Nuclear-Charge Screening in Positronium Formation from Helium Atoms

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Abstract
An analytical treatment of the electron screening effect within an active-electron model is given for positronium formation from helium atoms. A first-order distorted wave approximation with correct boundary conditions is applied to evaluate the transition amplitude. In the range of impact energy for which the introduced perturbative approach is valid, both the total and differential cross sections are calculated and the results for total cross sections are compared with the other calculations and with the available experimental data.

Keywords: Positronium formation; Distorted-wave approximation; Correct boundary conditions; Nuclear-charge screening

Introduction
There are many important applications for the positron scattering processes in physics, chemistry, medicine, materials science, materials engineering and other fields of science and technology [1,2]. For this fact, over the last few decades, a considerable amount of the experimental and theoretical works devoted to study of such processes. On the other hand, the positronium (Ps) atom, which presents a simple exotic bound state between matter and antimatter, has attracted a great deal of interest in theory and experiment for its significant role in production of antihydrogen atoms. The antihydrogen atoms in turn can be used for understanding of the validity of quantum electrodynamics and testing of the charge conjugate symmetries, the action of gravity on antimatter and charge-parity-time (CPT) invariance theorem (see for example Ref. [3] and references therein).

Among all the processes, a process which may occur during the positron-atom and/or positron-molecule collisions is the charge transfer or positronium formation process. Ps formation during the positron-helium collision is an example of the rearrangement collisions and has drawn the attention of a large number of theoreticians and experimentalists [4–29]. Since two active electrons in the target atom are involved in the interactions, the positron-helium collision process is really a four-body problem. However, for simplicity, most of the theoretical approaches, which have been formulated to explain the dynamics of the Ps formation in such a collision system, have been outlined based on a three-body model in which the passive electron is assumed to remain frozen in its initial state during the charge transfer process. A wide variety of approximations with various degrees of sophistication have been used to investigate this rearrangement scattering process. The first-order Born approximation (FBA) [11,12], eikonal approximation [12], first-order distorted wave formalism (DW1) [13], high-energy second-order...
Born (B2) [14], continuum distorted-wave (CDW) approach [12,15], the methods based on the Kohn and inverse Kohn variational procedures [16], two-state close-coupling approximation (CCA) [17], single- and two-centered convergent close-coupling (CCC) [18,19] method, classical trajectory Monte-Carlo (CTMC) technique [20], the target continuum distorted-wave approximation (TCDWA) [21], and the spherical coupled-channel method (SCC) [22] are some of the theories applied to calculate the positronium formation cross sections at different ranges of incident positron energy. Very recently a number of calculations have been reported on Ps formation in the collision of positron with helium atoms based on the momentum-space coupled-channel optical (CCO) method by Zhou and co-workers [23], second-order distorted-wave approximation (DWA2) by Sen and Mandal [24], two-center convergent close-coupling (CCC) and multiconfigurational two-center convergent close-coupling (MCCC) approaches by Utamuratov et al [26,27], first-order Coulomb-Born approximation (CBA) and a self-consistent correct boundary distorted-wave approximation (SCDW) by Ghanbari-Adivi [28,29]. Recently the total cross sections for Ps formation in other noble gas atoms e.g. Ne, Ar, Kr and Xe have been reported by Larricchia et al [30] and Marler et al [31]. Also, a number of theoretical works [32–35] have been concerned with the investigation of the Ps formation process in the impact of the positron on multielectron atomic targets. However, as far as we are aware, only a few of the above mentioned works [33,36] have been devoted to the angular distribution of the differential cross sections (DCS) for such processes. Also, the literature is poor in reporting cross sections for Ps formation from K and other inner shells of multielectron atoms.

Although, the Ps formation process, in ion-atom (molecule) collisions, is practically significant at lower energies from the threshold up to 100 eV, there are a large number of calculations [11-15,21,24,28,29] and measurements [4–8] for such a process at higher impact energies. Calculations for this region of the impact energy are generally based on the perturbative techniques which are valid at high energies. The present method is a very simple analytical work based on perturbative techniques that gives results in its validity region comparable with the results obtained from other more complicated perturbative methods. Also, among the theories on the Ps formation process, the convergent close-coupling (CCC) [25–27] calculations are in high agreement with the latest experiments for Ps formation cross section in helium. But CCC calculations are sophisticated and time-consuming while the present work in addition to its considerable simplicity, is more economic in terms of computation time in comparison with the more advanced theories such as CCC.

