# Unified Treatment of Positron Annihilation and Positronium Formation

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The effects of the positron ($e^+$) annihilation in $e^+$ scattering by the H atom are included directly in the Hamiltonian as an absorption potential, and hence the finite lifetimes $\Gamma_{ns}$ of positronium (Ps) in states $ns$ are automatically taken account of. The Schrödinger equation is solved using the hyperspherical close-coupling method. The annihilation and Ps formation are shown to be inseparable near the Ps($1s$) threshold $E_{\rm th}$; Ps formation constitutes just an indirect pathway to annihilation. The annihilation cross section, which would diverge near $E_{\rm th}$ if $\Gamma_{1s}$ were infinite, connects smoothly across $E_{\rm th}$ to the cross section for Ps formation, which is meaningful only at energies well above $E_{\rm th}$.

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A positron ($e^+$) colliding with an atom or a molecule may excite or ionize the target if the collision energy $E$ is high enough. If $e^+$ shares a common space with any of the target electrons ($e^-$) during the collision, the $e^+$-$e^-$ pair may annihilate and emit two or three $\gamma$-ray photons [1]. The positron may capture an electron forming an $e^+$-$e^-$ bound system called positronium (Ps) in a hydrogenlike state $(n, l)$ if $E$ exceeds a threshold $E_{\rm th}(n)$ $[= I - (6.8/n^2)$ eV, where $I$ is the ionization potential of the target]. This Ps eventually annihilates $\sim 10^{-10}$ s or longer after its formation in the same manner as the annihilation in the direct collision. The collision time under most experimental conditions is much shorter; $e^+$ with $E > 1$ eV can traverse a distance of 1 a.u. in $< 10^{-16}$ s. At any $E < E_{\rm th}(1s)$, Ps may still be formed virtually, or in a closed channel, and may annihilate. The virtual formation of Ps should be distinguished from the temporary formation of a resonance state of Ps bound by the residual ion near a particular energy $E \simeq E_{\rm res}$, and also from the formation of a virtual state, which has a small negative energy like a weakly bound state but has a wave function growing exponentially asymptotically.

The three kinds of channels, i.e., the direct (elastic and inelastic) channels, the quantum electrodynamical annihilation channel, and the Ps channels all couple and should be treated on equal footing, in principle. The annihilation cross section $\sigma_{\rm an}$, however, is usually much smaller than the elastic cross section. Also, annihilation occurs only if the $e^+$-$e^-$ distance $r$ vanishes. This allows a much simpler method of first obtaining the scattering wave function $\Psi$ (normalized to unit flux of the incident $e^+$) by neglecting annihilation, and then $\sigma_{\rm an}$ by [2]

$$\sigma_{\rm an} = (c/v)\pi r_0^2 Z_{\rm eff} = (c/v)\pi r_0^2 \langle \Psi \mid \delta(r) \mid \Psi \rangle. \quad (1)$$

Here, $r_0$ ($= e^2/m_e c^2$) is the classical electron radius, $c$ the velocity of light, $v$ the initial $e^+$ velocity, and $Z_{\rm eff}$, defined by the first equality, represents an effective number of target electrons contributing to annihilation.

Equation (1) is known to increase sharply and diverge as $E$ approaches $E_{\rm th}(1s)$ from below (Fig. 1). This was postulated by Laricchia and Wilkin [3] on the basis of their model annihilation rate. Indeed, Van Reeth and Humberston [4] confirmed this threshold divergence by

