Hyperspherical hidden crossing method applied to Ps(1s)-formation in low energy \(e^+ - H\), \(e^+ - Li\) and \(e^+ - Na\) collisions

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Abstract. The hyperspherical hidden crossing method with the correction term (HHCM\(^{\text{cor}}\)) has been used to calculate partial wave Ps(1s)-formation cross sections for low-energy \(e^+ - H\), \(e^+ - Li\) and \(e^+ - Na\) collisions. The St"uckelberg phase varies in a systematic way as a function of atomic number \(Z\), incident positron momentum \(k_+\), and total orbital angular momentum \(L\) and provides an explanation for the small S-wave cross section for all three systems.

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1. Introduction

The hyperspherical hidden crossing method (HHCM) was developed to treat collisions between three particles of arbitrary charge and mass [1]. The method is an approximation based on the one-Sturmian theory. Although fully quantum mechanical in origin, the expression for the cross sections involve Wentzel–Kramers–Brillouin (WKB) type functions $e^{i \int K(R) dR}$, where $R$ is the hyperradius, $K(R)$ is the wave number, and the integration path is in the complex $R$ plane.

There are a number of advantages to the HHCM. For low energy collisions, in most cases only the physically open channels are included in the calculation of the cross sections. In contrast, close coupling calculations must include a large number of closed channels to achieve convergence. With an insufficient number of channels, pseudoresonances may appear in the cross sections. Because the HHCM was formulated in hyperspherical coordinates, it is ideally suited for collisions involving rearrangement. Calculations which use a basis set centered on the target and on the atom resulting from the rearrangement can result in overcompleteness; this can lead to numerical instability. In the HHCM, a scattering transition $i \rightarrow j$ is mathematically represented as path in the complex plane. By virtue of its relative simplicity, the HHCM can provide important insights into the scattering process—insights that are masked by the complexity of more exact calculation.

In order to improve the accuracy of the cross sections obtained with the HHCM, a correction term was derived from the one-Sturmian theory [2]. The potentials with the correction term agree asymptotically with the close coupling potentials through order $1/R^2$ [3–5]. Including the correction term does not compromise the simplicity of the method; it simply provides an improved value for the wave vector $K(R)$. However, there is one undesirable consequence of using the correction term. The correction term diverges at the branch point, and therefore we include it only on the real axis. As a result, the cross section becomes path dependent. The correction term can be included in a consistent way by following the prescription for the paths given in [6]; we refer to these calculations as HHCM$^{+\text{cor}}$.

The HHCM has previously been applied with success to three-body collisions, including electron excitation [1] and impact ionization [1, 7–12]. Earlier HHCM calculations for Ps(1s) formation in $e^+ - H$ collisions included an asymptotic approximation to the correction term (for the P- and D-waves) and provided an explanation for the small S-wave Ps(1s)-formation cross section in terms of the St"uckelberg phase [2]. The HHCM was also used to treat near-threshold positron impact ionization of hydrogen [13]. The HHCM enables one to understand why the S-wave cross section for any process for $e^+ - H$ collisions (including ionization) that proceeds via the Ps(1s) formation channel is small. Although the HHCM was derived for three-body Coulomb systems, it has been successfully used to study the recombination of three identical bosons with zero range two-body potentials [14]. We previously used the HHCM to calculate partial wave Ps(1s)-formation cross sections for $e^+ - Li$ collisions [15]. Despite the success of these calculations, the application of the HHCM has been somewhat limited.

