed analytically,

$$M_F^{Dir}(k) = \frac{-2^{10} N_I N_F \pi^{5/2} b (\beta^2 - \gamma^2)}{(k^2 + \gamma^2)(k^2 + \beta^2)(k'^2 + b^2)^2} \left\{ \frac{2(b^2 - b + k'^2) - ab}{b(a+2)^3} + \frac{(a+b+2)(a+2b+2-k'^2/b) - k'^2}{[(a+b+2)^2 + k'^2]} \right\} + \{a \leftrightarrow b\}. \quad (13)$$

In the exchange matrix element the \vec{r}_3 integral again is easy, and it yields the following expression:

$$\frac{32\pi b N_I e^{-ar_2}}{(k'^2 + b^2)^2} [g(b, r_1) + g(b, r_2) - g(b, x) - 2g(b, 0)] + \{a \leftrightarrow b\}. \quad (14)$$

Each term in the expression for $M_F^{Exch}(k)$ separates in the same way as did the simple terms in $M_I^{Exch}(k)$. For example, the first term in Eq. (14) when inserted in Eq. (11b) yields

$$\frac{-32\sqrt{\pi} N_I N_F b}{(k'^2 + b^2)^2} \int_0^\infty dx x^2 \int d\vec{r}_1 g(b, r_1) e^{-(2r_1 + \rho_1/2)} j_0(kR_1) \times \int d\vec{r}_2 F(R_2) e^{-(ar_2 + \rho_2/2)} + \{a \leftrightarrow b\}, \quad (15)$$

and fairly straightforward numerical integration can evaluate it.

IV. RESULTS AND DISCUSSION

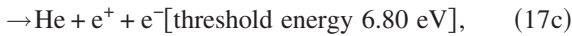
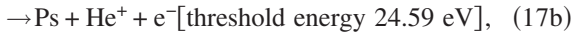
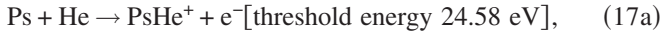
Once the two forms of matrix elements have been evaluated for a range of momenta k the total cross sections can be obtained from the formula

$$\sigma_{I,F}(k) = \frac{1}{4\pi} \frac{v'}{v} |M_{I,F}(k)|^2 a_0^2 = \frac{1}{\pi} \frac{\sqrt{k^2/2 - 1.806262}}{k} |M_{I,F}(k)|^2 a_0^2. \quad (16)$$

We show the results we have obtained in both I and F approximations in Table I and in Fig. 1. From the latter one can see that the two approximations are very close near threshold and up to their joint maximum, but they deviate considerably as k increases. Despite the rough quality of the present calculation—the Born approximation, the limitation to S waves, and the difference between post- and prior forms—the present results should be useful in designing experiments to produce and detect the positronium helide ion. Although there are now many theoretically verified particle-bound states containing at least one positron, there are only two such systems (besides positronium itself) that have been experimentally observed: the positronium negative ion [5], and positronium hydride [6]. We would like to think of positronium physics as not merely a mathematical subject, so we will add a brief discussion of possible experimental detection of positronium helide, with the hope that we may stimulate interest

in this reaction among our experimental colleagues.

Experimental verification of the formation of PsHe^+ is not simple in spite of the fact that the present reaction has a much larger cross section than does the radiative reaction discussed earlier [1]. This is partly because of its very small binding energy and partly because there are several competing reactions. It seems that the best way of verifying that this system has been produced by the reaction discussed here is to begin with a beam of Ps atoms of sharply defined energy and detect the outgoing electrons and their energy distribution. Several reactions generate outgoing electrons:



and some others involving excitation of either Ps or He atoms. But the electron energy of the first, interesting, reaction, Eq. (17a), is uniquely determined by conservation of energy (when we assume the helium nucleus is infinitely massive), while the other two, Eqs. (17b) and (17c), have three-body final states, and the electron must share its energy, giving rise to a continuum of electron energies. So one should look for a sharp electron energy to detect the formation of PsHe^+ .

Reaction (17b) may not interfere too badly with detection of the peak which lies slightly above the upper continuum limit. Unfortunately, the cross section [7] for reaction (17c) is several orders of magnitude larger than for the formation reaction (17a) in which we are interested, and the peak would lie buried in its continuum. This probably means that the only way that the peak signifying formation of PsHe^+ could be distinguished from the competing electron continuum would be if it were extremely narrow. This would require significant improvements in the energy control of Ps beams beyond the present state of the art [7]. One remaining possibility involves the use of an anticoincidence setup, which would reject any electrons that were accompanied by a positron; the rejection efficiency would need to be almost perfect.

ACKNOWLEDGMENTS

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APPENDIX

The evaluation of the last term in the matrix element $M_I^{Exch}(k)$ appearing in Eq. (9) is somewhat more difficult than the others, since the integrand does not separate conveniently into a product of functions of \vec{r}_1 and \vec{r}_2 as the others do. We used two different techniques to simplify this integration. The first is quite similar to the method described in the Appendix of our previous paper [9] and involves a parametric integral. The second is simpler, involving an expansion in Legendre polynomials which turns out to converge extremely rapidly.

Taking the vector \vec{x} as the polar axis, we expand in the usual way:

$$\begin{aligned} \frac{1}{r_{12}} &= \sum_L \frac{r_{<}^L}{r_{>}^{L+1}} P_L(\hat{r}_1 \cdot \hat{r}_2) \\ &= \sum_L \frac{r_{<}^L}{r_{>}^{L+1}} \frac{4\pi}{2L+1} \sum_{m=-L}^L Y_{Lm}(\theta_1, \phi_1) Y_{Lm}^*(\theta_2, \phi_2), \quad (A1) \end{aligned}$$

where the symbols $<$ and $>$ refer to the lesser and greater of the pair r_1 and r_2 , respectively. The advantage of this expansion lies in the fact that each term in the sum has the two coordinates separated. When this expansion is inserted into the integral in Eq. (9) it becomes clear that only those terms with $m=0$ survive, since the rest of the integrand involves the polar angle only. For this reason Eq. (9) can be rewritten as

$$\begin{aligned} M_I^{Exch}(k)|_{12} &= -\frac{128\pi^2 b N_I N_F}{\sqrt{2}(k'^2 + b^2)^2} \sum_L \int_0^\infty dx x^2 \int d\vec{r}_2 \phi_{Ps}(\rho_2) \\ &\quad \times F(R_2) e^{-ar_2} P_L(\hat{x} \cdot \hat{r}_2) \int d\vec{r}_1 \psi_{He^+}(r_1) j_0(kR_1) \\ &\quad \times \phi_{Ps}(\rho_1) P_L(\hat{x} \cdot \hat{r}_1) \frac{r_{<}^L}{r_{>}^{L+1}} + \{a \leftrightarrow b\}. \quad (A2) \end{aligned}$$

Now each of the $d\vec{r}_i$ integrals involves integration over the polar angle and the radius only and depends on the magnitude of x . The usefulness of this way of calculating depends on the speed of convergence in L ; in the present case only three terms were necessary. Both methods gave essentially the same values.

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