Inseparable positron annihilation and positronium formation in positron-atom collisions: Description in terms of an absorption potential

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(Received 11 June 2003; published 23 October 2003)

Pair annihilation in the elementary process of positron (e^+) collisions with atoms is discussed in terms of an imaginary, absorption potential. This potential represents the QED effect of both direct annihilation during the collision and the indirect one via positronium (Ps) formation in a unified manner. These two mechanisms are inseparable from each other near the threshold for positronium formation, where the collision time becomes comparable to or even longer than the lifetime of the positronium. The theory is applied to the e^+-H collisions. The dominant *s*-wave annihilation cross section follows the Baz' threshold law near the thresholds $E_{\rm th}(1s\ ^{1,3}S)$ for the formation of Ps$(1s\ ^{1,3}S)$. Simple relations between the singlet and triplet cross sections are derived. The spin-averaged annihilation cross section rises sharply but continuously, first across $E_{\rm th}(1s\ ^1S)$, and then across $E_{\rm th}(1s\ ^3S)$, which lies at 0.841 meV above $E_{\rm th}(1s\ ^1S)$. The cross section would diverge at $E_{\rm th}(1s\ ^1S)$ and $E_{\rm th}(1s\ ^3S)$ in the conventional theory where Ps is assumed to have an infinite lifetime. The change of the annihilation probability as the Ps leaves H^+, is studied by decomposing it into the contributions from direct and indirect annihilation and from the interference between them.

DOI: 10.1103/PhysRevA.68.042716 PACS number(s): 34.85.+x, 36.10.Dr, 03.65.Nk

I. INTRODUCTION

When a free positron e^+ and a free electron e^- occupy a common position, they annihilate at some rate emitting two γ-ray photons if they form a singlet pair ($S=0$), and three if triplet ($S=1$) [1–3]. In a bound hydrogenlike system e^+-e^- or positronium (Ps), the nonzero value of the wave function at the coalescence point causes pair annihilation in an ns state. The lifetimes $\tau(ns\ ^1S)$ of parapositronium Ps$(ns\ ^1S)$ against 2γ annihilation are $1.24\times10^{-10}n^3$ s. Those of orthopositronium Ps$(ns\ ^3S)$ against 3γ annihilation are as long as $1.39\times10^{-7}n^3$ s. Those of non-*s* states are much longer. Annihilation occurs also in the field of other particles. Thus, a positron colliding with an atom or a molecule may annihilate with a bound electron. This is the direct mechanism of pair annihilation in collision. If a positronium is formed in this collision, it also annihilates mainly after the collision is over, which is the indirect mechanism.

The quantum electrodynamical phenomenon of pair annihilation may be described quantum mechanically as particle loss due to an effective absorption potential $-iH'$ proportional to $\delta(\mathbf{r})$, where $\mathbf{r}$ is the distance vector between the positron and the electron [4,5]. In the standard theory, however, the elementary processes of positron-atom scattering are described in terms of the Hamiltonian H_0 including only the Coulomb potentials and not the absorption potential $-iH'$ [3,6]. The scattering wave function Ψ_0 thus obtained is used to calculate the expectation value of H', which is proportional to the rate of pair annihilation during the collision. This approximation is usually justified by the extremely small probability of pair annihilation during the collision, or by the much shorter collision time $\tau_{\rm coll}$ than the lifetime $\tau(nl)$ of a positronium under most experimental conditions; a positron with a kinetic energy $E>1$ eV, e.g., can traverse a distance of 1 a.u. in less than 10^{-16} s.

In fact, the annihilation cross section due to this method diverges as the positron energy E approaches, from below, the threshold $E_{\rm th}$ for positronium formation [5,7–10]. Just above $E_{\rm th}$, the positronium-formation cross section rises sharply from zero [5,8–11], as Wigner's threshold law predicts [12]. This threshold behavior of the annihilation and positronium-formation cross sections derives from the approximation of the infinite positronium lifetime, or from the neglect of the absorption potential $-iH'$ in the scattering calculation.

It is theoretically known, however, that a threshold law is changed, in general, if the species formed in the new open channel has a finite lifetime τ [13]. This is because, in this case, the threshold $E_{\rm th}$ is blurred by the energy width Γ associated with this lifetime by the uncertainty principle $\Gamma=\hbar/\tau$. Thus, Baz' [13] derived a formula

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$$\sigma_0 \simeq C_0 \mathrm{Re}[\{\Gamma(\epsilon+i)\}^{1/2}] + C_0' \tag{1}$$

for the *S*-wave contribution to the cross section for the new channel at energies E near E_{th}, where [14]

$$\epsilon \equiv (E - E_{\mathrm{th}})/(\Gamma/2). \tag{2}$$

In Eq. (1), C_0 and C_0' are constants independent of ϵ. This equation reproduces the Wigner threshold law [12] for $\epsilon \gg 1$, and naturally, also for $\Gamma \to 0$. This equation may be easily shown to reduce to

$$\begin{aligned}\sigma_0 &\simeq C_0(\Gamma/2)^{1/2}[(\epsilon^2+1)^{1/2}+\epsilon]^{1/2} + C_0', \\ &= C_0(\Gamma/2)^{1/2}[(\epsilon^2+1)^{1/2}-\epsilon]^{-1/2} + C_0'.\end{aligned} \tag{3}$$

The account for the finite Γ in the derivation of Eqs. (1) and (3) is equivalent, in terms of positron-atom collisions, to the allowance for $-iH'$ in the positronium-formation channels at large distances between positronium and the residual ion. On the other hand, we recently introduced $-iH'$ directly into the Schrödinger equation to treat positron scattering by the hydrogen atom [5], as one should do for accurate calculations. In this theory, the annihilation and positronium formation in the conventional sense are inseparable. For $E \simeq E_{\mathrm{th}}$, the interference between the direct and indirect annihilation mechanisms becomes especially important. The conventional theory breaks down at these energies, since the effective collision time becomes comparable to or even longer than the positronium lifetime when $E \simeq E_{\mathrm{th}}$; the effective velocity of the relative ion-positronium motion is $\sim |E - E_{\mathrm{th}}|^{1/2}$ a.u. near E_{th}. The present paper develops further detailed theory of the dynamics of pair annihilation due to the potential $-iH'$, illustrating it for positron collisions with the hydrogen atom.

