# Radiative attachment of a positron to atomic helium in the triplet state

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In this study we evaluate the cross section for forming the nonrelativistically bound state of a positron with the helium triplet atom by radiative attachment. Although this cross-section was expected to be small compared with a competing rearrangement process involving positronium and ground-state helium, this calculation is a first step which should be useful for experimental production of this interesting system

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## I. INTRODUCTION AND HISTORY

Following an unpublished suggestion by Karl Canter, an attempt was made long ago by one of us (RJD) and colleagues [1] to determine whether the system consisting of a positron and a helium atom in the triplet state $e^+\mathrm{He}(^3S^e)$ might be stable, at least in the nonrelativistic approximation. (It was already known [2] that there is no particle-stable state of a positron and the singlet ground state of helium.) The existence of such a state would be of special interest, since the attached positron could be in a triplet spin state with both of the atomic electrons and would therefore be forbidden to annihilate into two gamma rays; its lifetime against annihilation into three gamma rays would be of the order of microseconds. (The only other known positronic system that has such a long annihilation lifetime is triplet positronium, Ps.) The Hylleraas-type trial function used in Ref. [1] was inadequate, and binding was not established, but an encouraging note was the fact that binding did occur if the positron mass was reduced by only about 6%. It was also clear that the most efficient type of trial function for this problem would be based on the picture of a positronium atom loosely bound to a helium ion (and symmetrized), rather than a positron attached to a triplet helium atom. We will use this fact later.

More recently the stable existence of this system has been rigorously established [3], and the best published value [4] of the energy for dissociation into the ground states of Ps and $He^+$ is $1.1874\times10^{-3}$ Ry or 0.01616 eV. References [3] and [4] verify in detail the physical picture of the bound system discussed above. The difficulty experienced in Ref. [1] was clearly due to the very small value of the dissociation energy.

In Ref. [1] there was also a brief discussion of how to form this bound system, if it exists. A straightforward technique would be radiative attachment of positrons colliding with metastable helium atoms in their lowest triplet state. There are obvious reasons why this process is expected not to be very efficient—radiative reactions are usually slow, and moreover there is not much overlap between the compact wave function of triplet helium and the extended one corresponding to the very weakly bound Ps-$He^+$ system. In Ref. [1] the rearrangement reaction involving ground-state helium, $\mathrm{Ps}+\mathrm{He}\rightarrow[e^+\mathrm{He}(^3S^e)]+e^-$, was recommended. It should have an "atomic" sized cross section and correspond physically to a Ps atom, simply knocking out one of the atomic target electrons and replacing it. Still, this second process may not be so simple experimentally, since controlled beams of Ps are needed. In this paper we take the first step by calculating the cross section for the radiative process. We intend to investigate the rearrangement later.

## II. CALCULATION

The standard way [5] of calculating the cross-section for radiative attachment is to calculate first the cross section for photodetachment and then to apply the principle of detailed balance. In our case the photodetachment reaction is

$$h\nu+[e^+\mathrm{He}(^3S^e)]\rightarrow e^++\mathrm{He}(^3S^e),$$

and the matrix element describing it is

$$M=\int\int\int d\vec{r}_1 d\vec{r}_2 d\vec{x} e^{-i\vec{k}*\vec{x}}\psi(r_1,r_2)Q\Psi(r_1,r_2,x) \qquad (1)$$

where $x$ refers to the positron, $r_i$ $(i=1,2)$ refers to the two electrons, and $k$ is the wave number of the outgoing positron. We are making the dipole approximation and also assuming that a plane-wave approximation is adequate for the outgoing positron; since the final state is neutral helium, there is no long-range Coulomb potential to consider. We will compare two forms of the transition operator $Q$: the length form, $Q_L=\hat{\varepsilon}\cdot(\vec{x}-\vec{r}_1-\vec{r}_2)$, and the velocity form $Q_V=\hat{\varepsilon}\cdot(\nabla_x-\nabla_1-\nabla_2)$, where $\hat{\varepsilon}$ is the unit vector describing the polarization direction of the incoming photon. We are using atomic units with energies in Rydbergs, and we are keeping the helium nucleus fixed.