We have carried out a systematic study of Ps(1s) formation in positron collisions with H, Li and Na using the HHCM$^{+\text{cor}}$. The HHCM$^{+\text{cor}}$ results for $e^+ - H$ and $e^+ - Na$ reported here are new; we also include the previously published HHCM$^{+\text{cor}}$ $e^+ - Li$ results [6] for completeness. We examine the behavior of the St"uckelberg phase as a function of atomic number $Z$, incident positron momentum $k_\perp$, and total orbital angular momentum $L$ for the three atoms with a single $l = 0$ valence electron. For the alkalis, we use a model potential to describe the interaction of the valence electron and the positron with the ion core.
These scattering systems are important in their own right. e\(^+\) – H is a fundamental three-body collision system and is of interest in astrophysics [16–18]. There have been many theoretical calculations of the Ps-formation cross section in e\(^+\) – H collisions. The Kohn variational [19], algebraic coupled state (ACS) [20, 21], hyperspherical close coupling (HSCC) [22–25], close coupling [26–32] and convergent close coupling (CCC) [33, 34] methods have been used to calculate the Ps(1s)-formation cross section in the Ore gap (the energy range where only the elastic and Ps(1s)-formation channels are open). The Ps-formation cross section for e\(^+\) – H collision has been measured [35].

For the alkalis Li and Na, Ps(1s) formation is an exothermic process; there are few examples of simple collision systems in which there are two open channels even at zero incident energy. For e\(^+\) – A collisions, where A is the ground state of Li or Na, one can either use a frozen core Hartree Fock approximation or a model; that is, e\(^+\) – A is treated as an effective three-body collisions. At low energies, accurate Ps(1s)-formation cross sections for e\(^+\) – Li and e\(^+\) – Na have been obtained using Kohn variational [36], close coupling [29, 37, 38], HSCC [39] and the CCC [40, 41] methods. The Ps-formation cross section has been measured for both systems [42].

The paper is organized as follows. In section 2.1, we provide a brief review of the HHCM theory as formulated for three charged particles; in section 2.2, we give the correction term to the HHCM theory and describe how to incorporate the correction term in a consistent way. The application of HHCM and HHCM\(^{\text{corr}}\) to positron–alkali collisions is given in section 2.3. In section 3, we present our results for the partial wave cross section for Ps(1s) formation in e\(^+\) – H, e\(^+\) – Li and e\(^+\) – Na and compare with other calculations and experiment. We discuss our findings regarding the St"uckelberg phase and the insights provided by the HHCM\(^{\text{corr}}\). Concluding remarks are given in section 4. Atomic units are used throughout unless explicitly stated otherwise.

2. Theory and application

2.1. Hyperspherical hidden crossing method (HHCM) for three-body Coulomb systems

The HHCM theory [1] and its application to e\(^+\) – H scattering [2] is described in detail elsewhere. For e\(^+\) – H collisions, the position vector of the electron and positron with respect to the proton are \(\vec{r}_-\) and \(\vec{r}_+\), respectively. The hyperadius is R = \(\sqrt{r^-_+ + r^+_+}\), and the two hyperangles are \(\alpha = \tan^{-1}(r^-_+/r_+)\) and \(\theta = \cos^{-1}(\vec{r}_- \cdot \vec{r}_+)\) [23]. The hyperspherical adiabatic energy eigenvalues \(\epsilon_\mu(R)\) are obtained by solving

\[
\left[\Lambda^2 + 2RC(\alpha, \theta)\right] \varphi_\mu(R; \Omega) = 2\epsilon_\mu(R)R^2\varphi_\mu(R; \Omega),
\]

at fixed \(R\). \(\Lambda^2\) is the grand angular momentum operator, \(C(\alpha, \theta)\) is the reduced potential

\[
C(\alpha, \theta) = -\frac{1}{\sin \alpha} + \frac{1}{\cos \alpha} - \frac{1}{\sqrt{1 - \sin 2\alpha \cos \theta}},
\]

and \(\varphi_\mu(R; \Omega)\) are the hyperspherical adiabatic basis functions, which depend on the two hyperangles and the three Euler angles [23].