In the present work, a simple model is presented for presenting the interactions between the incident positron and the target nuclei plus the non-active electron participating in the collision of the positron with helium atoms. The effect of adding the short-range potential arising from the non-active electron to the internuclear potential in the boundary-corrected first-order distorted-wave approximation (DW) on the exact K-shell electron capture amplitude is investigated. The single-zeta Rothenhau-Hartree-Fock wave functions are used to calculate the screening potential as well as the rearrangement amplitude. The method presented in this article can be generalized to the more complicated cases involving targets with multiple non-active electrons by employing parametric differentiation. Atomic units are used unless otherwise stated.

Materials and Methods

As it was mentioned in previous section, positronium formation from a multi-electron atomic target is in fact a few-body problem. However, for simplicity one may approximate this process to a three-body problem. To this end, we treat the positronium formation as a single active electron process and assume that the relaxation times of the other passive electrons are greater than the collision time; subsequently, they remain frozen in their states during the collision process. Thus, in this three-body problem, a positron impinges on a bound subsystem composed of a massive target ion $T$ of effective charge $Z_T$ and mass $M_T$ and an active electron $e$. In the laboratory system, the problem can be described by any of the pairs of Jacobi coordinates $(r_p, R_p)$ or $(r_e, R_e)$. The electronic coordinates $r_p$ and $r_e$ refer to the target nuclei and the positron projectile respectively, while $R_p$ and $R_e$ respectively present the position vectors of the positron and positronium atom relative to the target ion.

According to a time-independent scattering formalism developed by Toshima et al [37] and Belkić [38] for a general three-body scattering problem, the charge transfer boundary-corrected distorted-wave amplitude in an ion-atom collision assumes the prior form of:

$$A_{D_W} = \langle \chi_f | -U_r | \chi_i \rangle,$$  \hspace{1cm} (1)

where $\chi_i$ and $\chi_f$ are products of phase factors (which ensure that the overall solutions satisfy the proper
asymptotic boundary conditions for distorting potentials $U_i$ and $U_j$ in the entrance and exit channels), plane-wave functions for heavy particle motion and bound-state electronic wave functions $\phi_i(r_j)$ and $\phi_j(r_i)$. These distorted wave functions can be written explicitly, in coordinate space, as:

\[
\chi_i(r_j, R_j) = \phi_i(r_j) \exp[i \mathbf{K}_i \cdot \mathbf{R}_j] \times \exp\left[\frac{iZ_r(Z_r-1)}{v_i} \ln(v_j R_j - v_i \cdot \mathbf{R}_j)\right],
\]

\[
\chi_j(r_i, R_i) = \phi_j(r_i) \exp[i \mathbf{K}_j \cdot \mathbf{R}_i] \times \exp\left[\frac{iZ_r(Z_r-1)}{v_j} \ln(v_j R_j - v_j \cdot \mathbf{R}_i)\right],
\]

in which $\mathbf{K}_i$ and $\mathbf{K}_j$ are the initial and final wave vectors for the relative motion in the corresponding channels, $v_i$ and $v_j$ are the initial and final velocities and $Z_r$ and $Z_r^*$ are the projectile-ion and the residual target-ion charges, respectively. Using the distorted waves appearing in Eqs. 2 and 3, the integral form of the transition amplitude is written as:

\[
A_{DW} = \iint d\mathbf{r}_p dR_p Z_r^* (r_j, R_j) V_i(r_j, R_j) \chi_i(r_j, R_j),
\]

where $V_i(r_j, R_j)$ is the perturbative interaction potential in the initial channel;

\[
V_i(r_j, R_j) = V_{PP}(R_p) + V_{PT}(r_j),
\]