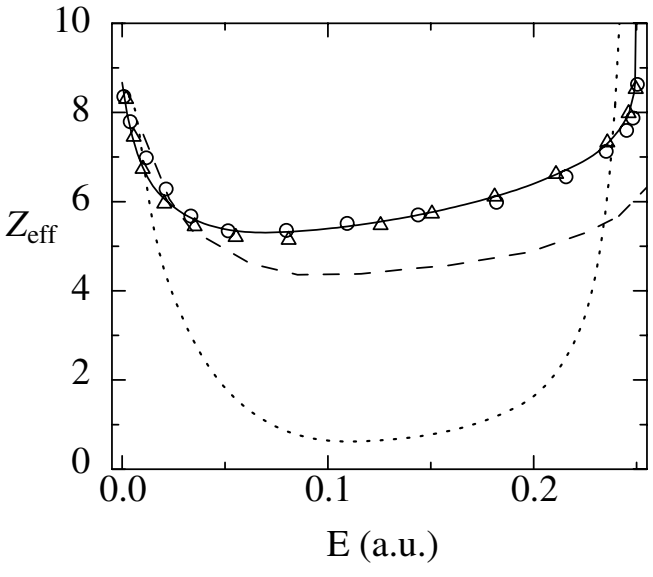


FIG. 1. The effective number $Z_{\rm eff}$ of electrons for annihilation in $e^+(E)$ + H($1s$) collisions below the Ps($1s$) threshold $E_{\rm th}(1s)$ ($= 6.8$ eV) calculated using Eq. (1). Solid curve: present HSCC calculation. Dotted curve: Laricchia and Wilkin [3]. ○: Van Reeth and Humberston [4]. △: Ryzhikh and Mitroy [5]. Dashed curve: Yamanaka and Kino [6].

  

detailed variational calculations for the $e^+ + \mathrm{H}$ collisions, though their results are grossly different from the Laricchia-Wilkin model. Ryzhikh and Mitroy [5] found that Eq. (1) they calculated using the momentum-space Lippmann-Schwinger equation lies within a few % difference from the result of Ref. [4] over the entire energy region. In particular, their results also show a sharp divergence toward $E_{\mathrm{th}}(1s)$. An application of the $S$-wave threshold law to Eq. (1) leads to the divergence as $(-\epsilon)^{-1/2}$ [7], where $\epsilon \equiv E - E_{\mathrm{th}}(1s)$, instead of the more rapid divergence as $(-\epsilon)^{-1}$ expected by Laricchia and Wilkin. The recent time-dependent close-coupling calculation by Yamanaka and Kino [6] fails to reproduce this remarkable threshold increase.

Variational calculations by Humberston *et al.* [8] reproduced the sharp threshold rise $\sim\epsilon^{1/2}$ of the Ps-formation cross section $\sigma_{\mathrm{Ps}}$ as predicted by the $S$-wave Wigner law [9]. However, the threshold is in fact blurred by the energy width $\Gamma(1s)$ ($= 5.29 \times 10^{-6}$ eV) of Ps($1s$), due mainly to the two-$\gamma$ annihilation lifetime $\tau(1s) = \hbar/\Gamma(1s)$. Hence, the Wigner law should be modified accordingly; see Refs. [10,11]. Gribakin and Ludlow [7] showed that this modification leads to the absence of any threshold divergence of $\sigma_{\mathrm{an}}$ or the threshold rise of $\sigma_{\mathrm{Ps}}$; they connect smoothly from one to the other across $E_{\mathrm{th}}(1s)$.

The analytic formulas due to the Wigner law and to its modification for decaying states as discussed in Ref. [7] are valid only very close to the threshold. Since the energy region of validity of these formulas is unknown, accurate numerical studies including the effects of the finite Ps lifetime would be highly desirable to elucidate the physics underlying the threshold behavior and to verify the modified threshold law. This modified law stems from the breakdown of approximation (1) for $\sigma_{\mathrm{an}}$ or $Z_{\mathrm{eff}}$ because of the great change in $\Psi$ due to annihilation near $E_{\mathrm{th}}$, or because of the extremely long collision time near $E_{\mathrm{th}}$, within which annihilation occurs considerably. We made a rigorous study of annihilation and Ps formation in $e^+$ impact on the H atom including the effects of the annihilation channel directly in the Hamiltonian. An accurate close-coupling calculation was achieved using the hyperspherical coordinates. It is clearly demonstrated that annihilation and Ps formation are inseparable near $E_{\mathrm{th}}(1s)$ and are describable in a unified manner.