II. THEORY

A. Absorption potential

The operator $-iH'$ for 2γ $(S=0)$ and 3γ $(S=1)$ annihilation of a free electron and a free positron is [1,2]

$$\begin{aligned}-i({}^{1,3}H') &= -i(\hbar c r_0^2)({}^{1,3}c)\alpha^S \delta(\mathbf{r}) \\ &= -i(e^2/a_B)({}^{1,3}c)\alpha^{S+3}\delta(\mathbf{r})\end{aligned} \tag{4}$$

to the lowest order, if the relative electron-positron motion, i.e., the motion in $\mathbf{r}$, is much slower than the velocity of light c. Here, α is the fine-structure constant,

$${}^1c = 2\pi \quad \text{and} \quad {}^3c = 8(\pi^2-9)/9, \tag{5}$$

r_0 $(=e^2/m_e c^2 = 2.82\times 10^{-13}$ cm) is the classical electron radius, and a_B is the Bohr radius. The 3γ annihilation is slower than the 2γ annihilation by a factor

$$\begin{aligned}\beta_{13} &\equiv \alpha^{-1}({}^1c/{}^3c) = 9\pi/[4\alpha(\pi^2-9)] \\ &= 1.114\times 10^3 = (0.898\times 10^{-3})^{-1}.\end{aligned} \tag{6}$$

The electron and the positron in a positronium move much slower than the velocity of light, and hence the potentials (4) may be used to describe the rates of 2γ annihilation and 3γ annihilation in Ps$(ns\ {}^{1,3}S)$ [1,2]. These potentials introduce an imaginary part

$$-\frac{i}{2}\Gamma(ns) = -i\langle \psi(ns)|H'|\psi(ns)\rangle \tag{7}$$

into the energy of Ps(ns) to the first order, $\psi(ns)$ being its wave function. The spin is omitted here, and also in the following, when the meaning is clear. The widths are

$$\begin{aligned}\Gamma(ns\ {}^1S) &= cr_0^2/2n^3 = 5.29\times 10^{-6} n^{-3}\ \text{eV}, \\ \Gamma(ns\ {}^3S) &= \Gamma(ns\ {}^1S)/\beta_{13} = 4.75\times 10^{-9} n^{-3}\ \text{eV}.\end{aligned} \tag{8}$$

The same absorption potential (4) may be used for low-energy positron scattering by atoms [4,5]; note that the potential field is weak enough for neglecting another kind of annihilation with emission of only one photon. According to the general theory of scattering by a time-independent complex potential at a real-valued energy [15], an imaginary potential leads to a nonunitary scattering matrix, and hence to the breakdown of the flux conservation. In terms of positron scattering, the cross section for flux absorption may be interpreted as the pair annihilation cross section ${}^{1,3}\sigma$, which can be determined from the flux loss, calculated from the complex phase shift in the case of a single-channel problem. It can be easily proved [15] that the same absorption or annihilation cross section is calculable also from the formula [16]

$${}^{1,3}\sigma = (2/v\hbar)\langle {}^{1,3}\Psi|{}^{1,3}H'|{}^{1,3}\Psi\rangle, \tag{9}$$

where v is the velocity of the incident positron. The scattering wave function ${}^{1,3}\Psi$ in Eq. (9) is normalized to the unit flux of the incident positrons and satisfies the Schrödinger equation

$$[{}^{1,3}H - E_t]{}^{1,3}\Psi = [H_0 - i({}^{1,3}H') - E_t]{}^{1,3}\Psi = 0 \tag{10}$$

for a real-valued total energy E_t of the whole system. Equation (9) is exact within the quantum-mechanical formulation. It was used in Ref. [5] to calculate the singlet cross section ${}^1\sigma$ for the $e^+ + \mathrm{H}$ collisions. Equation (9) also serves as a basis of various approximations.

For spin-unpolarized positron and atomic beams, the total annihilation cross section is calculated by [16]

$$\sigma_{\mathrm{tot}} = {}^1g\,{}^1\sigma + {}^3g\,{}^3\sigma, \tag{11}$$

where ${}^{1,3}g$ is the statistical weight of the spin state of the e^+-e^- pair, and therefore,

$${}^{1,3}g = (2S+1)/4. \tag{12}$$

An effective number Z_{eff} of target electrons contributing to singlet annihilation is customarily defined by

$$\sigma_{\mathrm{tot}} = (c/v)(\pi r_0^2) Z_{\mathrm{eff}}, \tag{13}$$

when ${}^3\sigma$ is negligible in comparison with ${}^1\sigma$.

B. The conventional perturbation theory

Since the absorption potential $-iH'$ usually affects the collision process only very weakly, the wave function ${}^{1,3}\Psi$ in Eq. (9) may be approximated by the solution Ψ_0 of the Schrödinger equation for the Coulomb N-body problem

$$(H_0 - E_t)\Psi_0 = 0, \tag{14}$$

so that the first-order perturbation approximation [3,6]

$${}^{1,3}\overline{\sigma}^{(\mathrm{an})} \equiv (2/v\hbar)\langle \Psi_0 | {}^{1,3}H' | \Psi_0 \rangle \tag{15}$$

follows [16,17]. Here, the bar on top of σ is meant to indicate that the absorption potential is neglected in the calculation of the scattering wave function. Equation (15) has long been used as a standard method of calculating the annihilation cross section.