We take very simple forms for the initial and final wave functions. The lowest triplet helium state is

$$\psi(r_1,r_2)=N_1\left[e^{-(ar_1+br_2)}-e^{-(br_1+ar_2)}\right], \qquad (2)$$

where the index $i=1$ and 2 refers to the two electrons, and the parameters minimizing the energy are $a=1.96863$ and $b=0.321007$. The normalization constant is

 

TABLE I. Comparison of certain matrix elements of the present model wave function with accurate ones from Ref. [4]

| Quantity | This work | Ref. [4] | % error |
|---|---|---|---|
| $\langle r_1\rangle=\langle r_2\rangle$ | 8.30609 | 8.02966 | 3.4 |
| $\langle \rho_1\rangle=\langle \rho_2\rangle$ | 9.37370 | 9.47212 | 1 |
| $\langle \delta(\vec{x})\rangle$ | $2.56\times10^{-4}$ | $9.70\times10^{-7}$ | large |
| $\langle \delta(\vec{r}_1)\rangle=\langle \delta(\vec{r}_2)\rangle$ | 1.27958 | 1.27317 | 0.5 |
| $\langle \delta(\vec{\rho}_1)\rangle=\langle \delta(\vec{\rho}_2)\rangle$ | 0.021409 | 0.018844 | 13.6 |
| $\langle x^2\rangle$ | 384.235 | 353.868 | 8.6 |

$$N_1=\frac{1}{\pi}\left[\frac{2}{(ab)^3}-\frac{128}{(a+b)^6}\right]^{-1/2}=0.119997. \tag{3}$$

This wave function gives a variational value of the energy $E=-4.32129$ Ry, as compared with the exact value of $E=-4.3506$ Ry. We construct the wave function that represents the bound system in the following way. We define the relative coordinate $\rho$ and the center of mass coordinate $R$ of the positronium atom as $\vec{\rho}_i=\vec{x}-\vec{r}_i$ and $\vec{R}_i=(\vec{x}+\vec{r}_i)/2$. Following our picture of the bound system as being described as the symmetrized product of a helium ion, a Ps atom, and an extended function describing the motion of the center of mass of the Ps atom, we write

$$\Psi(r_1,r_2,x)=N_2[F(R_1)\phi(\rho_1)\chi(r_2)-F(R_2)\phi(\rho_2)\chi(r_1)]. \tag{4}$$

Here the Ps wave function $\phi(\rho)=e^{-\rho/2}/\sqrt{8\pi}$, the helium ion wave function $\chi(r)=e^{-2r}\sqrt{8/\pi}$, and the relative motion wave function $F(R)=(e^{-\gamma R}-e^{-\beta R})/R$. This approximate wave function for the bound state has the qualitative features of the real system without including the correlation that is essential for computing realistic variational binding energy; we believe that it is adequate for a reasonable calculation of the cross-section of interest. To fix the values of the two parameters $\beta>\gamma$ we make use of some accurate results from Ref. [4]. To determine a value for $\gamma$ we note that the asymptotic form of $F(R)$ is exact if $\gamma=\sqrt{2B}$, where $B$ is the binding energy of the system relative to the Ps+$He^+$ threshold energy of $-4.5$ Ry. In Ref. [4], $B=0.0011874$ Ry, so we use the value $\gamma=0.048733$. To determine a value for the second parameter we required the expectation value of $x$ to agree with that given in Ref. [4]: $\langle x\rangle=15.7496$. This requirement fixed the value $\beta=0.248145$. With these values of the parameters, the normalization $N_2=0.085053$. As a check, we then calculated the expectation values of several additional operators (Table I), obtaining values close to that in Ref. [4] in most cases.

### A. The matrix element

By symmetry we can write the two forms of the matrix element as follows:

$$M_{\left\{\begin{smallmatrix}L\\V\end{smallmatrix}\right\}}(\vec{k})=2N_1N_2\int\int\int d^3x d^3r_1 d^3r_2\left[e^{-i\vec{k}\cdot\vec{x}}(e^{-(ar_1+br_2)}-e^{-(ar_2+br_1)})\begin{Bmatrix}Q_L\\Q_V\end{Bmatrix}F(R_1)\phi(\rho_1)\chi(r_2)\right]. \tag{4'}$$

We now change variables to the Jacobi set $\{\vec{R}_1,\vec{\rho}_1,\vec{r}_2\}$ after which the $Q$ operators take the forms $Q_L=\hat{\varepsilon}\cdot(\vec{\rho}_1-\vec{r}_2)$ and $Q_V=\hat{\varepsilon}\cdot(2\nabla_{\rho_1}-\nabla_2)$. The gradients in $Q_V$ are easily applied to the functions on the right giving $Q_V\Rightarrow-\hat{\varepsilon}\cdot(\hat{\rho}_1-2\hat{r}_2)$. Those parts of these two operators involving $\vec{r}_2$ make no contribution to the integral of Eq. (4), since all the other functions of that variable are scalars. After we carry out the simple integral over $d^3r_2$ the matrix elements take the form

$$M_{\left\{\begin{smallmatrix}L\\V\end{smallmatrix}\right\}}(\vec{k})=\frac{32\sqrt{2\pi}N_1N_2}{(2+b)^3}\int\int d^3Rd^3\rho e^{-i\vec{k}\cdot\vec{x}}e^{-ar}\times\begin{Bmatrix}\rho\\-1\end{Bmatrix}\hat{\varepsilon}\cdot\hat{\rho}F(R)\phi(\rho)-\{a\leftrightarrow b\}. \tag{5}$$