with $xy$ with $xy = Pe$, $PT$ is the two-body interaction potential between particles $x$ and $y$. The $Pe$ interaction is a Coulomb one as $V_{PP}(r_j) = \frac{Z_r}{r_j}$ and/or the $PT$ interaction is sum of a Coulomb long-range interaction due to interaction between the nuclei and the specified projectile and a short-range part due to the nuclear-screening effect of the passive electrons;

\[
\lim_{R_p \to \infty} V_{PP}(R_p) = \frac{Z_r}{R_p} (Z_r-1),
\]

and subsequently one finds;

\[
\lim_{r_j \to \infty, R_j \to \infty} V_i(r_j, R_j) = U_i(r_j, R_j) = \frac{Z_r^*(Z_r-2)}{R_p}
\]

Therefore, the transition amplitude introduced in Eq.1 satisfies the appropriate boundary conditions in the initial channel. For numerical calculations it is mandatory to present the $V_{PP}$ in a simpler analytical form. For positronium formation from helium atoms in their ground states, this potential is radially symmetrical. Using a single-zeta Hartree-Fock slater orbital equivalent to the $1s$ hydrogenic wave function with exponent parameter $\zeta = 1.6875$, the simple analytical expression

\[
V_{PP}(r_j) = \frac{Z_r[(Z_r-1) + (1 + \zeta R_p) \exp(-\sigma R_p)]}{R_p},
\]

with $\sigma = 2\zeta$ can be found for the projectile-target ion interaction. This potential, which includes two long- and short-range parts with the same sign, has the following closed form in the momentum space;

\[
V_{PP}(k) = \frac{1}{\sqrt{2}\pi} \left(\frac{2}{k^2 + \sigma^2} \right)^{3/2} \left(\frac{Z_r^2 - 1}{k^2 + \sigma^2} \right)
\]

If one ignores the screening effect of the non-active electron the short range term disappears from the transition matrix element presented in Eq. 1. For positrons incident on helium atoms $Z_r = Z_r^* = 1$, and so the boundary phases become equivalent to unit. Using this fact and applying the Fourier transform technique the transition amplitude can be written as;

\[
A_{DW} = A_{DW}^{(e)} + A_{DW}^{(b)},
\]

where

\[
A_{DW}^{(e)} = (2\pi)^{1/2} \int d\mathbf{k} \phi^*_j(\mathbf{k}) I^{(PP)}_j (\mathbf{k} - \mathbf{K}) \phi_j(\mathbf{J}),
\]

and

\[
A_{DW}^{(b)} = (2\pi)^{1/2} \int d\mathbf{k} \phi^*_j(\mathbf{k}) V_{PP}(\mathbf{k}) \phi_j(\mathbf{K} - \mathbf{J}).
\]
\( A^{(a)}_{\text{DW}} \) is the partial amplitude due to the attractive interaction of the positron and the active electron, while \( A^{(b)}_{\text{DW}} \) is the partial amplitude which includes both the repulsive interaction of the positron with target nuclei and the nuclear-screening effect of the passive electron. In Eqs. 12 and 13, \( \phi_1 ^{\text{f}} (\textbf{k}) \) and \( \phi_1 ^{\text{i}} (\textbf{k}) \) are the initial and final bound states of the active electron in momentum space and vectors \( \textbf{J} \) and \( \textbf{K} \) denote the momentum transferred to the target-ion and projectile, respectively.

In terms of these vectors, the momentum conservation takes the form \( \textbf{J} + \textbf{K} + \textbf{v}_f = 0 \).

Using the Schrödinger equation for the bound state of the electron in the final channel and inserting the \( 1s \) initial and final orbitals in the momentum space, the first partial amplitude can be reduced to

\[
A^{(a)}_{\text{DW}} = -4\pi \sqrt{2} \zeta_\gamma^{3/2} \frac{J^2 - 2\varepsilon_i}{(K^2 + \zeta_\gamma^2) (J^2 + \zeta_\gamma^2)} ,
\]

in which \( \varepsilon_i \) is the electron binding energy in its initial bound state and \( \zeta_\gamma \) is the exponent parameter of the \( 1s \) hydrogenic wave function for positronium atoms, \( \zeta_\gamma = \frac{1}{5} \).