In the scattering problem (14) for positron energy E, a positronium Ps(nl) with an internal energy $E(nl)$ may be formed above a threshold $E_{\mathrm{th}}(nl) = I + E(nl) = I - (e^2/4a_B n^2)$, where I is the ionization potential of the target. In fact, each level $E(nl)$ is split into fine and hyperfine levels. In particular, each S state is split into two hyperfine levels $E(ns\ {}^{1,3}S)$, so that the threshold may be written as $E_{\mathrm{th}}(ns\ {}^{1,3}S)$. For the ground state, the hyperfine splitting is $\Delta = E(1s\ {}^3S) - E(1s\ {}^1S) = 0.841$ meV $\gg \Gamma(1s\ {}^{1,3}S)$ [18]. Note that no spin-dependent operators are included in the Schrödinger equation (14), so that the hyperfine splitting has to be included artificially by shifting the energy scale for the triplet cross section by Δ from that for the singlet cross section.

Equation (15) is known to diverge as $[E_{\mathrm{th}} - E]^{-1/2}$ as the energy E tends to the threshold E_{th} from below. This divergence was confirmed, for example, by Van Reeth and Humberston [7] for singlet positron scattering by the hydrogen atom by variational calculations. Ryzhikh and Mitroy [8] used a momentum-space Lippmann-Schwinger equation and obtained results that converged to a 1–2% level of accuracy. Both their results and the hyperspherical close-coupling (HSCC) calculations for Eq. (15) by the present authors [5] agreed very well with the results of Ref. [7], reproducing the threshold divergence of Eq. (15) for the singlet case. The model annihilation rate postulated by Laricchia and Wilkin [19] also shows the divergence behavior, although more rapidly as $[E_{\mathrm{th}} - E]^{-1}$.

C. Threshold behavior

Wigner's law [12] predicts that the Lth partial-wave cross section for Ps($1s$) formation behaves as

$$\overline{\sigma}_L^{(\mathrm{Ps})} = C_L^{(\mathrm{Ps})}(\Gamma\epsilon)^{L+1/2} + (\mathrm{higher-order\ terms}) \tag{16}$$

for $\epsilon > 0$ near the threshold in the absence of $-iH'$, where the spin-dependent width $\Gamma(1s\ {}^{1,3}S)$ is denoted simply by Γ, and the spin-dependent reduced energy ${}^{1,3}\epsilon$ by ϵ. The S-wave first-order annihilation cross section $\overline{\sigma}_0^{(\mathrm{an})}$, which is the dominant contribution to $\overline{\sigma}^{(\mathrm{an})}$, behaves as

$$\overline{\sigma}_0^{(\mathrm{an})} = C_0^{(\mathrm{an})}(\Gamma/2)(\Gamma|\epsilon|)^{-1/2} + \mathrm{const} \tag{17}$$

for $\epsilon < 0$ near the threshold [5,7–10]. This may be derived from Eq. (15) by replacing Ψ_0 by its Ps($1s$) channel function, which is the only term in Ψ_0 that depends strongly on ϵ near the threshold.

We note that the effect of the imaginary potential on the scattering process is negligible at energies E that satisfy the relation $|E - E_{\mathrm{th}}(1s\ {}^{1,3}S)| \gg \Gamma(1s\ {}^{1,3}S)$, or $|\epsilon| \gg 1$, and therefore, it follows that

$${}^{1,3}\sigma_L \simeq {}^{1,3}\overline{\sigma}_L^{(\mathrm{Ps})} \quad \text{for} \quad \epsilon \gg 1,$$

$${}^{1,3}\sigma_L \simeq {}^{1,3}\overline{\sigma}_L^{(\mathrm{an})} \quad \text{for} \quad \epsilon \ll -1. \tag{18}$$

We note also that no spin effect is included in the Schrödinger equation (14) for determining ${}^{1,3}\overline{\sigma}_L^{(\mathrm{Ps})}$. Furthermore, the first-order approximation (15) is the same for both $S = 0$ and $S = 1$ except for the coefficient of the δ function in Eq. (4). Therefore, we have

$$\frac{{}^1\sigma_L}{{}^3\sigma_L} \simeq \frac{{}^1\overline{\sigma}_L^{(\mathrm{Ps})}}{{}^3\overline{\sigma}_L^{(\mathrm{Ps})}} = 1 \tag{19}$$

for $E - E_{\mathrm{th}}(1s\ {}^{1,3}S) \gg \Gamma(1s\ {}^1S)$, and

$$\frac{{}^1\sigma_L}{{}^3\sigma_L} \simeq \frac{{}^1\overline{\sigma}_L^{(\mathrm{an})}}{{}^3\overline{\sigma}_L^{(\mathrm{an})}} = \beta_{13} \tag{20}$$

for $E - E_{\mathrm{th}}(1s\ {}^{1,3}S) \ll -\Gamma(1s\ {}^1S)$. In these equations, the singlet and triplet cross sections are to be compared at a common energy value measured from each respective threshold $E_{\mathrm{th}}(1s\ {}^{1,3}S)$. The cross sections summed over L also satisfy relations similar to Eqs. (19) and (20).

The first term in the S-wave Baz' threshold formula (3) satisfies a simple relation

$$\frac{{}^1\sigma_0(\epsilon)}{{}^3\sigma_0(\epsilon)} \simeq \beta_{13}^{1/2}, \tag{21}$$

if ${}^1C_0 \simeq {}^3C_0$, where the singlet and triplet cross sections are to be compared at a common value of ϵ defined for each respective spin. Indeed, the relation ${}^1C_0 \simeq {}^3C_0$ follows if we assume that the cross section (3) satisfies Eq. (19) and that the first term is dominant in Eq. (3).

