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Effect of electron correlation on positronium formation in positron-helium scattering

P. Chaudhuri[1,a], S.K. Adhikari[1], B. Talukdar[2], and S. Bhattacharyya[2]

[1] Instituto de Física Teórica, Universidade Estadual Paulista 01.405-900 São Paulo, São Paulo, Brazil
[2] Department of Physics, Visva Bharati University, Santiniketan 731235, India

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Abstract. A three-parameter correlated wave function for the helium ground state is used to study the scattering reaction $e^+ + \mathrm{He} \to \mathrm{He}^+ + \mathrm{Ps}$, where Ps stands for positronium atom. An exact analytical expression is constructed for the first Born scattering amplitude for Ps formation from helium. Based on this numerical results are presented for both differential and total cross-sections. It is demonstrated that the inner electronic correlation of the target atom plays a crucial role in explaining the discrepency between theory and experiment.

PACS. 34.90.+q Other topics in atomic and molecular collision processes and interactions – 34.50.-s Scattering of atoms, molecules, and ions

Quite a long ago it was recognized by Wardle [1] that positron-helium scattering data depend crucially on the choice of the wave function. Despite that, most of the studies on the scattering reaction have been envisaged within the framework of independent-electron model of the atom [2]. Only recently van Reeth and Humberston [3] verified that even in a flexible variational formulation of the problem one needs to use a superior quality correlated helium wave function to get improved and better converged results for comparison with experiments [4]. These works tend to indicate that one of the tasks in studying positronium (Ps) formation in helium is to analyze the effect of electronic correlation on the scattering data. The present work is an effort in this direction.

By using a three-parameter correlated wave function we shall construct an exact analytical expression for the Ps formation cross-section for scattering of positrons off helium atom and present numerical results for differential and total cross-sections at incident energies 125, 250 and 500 eV respectively. It is not our intention to contest the results of reference [3] with regard to numerical accuracy. In contrast, we shall work within the framework of first Born approximation and try to gain some added realism for the effect of electron correlation on the Ps-formation cross-section.

The helium-wave function of our interest is given by

$$\psi(\mathbf{r}_i, \mathbf{r}_j, \mathbf{r}_{ij}) = \frac{1}{N} e^{-\alpha(r_i+r_j)} \chi(r_{ij}) Y_{00}(\hat{r}_i) Y_{00}(\hat{r}_j), \tag{1}$$

where the correlation function $\chi(r_{ij})$ is given by

$$\chi(r_{ij}) = 1 - \lambda e^{-\mu r_{ij}}, \tag{2}$$

with $\mathbf{r}_{ij} = \mathbf{r}_i - \mathbf{r}_j$. The suffixes i and j label the coordinates of the electrons of helium atom. N is the normalization constant given by

$$N^2 = \langle \psi | \psi \rangle = C \frac{\pi^2}{\alpha^3} \Big[\frac{1}{\alpha^3} - \frac{2\lambda}{(\mu+2\alpha)^5} (\mu^2 + 10\mu\alpha + 32\alpha^2) + \frac{\lambda^2}{8(\mu+\alpha)^5} (\mu^2 + 5\mu\alpha + 8\alpha^2) \Big], \tag{3}$$

with $C = (4\pi)^{-2}$. Here α, λ, μ are adjustable parameters.

In this work we shall use $i = 2$ and $j = 3$. As $r_{ij} \to \infty, \chi(r_{ij}) \to 1$. This expresses the separability of the wave function when the two electrons are far apart. As demanded by Hartree and Ingmann [5], we can allow $\chi(r_{ij})$ to assume a small finite value for $r_{ij} = 0$. The wave function (1) was used by two of us [6] to construct an exact analytical expression for the expectation value of the helium-atom Hamiltonian expressed in the inter-particle coordinates. With some relaxation for the cusp conditions, the variationally determined parameters could account for 67% of the correlation energy (E_{corr}). In a more detailed study for the ground state of helium and isoelectronic ions, Kleinekathofer *et al.* [7] found that 91% of E_{corr} can be recovered by demanding the exact correlation cusp condition. In this case μ in (1) becomes equal to 0.5 a.u.

It can not be denied that there exist in the literature [8] many more realistic wave functions than that in (1).

