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Collision between two ortho-positronium (Ps) atoms: A four-body Coulomb problem

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Abstract. The elastic collision between two ortho-positronium (e.g. $S = 1$) atoms is studied using an *ab-initio* static exchange model (SEM) in the centre of mass (CM) frame by considering the system as a four-body Coulomb problem where all the Coulomb interaction terms in the direct and exchange channels are treated exactly. A coupled channel methodology in momentum space is used to solve Lippman–Schwinger equation following the integral approach. A new SEM code is developed in which the Born–Oppenheimer (BO) scattering amplitude acts as input to derive the SEM amplitude adapting the partial wave analysis. The s-, p- and d-wave elastic phase shifts and the corresponding partial cross-sections for the spin alignment $S = 0$, i.e., singlet (+) and $S = 2$, i.e., triplet (−) states are studied. An augmented Born approximation is used to include the contribution of higher partial waves more accurately to determine the total/integrated elastic cross-section (σ), the quenching cross-section (σ_q) and ortho-to-para conversion ratio (σ/σ_q). The effective range theory is used to determine the scattering lengths and effective ranges in the s-wave elastic scattering. The theory includes the non-adiabatic short-range effects due to exchange.

Keywords. Positronium; elastic collision; exact exchange; CM frame; scattering length; quenching cross-section; non-adiabatic effects.

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1. Introduction

The scattering of two positronium (Ps) atoms is a problem of fundamental physical importance [1–17] and of relevance to the formation of the Ps_2 molecule [1–9] as well as current endeavours towards the production of Ps Bose–Einstien condensation (BEC) [1,10,11]. It is again useful for its applications in technology [18,19]. The Ps–Ps scattering problem is very difficult to treat theoretically as it is a four-body Coulomb problem. At lower energies, the particles are highly correlated. The proper symmetry of a two-Ps system

is a quite complicated group theoretical problem [4,5]. However, in scattering theory, when two ortho-Ps (e.g. $S = 1$) atoms collide, the total aligned spin of the system can be $S = 2$ when both the atoms are aligned in the same direction (e.g. polarized beam) and $S = 0$, if they are oppositely aligned. An *ab-initio* static exchange model (SEM) [20–25] is used to study the collision between two ortho-Ps atoms following a coupled channel methodology in the momentum space [20–26]. An integral approach to solve the non-relativistic Schrödinger equation e.g., the Lippman–Schwinger-type equations, is used to get coupled integral equations for different channels. The system is treated in the centre of mass (CM) frame considering it as a four-centre Coulomb problem [25,27]. All the Coulomb interaction terms in both the direct and exchange/rearrangement channels are treated exactly. In Ps–Ps system, all the four charges are of equal masses; in addition, the two electrons and two positrons are indistinguishable. So the exchange between two electrons and between two positrons are equally probable. As the system is treated in the CM frame, the exchange between only two positrons and between only two electrons are equivalent. Again, if both exchanges happen simultaneously, then the system is equivalent to the direct channel. So, effectively there are two direct channels and two exchange channels. So, the exchange between only the electrons is sufficient to describe the collision process. Accordingly, the spin-aligned $S = 2$ state as triplet $(-)$ and spin-aligned $S = 0$ state as singlet $(+)$ are described. The plus and minus signs in the bracket indicate that the space parts of the system wavefunction are symmetric and antisymmetric respectively. Accordingly, the total cross-section could be defined by taking one-fourth contribution from the singlet and three-fourth contribution from the triplet channels. However, a multiplicative factor greater than one may be required due to larger reaction rate for both the exchanges between the electrons and between the positrons. The theory by its nature, includes non-adiabatic short-range effects due to exchange between electrons as well as between positrons.

In a system of four charged particles, there are six Coulomb interaction terms. In the present system, two positron–electron interaction terms are used to define two Ps-atomic wavefunctions. So, effectively there are four Coulomb interaction terms between the atoms. The simplest first-Born matrix elements are nine-dimensional integrals. The analytical parts of the matrix elements are relatively easier to compute in direct channel due to the symmetry of system wavefunctions in the initial and final states; it is possible to get the closed form. But in the rearrangement channel when the electrons exchange their positions, the initial and final-state wavefunctions are not symmetric. It is extremely difficult to compute nine-dimensional space integration to include the effect of exchange/antisymmetry of the system electrons exactly. Using the Fourier transform and Bethe integral formulae, one can reduce the dimension of these matrix elements into tractable two-dimensional (X–Y) integrals with limits zero (0) to one (1). The positron–positron and two electron–positron interaction terms are relatively less difficult to compute due to the presence of two coupled terms. But the electron–electron correlation matrix element contains three coupled terms and is extremely difficult to transform into a tractable two-dimensional form. It was less difficult in Ps and H system [20]; due to very light mass of Ps it was a good approximation to consider the H-nucleus as the origin of the centre of mass and it was treated as a three-centre problem. By using a simple substitution of variables and accordingly changing the space of integration, it has been possible to transform the electron–electron exchange integral in the four-centre problem

into a nine-dimensional integral having only two coupled terms that can be reduced into a tractable similar two-dimensional form following exactly the same procedure as is used in other correlation terms.