(Here we have dropped the subscript as it is no longer needed.) By Fourier transforming the function of $r$ as follows

$$e^{-ar}=e^{-a|\vec{R}-\vec{\rho}/2|}=\frac{a}{\pi^2}\int d^3p\frac{e^{i\vec{p}\cdot(\vec{R}-\vec{\rho}/2)}}{(p^2+a^2)^2}, \tag{6}$$

we can formally separate the integrals over $d^3R$ and $d^3\rho$,

$$M_{\left\{\begin{smallmatrix}L\\V\end{smallmatrix}\right\}}(\vec{k})=\frac{16N_1N_2a}{\pi^2(2+b)^3}\int\frac{d^3p}{(p^2+a^2)^2}I(q)J_{\left\{\begin{smallmatrix}L\\V\end{smallmatrix}\right\}}(\vec{s})-\{a\leftrightarrow b\}, \tag{7}$$

where

$$I(q)=\int d^3Re^{i\vec{q}\cdot\vec{R}}F(R)=\frac{4\pi(\beta^2-\gamma^2)}{(q^2+\beta^2)(q^2+\gamma^2)}, \tag{8}$$

and

$$J_{\left\{\begin{smallmatrix}L\\V\end{smallmatrix}\right\}}(\vec{s})=\int d^3\rho e^{-i\vec{s}\cdot\vec{\rho}}\hat{\varepsilon}\cdot\hat{\rho}e^{-\rho/2}\begin{Bmatrix}\rho\\-1\end{Bmatrix}=128\pi i\hat{\varepsilon}\cdot\vec{s}\begin{Bmatrix}\frac{-8}{(1+4s^2)^3}\\\frac{1}{(1+4s^2)^2}\end{Bmatrix}. \tag{9}$$

[Here we have introduced two convenient definitions: $\vec{q}=\vec{p}+\vec{k}$ and $\vec{s}=(\vec{p}-\vec{k})/2$.] The angular part $\hat{\varepsilon}\cdot\vec{s}$ can be replaced by the expression $\hat{\varepsilon}\cdot\hat{k}(\hat{k}\cdot\vec{p}-k)/2$, after which the integral over $d^3p$ reduces to a two-dimensional integral over $p$ and $\mu=\hat{k}\cdot\hat{p}$. The angular integral can be evaluated analytically followed by the numerical evaluation of the radial integral, or the double integral can be done completely numerically. We have checked our work by carrying out both these procedures, which agreed completely. Notice that we can factor out the correlation between the polarization direction of the

photon and the direction of the outgoing positron and can write

$$M_{\begin{Bmatrix} L \\ V \end{Bmatrix}}(\vec{k}) = \hat{\varepsilon} \cdot \hat{k} \bar{M}_{\begin{Bmatrix} L \\ V \end{Bmatrix}}(k), \tag{10}$$

where the reduced matrix element $\bar{M}$ depends only on the magnitude of the momentum.

### B. The cross sections

The standard expressions [5] for the photodissociation cross sections, in both the velocity and length forms, can be written as follows:

$$\left.\frac{d\sigma_V(\vec{k})}{d\Omega}\right|_{photo} = (\hat{\varepsilon} \cdot \hat{k})^2 \frac{\alpha k}{\pi \omega} |\bar{M}_V|^2 a_0^2 \tag{11a}$$

and

$$\left.\frac{d\sigma_L(\vec{k})}{d\Omega}\right|_{photo} = (\hat{\varepsilon} \cdot \hat{k})^2 \frac{\alpha k \omega}{4\pi} |\bar{M}_L|^2 a_0^2. \tag{11b}$$

In these expressions $k$ is the wave number of the positron in units of $1/a_0$, $\omega$ is the photon energy in Rydbergs, and $\alpha$ is the fine-structure constant. Since we are really only interested in total cross sections, we can integrate over the angular factor and finally get the photodetachment results,

$$\sigma_V(k)|_{photo} = \frac{4\alpha k}{3\omega} |\bar{M}_V|^2 a_0^2 \tag{12a}$$

and

$$\sigma_L(k)|_{photo} = \frac{\alpha k \omega}{3} |\bar{M}_L|^2 a_0^2. \tag{12b}$$

