Enhancement of Positron-Atom Annihilation near the Positronium Formation Threshold

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The behavior of the positron-2γ annihilation rate on an atomic target near the positronium (Ps) formation threshold is determined. When the positron energy ε approaches the threshold $\varepsilon_{\rm thr}$ from below, the effective number of electrons contributing to the annihilation, $Z_{\rm eff}$, grows as $Z_{\rm eff} \simeq A/\sqrt{\varepsilon_{\rm thr} - \varepsilon}$, where A is related to the size of the Ps formation cross section, $\sigma_{\rm Ps} \simeq B\sqrt{\varepsilon - \varepsilon_{\rm thr}}$, by $A = B\sqrt{2\varepsilon_{\rm thr}}/32\pi$ (in atomic units). Taking account of the finite Ps lifetime eliminates the singularity in $Z_{\rm eff}$ and shows that close to threshold the positron annihilation cross section is identical to the para-Ps formation cross section.

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The behavior of cross sections near thresholds is of great interest, because it can be investigated analytically, as was demonstrated in the classic work by Wigner [1]. This and subsequent works [2] explained threshold features in many reactions, however, the behavior of the positron annihilation cross section near the positronium (Ps) formation threshold has not yet been established. This problem has become more pressing with the advent of variational calculations that are able to accurately calculate positron annihilation cross sections near the Ps formation threshold [3]. These calculations have revealed a discrepancy with the existing model of threshold behavior [4] (see below). In this Letter we have established the relation between the near-threshold energy dependence of the annihilation rate and Ps formation, and shown that, when the finite Ps lifetime is taken into account, the annihilation cross section connects smoothly with the Ps formation cross section. The solution found also applies to a general problem of a threshold law for creation of an unstable particle [5].

The scattering of positrons by atoms differs considerably from the case of electron scattering. This is due to the possibility of Ps formation and annihilation. For atoms whose ionization potentials I are lower than the Ps binding energy ($|E_{1s}| \approx 6.8$ eV), it is open at all positron energies. For atoms with $I > 6.8$ eV, e.g., noble gases, Ps formation is often the first inelastic scattering channel to open, with a threshold $\varepsilon_{\rm thr} = I - |E_{1s}|$. The positron can also annihilate with an atomic electron, which leads predominantly to the emission of two γ-quanta [6].

The positron annihilation rate in a gas of density n is usually expressed in terms of the effective number of electrons ($Z_{\rm eff}$) as $\lambda = \pi r_0^2 c Z_{\rm eff} n$ [7], which corresponds to the annihilation cross section

$$\sigma_a = \pi r_0^2 (c/v) Z_{\rm eff}\,, \tag{1}$$

where $r_0 = e^2/mc^2$ is the classical electron radius, c is the speed of light, and v is the incident positron velocity. Equation (1) defines $Z_{\rm eff}$ as the ratio of the positron annihilation cross section on the atom to the spin-averaged annihilation cross section on a free electron in the Born approximation. $Z_{\rm eff}$ can therefore be written as [7]

$$Z_{\rm eff} = \int \sum_{i=1}^{N} \delta(\mathbf{r}_i - \mathbf{r}) \times |\Psi(\mathbf{r}_1, \ldots, \mathbf{r}_N, \mathbf{r})|^2 \, d\mathbf{r}_1 \ldots d\mathbf{r}_N d\mathbf{r}\,, \tag{2}$$

where $\Psi(\mathbf{r}_1, \ldots, \mathbf{r}_N, \mathbf{r})$ is the full $(N + 1)$-particle wave function of the N electron coordinates $\mathbf{r}_i$ and positron coordinate $\mathbf{r}$. The wave function is normalized to a positron plane wave at large distances,

$$\Psi(\mathbf{r}_1, \ldots, \mathbf{r}_N, \mathbf{r}) \simeq \Phi_0(\mathbf{r}_1, \ldots, \mathbf{r}_N) e^{i\mathbf{k}\cdot\mathbf{r}}, \tag{3}$$

where $\Phi_0(\mathbf{r}_1, \ldots, \mathbf{r}_N)$ is the target ground-state wave function, and $\mathbf{k}$ is the incident positron momentum.