The present paper deals with the elastic collision between two ortho-Ps atoms, when both are in ground ($1s$) states. The eigenstate expansion method to define the system wavefunction and an approach like the Hartree–Fock variational method to project out different channels are used to get the coupled integro-differential equations. One can use iterative method to find the unknown coefficients used in eigenstate expansion with partial wave analysis. However, the number of coupled equations is restricted here by taking the number of bound states [26] into account. This is known as differential approach. In integral approach, one uses the help of Lippman–Schwinger equation to get the coupled integral equations [26]. Either the configuration space [27] or the momentum space [20–26] can be used to form the equations. However, in the momentum space formalism [20], the convergence problem is much easier to overcome than the coordinate space formalism. When the exchange amplitude is combined (adding or subtracting) with the direct first-Born amplitude, it is called the Born–Oppenhimer (BO) amplitude following the nomenclature of Ray and Ghosh [20] and accordingly the singlet (+) and triplet (−) channels are defined. The BO ($\pm$) amplitudes are used as inputs in the coupled channel methodology to derive the SEM amplitudes for the singlet (+) and triplet (−) channels, respectively. A partial wave analysis and angular momentum algebra are used to reduce the three-dimensional coupled integral equation to the one-dimensional form. The partial wave contributions: $L = 0$ is defined as the s-wave, $L = 1$ as the p-wave and so on. The s-, p-, d-wave elastic phase shifts, the corresponding s-, p-, d-wave elastic cross-sections, the integrated/total elastic cross-section, the quenching cross-section and ortho-to-para conversion ratio are evaluated. To calculate the integrated/total elastic cross-section (σ) more accurately to include the contribution of higher partial waves, an augmented Born approximation [20] is used. The effective range theory [28] is applied to derive the scattering length (a) and the effective range (r_0) utilizing the variation of the s-wave elastic phase shift (δ_0) with the incident energy. To get the scattering cross-section, one has to integrate the square of the amplitude over the scattering angle [$\Omega(\theta, \phi)$]. Accordingly, an efficient computer code is developed to compute the SEM amplitude utilizing Born–Oppenheimer (BO) amplitude as the input. It could be useful as the starting code to solve many challenging problems involving two-atomic collision.

2. Theory

The description of the present Ps–Ps system is given in figure 1. The vector $\vec{r}_1$ represents the relative coordinate between the positron $e_{\rm A}^+$ and the electron e_1^- in first Ps. Similarly, vector $\vec{r}_2$ represents the relative coordinate between the positron $e_{\rm B}^+$ and the electron e_2^- in second Ps. $\vec{R}$ and $\vec{r}$ represent the relative coordinates between two positrons $e_{\rm A}^+$ and $e_{\rm B}^+$ and between two electrons e_1^- and e_2^-, respectively. The initial and final-state wavefunctions of the system are defined as

$$\psi_{\rm i}(\vec{r}_1, \vec{r}_2, \vec{R}) = {\rm e}^{i\vec{k}_{\rm i}\cdot\vec{R}'}\phi_{1s}^{\rm A}(\vec{r}_1)\phi_{1s}^{\rm B}(\vec{r}_2), \tag{2.1a}$$

$$\psi_{\rm f}(\vec{r}_1, \vec{r}_2, \vec{R}) = (1 \pm P_{12}){\rm e}^{i\vec{k}_{\rm f}\cdot\vec{R}_{\rm f}}\phi_{1s}^{\rm A}(\vec{r}_1)\phi_{1s}^{\rm B}(\vec{r}_2), \tag{2.1b}$$

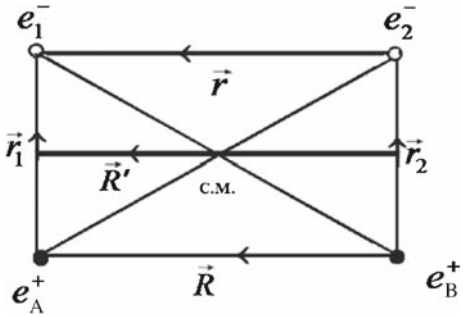

Figure 1. The picture of Ps–Ps system.

so that $\vec{k}_\mathrm{i}$ and $\vec{k}_\mathrm{f}$ represent the initial and final momenta of the system (e.g. momenta of the projectile Ps if the target Ps is taken at rest); $\phi_{1s}^\mathrm{A}(\vec{r}_1)$ and $\phi_{1s}^\mathrm{B}(\vec{r}_2)$ represent the ground-state wave functions of two Ps atoms; P_{12} is the exchange or antisymmetry operator. $\vec{R}'$ and $\vec{R}_\mathrm{f}$ represent the CM-coordinates of the system in the direct and exchange channels respectively and are defined as

$$\vec{R}' = \vec{R} + \frac{m_\mathrm{e}}{m_\mathrm{A}+m_\mathrm{e}}\vec{r}_1 - \frac{m_\mathrm{e}}{m_\mathrm{B}+m_\mathrm{e}}\vec{r}_2, \tag{2.2a}$$

$$\vec{R}_\mathrm{f} = \vec{R} + \frac{m_\mathrm{e}}{m_\mathrm{A}+m_\mathrm{e}}(\vec{r}_2 - \vec{R}) - \frac{m_\mathrm{e}}{m_\mathrm{B}+m_\mathrm{e}}(\vec{r}_1 + \vec{R}), \tag{2.2b}$$

when m_A, m_B are the masses of two positrons and m_e is the mass of the electron.