The hyperspherical adiabatic functions \(\varphi_\mu(R; \Omega)\) are expanded into states of total orbital angular momentum \(L\). This yields a set of coupled partial differential equations for the unknown expansion coefficients \(f^{(L)}_{\mu, I}(R; \alpha, \theta)\) (which are independent of the Euler angles):

\[
\sum_{J=0}^{L} H^{(L)}_{I, J} f^{(L)}_{\mu, I}(R; \alpha, \theta) = 2R^2 e^{(L)}_{\mu, I}(R) f^{(L)}_{\mu, I}(R; \alpha, \theta), \quad I = 0, 1, \ldots, L.
\]
$H_{i,j}^{(L)}$ are given in [8, 13]. Hereafter, we suppress the superscript $(L)$ for brevity. The eigenvalue $\varepsilon'_\mu(R)$ is related to the hyperspherical adiabatic energy eigenvalue by

$$\varepsilon'_\mu(R) = \varepsilon_\mu(R) + \frac{1}{8R^2}. \quad (4)$$

The corresponding wave vector is

$$K^2_\mu(R) = 2[E - \varepsilon'_\mu(R)], \quad (5)$$

where $E$ is the total energy of the three-body system.

In the energy range where there are only two open channels, it is necessary to calculate the eigenvalues $\varepsilon'_\mu(R)$ associated with the two levels $\mu = i, j$, where $\varepsilon'_\mu(R) < \varepsilon'_j(R)$. For hydrogen, $\mu = i$ corresponds $\varepsilon^i + H$ and $\mu = j$ corresponds to $Ps(1s) + H^+$. We solve the coupled equations given in equation (3) for $2R^2\varepsilon'_\mu(R)$ and $f_{\mu,i}(R; \theta, \phi)$, $\mu = i, j$ using the finite element method [43–45]. It is computationally intensive to solve a complex generalized eigenvalue problem for thousands of values of $R$. In order to maximize efficiency, we use Rayleigh quotient iteration [43]. We start at $R = 0$, where $2R^2\varepsilon'_\mu(R)$ and $f_{\mu,i}(R; \theta, \phi)$ corresponding to the levels $\mu = i, j$ are known analytically [46]. We then increase $R$ in small increments along the real axis, using the previous values of $2R^2\varepsilon'_\mu(R)$ and $f_{\mu,i}(R; \theta, \phi)$ as an initial guess for the new eigenpair. Since the energy levels are degenerate at $R = 0$, using the eigenvector as well as the eigenvalue is essential in order to split the degeneracies.

Once we have obtained $2R^2\varepsilon'_\mu(R)$ and $f_{\mu,i}(R; \theta, \phi)$ on the real axis, we search for the branch point on the Riemann surface $\varepsilon'(R)$. The designation $\mu = i, j$ is only meaningful on the real axis. Beginning at some point on the real axis and using the computed value of $2R^2\varepsilon'_\mu(R)$ and $f_{\mu,i}(R; \theta, \phi)$, we solve equation (3) along the perimeter of a large square in the complex plane using the same iterative technique to track $2R^2\varepsilon'(R)$. If the square includes the branch point between the two levels $i$ and $j$, $\varepsilon'(R) = \varepsilon'_j(R)$ upon returning to the starting point on the real axis. By systematically subdividing the square, we can locate the branch point to the desired accuracy.

In the HHCM formulation, the cross section for a transition between levels $i$ and $j$ is obtained by summing WKB-like functions $e^{i\int K(R) dR}$ over the two paths in the complex $R$ plane that lead to the transition [1]. The classical turning points on the two levels, $R_i^0$ and $R_j^0$, are defined by $\varepsilon'_\mu(R_i^0) = E$, $\mu = i, j$. For the first path, we integrate in from infinity to a point $R_i^0 \leq R_i^j$ along the real axis, using the negative branch of the wave vector $K_i(R)$; we then integrate clockwise around the branch point $R_b$ in the upper half plane, and back out to infinity using the positive branch of $K_j(R)$. For the second path, we integrate in from infinity on the negative branch of $K_i(R)$, enclose $R_b^c$ clockwise in the lower half plane, continue inward on the real axis to a point $R_j^0 \leq R_j^i$, and then integrate back out to infinity using the positive branch of $K_j(R)$. The branch cuts for $K_\mu(R)$ are chosen from $R_i^\mu$ to infinity.