Gribakin and Ludlow [9] introduced an imaginary part $-i\Gamma/2$ into the Ps($1s$) energy in the derivation of the threshold formulas (16) and (17). They found that the first term in $\overline{\sigma}_0^{(\mathrm{Ps})}$ of Eq. (16) for $\epsilon > 0$ is modified into the first equality in Eq. (3) (without C_0'), and the first term in $\overline{\sigma}_0^{(\mathrm{an})}$ of Eq. (17) for $\epsilon < 0$ into the second equality in Eq. (3) (without C_0'). This led them to conclude that the modified annihilation cross section below E_{th} connects smoothly to the modified positronium-formation cross section above E_{th}, though C_0' was not proved to be common to the two energy regions. Ludlow and Gribakin [10] used the Ps-channel wave function with a complex wave number in the conventional for-

mula (15) for the annihilation cross section. This also led to Eq. (3). This procedure can now be justified by using Eq. (9), which follows from the present formulation in terms of the absorption potential. Naturally, this argument proves that C_0' is indeed common to both $\epsilon<0$ and $\epsilon>0$.

To study the validity of the *S*-wave threshold formula (3) and the 2γ-3γ relation derived from it, and to study the behavior of the higher partial-wave cross sections, a rigorous treatment of the Schrödinger equation (10) is indispensable. A preliminary report of an initial attempt on the 2γ annihilation in positron scattering by the hydrogen atom, $e^+ + \mathrm{H}$, is found in Ref. [5]. Further results will be discussed in the following section.

III. CALCULATIONS AND RESULTS

A. Hyperspherical close-coupling method

Starting from the independent-particle coordinates $\mathbf{r}_1$ for e^+ and $\mathbf{r}_2$ for e^- relative to the proton p, we define the five-dimensional hyperangle $\Omega=(\tan^{-1}(r_2/r_1),\hat{\mathbf{r}}_1,\hat{\mathbf{r}}_2)$ and the hyperradius ρ satisfying

$$\rho^2=r_1^2+r_2^2. \tag{22}$$

An advantage of these hyperspherical coordinates (ρ,Ω), not enjoyed by $(\mathbf{r}_1,\mathbf{r}_2)$, is that only one variable out of the six-dimensional coordinate space runs over to infinity.

Early development [20–22] revealed the usefulness of adiabatic hyperspherical potentials, or the potential energy curves drawn as functions of the hyperradius ρ, in understanding the physics of bound and resonance states both visually and numerically in analogy with adiabatic potential curves of diatomic molecules. A remarkable improvement was then achieved by taking the nonadiabatic coupling into account, i.e., by solving the close-coupling equations in terms of (ρ,Ω), or the HSCC equations. The HSCC method has been used extensively and found to be a powerful tool for accurate studies of the dynamics of many kinds of three-body and even four-body systems; see, e.g., Refs. [22–25].

The convergence of the HSCC method with respect to the number of coupled channels has been found to be much faster than the conventional close-coupling method with the independent-particle coordinates. This rapid convergence is due to the HSCC's efficient account of the correlation effects between $\mathbf{r}_1$ and $\mathbf{r}_2$, which are partly included already in the single-channel approximation.

In general, a hyperradius ρ_c is defined as $\rho_c^2=M_cR_c^2+\mu_c r_c^2$ using a particular set of Jacobi coordinates $(\mathbf{R}_c,\mathbf{r}_c)$ and the reduced masses (M_c,μ_c) for the motion in $\mathbf{R}_c$ and in $\mathbf{r}_c$. This ρ_c turns out to be independent of the choice of Jacobi coordinates $(\mathbf{R}_c,\mathbf{r}_c)$. For the initial arrangement in $e^+ + \mathrm{H}$ scattering, the appropriate Jacobi coordinates is $(\mathbf{r}_1,\mathbf{r}_2)$, for which ρ_c coincides with ρ of Eq. (22). The Jacobi coordinates that are good for the arrangement $\mathrm{Ps}+p$ are the vector $\mathbf{r}$ from the proton to the center of mass of the positronium, and the electron-positron distance vector $\mathbf{r}=\mathbf{r}_2-\mathbf{r}_1$. In this case we have $\rho_c^2=2R^2+(1/2)r^2$, which is equal to Eq. (22). Thus, the transition from the arrangement $e^+ + \mathrm{H}$ to the arrangement $\mathrm{Ps}+p$ can be described in terms of a single reaction coordinate ρ throughout the collision. This is not the case if the independent-particle coordinates are used. This justifies the use of hyperspherical coordinates (ρ,Ω) for the whole Schrödinger equation (10) for the rearrangement collision.

The Hamiltonian H in Eq. (10) may be divided into the kinetic-energy operator in ρ, the absorption potential $-iH'$, and the rest, h_{ad} (see Ref. [20] for its explicit form), which is adiabatic in ρ. Thus, we have

$$H=-\frac{1}{2}\left[\frac{d}{d\rho^2}+\frac{5}{\rho}\frac{d}{d\rho}\right]+h_{\mathrm{ad}}-iH'. \tag{23}$$

The adiabatic channel functions $\{\varphi_i\}$ are defined by the eigenvalue equation

$$h_{\mathrm{ad}}(\Omega;\rho)\varphi_i(\Omega;\rho)=U_i(\rho)\varphi_i(\Omega;\rho), \tag{24}$$

where ρ is treated as the adiabatic parameter. The hyperradius ρ 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 the hydrogen atom or the positronium as $\rho\to\infty$.

In the HSCC method, the total wave function Ψ in the Schrödinger equation (10) is expanded as

$$\Psi(\rho,\Omega)=\sum_i \rho^{-5/2}F_i(\rho)\varphi_i(\Omega;\rho), \tag{25}$$

which leads to coupled radial equations [23]

$$\left[-\frac{1}{2}\frac{d^2}{d\rho^2}+U_i(\rho)-E_t\right]F_i(\rho)+\sum_j (V_{ij}-iH'_{ij})F_j(\rho)=0. \tag{26}$$

Here, $E_t=E-1/2$, and V_{ij} is the nonadiabatic coupling stemming from the differential operators on the right-hand side of Eq. (23). Equations (26) for the complex functions $\{F_i(\rho)\}$ are solved up to a large value of ρ, where the solutions are matched with the asymptotic form expressed in $(\mathbf{r}_1,\mathbf{r}_2)$ and satisfying the scattering boundary conditions.