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[a] e-mail: `puspita@ift.unesp.br`

However, to have a deeper understanding for the influence of target on the scattering reaction, it is desirable to deal with simple wave functions which can account for the essential important features of the exact wave functions. In view of this we envisage in terms of (1) an analytical study for the Ps-formation from helium. We believe that the present endeavour will help to provide a clear visualization for the effect of electron correlation on this rearrangement collision process.

In atomic units, the first Born scattering amplitude for Ps-formation from helium is given by

$$f^B(\mathbf{k}',\mathbf{k}) = \frac{1}{\pi}\int \phi^*(\mathbf{r}_3)\omega^*(\mathbf{r}_{12})e^{-i\mathbf{k}'\cdot\mathbf{S}_{12}}V(\mathbf{r}_1,\mathbf{r}_2,\mathbf{r}_3) \times\psi(\mathbf{r}_2,\mathbf{r}_3,\mathbf{r}_{23})e^{i\mathbf{k}\cdot\mathbf{r}_1}\,d\mathbf{r}_1\,d\mathbf{r}_2\,d\mathbf{r}_3, \tag{4}$$

where

$$V(\mathbf{r}_1,\mathbf{r}_2,\mathbf{r}_3) = \left(\frac{2}{r_1} - \frac{2}{r_2} + \frac{1}{r_{23}} - \frac{1}{r_{13}}\right). \tag{5}$$

In writing (4) we denote the incident positron and two atomic electrons as particles 1, 2 and 3. Here ψ, ϕ are the wave functions of the target helium atom and ionized helium in the ground state and ω that of the positronium atom with

$$\mathbf{S}_{12} = \frac{1}{2}(\mathbf{r}_1 + \mathbf{r}_2); \qquad \mathbf{r}_{12} = \mathbf{r}_1 - \mathbf{r}_2. \tag{6}$$

The wave number of the positron, $\mathbf{k}$, and that of the positronium, $\mathbf{k}'$ are related through conservation of energy by

$$k^2 + 2E_{\text{He}} = \frac{1}{2}k'^2 - 4.5 \tag{7}$$

where E_{He} is the expectation value of the Hamiltonian of He atom using (1).

In the above we have used the post form of interaction to write the scattering amplitude $f^B(\mathbf{k}',\mathbf{k})$. However, we could use the prior form as well. In the first Born approximation the two forms of the amplitude will give identical results provided an exact bound-state wavefunction is used for the helium atom. Since the present study is envisaged to give an estimate for the effect of initial target-state correlation on PS formation by employing only a reasonably accurate wavefunction, we preferred the post form of interaction which, in the rearrangement channel, is obtained by post operation of the operator $H - E$ on the final plane-wave state

$$\Phi_f(\mathbf{r}_1,\mathbf{r}_2,\mathbf{r}_3) = \phi(\mathbf{r}_3)\omega(\mathbf{r}_{12})\exp(i\mathbf{k}'\cdot\mathbf{s}_{12}).$$

Here, H is the Hamiltonian of the scattering system and E its total energy conserved during the scattering process. The prior form of interaction is obtained, on the other hand, by the operation of $(H - E)$ on the plane-wave state

$$\Phi_i(\mathbf{r}_1,\mathbf{r}_2,\mathbf{r}_3) = \Psi(\mathbf{r}_2,\mathbf{r}_3)\exp(i\mathbf{k}\cdot\mathbf{r}_1)$$

in the incident channel.

To evaluate the amplitude in (4) we work with the hydrogenic wave function for the ionized helium in the form $e^{-Zr_3}|_{Z=2}$. Positronium wave function is taken in the form $e^{-\mu S_{12}}\,|_{\mu=0.5}$. Also we use the Fourier transformation

$$e^{-\mu r_{ij}} = \frac{\mu}{\pi^2}\int \frac{e^{i\mathbf{p}\cdot(\mathbf{r}_i-\mathbf{r}_j)}}{(\mu^2+p^2)^2}\,d\mathbf{p}. \tag{8}$$

Then the radial equation in (4) become separable and can be evaluated in terms of elementary integral

$$\int e^{-ar+i\mathbf{b}\cdot\mathbf{r}}\,d\mathbf{r} = \frac{8\pi a}{(a^2+b^2)^2}\,\cdot \tag{9}$$