Inserting the wave functions in momentum space describing the corresponding bond states of the active electron and using the Lewis integral,

\[
L(\lambda_1, \lambda_2, \lambda_3) = \int \frac{dk}{|\textbf{k} - \textbf{K}|^2 + \lambda_1^2} \times \frac{1}{k^2 + \alpha^2} \times \frac{1}{|\textbf{k} + \textbf{J}|^2 + \lambda_2^2} \times \frac{1}{|\textbf{k} + \textbf{J}'|^2 + \lambda_3^2} \times \frac{1}{|\textbf{k} + \textbf{K}'|^2 + \lambda_4^2} ,
\]

\[
= \pi^2 (\alpha^2 - \beta^2)^2 \ln \left( \frac{\alpha + (\alpha^2 - \beta^2)^{1/2}}{\alpha - (\alpha^2 - \beta^2)^{1/2}} \right) ,
\]

with

\[
\alpha = (K^2 + \lambda_1^2 + \lambda_2^2) \lambda_3,
\]

\[
+ (J^2 + \lambda_1^2 + \lambda_3^2) \lambda_4 ,
\]

\[
\beta = [K^2 + (\lambda_1^2 + \lambda_2^2)^2] [J^2 + (\lambda_1^2 + \lambda_3^2)^2] ,
\]

and employing the parametric partial derivatives of the Lewis integral, \( L(\lambda_1, \lambda_2, \lambda_3) \), one can write the second partial amplitude including the nuclear screening effect as;

\[
A^{(b)}_{\text{DW}} = \frac{2\sqrt{2}}{\pi} \zeta_\gamma^{3/2} \left\{ (Z_f - 1) \frac{\partial L(\lambda_1, \lambda_2, \lambda_3)}{\partial \lambda_2 \partial \lambda_3} \right|_{\lambda_1 = \phi} + \partial^2 L(\lambda_1, \lambda_2, \lambda_3) \right|_{\lambda_1 = \phi} - \zeta_\gamma \right|_{\lambda_1 = \phi} ,
\]

With the analytical forms of the partial amplitudes, the closed form of the transition amplitude given in Eq.11 is readily evaluated. This procedure can also be simply generalized to the positronium formation from K shell of other atomic targets with multiple non-active electrons.

### Results and Discussion

In this section, the differential and total cross sections for positronium formation from helium atoms in their ground states are presented. Differential electron transfer cross sections are shown in Fig. 1 for positrons incident at 100, 200 and 500 eV energies on the helium atoms. The general features of the differential cross sections are similar to those obtained from the first-order Born approximation for electron capture from hydrogen atoms by impact of fast protons [39]. All the curves, for the angular distribution of the differential cross sections, show a large kinematical peak in the forward direction followed by a deep dip at about 20–25° and then decaying smoothly at larger angles. The origin of the dip occurring in the curves seems to be the cancelation of the partial amplitudes in the transition matrix element due to the attractive positron-electron and the repulsive positron-target nuclei potentials. In the forward direction the attractive positron-electron term dominates the matrix element and at larger angles beyond the dip the repulsive positron-target nuclei term dominates and give rise to the tail of the distribution. It is obvious that the smaller scattering angles are corresponding to large impact parameters where the positron-electron interaction dominates, while the large scattering angles correspond to the small impact parameters for which the reaction is more penetrating and consequently the repulsive positron-target nuclei interaction dominates. The dark angle (the angle in which the cancelation occurs and the dip appears) shifts toward the smaller scattering angles and the width of the dark zone decreases as the impact energy increases. This is reasonable, because for a fixed impact parameter, as the impact energy increases the reaction
becomes more penetrating and the role of the repulsive interaction becomes more pronounced.