The usual formulation for rearrangement collisions in terms of independent-particle coordinates leads to coupled *integro-differential* equations because of the different variables for describing different arrangements. On the other hand, Eqs. (26) are coupled *differential* equations, which are much easier to solve.

B. Partial-wave annihilation cross sections

In expansion (25), we retained only those channels converging to $\mathrm{H}(n=1,2)$ or $\mathrm{Ps}(n=1,2)$ in the asymptotic limit since the HSCC expansion is known to converge rapidly, and since we are concerned with energies E close to the threshold E_{th} for the channel $\mathrm{Ps}(1s\,^{1,3}S)+p$. In this energy region well below the $\mathrm{H}(2p)$ and $\mathrm{Ps}(2p)$ thresholds, the total angular momentum L is equal to that of the incident e^+ and to that of the asymptotic Ps-p motion.

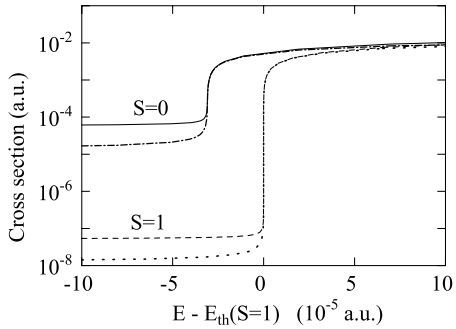

FIG. 1. The singlet ($S=0$) and triplet ($S=1$) annihilation cross sections ${}^{1,3}\sigma$ (full and broken curves) and their S-wave components ${}^{1,3}\sigma_0$ (dot-dashed and dotted curves) plotted as functions of the incident positron energy E measured from the threshold $E_{\rm th}(S=1)$ of the formation of an ortho(triplet)-positronium. The total annihilation cross section for an unpolarized positron beam is calculable by $({}^1\sigma+3\,{}^3\sigma)/4$.

Figure 1 shows the whole picture of the singlet ($S=0$) and triplet ($S=1$) annihilation cross sections ${}^{1,3}\sigma$ of Eq. (9) near the thresholds $E_{\rm th}(1s\,{}^{1,3}S)$, together with their S-wave components ${}^{1,3}\sigma_0$. The singlet cross section ${}^1\sigma$ rises sharply close to $E_{\rm th}(1s\,{}^1S)$, and then does the triplet cross section ${}^3\sigma$ close to $E_{\rm th}(1s\,{}^3S)$, which lies above $E_{\rm th}(1s\,{}^1S)$ by Δ ($=0.841$ meV). As discussed in Sec. II C, the ratios ${}^1\sigma/{}^3\sigma$ and ${}^1\sigma_0/{}^3\sigma_0$ approach β_{13} ($=1.114\times10^3$) on the left of the threshold [see Eq. (20)], and they approach 1.0 on the right [see Eq. (19)]. The magnitudes of the sudden but smooth rise of ${}^3\sigma$ and ${}^1\sigma$ near the threshold, therefore, also have a ratio of β_{13}.

The S-wave contributions ${}^{1,3}\sigma_0$ to ${}^{1,3}\sigma$ are plotted as full curves in Fig. 2 versus the reduced energy ϵ of Eq. (2), whose meaning is different depending on the spin S. In the energy region across the threshold $\epsilon=0$ covered in Fig. 2,

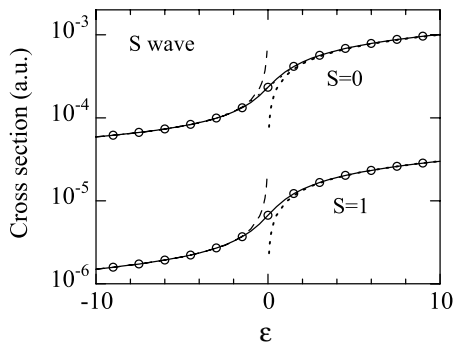

FIG. 2. The near-threshold S-wave singlet ($S=0$) and triplet ($S=1$) annihilation cross sections plotted versus the reduced energy ϵ of Eq. (2). Note that the threshold energy $E_{\rm th}$ and the width Γ in definition (2) differ depending on the spin S. Full curves: ${}^{1,3}\sigma_0$ calculated including the absorption potential $-iH'$. Dotted curves for $\epsilon>0$: positronium formation cross section ${}^{1,3}\overline{\sigma}_0^{\rm (Ps)}$ calculated without $-iH'$ in the conventional manner. Broken curves for $\epsilon<0$: annihilation cross section ${}^{1,3}\overline{\sigma}_0^{\rm (an)}$ [see Eq. (15)] calculated in the conventional manner. Circles: Baz's threshold formula (3) fitted to the full curves.