The three-dimensional integrals over $\mathbf{p}$ appear in the Lewis form [10]. We finally obtain

$$f^B(\mathbf{k}',\mathbf{k}) = \frac{1}{\pi^2}[(I_1 + I_2) - \lambda(I_3 + I_4)], \tag{10}$$

where

$$I_1 = A - B, \tag{11}$$

$$I_2 = C - D, \tag{12}$$

$$I_3 = E - F, \tag{13}$$

$$\text{and}\quad I_4 = G - H. \tag{14}$$

The results for B, C, F and H are found in closed analytic form. Defining a general notation

$$Q_{mn}(\mu,\boldsymbol{\zeta}_i;x,\mathbf{y}) = \frac{1}{(\mu^2+\zeta_i^2)^m(x^2+y^2)^n}$$

we can write them as

$$B = \frac{512\pi^3\mu}{(\alpha+2)^3}\;Q_{21}(\mu,\boldsymbol{\zeta}_i;\alpha,\mathbf{K}), \tag{15}$$

$$C = \frac{256\pi^4\mu}{\pi(\alpha+2)^3}\;\big[Q_{21}(\mu,\boldsymbol{\zeta}_i;\alpha,\mathbf{K}) - \{(\alpha+2)(2\alpha+2)+1\}Q_{21}(\mu,\boldsymbol{\zeta}_i;2\alpha+2,\mathbf{K})\big], \tag{16}$$

$$F = \frac{512\pi^3\mu(\alpha+2)}{(\alpha^2+\zeta_f^2)}\;Q_{22}(\mu,\boldsymbol{\zeta}_i;\alpha+2,\boldsymbol{\zeta}_i), \tag{17}$$

and

$$H = \frac{256\pi^3\alpha(\alpha+2)}{(\alpha^2+\zeta_f^2)}\;Q_{12}(\mu,\boldsymbol{\zeta}_i;\alpha+2,\boldsymbol{\zeta}_i). \tag{18}$$

The rest of the quantities in (10) are given in the Lewis form to read [9]

$$A = \frac{128\pi}{(\alpha+2)^3}\lim_{\beta\to 0}L_{110}(\mu;\boldsymbol{\zeta}_f,\alpha;\boldsymbol{\zeta}_i,\beta), \tag{19}$$

$$D = \frac{64\pi}{(\alpha+2)^3}\Bigg[\lim_{\beta\to 0}\lim_{Z_2\to\alpha}L_{110}(\mu;\boldsymbol{\zeta}_f,Z_2;\boldsymbol{\zeta}_i,\beta) - \frac{1}{2}\lim_{Z_2,Z_3\to\alpha}(Z_3+2)L_{111}(\mu;\boldsymbol{\zeta}_f,Z_2;\boldsymbol{\zeta}_i,Z_3+2) - \lim_{Z_2,Z_3\to\alpha}L_{110}(\mu;\boldsymbol{\zeta}_f,Z_2;\boldsymbol{\zeta}_i,Z_3+2)\Bigg], \tag{20}$$

$$E=\frac{128\pi\alpha}{\left(\alpha^2+\zeta_f^2\right)^2}\lim_{\beta\to 0}L_{110}(\mu;0,\alpha+2;\boldsymbol{\zeta}_i,\beta),\tag{21}$$

and

$$G=\frac{64\pi\mu}{\left(\mu^2+\zeta_i^2\right)^2}\lim_{Z_2,Z_3\to\alpha}L_{011}(\mu;\mathbf{K},Z_2;0,Z_3+2).\tag{22}$$

where the notation

$$L_{lmn}(\mu;\boldsymbol{\zeta}_f,\alpha;\boldsymbol{\zeta}_i,\beta)=\frac{\partial^l}{\partial\mu^l}\frac{\partial^m}{\partial\alpha^m}\frac{\partial^n}{\partial\beta^n}L_{000}(\mu;\boldsymbol{\zeta}_f,\alpha;\boldsymbol{\zeta}_i,\beta)\tag{23}$$

with

$$L_{000}(\mu,\boldsymbol{\zeta}_f,\alpha;\boldsymbol{\zeta}_i,\beta)=\int\frac{1}{(p^2+\mu^2)(\mid\mathbf{p}+\boldsymbol{\zeta}_f\mid^2+\alpha^2)}\times\frac{1}{(\mid\mathbf{p}+\boldsymbol{\zeta}_i\mid^2+\beta^2)}\,d\mathbf{p}.\tag{24}$$

In writing the above eight equations we have used the notation

$$\boldsymbol{\zeta}_f=\frac{\mathbf{k}'}{2},\ \boldsymbol{\zeta}_i=\mathbf{k}-\frac{\mathbf{k}'}{2}\ \text{ and }\ \mathbf{K}=\mathbf{k}-\mathbf{k}'.\tag{25}$$