In elastic scattering $|\vec{k}_\mathrm{i}| = |\vec{k}_\mathrm{f}|$; so only the direction of the final momentum $\vec{k}_\mathrm{f}$ changes due to scattering. The Coulomb interaction between the atoms in the direct and exchange channels are expressed as

$$V_\mathrm{Direct}(\vec{R},\vec{r}_1,\vec{r}_2) = \frac{e_\mathrm{A}^+e_\mathrm{B}^+}{|\vec{R}|} - \frac{e_\mathrm{A}^+e_2^-}{|\vec{R}-\vec{r}_2|} - \frac{e_\mathrm{B}^+e_1^-}{|\vec{R}+\vec{r}_1|} + \frac{e_1^-e_2^-}{|\vec{R}+\vec{r}_1-\vec{r}_2|}, \tag{2.3a}$$

$$V_\mathrm{Exchange}(\vec{R},\vec{r}_1,\vec{r}_2) = \frac{e_\mathrm{A}^+e_\mathrm{B}^+}{|\vec{R}|} - \frac{e_\mathrm{A}^+e_1^-}{|\vec{r}_1|} - \frac{e_\mathrm{B}^+e_2^-}{|\vec{r}_2|} + \frac{e_1^-e_2^-}{|\vec{R}+\vec{r}_1-\vec{r}_2|}, \tag{2.3b}$$

respectively. Here the magnitudes of all the Coulomb terms in the numerators in eqs (2.3a) and (2.3b) are equal to unity in atomic unit (a.u.). The formally exact Lippman–Schwinger-type coupled integral equation for the scattering amplitude in momentum space [26] is given by

$$f^\pm_{n'1s,n1s}(\vec{k}_\mathrm{f},\vec{k}_\mathrm{i}) = B^\pm_{n'1s,n1s}(\vec{k}_\mathrm{f},\vec{k}_\mathrm{i}) - \frac{1}{2\pi^2}\sum_{n''}\int \mathrm{d}\vec{k}''\frac{B^\pm_{n'1s,n''1s}(\vec{k}_f,\vec{k}'')\,f^\pm_{n''1s,n1s}(\vec{k}'',\vec{k}_i)}{\vec{k}^2_{n''1s}-\vec{k}''^2+i\varepsilon}. \tag{2.4}$$

Here $B^\pm$ are the well-known Born–Oppenheimer (BO) scattering amplitude [20–25] in the singlet (+) and triplet (−) channels, respectively. Similarly, $f^\pm$ indicate the unknown

SEM scattering amplitudes for the singlet and triplet channels. The BO amplitude is defined as

$$B^{\pm}_{n'1s,n1s}(\vec{k}_{\rm f},\vec{k}_{\rm i}) = -\frac{\mu}{2\pi}\int {\rm d}\vec{R}{\rm d}\vec{r}_1{\rm d}\vec{r}_2\psi^*_{\rm f}(\vec{R},\vec{r}_1,\vec{r}_2) \times V(\vec{R},\vec{r}_1,\vec{r}_2)\psi_{\rm i}(\vec{R},\vec{r}_1,\vec{r}_2), \tag{2.5}$$

when μ is the reduced mass of the system. The four Coulomb interaction terms in eqs (2.3a) and (2.3b) are: the first term is the nucleus–nucleus (NN) interaction, the fourth term is the electron–electron (e_1e_2) interaction in both the channels; the second term is the interaction between the nucleus $e^+_{\rm A}$ and the electron e^-_2 (Ae_2) in the direct channel and the interaction between the nucleus $e^+_{\rm A}$ and the electron e^-_1 (Ae_1) in the exchange channel and the third term is the interaction between the nucleus $e^+_{\rm B}$ and the electron e^-_1 (Be_1) in direct channel and the interaction between the nucleus $e^+_{\rm B}$ and the electron e^-_2 (Be_2) in the exchange channel.

The explicit form of the first term in the direct ($F^{NN}_{\rm B}$) and exchange ($F^{NN}_{\rm O}$) channels are:

$$F^{NN}_{\rm B} = -\frac{\mu}{2\pi}\int {\rm d}\vec{R}{\rm d}\vec{r}_1{\rm d}\vec{r}_2{\rm e}^{-i\vec{k}_{\rm f}\cdot\vec{R}'}\phi^{\rm A^*}_{1s}(\vec{r}_1)\phi^{\rm B^*}_{1s}(\vec{r}_2) \times\frac{1}{R}{\rm e}^{i\vec{k}_{\rm i}\cdot\vec{R}'}\phi^{\rm A}_{1s}(\vec{r}_1)\phi^{\rm B}_{1s}(\vec{r}_2), \tag{2.6a}$$

$$F^{NN}_{\rm O} = -\frac{\mu}{2\pi}\int {\rm d}\vec{R}{\rm d}\vec{r}_1{\rm d}\vec{r}_2{\rm e}^{-i\vec{k}_{\rm f}\cdot\vec{R}_{\rm f}}\varphi^{\rm A^*}_{1s}(\vec{R}-\vec{r}_2)\phi^{\rm B^*}_{1s}(\vec{R}+\vec{r}_1) \times\frac{1}{R}{\rm e}^{i\vec{k}_{\rm i}\cdot\vec{R}'}\phi^{\rm A}_{1s}(\vec{r}_1)\phi^{\rm B}_{1s}(\vec{r}_2), \tag{2.6b}$$

respectively. Similarly, the fourth electron–electron correlation terms for the direct and exchange channels are

$$F^{e_1e_2}_{\rm B} = -\frac{\mu}{2\pi}\int {\rm d}\vec{R}{\rm d}\vec{r}_1{\rm d}\vec{r}_2{\rm e}^{-i\vec{k}_{\rm f}\cdot\vec{R}'}\varphi^{\rm A^*}_{1s}(\vec{r}_1)\phi^{\rm B^*}_{1s}(\vec{r}_2)\frac{1}{|\vec{R}+\vec{r}_1-\vec{r}_2|} \times{\rm e}^{i\vec{k}_{\rm i}\cdot\vec{R}'}\phi^{\rm A}_{1s}(\vec{r}_1)\phi^{\rm B}_{1s}(\vec{r}_2), \tag{2.7a}$$

$$F^{e_1e_2}_{\rm O} = -\frac{\mu}{2\pi}\int {\rm d}\vec{R}{\rm d}\vec{r}_1{\rm d}\vec{r}_2{\rm e}^{-i\vec{k}_{\rm f}\cdot\vec{R}_{\rm f}}\phi^{\rm A^*}_{1s}(\vec{R}-\vec{r}_2)\phi^{\rm B^*}_{1s}(\vec{R}+\vec{r}_1)\frac{1}{|\vec{R}+\vec{r}_1-\vec{r}_2|} \times{\rm e}^{i\vec{k}_i\cdot\vec{R}'}\phi^{A}_{1s}(\vec{r}_1)\phi^{\rm B}_{1s}(\vec{r}_2), \tag{2.7b}$$

respectively.