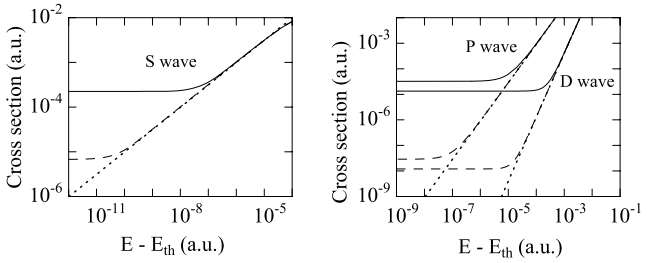

FIG. 3. The partial-wave ($L=0,1,2$) singlet (full curves) and triplet (broken curves) annihilation cross sections ${}^{1,3}\sigma_L$ plotted versus the incident positron energy E measured from the threshold $E_{\rm th}$ for the production of positronium. Note that the thresholds $E_{\rm th}$ for the full and broken curves are different by $\Delta=0.841$ meV.

the fitting (represented by the circles) of the Baz' formula (3) to the full curves is seen to be quite accurate, and the simple relation (21) is observed quite well. The annihilation cross sections ${}^{1,3}\overline{\sigma}_0^{\rm (an)}$ (broken curves) calculated in the conventional manner (15) digress from the full curves close to the threshold $E_{\rm th}$ and diverge. The positronium formation cross sections ${}^{1,3}\overline{\sigma}_0^{\rm (Ps)}$ (dotted curves) calculated in the conventional manner start to grow from $E_{\rm th}$ according to the Wigner law (16), and approach the full curves as well as the Baz' law (3).

The three lowest partial-wave cross sections ${}^{1,3}\sigma_L$ for singlet (full curves) and triplet (broken curves) annihilation are shown in Fig. 3 in a broader energy region than Fig. 2 above the thresholds. The singlet and triplet thresholds are adjusted to lie at the same position in Fig. 3. As is evident from the data in Fig. 2 at $\epsilon=0$, the ratio ${}^1\sigma_0(E={}^1E_{\rm th})/{}^3\sigma_0(E={}^3E_{\rm th})$ of the S-wave cross sections is $\beta_{13}^{1/2}$, and the ratio ${}^1\sigma_0(E)/{}^3\sigma_0(E)$ approaches 1.0 as the energy E increases; see Eq. (19). The higher-partial-wave cross sections start from a constant value that depends on S and L but satisfying Eq. (20), remain constant near the threshold, and gradually approach the Wigner-type form (16) independent of the spin S due to the relation (19). Because of the Wigner law, the cross sections for the higher partial waves, which are the smaller close to the threshold, eventually dominate over the lower partial waves as E increases.

The partial-wave cross sections ${}^{1,3}\sigma_L$ below the threshold are presented in Fig. 4. Here, the triplet cross sections (broken curves) are multiplied by a factor β_{13}, while the singlet ones (full curves) are not, since the ratio ${}^1\sigma_L/{}^3\sigma_L$ should approach β_{13} well below the threshold $E_{\rm th}$. The P- and D-wave cross sections become almost independent of the spin after this normalization. The S-wave cross sections ${}^1\sigma_0$ and $\beta_{13}\,{}^3\sigma_0$ are almost the same at low energies, having a broad minimum and then growing nearly as $\propto(E_{\rm th}-E)^{-1/2}$. The annihilation cross sections ${}^1\overline{\sigma}_0^{\rm (an)}$ and $\beta_{13}^3\overline{\sigma}_0^{\rm (an)}$ (dotted curve) calculated using Eq. (15) diverge in this way as was explained earlier. The singlet cross section ${}^1\sigma_0$ digresses from the dotted curve around 10^{-7} a.u. below the threshold, and then $\beta_{13}\,{}^3\sigma_0$ does so around 10^{-10} a.u. below the threshold, thus avoiding divergence. The S-wave cross sections are dominant close to the threshold, but the P wave

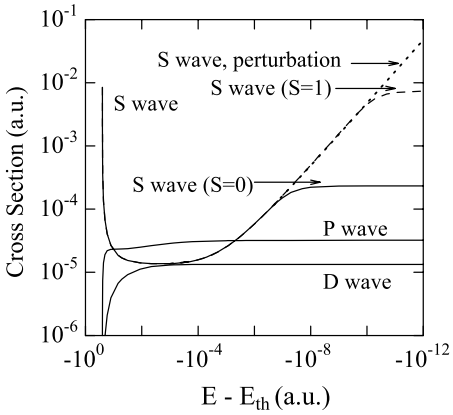

FIG. 4. The partial-wave ($L=0,1,2$) singlet (full curves) and triplet (broken curves) annihilation cross sections plotted versus the incident positron energy E measured from the threshold $E_{\rm th}$ for the production of positronium. The triplet cross sections are multiplied by a constant $\beta_{13}\simeq 1.114\times 10^3$. The dotted curve is the S-wave result ${}^{1,3}\overline{\sigma}_0^{(\rm an)}$ obtained in the conventional manner [see Eq. (15)]. For P and D waves, the full and broken curves are indistinguishable in the figure. Note that the thresholds $E_{\rm th}$ for the full and broken curves are different, and therefore, that the actual positron energies for the singlet and triplet scattering for a common value of the abscissa are different from each other.

dominates over the S wave for 0.15 a.u.$<E<E_{\rm th}-5.0\times 10^{-5}$ a.u.

The validity of Baz's threshold formula (3) has been tested by fitting it to the calculated S-wave annihilation cross section and by taking the ratio of the fitted to the calculated value at each E. This ratio is plotted in Fig. 5 for the singlet (full curve) and triplet (broken curve) cross sections. For both spins, the formula is found to be fairly accurate for $|E-E_{\rm th}|<10^{-6}$ a.u.

C. Annihilation in the positronium channel

A remark is due here on the role of the imaginary coupling potential $-iH'_{ij}$ included in Eq. (26). This potential is extremely weak compared with the Coulomb potentials. Nevertheless, this coupling persists up to the asymptotic region of ρ, affecting the properties of the asymptotic channel functions. For Ps-p channels, large values of ρ correspond to large Ps-p distances R, and the integration over Ω at large ρ corresponds to that over $(\hat{\mathbf{R}},\mathbf{r})$. Therefore, all the matrix elements

$$H'_{ij}=\langle \mathrm{Ps}(ns)+p|H'|\mathrm{Ps}(n's)+p\rangle_\Omega$$

that couple s-state positronium channels, including the diagonal elements, approach constants as $\rho\to\infty$ because of the nonzero s-state wave functions $\psi_{\rm Ps}$ at $r=0$.