For numerical computation we have used the Lewis integral [10] given by

$$\begin{aligned}L_{000}(\mu;\mathbf{q}_1,a;\mathbf{q}_2,b)&=\int\frac{1}{(p^2+\mu^2)(|\mathbf{p}-\mathbf{q}_1|^2+a^2)}\times\frac{1}{(|\mathbf{p}-\mathbf{q}_2)|^2+b^2)}\,d\mathbf{p}\\&=\frac{\pi^2}{\xi^{1/2}}\log\left[\frac{(\beta+\xi^{1/2})}{(\beta-\xi^{1/2})}\right],\end{aligned}\tag{26}$$

$$\xi=\alpha\gamma-\beta^2\tag{27}$$

$$\alpha\gamma=\{(\mathbf{q}_1-\mathbf{q}_2)^2+(a+b)^2\}\{q_1^2+(\mu+a)^2\}\times\{q_2^2+(b+\mu)^2\}\tag{28}$$

$$\beta=\mu\{(\mathbf{q}_1-\mathbf{q}_2)^2+(a+b)^2\}+b\{q_1^2+(\mu+a)^2\}+a\{q_2^2+(\mu+b)^2\}-4ab\mu.\tag{29}$$

Based on the analytical expression for $f^B(\mathbf{k}',\mathbf{k})$ we have computed for differential $(d\sigma/d\Omega)$ and total (σ) cross-sections. We have chosen to work with $\alpha=1.8145$ and $\lambda=\mu=0.5$ a.u. for which E_{He} was found to be 2.900 a.u. [7]. The result for $(d\sigma/d\Omega)$ (in units of a_0^2) at projectile energies $E_i=500$ eV, 250 eV and 125 eV are shown in Figures 1, 2 and 3. In addition to the values of $(d\sigma/d\Omega)$ calculated on the basis of our correlated wave function (solid line), we have also plotted in each figure the corresponding results obtained by using (i) Hartree-Fock-Roothan function [11] (dashed line) and (ii) our present wave function in the limit of no correlation, $\lambda=0$ (dotted line).

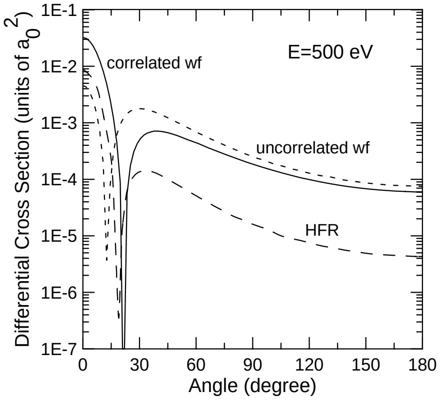

Fig. 1. Differential cross-section (in units of a_0^2) for positronium formation in e^+-He scattering at incident energy $E_i=500$ eV using (i) correlated wave function (1) (solid line), (ii) wave function (1) in the limit of no correlation (dotted line), and (iii) Hartree-Fock-Roothan (HFR) wave function (dashed line).

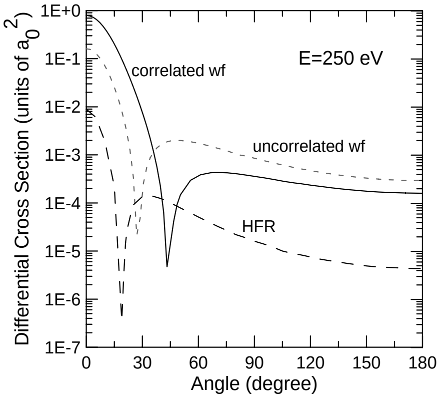

Fig. 2. Differential cross-section (in units of a_0^2) for positronium formation in e^+-He scattering at incident energy $E_i=250$ eV using (i) correlated wave function (1) (solid line), (ii) wave function (1) in the limit of no correlation (dotted line), and (iii) Hartree-Fock-Roothan (HFR) wave function (dashed line).