The modulus square of the sum of the WKB-like functions over the two paths is

$$|e^{i\int_{path_1} K(R) dR} + e^{i\int_{path_2} K(R) dR}|^2 = 4P^L_{ij} \cos^2 \Delta^L_{ij}, \quad (6)$$

where $P^L_{ij}$ is the one-way transition probability,

$$P^L_{ij} = \exp \left[-2 \text{Im} \int_c K(R) dR \right] \quad (7)$$
and $\Delta_{ij}^L$ is the Stückelberg phase

$$\Delta_{ij}^L = \text{Re} \int_c K(R) \, dR$$

[2, 6, 15]. (The superscript $L$ on $K(R)$ has been suppressed.) The contour $c$ that appears in equations (9) and (10) starts at $R'_i$, goes clockwise around $R_b$, and ends at $R'_j$. The value for the transition probability and the Stückelberg phase are independent of the details of the contour.

The HHCM cross section for Ps(1s) formation (in units of $\pi a_0^2$) is given by

$$\sigma_{Ps}^L = \frac{(2L + 1)}{k^2} |\tilde{S}_{ij}^L|^2,$$  \hspace{1cm} (9)

where $k$ is the incident positron momentum and

$$|\tilde{S}_{ij}^L|^2 = 4 P_{ij}^L (1 - P_{ij}^L) \sin^2 \Delta_{ij}^L$$  \hspace{1cm} (10)

[2, 6, 15]. $\tilde{S}_{ij}^L$ is the S-matrix element for a transition between levels $i$ and $j$.

2.2. Correction term to HHCM

The HHCM is an approximation based on the one-Sturmian theory [1]. Within the framework of the one-Sturmian theory, one can derive a correction term when $\epsilon'_\mu(R)$ is a slowly varying function of $R$, such as for large real $R$ [2]. The correction term includes the Langer factor and the usual diagonal non-adiabatic matrix element. The eigenvalue and the wave vector including the correction term are

$$\tilde{\epsilon}'_{\mu}(R) = \epsilon'_\mu(R) - \frac{1}{8R^2} - \frac{1}{2} \left\langle \varphi_{\mu} \left| \frac{\partial^2 \varphi_{\mu}}{\partial R^2} \right| \right\rangle$$

(11)

and

$$\tilde{K}_{\mu}^2(R) = 2[E - \tilde{\epsilon}'_{\mu}(R)].$$

The classical turning points are now given by $\tilde{\epsilon}'_{\mu}(\tilde{R}_\mu') = E, \mu = i, j$. Using the correction term for large real $R$ improves the HHCM approximation, and in general lowers the partial wave cross sections. We chose not to use the correction term anywhere in the complex plane because it diverges at the branch points. In figure 1(a), we show the eigenvalues for the two channels $e^+ - \text{H}$ and Ps(1s) + $\text{H}^+$. For hydrogen, there are no avoided crossings for level $i$ or $j$. In table 1 we give the branch points $R_b$ for $0 \leq L \leq 3$ and the classical turning points $\tilde{R}_i'$, $\mu = i, j$. (The value quoted for $R_b$ is the center of a square which contains the branch point and whose sides are 0.10.)

There is a very slight barrier in the potential curve for $\tilde{\epsilon}'_j(R), L = 1$ (figure 1(b)), which effects only the near-threshold region for Ps(1s) formation. At the lowest incident positron momentum we considered ($k_e = 0.712$), there are two additional classical turning points $\tilde{R}_j' = 11.8$ and 13.6 that are associated with the barrier. We considered the transmission through the barrier and over the barrier using the analysis in [2]; the barrier is approximated by an inverted harmonic oscillator potential.