In Ref. [4] Laricchia and Wilkin proposed a simple phenomenological model for $Z_{\rm eff}$. In particular, they approximated the lifetime of virtual Ps by the uncertainty principle,

$$\Delta t \simeq |\varepsilon - I - E_{1s}|^{-1} \tag{4}$$

(atomic units, $\hbar = m = |e| = 1$, are used henceforth), and predicted the following energy dependence of the annihilation rate near Ps formation threshold [8]:

$$Z_{\rm eff} \propto \Delta t \simeq |\varepsilon - \varepsilon_{\rm thr}|^{-1}. \tag{5}$$

Numerical calculations have confirmed that virtual Ps does lead to increased annihilation near the threshold [3], but, as we show below, the actual rate of increase is much slower, $Z_{\rm eff} \propto (\varepsilon_{\rm thr} - \varepsilon)^{-1/2}$. Qualitatively, the problem is that Eq. (4) assumes that virtual Ps is formed with a zero kinetic energy and momentum $K = 0$. However, due to the momentum-coordinate uncertainty principle, this would have meant that the virtual Ps is spread over the whole space.

Although $Z_{\rm eff}$ represents the annihilation cross section, Eq. (2) has the form of a transition amplitude. This allows one to represent $Z_{\rm eff}$ by a many-body theory diagrammatic expansion [9,10]. It enables one to identify the contribution of annihilation within the virtual Ps to $Z_{\rm eff}$ (Fig. 1). This diagram gives a relatively small contribution to $Z_{\rm eff}$

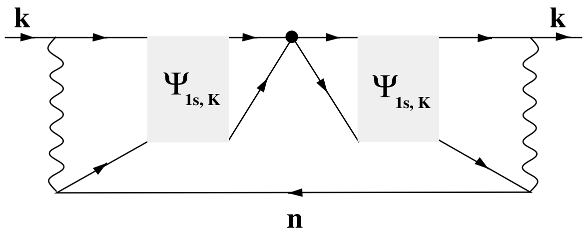

FIG. 1. The contribution of virtual Ps to Z_{eff}. The shaded blocks $\Psi_{1s,\mathbf{K}}$ represent propagation of the (virtual) ground-state Ps, formed when the positron ($\mathbf{k}$) picks up an electron from an atomic orbital n. The wavy lines are the electron-positron Coulomb interaction V, and the solid circle is the annihilation vertex.

at low positron energies [10], however, it is the only one which is singular at the Ps formation threshold.

The diagram in Fig. 1 corresponds to the following expression:

$$\Delta Z_{\text{eff}} = \int \frac{\langle n, \mathbf{k}|V|\Psi_{1s,\mathbf{K}}\rangle |\varphi_{1s}(0)|^2 \langle \Psi_{1s,\mathbf{K}}|V|\mathbf{k}, n\rangle}{(\varepsilon + \epsilon_n - E_{1s} - K^2/4)^2} \times \frac{d^3K}{(2\pi)^3}, \tag{6}$$

where $\varepsilon \equiv k^2/2$ is the incident positron energy, $\langle \Psi_{1s,\mathbf{K}}|V|\mathbf{k}, n\rangle$ is the Ps formation amplitude [11], φ_{1s} is the wave function of the internal motion of Ps [$\varphi_{1s}(0) = (8\pi)^{-1/2}$ a.u.], $\mathbf{K}$ is the Ps center-of-mass momentum, and ε_n is the energy of the atomic orbital n ($\varepsilon_n = -I$ for the removal of the outermost electron).