The second and third terms in the direct and the exchange channels are

$$F^{{\rm A}e_2}_{\rm B} = -\frac{\mu}{2\pi}\int {\rm d}\vec{R}{\rm d}\vec{r}_1{\rm d}\vec{r}_2{\rm e}^{-i\vec{k}_{\rm f}\cdot\vec{R}'}\phi^{\rm A^*}_{1s}(\vec{r}_1)\phi^{\rm B^*}_{1s}(\vec{r}_2)\frac{(-1)}{|\vec{R}-\vec{r}_2|} \times{\rm e}^{i\vec{k}_{\rm i}\cdot\vec{R}'}\phi^{\rm A}_{1s}(\vec{r}_1)\phi^{\rm B}_{1s}(\vec{r}_2), \tag{2.8a}$$

$$F^{{\rm A}e_1}_{\rm O} = -\frac{\mu}{2\pi}\int {\rm d}\vec{R}{\rm d}\vec{r}_1{\rm d}\vec{r}_2{\rm e}^{-i\vec{k}_{\rm f}\cdot\vec{R}_{\rm f}}\varphi^{\rm A^*}_{1s}(\vec{R}-\vec{r}_2)\phi^{E^*}_{1s}(\vec{R}+\vec{r}_1)\frac{(-1)}{|\vec{r}_1|}{\rm e}^{i\vec{k}_{\rm i}\cdot\vec{R}'} \times\phi^{\rm A}_{1s}(\vec{r}_1)\phi^{\rm B}_{1s}(\vec{r}_2), \tag{2.8b}$$

$$F_{\mathrm{B}}^{\mathrm{Be}_1} = -\frac{\mu}{2\pi}\int \mathrm{d}\vec{R}\mathrm{d}\vec{r}_1\mathrm{d}\vec{r}_2 \mathrm{e}^{-i\vec{k}_{\mathrm{f}}\cdot\vec{R}'}\phi_{1s}^{\mathrm{A}^*}(\vec{r}_1)\phi_{1s}^{\mathrm{B}^*}(\vec{r}_2)\frac{(-1)}{|\vec{R}+\vec{r}_1|}$$
$$\times \mathrm{e}^{i\vec{k}_{\mathrm{i}}\cdot\vec{R}'}\phi_{1s}^{\mathrm{A}}(\vec{r}_1)\phi_{1s}^{\mathrm{B}}(\vec{r}_2), \tag{2.9a}$$

$$F_{\mathrm{O}}^{\mathrm{Be}_2} = -\frac{\mu}{2\pi}\int \mathrm{d}\vec{R}\mathrm{d}\vec{r}_1\mathrm{d}\vec{r}_2 \mathrm{e}^{-i\vec{k}_{\mathrm{f}}\cdot\vec{R}_{\mathrm{f}}}\phi_{1s}^{\mathrm{A}^*}(\vec{R}-\vec{r}_2)\phi_{1s}^{\mathrm{B}^*}(\vec{R}+\vec{r}_1)\frac{(-1)}{|\vec{r}_2|}$$
$$\times \mathrm{e}^{i\vec{k}_{\mathrm{i}}\cdot\vec{R}'}\phi_{1s}^{\mathrm{A}}(\vec{r}_1)\phi_{1s}^{\mathrm{B}}(\vec{r}_2). \tag{2.9b}$$

The most difficult term is the integral in eq. (2.7b) i.e., the electron–electron correlation with exchange; it contains three completely different coupled terms and two uncoupled terms in a nine-dimensional integral. The total elastic cross-section (σ) is defined as

$$\frac{\mathrm{d}\sigma}{\mathrm{d}\Omega} = \frac{3}{4}\left|f^-\right|^2 + \frac{1}{4}\left|f^+\right|^2 \tag{2.10}$$

and the quenching cross-section (σ_{q}) is defined as

$$\frac{\mathrm{d}\sigma_{\mathrm{q}}}{\mathrm{d}\Omega} = \frac{1}{16}\left|f^- - f^+\right|^2. \tag{2.11}$$

The conversion ratio ($\sigma_{\mathrm{q}}/\sigma$) is a parameter to quantify the fraction of total cross-section transformed into para-Ps that could be measured. To calculate the integrated/total elastic cross-section more accurately, an augmented Born approximation is used. Here the contributions of higher partial waves are replaced by the equivalent first Born term using the formulation

$$\sigma = \sum_l \sigma_l + \sigma^{\mathrm{BO}} - \sum_l \sigma_l^{\mathrm{BO}}, \tag{2.12}$$

if σ_l is the partial cross-section using SEM; σ^{BO} and $\sigma_l^{\mathrm{BO}}$are the total and partial BO cross-sections, respectively.