While it is desirable to use equation (12) for real $R$, the drawback is that the cross section becomes path dependent. Previously, we developed a procedure for choosing the two paths so that the correction term is treated in a consistent way for both levels associated with the
transition [6]. For the first path, we come in from infinity on the real axis to the point \( \tilde{R}_i \) using \( \tilde{K}_i (R) \); we encircle \( R_b \) clockwise using \( K (R) \), and return to \( \tilde{R}_i \); we then go back out to infinity on the real axis using \( \tilde{K}_j (R) \). We deform the contour integral of \( \tilde{K} (R) \) to ensure that only the branch point connecting levels \( i \) and \( j \) is encircled. The second path is similar except that we encircle \( R^*_b \). In figure 2, we show the two paths (including the deformation) on the Reimann surface \( \varepsilon' (R) \) for \( L = 0 \). We refer to calculations which include the correction term as HHCM+cor.

One of the attractive features of this approach for including the correction term is that there is no appreciable change, if any, in the Stöckelberg phase. This is important because one of the main advantages of the HHCM method is that the Stöckelberg phase can provide valuable information about scattering process. The correction term tends to lower the one-way transition probability \( P^{L}_{ij} \) and the Ps(1s)-formation cross section.

2.3. HHCM and HHCM+cor for positron–alkali collisions

Although the HHCM was formally derived for three charged particles [1], it can be used to treat effective three-body collision systems. We present below the application of the HHCM and the HHCM+cor to \( e^+ - A \) collisions, where \( A \) is the ground state of Li [6, 15] or Na.
We treat the incoming positron $e^+$, the valence electron $e^-$, and the positive ion core $A^+$ as an effective three-body Coulomb system. $\vec{r}_+$ and $\vec{r}_-$ now represent the position vector of the positron and electron with respect to the core.

We use the Peach model potential \[47, 48\] to describe the electron–ion and positron–ion interaction,

$$V_{e^+ - A^+} = \pm \frac{1}{r_\pm} \left( \frac{Z - 1}{r_\pm} \right) e^{-\gamma r_\pm} \left[ 1 + \delta r_\pm + \delta' r_\pm^2 \right] - \frac{\alpha_d}{2r_\pm^3} \omega_2(\beta r_\pm) - \frac{\alpha'_d}{2r_\pm^3} \omega_3(\beta' r_\pm),$$

(13)

$\omega_n(x)$ is a cutoff function and the quadrupole term was included only for Na. $\alpha_d$ is the static dipole polarizability \[49, 50\] and the other parameters given \[47, 48\] were optimized to reproduce the observed energy levels. Any model potential which gives the correct nodal structure for the physical ground state, by necessity has spurious low-lying energy levels. The potential curves corresponding to these spurious levels were ignored in the HHCM$^{\text{cor}}$ calculation. The electron–positron interaction includes terms analogous to the dielectronic correction,

$$V_{e^+ - e^-} = \frac{1}{|\vec{r}_+ - \vec{r}_-|} + \frac{\alpha_d}{2r_+^3r_-^3} \cos \theta \sqrt{\omega_2(\beta r_+)\omega_2(\beta r_-)} + \frac{\alpha'_d}{2r_+^3r_-^3} \left( 3 \cos^2 \theta - 1 \right) \sqrt{\omega_3(\beta' r_+)\omega_3(\beta' r_-)}. $$

(14)

(For lithium $\alpha'_d = 0$.) We verified the accuracy of the interactions given in equations (13) and (14) by calculating the binding energy of the weakly bound effective three-body systems, $e^+\text{Li}$ \[51\] and $e^+\text{Na}$ \[52\].

The reduced potential for the positron-alkali system used in the HHCM$^{\text{cor}}$ calculations,

$$C(R; \theta, \phi) = R \left[ V_{e^+ - A^+}(R; \theta, \phi) + V_{e^+ - A^+}(R; \theta, \phi) + V_{e^+ - e^-}(R; \theta, \phi) \right]$$

(15)

depends on the parameter $R$.
Ps(1s) formation is an exothermic reaction for ground state lithium Li(2s) and sodium Na(3s); that is, the channel $\text{Ps}(1s) + A^+(\mu = i)$ lies energetically below the incident channel $e^+ − A(\mu = j)$. For the alkali atoms, we calculate the transition probability and St"uckelberg phase for the transition $\text{Ps}(1s) + A^+ \rightarrow e^+ + A$. However, we can exploit the symmetry of the S-matrix ($|\tilde{S}_{Li}^{\mu}|^2 = |\tilde{S}_{ji}^{\mu}|^2$) to compute the Ps(1s)-formation cross section according to equation (9).