At threshold, $\varepsilon + \epsilon_n - E_{1s} \equiv \varepsilon - \varepsilon_{\text{thr}} \to 0$ and $K \ll 1$ dominate the integral. For $K \to 0$ the amplitude $\langle \Psi_{1s,\mathbf{K}}|V|\mathbf{k}, n\rangle$ is constant and independent of the direction of $\mathbf{K}$, since s-wave Ps formation is dominant [12]. The amplitude can therefore be taken out,

$$\Delta Z_{\text{eff}} = \frac{|\langle \Psi_{1s,0}|V|\mathbf{k}, n\rangle|^2}{64\pi^4} \int \frac{d^3K}{(\varepsilon - \varepsilon_{\text{thr}} - K^2/4)^2}. \tag{7}$$

After elementary integration we obtain the following threshold behavior:

$$Z_{\text{eff}} \simeq \frac{1}{8\pi^2} \frac{|A_{\text{Ps}}|^2}{\sqrt{\varepsilon_{\text{thr}} - \varepsilon}}, \tag{8}$$

where $A_{\text{Ps}} \equiv \langle \Psi_{1s,0}|V|\mathbf{k}, n\rangle$ is the Ps formation amplitude at threshold, or for the annihilation cross section (1),

$$\sigma_a \simeq \frac{r_0^2 c}{8\pi k} \frac{|A_{\text{Ps}}|^2}{\sqrt{\varepsilon_{\text{thr}} - \varepsilon}}, \tag{9}$$

where $k = \sqrt{2\varepsilon_{\text{thr}}}$ is the positron momentum at threshold.

The Ps formation cross section is given by the golden rule as

$$\sigma_{\text{Ps}} = \frac{2\pi}{k} \int |\langle \Psi_{1s,\mathbf{K}}|V|\mathbf{k}, n\rangle|^2 \delta\left(\varepsilon_{\text{thr}} + \frac{K^2}{4} - \varepsilon\right) \times \frac{d^3K}{(2\pi)^3}. \tag{10}$$

Near threshold this gives

$$\sigma_{\text{Ps}} = \frac{4}{\pi k} |A_{\text{Ps}}|^2 \sqrt{\varepsilon - \varepsilon_{\text{thr}}}, \tag{11}$$

which is simply Wigner's threshold law [1]. Note that, apart from the reciprocal energy dependences, both the annihilation rate and cross section, Eqs. (8) and (9), and the Ps formation cross section, Eq. (11), are proportional to the same squared Ps formation amplitude. Note also that both threshold laws are due to the s-wave Ps formation.

The above formulas can also be derived in a more conventional fashion by considering the asymptotic form of the wave function of the positron-atom system above and below threshold. For simplicity we will present the derivation for a one-electron atom. The generalization to many-electron systems is straightforward. Above threshold, the wave function takes the asymptotic form,

$$\Psi(\mathbf{r}_1, \mathbf{r}) \simeq \Phi_0(\mathbf{r}_1)\left[e^{i\mathbf{k}\cdot\mathbf{r}} + f\frac{e^{ikr}}{r}\right] + f_{\text{Ps}} \frac{e^{iKR}}{R} \varphi_{1s}(\boldsymbol{\rho}), \tag{12}$$

where f is the positron elastic scattering amplitude, f_{Ps} is the Ps formation amplitude, $\mathbf{R} = (\mathbf{r}_1 + \mathbf{r})/2$ is the Ps center of mass, and $\boldsymbol{\rho} = \mathbf{r}_1 - \mathbf{r}$ is the internal Ps coordinate.

The differential Ps formation cross section is given by $d\sigma_{\text{Ps}}/d\Omega = (K/Mk)|f_{\text{Ps}}|^2$, where $M = 2$ is the mass of the Ps atom, and $K = [2M(\varepsilon - \varepsilon_{\text{thr}})]^{1/2}$. Close to threshold the slow Ps is formed primarily in the s wave, and the total Ps formation cross section is

$$\sigma_{\text{Ps}} = \frac{4\pi\sqrt{\varepsilon - \varepsilon_{\text{thr}}}}{k} |f_{\text{Ps}}|^2. \tag{13}$$