This leads to two significant consequences. First, for the definition of the asymptotically correct channels, the positronium states have to be redefined by diagonalizing the coupling matrix $-iH'$ at large ρ, or by taking linear combinations of the wave functions $\psi_{\rm Ps}(ns)$, so that no coupling potentials may exist asymptotically between any pair of the redefined channels.

Second, each element of the diagonalized coupling matrix $-iH'$ introduces an imaginary part into the positronium energy. This introduces a small imaginary part into the kinetic energy of the relative Ps-p motion: $K^2/4=(\Gamma/2)(\epsilon+i)$. The wave number K is complex even for $\epsilon>0$ and may be written as $K_{\rm re}+iK_{\rm im}$. It immediately follows that $K_{\rm re}K_{\rm im}=\Gamma$ and that

$$K_{\rm re}=\Gamma^{1/2}[(\epsilon^2+1)^{1/2}+\epsilon]^{1/2},$$

$$K_{\rm im}=\Gamma^{1/2}[(\epsilon^2+1)^{1/2}-\epsilon]^{1/2}. \tag{27}$$

The asymptotic positronium-channel function

$$\Phi=\psi_{\rm Ps}(\mathbf{r})f(\epsilon)\exp(iK\rho)/\rho \quad (\rho\simeq R) \tag{28}$$

outgoing with an amplitude $f(\epsilon)$ decreases with R as $\exp(-K_{\rm im}R)/R$, meaning that it is now 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 the positronium annihilates.

The behavior of the annihilation cross section for $E\simeq E_{\rm th}$ may be examined by inserting Eq. (28) into the wave function $\mathbf{\Psi}$ in Eq. (9), the rest of $\mathbf{\Psi}$ being slowly varying with E close to $E_{\rm th}$. After the integration over Ω, the S-wave cross section is found to be proportional to

$$\Gamma|f_0|^2\int^\infty d\rho\,\exp(-2K_{\rm im}\rho)=\Gamma|f_0|^2/(2K_{\rm im})+\text{const}$$

$$=|f_0|^2(K_{\rm re}/2)+\text{const}, \tag{29}$$

except for a term more slowly varying with ϵ. Here, f_0 is the S-wave amplitude, which is almost independent of ϵ close to $\epsilon=0$. The integral (29) combined with Eq. (27) reproduces Baz's formula (3). If $\mathbf{\Psi}$ is replaced by $\mathbf{\Psi}_0$ as in the conventional method, the extremely small $K_{\rm im}(\propto[E_{\rm th}-E]^{1/2})$ at energies E below and very near $E_{\rm th}$ makes the cross section extremely large.

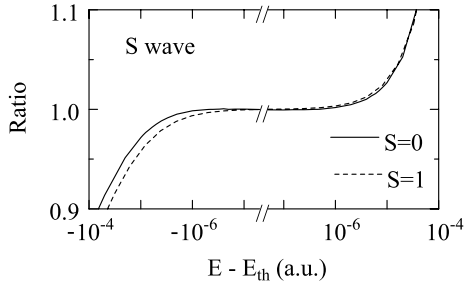

FIG. 5. The accuracy of the fitting of Baz's formula (3) to the calculated S-wave singlet (full curve) and triplet (broken curve) annihilation cross sections. The ratio of the fitted Baz' formula to the calculated results is plotted against the incident positron energy E measured from the threshold $E_{\rm th}$ for the production of positronium.

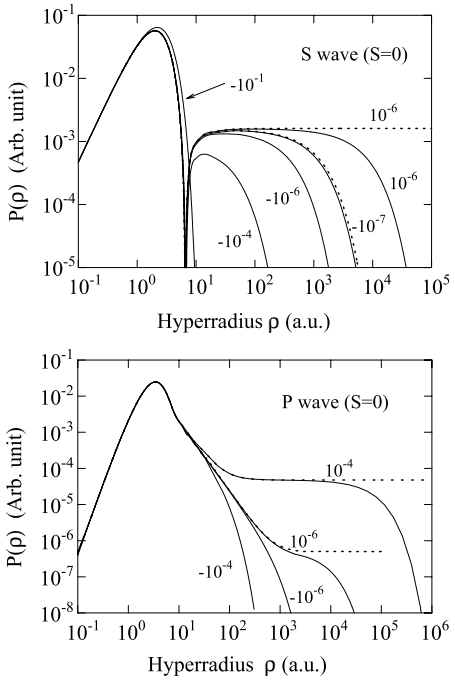

FIG. 6. The singlet annihilation function ${}^1P(\rho)$ of Eq. (30) as a function of the hyperradius ρ. Full curves: with inclusion of the absorption potential $-iH'$. Dotted curves: without $-iH'$. The number on each curve is the positron energy E in a.u. measured from the threshold ${}^1E_{\rm th}$ for the production of para-Ps$(1s)$. (a) $L=0$. The leftmost full and dotted curves, which are almost indistinguishable from each other, are common to all cited energies except for -10^{-1} a.u. (b) $L=1$.

A procedure in the present time-independent approach that corresponds to tracking the time evolution of the collision system would be to study the annihilation function ${}^{1,3}P(R;E)$ defined by carrying out the integration (9) over the whole space except for R. Alternatively, one may define the annihilation function ${}^{1,3}P(\rho;E)$ in terms of the hyperspherical coordinates by

$$
\begin{aligned}
{}^{1,3}\sigma(E) &= \int {}^{1,3}P(\rho;E)d\rho \\
&= \frac{2}{v\hbar}\int \rho^5 d\rho \langle {}^{1,3}\Psi | {}^{1,3}H' | {}^{1,3}\Psi \rangle_\Omega . \qquad (30)
\end{aligned}
$$

The first-order annihilation function may be obtained by replacing Ψ in Eq. (30) by Ψ_0 of Eq. (14).