The very steep slope in the extreme forward directions and then a more gradual decrease of the angular distribution with larger angles is a feature which presents in all the angular distributions plotted in parts (a) and (b) of Fig. 1. All of the distributions decrease in magnitude with increase in the incident energy. Fig. 1 also compares the present results with the corresponding calculations performed based on the Coulomb-Born approximation (CBA) with $Z_T = 2$ and from the distorted wave approach using the Green, Sellin and Zocher (GSZ) potential describing the positron-target ion interaction [29,40]. The latter method is a first-order approximation with correct boundary conditions which satisfies the post-prior symmetry and hereafter is referred to as the SCDW method. At each of the specified incident energies, for scattering angles smaller than the dark angle, the results obtained from the present method are very close to the corresponding results obtained from the other two formalisms mentioned above. For a specified energy, in this range of the scattering angles, the differences between the curves of the present results and those obtained from CBA are very marginal for a specified energy. But for scattering angles beyond the dark angle, the differences between the curves become more pronounced. In this angular region, the present results are higher than those of CBA which in turn are larger than those of the SCDW method. As the incident energy increases, the curves of CBA and SCDW become more close to each other but they still differ significantly from the present results. These facts show that the nuclear-screening effect of the passive electrons is ignorable at small scattering angles, while it plays a more important role at the scattering angles larger than the dark angle. This last feature can be extracted directly from the formalism presented in section 2. Since the long- and short-range terms of the $V_{FR}(|R|)$ in Eq. 10 have the same sign, the attractive positron-electron interaction will be canceled more by the additional screening term due to the non-active electron. Also, it is an easy practice to show that the effectiveness of the screening depends on the momentum transfer to the positron and the screening becomes more effective with increase in the momentum transfer. Therefore, at small scattering angles the momentum transfer is small and the cross sections approximately coincide to those of the CBA [28] and SCDW [29] formalisms. As the scattering angle becomes larger, the momentum transfer increases and the screening affects the cross sections more significantly.

The spatial distribution of the passive electron produces not only a radial electron correlation due to its affect on the spatial distribution of the active electron in the preparation of the initial bound state but also an indirect dynamical correlation due to its influence on the charge transfer amplitude by the screening potential. Two terms are included in the shielding potential; the first term causes a Coulomb dynamical correlation and corresponds to the consideration of the non-active electron as being exactly placed on the target nucleus position and the second one causes a non-Coulomb correlation and affects the evolution of the positron during the collision at finite distances. These two terms, in fact, are the partial aspects of the influence of the passive electron on the dynamics of the capture reaction. The short-range part has more affect on the transition amplitude at small impact parameters or at

![Figure 1](Color online) Angular distribution of the differential positronium formation cross sections for positron incident at 100, 200 and 500 eV on helium atoms.
larger scattering angles. It is expected that if the short-range part is removed from the interaction potential and the correct boundary conditions yet be satisfied, the present differential cross sections coincide to those of the Coulomb-Born approximation. But the existence of this short-range interaction makes some considerable differences between the CBA as well as the SCDW and the present calculations. Fig. 2 shows the influences of the Coulomb and non-Coulomb correlations on positronium formation differential cross sections at 100 eV. Without considering the active electron, the kinematical peak at the extreme forward scattering angles disappears and a peak occurs at the same angular region in which the unphysical dip appears. Adding the Coulomb correlation to the interaction potentials gives the results which are very close to those of the CBA. Considering only the non-Coulomb correlation gives some results which are similar in shape to but larger in magnitude than those which result when only the Coulomb correlation is considered. Considering both of the correlations shifts the unphysical dip a little toward the smaller scattering angles and increases considerably the value of the cross sections at larger scattering angles.