By comparison with Eq. (11) we find that [13]

$$A_{\text{Ps}} \equiv -\pi f_{\text{Ps}}. \tag{14}$$

Below threshold, the Ps formation channel is closed, the Ps momentum becomes imaginary, $K = i|K| = i[2M(\varepsilon_{\text{thr}} - \varepsilon)]^{1/2}$, and the asymptotic part of the wave function (12) corresponding to virtual Ps formation is then

$$f_{\text{Ps}} \frac{e^{-|K|R}}{R} \varphi_{1s}(\boldsymbol{\rho}). \tag{15}$$

For the positron energies approaching threshold, $|K| \to 0$, the range of typical virtual Ps center-of-mass distances becomes large, $R \sim |K|^{-1} \gg 1$ a.u., and the contribution of this term in Z_{eff}, Eq. (2), becomes dominant. By substituting it into Eq. (2) we have

$$Z_{\text{eff}} \simeq \int \delta(\boldsymbol{\rho}) |f_{\text{Ps}}|^2 e^{-2|K|R} R^{-2} |\varphi_{1s}(\boldsymbol{\rho})|^2 d\mathbf{R}\, d\boldsymbol{\rho}, \tag{16}$$

where we have changed the integration variables from $\mathbf{r}_1$ and $\mathbf{r}$ to $\mathbf{R}$ and $\boldsymbol{\rho}$. The asymptotic forms (12) and (15) are valid only when the positron is outside the atom. However, since large distances R give the major contribution to the integral in (16), we can formally extend the integration to the whole space. The contribution of small distances

$r \sim 1$, as well that of the first term in (12), remain finite at threshold. Integrating over $\mathbf{R}$ and $\boldsymbol{\rho}$ in Eq. (16), we have

$$Z_{\rm eff} \simeq \frac{|f_{\rm Ps}|^2}{8\sqrt{\varepsilon_{\rm thr} - \varepsilon}}, \tag{17}$$

in exact agreement with Eq. (8). A term similar to (15) was used in variational calculations of positron scattering on H and He to improve the convergence near threshold [14]. The derivation above explains why it also leads to the near-threshold rise of $Z_{\rm eff}$, as noticed in Ref. [3].

As an illustration, let us compare our threshold law to the accurate numerical $Z_{\rm eff}$ for hydrogen [3]. In hydrogen the s-wave Ps is formed by the s-wave positron. Figure 2 shows that, in accordance with Eq. (8), the numerical s-wave $Z_{\rm eff}$ is a linear function of $(\varepsilon_{\rm thr} - \varepsilon)^{-1/2}$ close to threshold. To verify the coefficient in the $(\varepsilon_{\rm thr} - \varepsilon)^{-1/2}$ dependence we use the Ps formation cross section obtained by the same authors [14] and extract $|A_{\rm Ps}|^2 = 0.53$. After substitution into Eq. (8) and the addition of a constant background (not accounted for by this equation), we see that our analytical form gives an excellent description of the numerical s-wave $Z_{\rm eff}$ (Fig. 2). Figure 2 also shows that the addition of higher positron partial waves does not change the slope of the $(\varepsilon_{\rm thr} - \varepsilon)^{-1/2}$ dependence and only adds to the constant background.

The threshold law for $Z_{\rm eff}$ is applicable in a narrow energy range below threshold, comparable to that of the Wigner law for $\sigma_{\rm Ps}$ above it. For hydrogen this range is $|K| \lesssim 0.03$ a.u., or $|\varepsilon - \varepsilon_{\rm thr}| \lesssim 0.01$ eV. On the other hand, at $\varepsilon - \varepsilon_{\rm thr} \to 0$, Eqs. (8) and (9) predict a nonphysical infinity, which would contradict unitarity of the S matrix. Therefore, one cannot use them too close to the threshold.

The problem is that the above formulas have been derived by assuming that the reaction product, Ps, is a stable