3. Methodology

A highly efficient computer code is developed using the FORTRAN programming language and numerical analysis. The code calculates the elastic phase shifts and the corresponding cross-sections for both the singlet (+) and the triplet (−) channels. Two sets of coupled one-dimensional integral equation, f_L^+ corresponding to the symmetric space part and f_L^- corresponding to antisymmetric space part are solved parallelly in the same code using the matrix inversion method for each partial wave (L). The pole term in the coupled integral eq. (2.4) is evaluated using the formulation with delta function and principal value parts so that

$$\frac{1}{\vec{k}_n^2 - \vec{k}''^2 + i\varepsilon} = -i\pi\delta(\vec{k}_n^2 - \vec{k}''^2) + \frac{P}{\vec{k}_n^2 - \vec{k}''^2}. \tag{3.1}$$

The principal value integral from zero to infinity has been replaced by

$$\int_0^\infty \mathrm{d}k'' = \int_0^{2k_n} \mathrm{d}k'' + \int_{2k_n}^\infty \mathrm{d}k''. \tag{3.2}$$

Even number of Gaussian points in the interval 0–$2k_n$ are used to avoid the singularity problem at $k'' = k_n$. The Gauss–Legendre quadratures are used to perform two-dimensional integrations in $B^{\pm}$ and the θ integration numerically in the present code. All the integrations converged properly if $k \leq 10$ a.u. The convergence is studied very carefully to integrate over the scattering angle (θ) and the variables in the two-dimensional integrals (X and Y), by varying the number of Gauss–Legendre quadratures. To study the correctness of the partial wave analysis method, the same partial wave analysis is applied to calculate the BO amplitude. It is verified that the BO amplitude obtained by partial wave analysis method and by the non-partial wave method are equal. More partial waves are required to get the converged data at higher energies. To include the contribution of the higher partial waves as accurately as possible in the integrated cross-section, an augmented Born approximation [20–25] is used in the present code. To apply the augmented Born method, we need to compare the SEM amplitude with the corresponding BO amplitude for each partial wave (L). As L increases, the difference between the two decreases gradually. When both are almost equal, only then it can replace the higher partial wave contribution of SEM amplitude by the equivalent BO amplitude. It is possible to get reliable data upto $k \leq 10$ a.u. i.e., the energy $E = 1360$ eV in Ps–Ps scattering using a coupled channel methodology.

To determine the s-wave elastic scattering lengths (a^+ and a^-), the effective range theory that expresses s-wave elastic phase shift (δ_0) as a function of scattering length (a) and projectile energy ($\sim k^2$) so that

$$k \cot \delta_0 = -\frac{1}{a} + \frac{1}{2} r_0 k^2 + O(k^4), \tag{3.3}$$

is useful, when k is the magnitude of the incident momentum in atomic unit and r_0 is the effective range. The incident energy is related to k by the relation $E\,(\text{eV}) = (27.21k^2/2\mu)$. The negative scattering length ($a < 0$), means that there is no possibility of binding in the system. But the positive scattering length ($a > 0$) means that a binding is physically possible; so it indicates the possibility of Feshbach resonances and the BEC formation. A rapid change in phase shift by π radian in a very narrow energy interval is an indication of the presence of a Feshbach resonance [23,24,28]; but the resonance should be reflected in the s-wave partial cross-sections too. So in the present code, the partial cross-sections are derived directly from the real and imaginary parts of the partial amplitudes by avoiding the phase shifts. The presence of a Feshbach resonance indicates a binding in the system. To study resonances, a very large number of mesh points in a very narrow energy interval is necessary. So a good computation facility is required for the purpose.

4. Results and discussion

A new code is developed to study the elastic collision between two ortho-Ps atoms (when both are in ground states) using the *ab-initio* SEM theory. Here the CM frame is used to study the four-body Coulomb problem of equal masses. In the new code, the BO amplitude acts as input to derive the unknown SEM amplitude. All the Coulomb interaction terms in both the direct and exchange channels to derive the BO amplitude are calculated exactly. The theory is useful to include the non-adiabatic short-range effects due to exchange. The detailed data obtained by using the present new code are being reported.

The s-wave elastic phase-shifts of both the total spin-aligned states: $S = 0$ for the singlet $(+)$ and $S = 2$ for the triplet $(-)$ are presented in figure 2 and the corresponding s-wave partial cross-sections are plotted in figure 3 against the incident momenta $k = 0.1-0.6$ a.u. at the energy region below the threshold. These data are compared with the data of Ivanov *et al* [14] in figure 2 and are almost similar to the data reported earlier [13] using similar type of calculation but approximating the electron–electron exchange term. In table 1, the s-, p- and d-wave elastic phase shifts and in table 2, the corresponding s-, p- and d-wave partial cross-sections are presented following the present exact exchange analysis. It should be noted that all the p-wave (odd parity) phase shifts are zero or $\pm\pi$ radian and all the p-wave cross-sections are zero.

In the present new code, when the most difficult electron–electron interaction matrix element is approximated by the positron–positron interaction matrix element, the s- (even parity) and d- (even parity) wave data are exactly the same with the exact exchange analysis data of tables 1 and 2, but all the p-wave (odd parity) data are very different and partial cross-sections are not zero or close to zero. The present s-, p- and d-wave data using the approximate form for the electron–electron exchange term are presented in tables 3 and 4. Comparing the phase-shift data of tables 1 and 3 and partial cross-sections data of tables 2 and 4, it is evident that the approximation to define the electron–electron exchange term introduced a large error to calculate the contribution of the highly important p-wave (odd parity) e.g., the non-spherical orbitals.