In figure 3(a), we show the potential curves $\tilde{\varepsilon}_\mu(R)$ for $e^+ + \text{Na}$. Unlike hydrogen, there are avoided crossings for levels $i$ and $j$, and between $i$ and $j$. The diagonal non-adiabatic matrix element in the correction term is large at the avoided crossings and $\tilde{\varepsilon}_\mu(R)$ can have a sharp peak in the vicinity of the crossing. In figure 3(b), we show the behavior of $\varepsilon'_\mu(R)$ and $\tilde{\varepsilon}'_\mu(R)$ for Na ($L = 3$) near an avoided crossing $R_{i}^{\text{ac}} = R_{j}^{\text{ac}} = 0.985$. For the paths that were used in the calculation, the value of $\tilde{R}'_\mu$ is always greater than the value of $R$ at the avoided crossings. In table 2, we give the values for the branch points $R_b$ and the classical turning points $\tilde{R}'_\mu$, $\mu = i, j$.

![Figure 3](http://www.njp.org/)

**Figure 3.** (a) Potential curves $\tilde{\varepsilon}_\mu(R)$ for $\text{Ps}(1s) + \text{Na}^+ (\mu = i)$ and $e^+ + \text{Na}(3s)(\mu = j)$. The horizontal lines indicate the energy range corresponding to $0.04 \leq k_+ \leq 0.393$. (b) $\varepsilon'_\mu(R)$ and $\tilde{\varepsilon}'_\mu(R)$ for the $L = 3$ near the avoided crossing between levels $i$ and $j$ at $R_{i}^{\text{ac}} = R_{j}^{\text{ac}} = 0.985$.

### 3. Results

The HHCM$^{\text{cor}}$ was used to calculate the lowest four partial wave Ps(1s)-formation cross sections for low-energy positron collisions with H, Li and Na. We present results in the energy range where there are only two open channels, elastic scattering and Ps(1s) formation. We also discuss the behavior of the St"uckelberg phase as a function of atomic number $Z$, incident positron momentum $k_+$, and the total orbital angular momentum $L$. We compare the HHCM$^{\text{cor}}$ cross sections with the results from other theoretical calculations and with the experimental measurements.
Table 2. The branch points $R_b$ associated with the two levels $Ps(1s) + A^+(\mu = i)$ and $e^+ + A (\mu = j)$, and the classical turning points $\tilde{R}_f^L$ for $0.05 \leq k_+^L \leq 0.368$ and $0.04 \leq k_+^{Na} \leq 0.393$.

| $A$ | $L$ | $R_b$ | $\tilde{R}_f^L$ | $\tilde{R}_f^j$ |
|-----|-----|-------|----------------|----------------|
| Li  | 0   | 10.90 + i4.70 | 3.51 - 3.12 | 12.5 - 7.45 |
|     | 1   | 10.90 + i4.70 | 4.34 - 3.74 | 27.0 - 8.25 |
|     | 2   | 10.80 + i4.80 | 6.21 - 4.89 | 48.9 - 9.00 |
|     | 3   | 10.65 + i5.00 | 10.1 - 6.67 | 70.0 - 10.5 |
| Na  | 0   | 10.65 + i4.85 | 3.96 - 3.50 | 12.7 - 7.15 |
|     | 1   | 10.65 + i5.05 | 4.67 - 4.01 | 39.8 - 7.73 |
|     | 2   | 10.55 + i5.15 | 6.27 - 4.99 | 65.2 - 8.59 |
|     | 3   | 10.45 + i5.35 | 9.27 - 6.46 | 90.9 - 10.0 |

Figure 4. (a) HHCM$^{cor}$ $Ps(1s)$ formation partial wave cross sections for $e^+ - H$ are compared with the HSCC and ACS results. (b) HHCM$^{cor}$ $Ps(1s)$-formation cross section (summed over the lowest for partial waves) is compared with the HSCC, ACS and CCC total $Ps(1s)$-formation cross sections and experimental measurements.