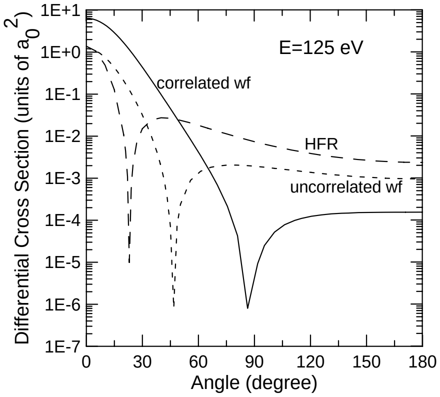

Fig. 3. Differential cross-section (in units of a_0^2) for positronium formation in e^+-He scattering at incident energy $E_i=125$ eV using (i) correlated wave function (1) (solid line), (ii) wave function (1) in the limit of no correlation (dotted line), and (iii) Hartree-Fock-Roothan (HFR) wave function (dashed line).

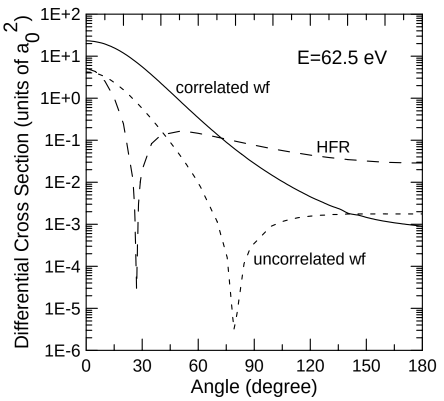

Fig. 4. Differential cross-section (in units of a_0^2) for positronium formation in e^+−He scattering at incident energy $E_i = 62.5$ eV using (i) correlated wave function (1) (solid line), (ii) wave function (1) in the limit of no correlation (dotted line), and (iii) Hartree-Fock-Roothan (HFR) wave function (dashed line).

Table 1. Ps formation cross-section in units of πa_0^2 for different incident positron energies.

E_i (eV)	σ_{corr}	σ_{ucorr}	σ_{HFR}
125	0.6091	0.0879	0.0774
250	0.0416	0.0093	0.0061
500	0.0018	0.0019	0.0003

For the sake of brevity, we label these cross-sections as $(d\sigma/d\Omega)_{corr}$, $(d\sigma/d\Omega)_{HFR}$ and $(d\sigma/d\Omega)_{ucorr}$. A general feature of our results is that the inter-electronic correlation pushes the dip of the cross-section to larger angles, the effect being more pronounced at low energies and also that in the forward direction, $(d\sigma/d\Omega)_{corr}$ is greater than each of $(d\sigma/d\Omega)_{HFR}$ and $(d\sigma/d\Omega)_{ucorr}$ at all energies. We have verified that the dip in $(d\sigma/d\Omega)_{corr}$ disappears altogether for $E_i \leq 62.5$ eV (Fig. 4). While it is tempting to attribute the difference between the numbers for $(d\sigma/d\Omega)_{corr}$ and those for $(d\sigma/d\Omega)_{HFR}$ and $(d\sigma/d\Omega)_{ucorr}$ to the effect of correlation, the disagreement between the values of $(d\sigma/d\Omega)_{HFR}$ and $(d\sigma/d\Omega)_{ucorr}$ deserves some additional comments. For $\lambda = 0$, the wave function (1) goes over to the conventional orbital product of two hydrogenic wave functions which gives reasonable results (when compared with Hartree-Fock results) for E_{He} with $\alpha = 1.69$. But our chosen value of α is 1.8145. Thus we can not expect agreement between the two sets of data.

In Table 1 we display our results for the total cross-section. For $E_i = 125$ eV and 250 eV, the values of σ_{corr} are roughly one order of magnitude larger than the corresponding results for σ_{ucorr}. It is of interest to note that experiments [12] demand for such augmented data and the difference between the theory and experiment can not be settled only by going over to higher order purterbative calculation [13]. For $E_i = 500$ eV, the results of σ_{corr} and σ_{ucorr} do not differ appreciably. This is understandable since at such high energies the correlation effect can be expected to be negligible. However, we can not explain why in this energy σ_{ucorr} and σ_{HFR} differ by an order of magnitude.

Finally, we conclude by noting that the type of demonstration presented by us for the importance of correlation effect should be pursued in more realistic calculation for Ps-formation from helium. It is pertinent to note that the first-order approximation for rearrangement collisions involving the heavy-particles should, in general, be augmented with higher order matrix elements of the perturbation series. However for light particles, such as positrons, good estimates of the first order cross-section at higher incident energies would indicate the worthiness of the approach for higher order calculations.

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