In addition, a very large number of energy mesh points in the energy interval 0.13–5.10 eV are used to calculate the s-wave elastic phase shifts and the corresponding cross-sections in search of Feshbach resonances using the exact analysis of exchange,

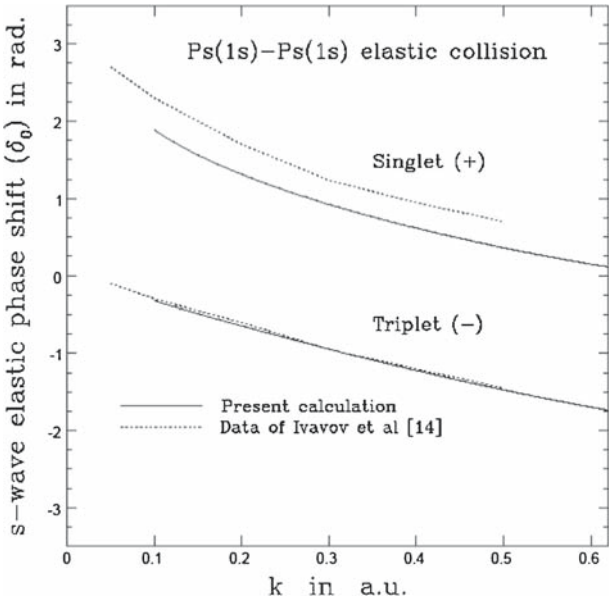

Figure 2. The s-wave elastic phase shifts in radian for both singlet $(+)$ and triplet $(-)$ channels in Ps($1s$)–Ps($1s$) scattering against the incident momentum k in a.u.

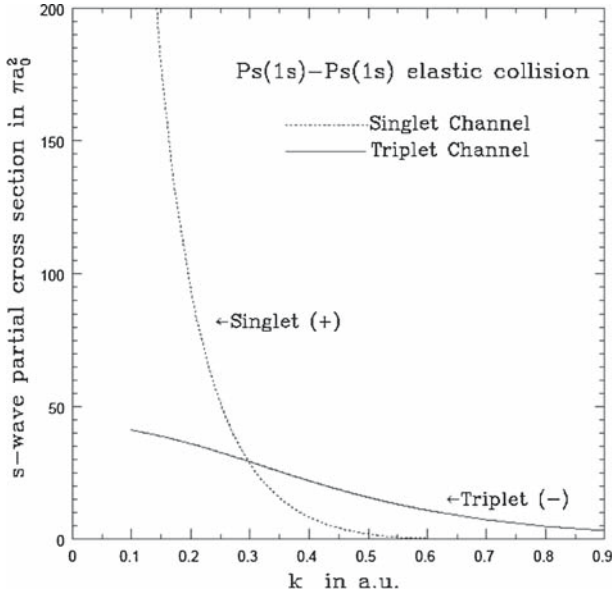

Figure 3. The s-wave elastic cross-sections in πa_0^2 for both singlet (+) and triplet (−) channels in Ps(1s)–Ps(1s) scattering against the incident momentum k in a.u.

but no resonances are found in the system studying both the singlet and triplet partial phase shifts and the corresponding cross-sections.

To get scattering lengths ($a^{\pm}$) for the s-wave elastic collision, k cot δ_0 is plotted against k^2 in figure 4 for both the spin alignment $S = 0$, singlet (+) and $S = 2$, triplet (−) following the effective range theory. In triplet channel, the curve is almost straight line but in singlet channel it is slightly curved. It signifies that the contribution of the higher-order terms ($\sim k^4$) in the effective range theory is negligible in triplet

Table 1. The s-, p- and d-wave phase shifts in radian for both the singlet (+) and triplet (−) channels in Ps(1s)–Ps(1s) elastic scattering.

	Singlet (+) phase shift in radian Ps(1s)–Ps(1s) system			Triplet (–) phase shift in radian Ps(1s)–Ps(1s) system		
k (a.u.)	s-wave	p-wave	d-wave	s-wave	p-wave	d-wave
0.1	1.887	3.142	3.141	−0.325	−3.142	−3.141
0.2	1.313	3.142	3.141	−0.643	−3.142	−3.141
0.3	0.926	3.142	3.138	−0.944	−3.142	−3.137
0.4	0.616	3.142	3.129	−1.222	−3.142	−3.127
0.5	0.359	3.142	3.114	−1.474	−3.142	−3.109
0.6	0.147	3.142	3.095	−1.697	−3.142	−3.085
0.7	3.118	3.142	3.073	−1.892	−3.142	−3.059
0.8	2.986	3.142	3.052	−2.059	−3.142	−3.035
0.9	2.890	3.142	3.035	−2.200	−3.142	−3.017

Table 2. The s-, p- and d-wave cross-sections in πa_0^2 for both the singlet (+) and triplet (−) channels in Ps($1s$)–Ps($1s$) elastic scattering.

	Singlet (+) cross-section in πa_0^2 Ps($1s$)–Ps($1s$) system			Triplet (−) cross-section in πa_0^2 Ps($1s$)–Ps($1s$) system		
k (a.u.)	s-wave	p-wave	d-wave	s-wave	p-wave	d-wave
0.1	361.227	0.000	0.0000	41.016	0.000	0.0000
0.2	93.524	0.000	0.0002	35.966	0.000	0.0002
0.3	28.383	0.000	0.003	29.147	0.000	0.004
0.4	8.350	0.000	0.019	22.081	0.000	0.026
0.5	1.978	0.000	0.059	15.850	0.000	0.083
0.6	0.240	0.000	0.122	10.934	0.000	0.177
0.7	0.044	0.000	0.191	7.349	0.000	0.278
0.8	0.149	0.000	0.248	4.874	0.000	0.351
0.9	0.306	0.000	0.281	3.229	0.000	0.378