It is well-known that the Thomas mechanism is a two-step classical process. If the impact energy be high enough, the wave packet of the projectile is small and the classical behavior of the scattering system is more evident. Thus, for such energies, it is reasonable to expect that the Thomas mechanism cause a local maximum around the Thomas angle in the electron capture differential cross sections. It is worthy to notify that the first-order perturbative formalisms which are applicable at intermediate energies are not capable of explaining the Thomas double scattering process. Therefore, the second local maximum appearing in curves after the unphysical dip should not be confused with the Thomas peak. Considering the higher order terms of the perturbative series smooths out the unusual sharp dip and the local maximum after it. As is known from heavy particle studies, CDW approximation contains some terms of the double scattering mechanism which give rise to this feature [12]. Since the CDW model outlined by Bransden et al [12] explicitly includes the second-order continuum intermediate states, it reproduces the Thomas peak at the expected angle of 45° for positronium formation from helium atoms. However, as it shown in Figure 3, both the post and prior forms of the CDW formalism proposed by Bransden et al [12] do not give reliable results for total cross sections especially at lower energies. In Fig. 3, the present results are compared with the first Born, eikonal and CDW formalisms. As can be seen from this figure, the present results are a little larger than those of the post eikonal formalism at all energies. In spite of the fact that post and prior CDW formalisms show the Thomas peak in the angular distribution of the differential cross sections, our results for the total cross sections are more reliable than those of the CDW formalism. All the curves presented in Fig. 3 converge at higher energies.
In Fig. 4, we compare the present calculated total cross sections with other calculations and the available measurements for incident energies of 50 through 250 eV. The present theoretical results for $1s \rightarrow 1s$ transitions have all been multiplied by 1.202 to account for excited-state capture. The comparisons made in part (a) show that the present results are higher than those of CBA and SCDW at smaller impact energies. As the incident energy increase, the theoretical curves converge. Also, it can be seen that the present results are larger than all the measurements for energies lower than 70 eV, while they are smaller than data from Fromme et al [5] and Diana et al [6] for impact energies higher than 80 eV. The best agreement occurs between the present results and the data from Overton et al [7] for energies larger than 80 eV. Also for these energies, the agreement between our results and the data from Murtagh [8] is reasonably good. Recently, the positronium-formation cross sections for positrons scattered by helium within the impact energy ranging from 10 to 60 eV were measured using a high-resolution trap-based pulsed positron beam [25]. A part of those measurements (for incident energy of 50-60 eV) is presented in Fig. 4. A Convergent close-coupling (CCC) formalism was also used to calculate the total cross section at the same range of the impact energy [25]. The results are shown in Fig. 4, part (a). The present calculations are larger than the above mentioned measurements and the CCC calculations for energies between 50-60 eV. This is reasonable because the calculations based on the perturbative formalisms are not so valid for lower scattering energies, but they will be more accurate as the impact energy increases.

In part (b) of Fig. 4, we compare the present calculations with the corresponding results obtained from CDW [15], CCC [19], CCO [23] and DWA2 [24] theories. Again, for energies below 80 eV, the present curve is higher than those of all these theories. For energies higher than 80 eV, the present results are very closed to the results obtained from CCO [23]. For energies higher than 150 eV all the curves converge. In any case, the agreement between the present calculations and the counted more sophisticated theories is very good. It is worthy to notice that although the present computations are very simple and economic in time, their results are comparable with the other theories and give a good description of the measured total cross sections for energies higher than 80 eV.

In summary, we have presented a distorted-wave formalism with correct boundary conditions for the calculation of the differential and total cross sections of positronium formation in the collision of positron with helium atoms. The method includes the effect of the nuclear screening of the non-active electron. The features observed in the angular distribution of the calculated differential cross sections are similar to those obtained from the first-order Born approximation for electron capture from hydrogen atoms by fast protons. The effectiveness of the screening is an increasing function of the momentum transfer. This function increases for larger scattering angles implying smaller distances. Although, it may be said that the present distorted-wave method is very simplistic for today's standards, it is analytical and very fast. This simplistic method gives the results for the differential cross sections with similar features to other first-order perturbative methods and reliable results for total cross sections at higher scattering energies for which the first-
order perturbative approximations are valid. Although the CDW formalism proposed by Bransden et al. [12] shows the Thomas peak at the expected angle of 45°, it does not give reliable results for total cross sections at least at energies lower than 100 eV. In spite of the simplicity and quickness of the computations of our method, the obtained results for the integrated cross sections are in reasonable agreement with the calculations from similar theories such as CBA and SCDW and also from the more sophisticated formalisms such as SCC, CCC, CCO and DWA2. Also, the agreement between the present integrated cross sections and the available measurements are reasonably good for incident energies between 80 to 250 eV.

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