3.1. HHCM$^{cor}$ $Ps(1s)$-formation cross sections

In figure 4(a) we show the HHCM$^{cor}$ partial wave cross sections $\sigma_{Ps}^L$, $L = 0, 1, 2, 3$ for $e^+ - H$ with incident positron momentum $0.712 \leq k_+ \leq 0.866$, which is in the Ore gap. For comparison, we also give the results of the HSCC [22] and the enlarged eight state (E8S) ACS calculations. The S-wave cross section is nearly zero over the entire energy range for all three calculations. There is reasonable agreement between the HHCM$^{cor}$ and the HSCC and ACS calculations for $L \geq 1$. In figure 4(b), we show the HHCM$^{cor}$ cross section (summed over the lowest four partial waves) as a function of the incident positron energy $E_+$ (in eV). On the same figure,
Figure 5. (a) HHCM$^{\text{cor}}$ Ps(1s) formation partial wave cross sections for $e^+ - \text{Li}$ are compared with the HSCC and CCA results. (b) HHCM$^{\text{cor}}$ and HSCC Ps(1s)-formation cross sections (summed over the lowest for partial waves) are compared with the HSCC and CCC total Ps(1s)-formation cross sections and experimental measurements.

we show the HSCC [22], the ACS [20] and the CCC [34] total Ps(1s)-formation cross sections. The ACS cross section, summed over the first four partial waves (not shown), is nearly identical to the ACS total Ps(1s)-formation cross section, indicating that the contribution from the partial waves for $L \geq 4$ is relatively small. The HHCM$^{\text{cor}}$ cross section is in good agreement with the other calculations, and all four calculations are consistent with the experimental results [35], although the measurement at the lowest energy (7 eV) is higher than the theoretical predictions.

In figures 5(a) and (b), we show similar results for $e^+ - \text{Li}$ collisions, with incident momentum $0.05 \leq k_+ \leq 0.368$. The partial wave cross sections are compared with a HSCC calculation [39] and an 14-state close coupling approximation (CCA) calculation [37]. As in the case of hydrogen, the S-wave cross section is very small away from the threshold region. (The S-wave cross section for the alkali atoms is infinite right at threshold because Ps(1s) formation is exothermic.) All three calculations are in reasonable agreement for P-wave and D-wave, except that the CCA $\sigma_{p_3}^2$ has a resonant structure. The HHCM$^{\text{cor}}$ $\sigma_{p_3}^3$ appears to be too large, relative to the HSCC. This overestimation of $\sigma_{p_3}^3$ may due to the fact that $R_i$ is large for this case, which means that the effect of the correction term is diminished. In figure 5(b) we compare the HHCM$^{\text{cor}}$ and HSCC cross sections, both summed over the lowest four partial waves. On the same figure, we show the HSCC and the CCC [40] total Ps(1s)-formation cross sections; also shown are the experimental measurements [41], which are the lower bounds to the cross section. In the case of $e^+ + \text{Li}$, the HSCC results suggest that the higher partial waves ($L \geq 4$) make a significant contribution to the total Ps(1s)-formation cross section.

The HHCM$^{\text{cor}}$ results for $e^+ + \text{Na}$ are shown in figures 6(a) and (b) for the incident positron momentum range $0.04 \leq k_+ \leq 0.393$. In figure 6(a), we compare the HHCM$^{\text{cor}}$ and the HSCC [39] partial wave ($0 \leq L \leq 3$) Ps(1s)-formation cross sections. Again, the S-wave