($S = 2$) channel but it is not negligible in singlet ($S = 0$) channel. In table 5, the computed scattering lengths and effective ranges are presented for both the singlet and triplet channels. They are again compared with the available data [10,12–15]. Adhikari [12] and Chakraborty *et al* [13] used similar type of coupled channel approach. Adhikari [12] used a model potential to define the exchange effect and Chakraborty *et al* [13] used an approximation to describe the electron–electron exchange term. The present data with exact exchange analysis are very close to the similar data reported in ref. [13]. It may appear that it is possible to approximate the most difficult electron–electron exchange term in Ps($1s$)–Ps($1s$) system by the positron–positron exchange term because both the electron and positron have equal masses and both the Ps atoms are in $1s$ state which is spherically symmetric and the central potential $V(\mathbf{r})$ is used, but the present detailed results made the idea that no approximate method is acceptable even for Ps($1s$)–Ps($1s$) elastic

Table 3. The s-, p- and d-wave phase shifts in radian for both the singlet (+) and triplet (−) channels in Ps($1s$)–Ps($1s$) elastic scattering approximating the electron–electron interaction term.

	Singlet (+) phase shift in radian Ps($1s$)–Ps($1s$) system			Triplet (−) phase shift in radian Ps($1s$)–Ps($1s$) system		
k (a.u.)	s-wave	p-wave	d-wave	s-wave	p-wave	d-wave
0.1	1.887	0.0153	3.141	−0.326	−0.0064	−3.141
0.2	1.313	0.1210	3.141	−0.643	−0.0433	−3.141
0.3	0.926	0.3564	3.138	−0.944	−0.1154	−3.137
0.4	0.616	0.5967	3.129	−1.222	−0.2086	−3.127
0.5	0.359	0.7125	3.114	−1.474	−0.3053	−3.109
0.6	0.147	0.7245	3.095	−1.697	−0.3917	−3.085
0.7	3.118	0.6843	3.073	−1.892	−0.4587	−3.059
0.8	2.986	0.6233	3.052	−2.059	−0.5019	−3.035
0.9	2.890	0.5568	3.035	−2.200	−0.5198	−3.017

scattering. It is again mentioned in an earlier presentation [29] that the use of non-spherical orbitals (e.g., p-states) in the coupled channel method using an approximate form for the electron–electron exchange term would introduce large errors.

In figure 5, the integrated/total elastic cross-section σ using the augmented Born approximation and the quenching cross-section σ_q for the Ps($1s$)–Ps($1s$) elastic scattering are presented in the energy region 0–150 eV. A resonance-like structure – a deep and a peak – appears in the energy region 20–30 eV in both the total elastic and quenching cross-sections in figure 5. In figure 6, the ortho-to-para conversion ratios (σ/σ_q) are plotted

Table 4. The s-, p- and d-wave cross-sections in πa_0^2 for both the singlet (+) and triplet (−) channels in Ps($1s$)–Ps($1s$) elastic scattering approximating the electron–electron interaction term.

	Singlet (+) cross-section in πa_0^2 Ps($1s$)–Ps($1s$) system			Triplet (−) cross-section in πa_0^2 Ps($1s$)–Ps($1s$) system		
k (a.u.)	s-wave	p-wave	d-wave	s-wave	p-wave	d-wave
0.1	361.227	0.282	0.0000	41.016	0.0492	0.0000
0.2	93.524	4.368	0.0002	35.966	0.5620	0.0002
0.3	28.383	16.232	0.003	29.147	1.7692	0.004
0.4	8.350	23.685	0.019	22.081	3.2178	0.026
0.5	1.978	20.513	0.059	15.850	4.3372	0.083
0.6	0.240	14.641	0.122	10.934	4.8572	0.177
0.7	0.044	9.787	0.191	7.349	4.8024	0.278
0.8	0.149	6.389	0.248	4.874	4.3393	0.351
0.9	0.306	4.137	0.281	3.229	3.6558	0.378

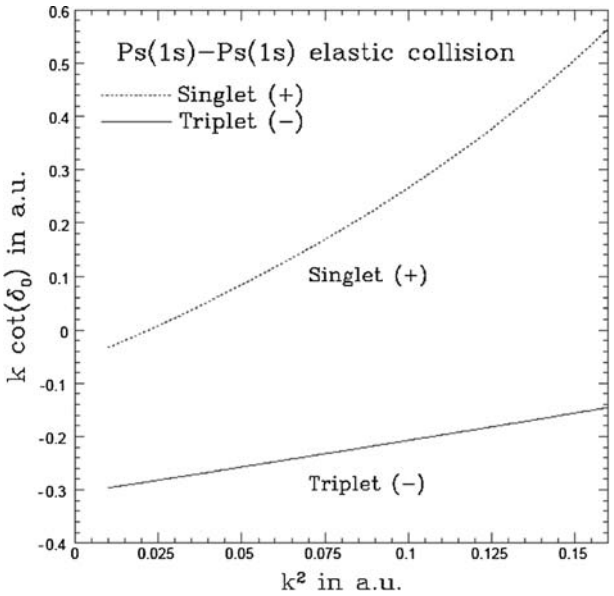

Figure 4. The plot of $k \cot \delta_0$ vs. k^2 in a.u. for both the singlet (+) and triplet (−) spin states of the two system electrons in Ps($1s$)–Ps($1s$) elastic scattering.