The S- and P-wave annihilation functions $P_L(\rho;E)$ for singlet collisions at energies E near $E_{\rm th}$ are plotted in Figs. 6(a) and 6(b). Both the results from the wave function calculated with and without the inclusion of the absorption potential $-iH'$ are compared with each other. The small-ρ part of the annihilation functions $P_L(\rho;E)$ is contributed mainly by the direct collision channels in $\mathbf{\Psi}$ (or its approximation $\mathbf{\Psi}_0$) in Eq. (30), and is nearly independent of E close to $E_{\rm th}$. The decay of the positronium-channel wave function with the increase of ρ, or R, becomes slower and slower as E approaches $E_{\rm th}$ from below [see Eq. (29)], and therefore, the

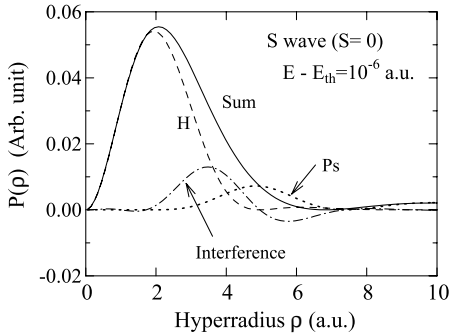

FIG. 7. The ${}^1S$-wave annihilation function ${}^1P(\rho)$ for scattering at an energy of 10^{-6} a.u. above the positronium formation threshold $E_{\rm th}$, decomposed into the contributions from the direct channel (H), positronium formation channel (Ps), and the interference between the two.

contribution to $P_L(\rho;E)$ from this channel extends to a region of larger and larger ρ (or R). This contribution to the S-wave cross section depends strongly on E, which is the main reason for the rapid increase of the threshold formula (3) across $E_{\rm th}$ as is seen in Figs. 1 and 2. For the P wave, $K_{\rm im}$ in Eq. (29) is just the same as for the S wave, and therefore, the ρ dependence of $P_1(\rho;E)$ looks similar to $P_0(\rho;E)$. The scattering amplitude f_0, however, is to be replaced by f_1 in Eq. (29). Since $|f_1|^2 \propto |E-E_{\rm th}|$ at E near $E_{\rm th}$, this prevents the P-wave cross section to grow large near $E_{\rm th}$.

Above $E_{\rm th}$, the positronium channel is open in the absence of the absorption potential $-iH'$, and the positronium formed in this channel keeps annihilating at any large distances ρ or R up to infinity for any partial wave; see the dotted curves in Figs. 6(a) and 6(b). On the other hand, in the presence of $-iH'$, this channel is closed, and the annihilation functions for this case (full curves) drop eventually, thus clearly deviating from the dotted curves.

The annihilation function $P(\rho;E)$ in Eq. (30) may be decomposed into three contributions, namely, that from the direct-collision channels in Ψ, that from the Ps-formation channels, and the cross terms (or the interference terms) between the two kinds of channels. This decomposition is arbitrary to some extent since the channels are well-defined only in the asymptotic regions of the configuration space; in the region where the collision partners lie close to each other, the total wave function may be expanded in terms of any complete set of basis functions. Nevertheless, it would be interesting to decompose $P(\rho;E)$ using the present definition of channels in terms of the hyperspherical coordinates.

Figure 7 shows the contributions to $P(\rho;E)$, thus defined, from direct annihilation (curve H), positronium formation (curve Ps), and the interference between them, at E slightly above $E_{\rm th}$. At this energy, the direct annihilation has a large peak at small values of ρ, and after it decreases, annihilation via positronium formation starts to contribute and keeps doing so until very large values of ρ. A significant interference term is clearly seen at intermediate values of ρ. Its absolute magnitude depends on the particular definition of the channels, but Fig. 7 illustrates at least the inseparability of the two different mechanisms of annihilation at energies E close to $E_{\rm th}$.

IV. SUMMARY

In conclusion, the introduction of an imaginary, absorption potential into the Schrödinger equation has allowed a natural description of the QED effect of pair annihilation in positronium and in positron scattering by atoms. This formulation is equivalent to the allowance for the finite lifetime of positronium formed either virtually or actually in the positron impact process. Annihilation in the direct collision and indirect annihilation via the formation of positronium are thus treated theoretically on equal footing. The direct mechanism is dominant well below the threshold energy $E_{\rm th}$ for positronium formation, and well above it the indirect one is dominant. Close to $E_{\rm th}$, however, the two mechanisms are inseparable, and the interference between them is found to be strong. Calculations for the system $e^+ + \mathrm{H}$ based on this formulation have reproduced the threshold formula for the production of unstable species derived by Baz'. The explicit allowance for the finite lifetime of positronium washes out the unphysical divergence of the annihilation cross section following from the conventional theory, in which the positronium is assumed as completely stable. Some simple relations between the cross sections for the singlet and triplet pair annihilation have been derived from the present formulation and the Baz' formula.

The recent development in the experimental techniques for the elementary processes of positron-atom/molecule collisions is remarkable. Measurements with an energy resolution of the positron beam of ~ 25 meV are now possible [26]. With the expectation of further progress in the near future, rich physics in the dynamics of these elementary processes deserves unraveling also theoretically, as in the present work. The annihilation process may be tracked as the time elapses during the collision if one solves the time-dependent Schrödinger equation with wave-packet propagation, as is increasingly popular in atomic and molecular processes in recent years. A wave packet, however, consists of components with a band of kinetic energies, and has a limitation of easily blurring or washing out and missing narrow resonances and sharp threshold structures such as the ones treated in this paper.

ACKNOWLEDGMENTS

This work was supported in part by the Ministry of Education, Science, Sports, and Technology, Japan (M.K., I.S.), Japan-US Collaborative Program, the JSPS (M.K.), and the collaborative program of NIFS (A.I., M.K.).

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