To convert these results to cross-sections for radiative attachment by detailed balance we multiply by $(p_\omega/p_k)^2$, where the numerator is the momentum of the outgoing photon, and the denominator is the momentum of the incoming positron. The result is

$$\left(\frac{p_\omega}{p_k}\right)^2 = \frac{\left[\dfrac{\omega e^2}{2a_0 c}\right]^2}{\left[\dfrac{\hbar k}{a_0}\right]^2} = \frac{\alpha^2 \omega^2}{4k^2}, \tag{13}$$

and the final expressions for the radiative attachment cross-sections are

$$\sigma_V(k)|_{attach} = \frac{\alpha^3 \omega}{3k} |\bar{M}_V|^2 a_0^2 \tag{14a}$$

and

$$\sigma_L(k)|_{attach} = \frac{\alpha^3 \omega^3}{12k} |\bar{M}_L|^2 a_0^2. \tag{14b}$$

The emitted photon energy is $\omega = k^2 + E[\mathrm{He}(^3S^e)] - E[e^+\mathrm{He}(^3S^e)] = k^2 + 0.1508$.

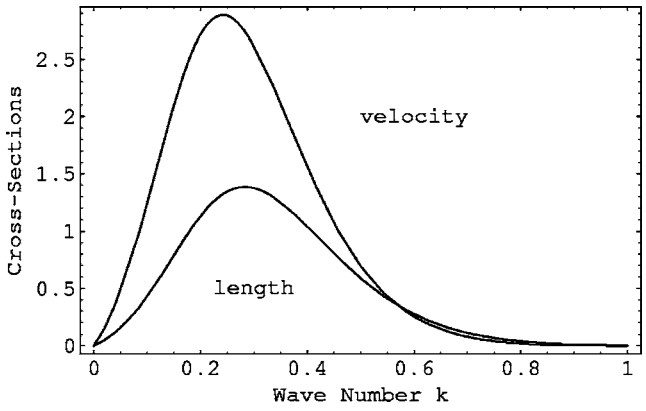


FIG. 1. Radiative attachment cross sections, both velocity and length forms, in barns.

## III. RESULTS AND DISCUSSION

In Fig. 1 and Table II we show the results of the calculation, giving the radiative attachment cross sections, both velocity and length forms, for positron incident energies up to 1 Rydberg ($k \leqslant 1$). Because the cross-sections are very small it is convenient to give the results in barns, units of $10^{-24}$ cm$^2$. The two forms have the same general shape, but they differ significantly, with the velocity form exceeding the length form over the lower half of the range.

As we had expected, these small cross sections probably make this radiative attachment process experimentally quite

TABLE II. Cross sections in barns for both the velocity and the length forms.

| $k$ | $\sigma_V$ | $\sigma_L$ |
|---|---|---|
| 0 | 0 | 0 |
| 0.05 | 0.482 | 0.157 |
| 0.1 | 1.231 | 0.425 |
| 0.15 | 2.098 | 0.789 |
| 0.2 | 2.723 | 1.134 |
| 0.25 | 2.884 | 1.345 |
| 0.3 | 2.618 | 1.375 |
| 0.35 | 2.113 | 1.252 |
| 0.4 | 1.559 | 1.041 |
| 0.45 | 1.071 | 0.806 |
| 0.5 | 0.695 | 0.589 |
| 0.55 | 0.430 | 0.411 |
| 0.6 | 0.254 | 0.275 |
| 0.65 | 0.144 | 0.178 |
| 0.7 | 0.078 | 0.112 |
| 0.75 | 0.040 | 0.068 |
| 0.8 | 0.019 | 0.040 |
| 0.85 | 0.008 | 0.023 |
| 0.9 | 0.003 | 0.012 |
| 0.95 | 0.0006 | 0.0061 |
| 1 | 0.00001 | 0.0027 |

difficult. Nevertheless, it only requires a low-energy beam of positrons and a target of metastable helium atoms, whose lifetime is very long. The competing process, stripping of positronium atoms in collision with ground-state helium, should have a larger cross section, and does not need to use excited helium atoms, but uses a beam of positronium atoms, whose lifetime is quite short and whose energy is harder to control. Our next task is to try to evaluate the cross section for this alternate process, in order to make recommendations for experimental follow-up.

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