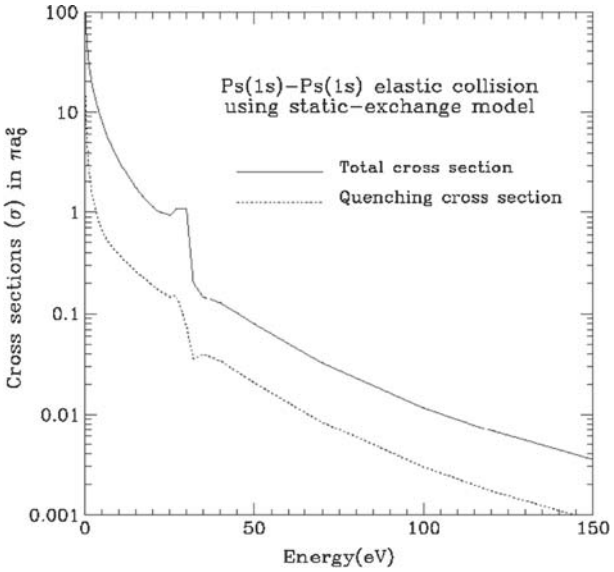

Figure 5. The variation of integrated/total elastic cross-sections and the quenching cross-section in πa_0^2 of Ps($1s$)–Ps($1s$) scattering with energy in eV.

against the incident energy and compared with the Ps–H system. It is evident from the figure that most of the annihilations occur at lower energies (below 50 eV). All the data presented in figures 5 and 6 are completely new and no data are available to compare them.

In addition, the present code is useful not only to study Ps($1s$)–Ps($1s$) collision, but also to study any two hydrogen-like atomic collisions. Using the present code and substituting the values of reduced mass and parameters of the wavefunctions of the Ps($1s$)–H($1s$) system, all the data of Ps($1s$)–H($1s$) elastic collision [20] were reproduced. The SEM is the simplest coupled channel model that includes only the non-adiabatic short-range effects due to exchange but no long-range interaction. In the coupled channel methodology [30], to include the effect of short-range forces, atomic s-states are useful, whereas to include the effect of long-range dipole–dipole van der Waals interaction, atomic p-states are useful [21–23,30]. So, one needs to improve the present code including the excitation and continuum channels by following the coupled channel methodology to get more reliable data at low and cold energies.

Table 5. The computed scattering lengths and ranges in a.u. for both the singlet and triplet spin states of system electrons in Ps($1s$)–Ps($1s$) elastic scattering.

Ps($1s$)–Ps($1s$) collision	Singlet (+)		Triplet (−)	
	Present data	Data of others	Present data	Data of others
Scattering length (a) (a.u.) →	9.35	5.7 [10], 7.46 [12], 10.96 [13], 8.44 [14], 8.26 [15], 9.15 [16]	3.25	1.91 [10], 1.56 [12], 3.28 [13], 3.00 [14], 3.02 [15], 3.0 [16]
Effective range (r_0) (a.u.) →	7.36	7.27 [13]	2.00	1.96 [13]

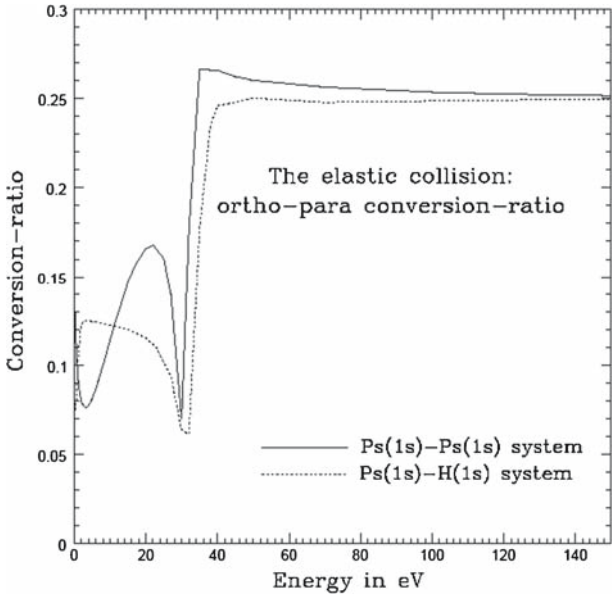

Figure 6. The comparison of the variation of ortho-to-para conversion ratios (σ_q/σ) of Ps($1s$)–Ps($1s$) and Ps($1s$)–H($1s$) systems with energy.

5. Conclusion

In conclusion, an *ab-initio* static exchange model (SEM) with a new computer code using FORTRAN programming language, is developed by following the coupled channel methodology in momentum space to study Ps($1s$)–Ps($1s$) elastic collision by considering the system as a four-body Coulomb problem in the CM frame. Both the spin-aligned $S = 0$, the singlet $(+)$ and $S = 2$, the triplet $(-)$ states are studied. All the Coulomb interaction terms in both the direct and exchange channels are calculated exactly. The present code is again useful to study any two hydrogen-like atomic collisions and the alkali atomic collisions at low and cold energies. The s-, p- and d-wave elastic phase shifts and the corresponding partial cross-sections are reported for the first time using the exact analysis of all the Coulomb interaction terms. The present data are compared with the available s-wave data using similar but approximate methods and are in close agreement. All p-wave (odd parity) phase shifts are $\pm\pi$ and the corresponding cross-sections are zero in the present exact exchange analysis. The integrated/total elastic cross-section (σ), the quenching cross-section (σ_q) and the conversion ratio (σ/σ_q) for the system are reported for the first time. The data indicate the importance of quenching processes at lower energies below 50 eV. Ortho-to-para conversion ratio is a useful quantity that could be measured. In addition, a thorough search is made in search of Feshbach resonances but no resonances are found in the system. Both the scattering lengths are found positive. It is necessary to extend the code for more reliable data including the excitation and continuum channels with exact analysis of all the Coulomb interaction terms.

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