The effects of the annihilation channel on the other channels may be described by an absorption potential

$$H' = -2ic\pi r_0^2 \delta(r) = -2i\pi r_0^{3/2}\delta(r) \tag{2}$$

in atomic units [12], which are used in the following. This potential reproduces the width $\Gamma(1s)$ for two-photon or two-$\gamma$ annihilation of para-Ps($1s$) as the first-order perturbation energy of the Ps($1s$) wave function $\psi_{\mathrm{Ps}}(\mathbf{r})$:

$$\langle \psi_{\mathrm{Ps}} | H' | \psi_{\mathrm{Ps}} \rangle = -ir_0^{3/2}/4 = -i\Gamma/2. \tag{3}$$

The width for the three-$\gamma$ annihilation of ortho-Ps($1s$) is much narrower and is negligible. This $H'$ reproduces the width of any state Ps($ns$) and also causes direct-collision annihilation properly. The Hamiltonian $H$ is the sum of $H'$ and the Coulomb three-body Hamiltonian $H_0$:

$$H = H_0 + H'. \tag{4}$$

The hyperspherical close-coupling (HSCC) method has been extensively used for $e^-$ and $e^+$ collisions with hydrogenlike atoms, photoionization of He-like atoms, and other three-body and four-body dynamics [13,14], and has been successful in observing new phenomena and in providing rationales of underlying physics. Here we apply this method to the $e^+$-H system. Let $\mathbf{r}_1$ be the position vector of $e^+$ relative to the proton $p$ and $\mathbf{r}_2$ be that of $e^-$, and hence $\mathbf{r} = \mathbf{r}_1 - \mathbf{r}_2$. The hyperradius $\rho$ is defined by $\rho^2 = r_1^2 + r_2^2$. The six-dimensional coordinate system $(\mathbf{r}_1, \mathbf{r}_2)$ is replaced by the set of hyperspherical coordinates $(\rho, \Omega)$ with a five-dimensional angular coordinate $\Omega$. The Hamiltonian $H_0$ in these coordinates reads as

$$H_0 = -\frac{1}{2}\left[\frac{d^2}{d\rho^2} + \frac{5}{\rho}\frac{d}{d\rho}\right] + h_{\mathrm{ad}}(\rho;\Omega), \tag{5}$$

with the adiabatic Hamiltonian

$$h_{\mathrm{ad}}(\rho;\Omega) = \frac{\Lambda^2(\Omega)}{2\rho^2} + V(\rho;\Omega), \tag{6}$$

which is $H_0$ for fixed $\rho$. Here, $\Lambda$ is the grand angular momentum operator [13,14], and $V(\rho;\Omega)$ is the sum of the two-body Coulomb potentials. The adiabatic channel functions $\{\varphi_i\}$ are defined by the eigenvalue equation

$$h_{\mathrm{ad}}(\rho;\Omega)\varphi_i(\rho;\Omega) = U_i(\rho)\varphi_i(\rho;\Omega), \tag{7}$$

where $\rho$ is treated as the adiabatic parameter. It becomes large when either the $e^+$-H or the Ps-$p$ distance becomes large. Thus each eigenvalue $U_i$ approaches a bound-state energy of either H or Ps as $\rho \to \infty$. For diagonalizing $h_{\mathrm{ad}}$, we used variationally optimized Slater-type orbitals (STOs), i.e., $21s$, $17p$, and $13d$ STOs centered on $e^+$, and $21s$, $17p$, $13d$, and $9f$ STOs on $p$. The accuracy of $U_i$ is better than ten (six) digits at large (smaller) values of $\rho$.

The total wave function $\Psi(\rho;\Omega)$ is expanded as

$$\Psi(\rho;\Omega) = \sum F_i(\rho)\varphi_i(\rho;\Omega) \tag{8}$$

in terms of the functions $\{\varphi_i(\rho;\Omega)\}$. The HSCC equations for the complex functions $\{F_i(\rho)\}$ derived from this expansion have both the nonadiabatic coupling matrix and a pure imaginary coupling matrix resulting from $H'$. The coupled equations are solved up to a large value of $\rho$ (3000 in this work), where the solutions are projected onto the asymptotic form in the Jacobi coordinates satisfying the scattering boundary conditions. The scattering

matrix thus obtained represents the flux loss due to $H'$, which defines the absorption or annihilation cross section $\sigma_{an}$. In expansion (8), we retained only those channels converging to H($n = 1, 2$) or Ps($n = 1, 2$) in the asymptotic limit since we are concerned with energies for which only the channel Ps($1s$) + $p$ may be open in addition to the initial channel $e^+ + H(1s)$. Thus the total angular momentum $L$ is equal to that of the incident $e^+$ and to that of the asymptotic Ps-$p$ motion.