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cross section is nearly zero away from threshold. The HHCM^{cor} overestimates the $L = 3$ partial wave contribution at higher energies. In figure 6(b), we compare the HHCM^{cor} and HSCC cross section, summed over the lowest four partial waves; also shown are the HSCC and CCC total Ps(1s)-formation cross sections. All three calculations are in very good agreement near threshold. Although the experimental measurement [42] of the Ps(1s)-formation cross section at 1.81 eV is in reasonable agreement with the theory, the results at lower energy increase in magnitude, while all three theoretical calculations predict a dramatic decrease in the cross section near threshold. The surprisingly good agreement between the HHCM^{cor} and the HSCC calculations is a fortuitous combination of the large HHCM^{cor} $L = 3$ partial wave cross section and the neglect of the contribution from higher partial waves.

3.2. Stückelberg phase

One of the most useful outcomes of the HHCM calculations is the insight that the method can provide about the scattering mechanism. For all three atoms, the S-wave cross section for Ps(1s) formation is extremely small away from threshold. This can be understood in terms of the Stückelberg phase $\Delta^{ij}_L$ (equation (8)). In figure 7, we show a plot of $\Delta^{ij}_L$ for H, Li and Na for the lowest four partial waves. For all three atoms, the phase is close to $\pi$ for $L = 0$, despite the fact that the branch points and classical turning points for the two alkali atoms are quite different from those for hydrogen (see tables 1 and 2). The phase of $\pi$ means that the two amplitudes corresponding to the different paths leading to Ps(1s) formation interfere destructively. This finding supports an earlier prediction that for the $L = 0$ rearrangement transition from the ground S-state of one atom to the ground S-state of a different atom, the Stückelberg phase

Figure 6. HHCM^{cor} Ps(1s) formation partial wave cross sections for e$^+ − $Na are compared with the HSCC results. (b) HHCM^{cor} and HSCC Ps(1s)-formation cross sections (summed over the lowest for partial waves) are compared with the HSCC and CCC total Ps(1s)-formation cross sections and experimental measurements.
Figure 7. The St"uckelberg phase $\Delta_{ij}^L$ ($0 \leq L \leq 3$) for $e^+ - H$, $e^+ - Li$ and $e^+ - Na$.

should be nearly an integer multiple of $\pi$ [53]. Ostrovsky [54] found that for the transition $d\mu(1s) + t \to d + t\mu(1s)$, the St"uckelberg phase $\Delta_{ij}^0 \approx 2\pi$.

For hydrogen, the St"uckelberg phase varies slowly as a function of $k_+$ and decreases from $\pi$ to $\frac{1}{2}\pi$ with increasing $L$. For $L = 2$, the phase is close to $\frac{1}{2}\pi$ and the amplitudes corresponding to the two paths interfere constructively. The cross section $\sigma_{Ps}^2$ is relatively large away from the threshold region. One can also predict from figure 7 that the next few partial waves will have a small phase. For the alkalis, the St"uckelberg phase for $L = 2$ and $L = 3$ is close to $\frac{1}{2}\pi$ and the corresponding partial wave cross sections are relatively large away from the threshold region. A St"uckelberg phase $\Delta_{ij}^L$ close to $\frac{1}{2}\pi$ is not a guarantee that the cross section will be large.

4. Conclusion

The accuracy of the HHCM$^{\text{cor}}$ Ps(1s)-formation cross sections is quite remarkable given the fact that the HHCM$^{\text{cor}}$ is an approximate theory which only includes the two channels involved in the transition. The HSCC, CCC, CCA and ACS calculations, which are based on more exact theories, include a much larger number of channels. The HHCM$^{\text{cor}}$ also provides an explanation for the small S-wave Ps(1s)-formation cross section in terms of the St"uckelberg phase for all three systems.

The HHCM was derived only for three charged particles [1]. The HHCM results for the recombination of three identical bosons indicate that the method can be extended to non-Coulomb systems [14]. The calculation of the HHCM$^{\text{cor}}$ Ps(1s)-formation cross section for positron–alkali atom collisions shows that the method can also be used to treat effective
three-body Coulomb systems. This suggests that the applicability of the HHCM is not limited to three charged particles.

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