For Ps-$p$ channels, large $\rho$ correspond to large Ps-$p$ distances $R$, and the integration over $\Omega$ is practically that over $(r, \hat{\mathbf{r}}, \hat{\mathbf{R}})$. Hence, all the matrix elements $\langle \mathrm{Ps}(ns) + p|H'|\mathrm{Ps}(n's) + p\rangle_\Omega$ coupling $s$-state Ps channels remain to be imaginary constants for large $\rho$ because of the nonzero $s$-state wave functions $\psi_{Ps}(r = 0)$. This introduces a small imaginary part into the kinetic energy $K^2/2M[ = \epsilon + i\Gamma(1s)/2]$ of the relative Ps($1s$)-$p$ motion, for example, where $M$ ( = 2.0) is the Ps mass. The wave number $K$ is complex even for $\epsilon > 0$ and may be written as $K_{re} + iK_{im}$. The asymptotic channel function

$$\Phi = \psi_{Ps}(\mathbf{r}) f(\epsilon) \exp(iKR)/R \tag{9}$$

outgoing with an amplitude $f(\epsilon)$ decreases slowly as $\exp(-K_{im}R)/R$, changing this channel into a closed channel even for $\epsilon > 0$. Normal closed channels have no influence on the flux conservation. The closed channels associated with Ps($ns$), however, cause flux loss through the $H'$ coupling with open channels. There is no well-defined Ps($ns$) formation in the present theory even when the collision is practically over before Ps annihilates.

The imaginary part of $K^2/2M$ leads to a relation $K_{im}K_{re}/M = \Gamma/2$, or $(K_{re}/M)\tau = (2K_{im})^{-1}$. The left-hand side is the distance $R_{an}$(t.d.) that Ps travels within its lifetime in the time-dependent picture. The right-hand side is the distance $R_{dec}$(t.ind.) in which the time-independent Ps-channel probability $|\Phi|^2R^2dR \propto \exp(-2K_{im}R)dR$ decays by $1/e$. Thus $R_{dec}$(t.ind.) is equal to the Ps annihilation distance $R_{an}$(t.d.). If $\epsilon \gg \Gamma$, then the effects of the imaginary energy are relatively weak, and the closed Ps($ns$) channels are almost open since $K_{im}/K_{re} \sim \Gamma/4\epsilon \ll 1$. The Ps-$p$ interactions are negligibly weak for $R > R_{an}$(t.d.), i.e., the collision is practically over before Ps($ns$) annihilates; Ps($ns$) is observable in principle before annihilation if $\epsilon \gg \Gamma$. On the other hand, if $\epsilon$ is comparable to $\Gamma$, the Ps-$p$ motion is so slow that Ps($ns$) annihilates during the collision, which constitutes indirect annihilation. Both the direct and indirect annihilation mechanisms lead to a common final channel, and hence, they interfere with each other. The cross sections for the direct and indirect annihilation are inseparable because of this interference.

In the absence of $\Gamma$, it follows that $K = i(2M|\epsilon|)^{1/2}$ ($\equiv i\kappa$) for $\epsilon < 0$. For $\epsilon$ close to 0, the dominant contribution to the integral of Eq. (1) comes from the region of $R$ where the Ps-channel function takes an asymptotic form (9) with $\exp(iKR) = \exp(-\kappa R)$. The amplitude $f(\epsilon)$ is nearly independent of $\epsilon$ for small $|\epsilon|$ for $S$ wave, according to the Wigner law [9]. Thus the $S$-wave contribution to $\sigma_{an}$ of Eq. (1), proportional to the integral of $\Gamma|f|^2\exp(-2\kappa R)$ over $R$, behaves as $\propto \kappa^{-1}$ or as $\propto |\epsilon|^{-1/2}$. This integral represents the cumulative intra-Ps annihilation as Ps leaves away from the proton until the channel wave function $\exp(-\kappa R)/R$ decays. The extremely slow decay of the wave function near $\epsilon = 0$, together with the nearly constant $f$, is the origin of the $S$-wave threshold divergence. For higher partial waves $L > 0$, the amplitude behaves as $|f|^2 \propto |\epsilon|^L$, and therefore, the contribution to the integral of Eq. (1) from the asymptotic $R$-region vanishes as $|\epsilon| \to 0$. Other contributions to this integral must be smoothly varying across $\epsilon = 0$. Thus all partial-wave cross sections other than the $S$ wave must be nearly constant close to $\epsilon = 0$.

We first carried out HSCC calculations of $\sigma_{an}$ based on Eq. (1) by neglecting $H'$. Figure 1 compares the calculated $Z_{eff}$ for $\epsilon < 0$ with those in the literature. The present $Z_{eff}$ agrees well with those by Van Reeth and Humberston [4] and by Ryzhikh and Mitroy [5] within 5%. The work of Laricchia and Wilkin [3] has been critically assessed earlier [5,7], and no further comment is due here. The result obtained by Yamanaka and Kino [6], using a time-dependent version of Eq. (1), disagrees significantly with other accurate calculations. Their result increases only weakly near $E_{th}(1s)$ and connects smoothly across the threshold. This is because they took no explicit account of the Ps channels. Even if they had done so, no divergence would have occurred since they enclosed the whole system in a finite, absorbing box, which would have strongly cut off the weakly closed Ps-channel.

Figure 2(a) compares the partial-wave contributions to the annihilation cross sections calculated with explicit account of the absorption potential $H'$ in the HSCC equations [$\sigma_{an}(L)$] and without it [$\tilde{\sigma}_{an}(L)$]. The Ps-formation cross section $\sigma_{Ps}$ calculated without $H'$ is also included. Note that the dominant contribution to $\sigma_{Ps}$ comes from the $S$ wave, and there is only a minute $L > 0$ contribution. The $S$-wave annihilation cross section $\sigma_{an}(S)$ is seen to bridge smoothly from $\tilde{\sigma}_{an}(S)$ well below $E_{th}(1s)$ to $\sigma_{Ps}(S)$ well above $E_{th}(1s)$. The direct annihilation dominates over the indirect annihilation via virtual Ps formation well below $E_{th}(1s)$. The concept of Ps($1s$) formation makes sense only well above $E_{th}(1s)$, and as the energy nears $E_{th}(1s)$, it becomes meaningless to separate Ps formation from direct annihilation. Figure 2(b) shows $\sigma_{an}(L)$ and $\sigma_{Ps}(L)$ in a broader energy range for $\epsilon > 0$ together with those from the $S$-wave analytic formula of Gribakin and Ludlow [7]. This analytic formula explains $\sigma_{an}(S)$ only in a narrow region of $\sim 5 \times 10^{-7} < \epsilon < 10^{-4}$, but deviates from $\sigma_{an}(S)$ outside of it.

None of the contributions $\sigma_{an}(L > 0)$ exhibits a threshold increase. Furthermore, each $\sigma_{an}(L)$ is almost the same

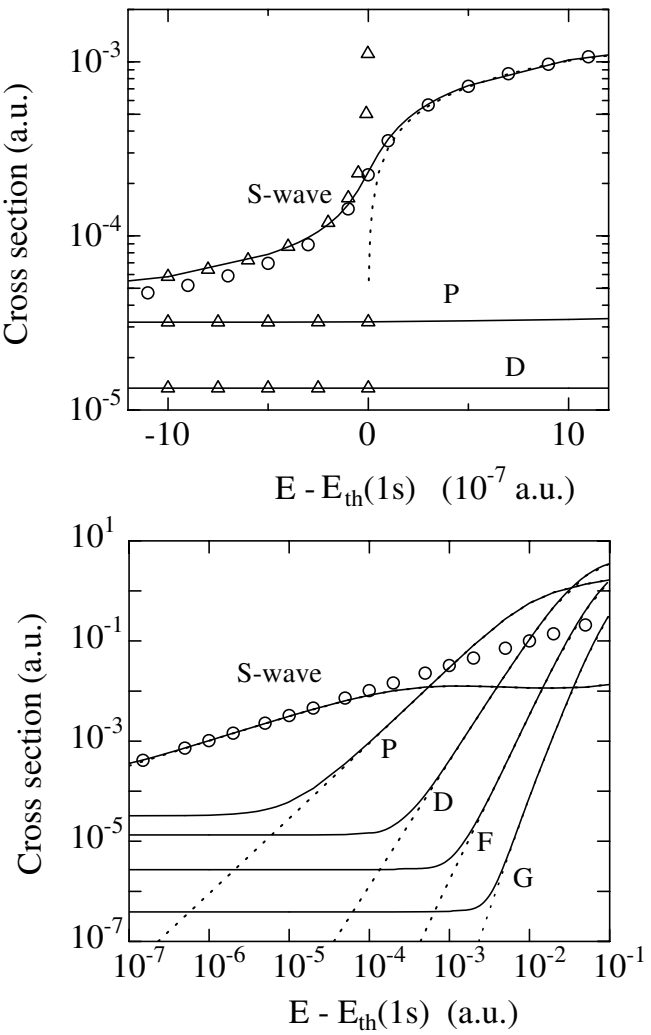


FIG. 2. Partial-wave ($L$) cross sections for annihilation in $e^+(E) + \mathrm{H}(1s)$ collisions near the Ps($1s$) threshold $E_{\mathrm{th}}(1s)$. Solid curves: $\sigma_{\mathrm{an}}(L)$ from HSCC calculations including the absorption potential $H'$. $\triangle$: $\tilde{\sigma}_{\mathrm{an}}(L)$ from HSCC calculations using Eq. (1). Dotted curves: $\sigma_{\mathrm{Ps}}(L)$ for Ps($1s$) formation calculated without $H'$; the total cross section $\sigma_{\mathrm{Ps}}$ is indistinguishable from $\sigma_{\mathrm{Ps}}(L=0)$. $\bigcirc$: analytic $S$-wave threshold law [7] normalized to the HSCC result at $E - E_{\mathrm{th}}(1s) = 0$. (a) Energy region close to $E_{\mathrm{th}}(1s)$. (b) $E > E_{\mathrm{th}}(1s)$ over a broader region.

as $\tilde{\sigma}_{\mathrm{an}}(L)$, which is a constant independent of $E$ near $E_{\mathrm{th}}(1s)$, as is shown earlier in this paper as a generalization of the $|\epsilon|^{-1/2}$ law [7] of $\tilde{\sigma}_{\mathrm{an}}(S)$. The Ps-formation cross sections $\sigma_{\mathrm{Ps}}(L)$, represented by dotted curves in Fig. 2(b), follow straight lines for small $\epsilon$, satisfying the Wigner threshold law $\epsilon^{L+1/2}$. This figure clearly illustrates the smooth transition of $\sigma_{\mathrm{an}}(L)$ from the direct annihilation to the nearly well-defined Ps formation across the threshold not only for $S$ wave but also for all higher partial waves. The cross sections $\sigma_{\mathrm{an}}(L)$ bend over from the $\epsilon^{L+1/2}$ form at higher $\epsilon$. For small $|\epsilon|$, the dominant contributions to $\sigma_{\mathrm{an}}$, $\tilde{\sigma}_{\mathrm{an}}$, and $\sigma_{\mathrm{Ps}}$ come from the $S$ wave, and the partial-wave contributions decrease rapidly as $L$ increases. As $\epsilon$ ($> 0$) grows larger, the more rapidly increasing $P$-wave contribution $\sigma_{\mathrm{an}}(P) \sim \sigma_{\mathrm{Ps}}(P)$ ($\propto \epsilon^{3/2}$) supersedes the $S$ wave, and then the $D$ wave ($\propto \epsilon^{5/2}$) overcomes the $P$ wave at even higher $\epsilon$.

In summary, we have shown for the first time a unified theoretical treatment of pair annihilation and Ps formation in $e^+ + \mathrm{H}$ scattering, which are inseparable from each other in principle, by including an absorption potential in the Hamiltonian and thus by taking account of the finite lifetime of Ps($ns$) in effect. The conventional method of calculating the annihilation cross section based on Eq. (1) breaks down near a threshold of Ps formation.

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