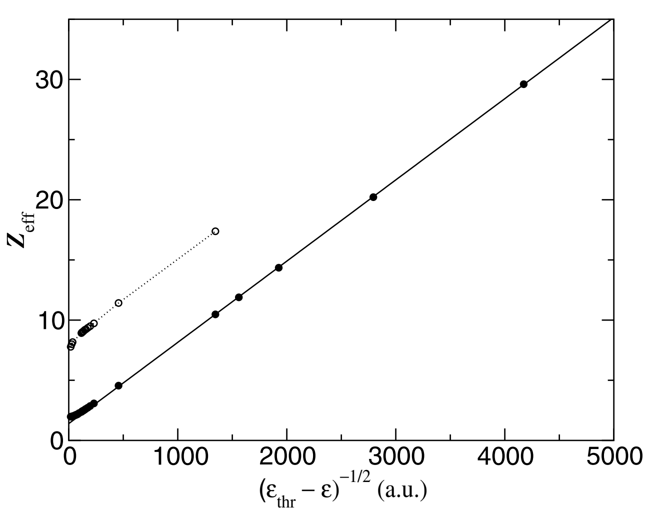

FIG. 2. Solid circles, numerical $Z_{\rm eff}$ (s wave) from Ref. [3]; solid line is Eq. (8), with $|A_{\rm Ps}|^2 = 0.53$ and background $Z_{\rm eff} = 1.4$ added. Open circles are total $Z_{\rm eff}$ (s, p, and d waves) from Ref. [3].

particle. However, Ps has a finite lifetime. The lifetime of Ps depends upon its total spin S. The $S = 0$ state, para-Ps, decays into 2γ. The $S = 1$ state, ortho-Ps, decays with the emission of 3γ, at a rate 10^3 times smaller than para-Ps [6]. We will therefore only account for the annihilation of para-Ps in the following analysis, which is correct as long as positron-atom annihilation into 2γ is considered.

The finite para-Ps lifetime results in its ground-state energy acquiring a small imaginary part,

$$E_{1s} \to E_{1s} - i\Gamma/2, \tag{18}$$

where $\Gamma = r_0^2 c/2 \approx 2 \times 10^{-7}$ a.u. is the para-Ps annihilation width [6]. Equation (7) now becomes

$$\Delta Z_{\rm eff} = \frac{|\langle \Psi_{1s,0}|V|\mathbf{k}, n\rangle|^2}{64\pi^4} \int \frac{d^3K}{(\Delta\varepsilon - K^2/4)^2 + \Gamma^2/4}, \tag{19}$$

where $\Delta\varepsilon \equiv \varepsilon - \varepsilon_{\rm thr}$. After an elementary integration we have

$$Z_{\rm eff} \simeq \frac{|A_{\rm Ps}|^2}{8\pi^2[\frac{1}{2}(\sqrt{\Delta\varepsilon^2 + \Gamma^2/4} - \Delta\varepsilon)]^{1/2}}. \tag{20}$$

The annihilation cross section then becomes

$$\sigma_a \simeq \frac{r_0^2 c|A_{\rm Ps}|^2}{8\pi k[\frac{1}{2}(\sqrt{\Delta\varepsilon^2 + \Gamma^2/4} - \Delta\varepsilon)]^{1/2}}. \tag{21}$$

For the Ps formation the finite para-Ps width means that we must interpret the δ function in Eq. (10) in the following way [12]:

$$\delta\left(\frac{K^2}{4} - \Delta\varepsilon - \frac{i\Gamma}{2}\right) \to \frac{1}{\pi} \frac{\Gamma/2}{(\Delta\varepsilon - K^2/4)^2 + \Gamma^2/4}. \tag{22}$$

Integrating this expression in Eq. (10), and taking into account that the probability of forming $S = 0$ state is $\frac{1}{4}$, we obtain the para-Ps formation cross section as

$$\sigma_{\text{para-Ps}} \simeq \frac{|A_{\rm Ps}|^2}{\pi k}\left[\frac{1}{2}(\sqrt{\Delta\varepsilon^2 + \Gamma^2/4} + \Delta\varepsilon)\right]^{1/2}. \tag{23}$$

A similar formula was obtained using a different method by Baz' [5], who considered the general problem of the threshold behavior for the creation of an unstable particle.

Away from threshold, $|\Delta\varepsilon| \gg \Gamma$, Eqs. (20) and (21) reproduce Eqs. (8) and (9), respectively (for $\Delta\varepsilon < 0$), and Eq. (23) becomes Eq. (11) for $\Delta\varepsilon > 0$. Close to threshold, for $|\Delta\varepsilon| \sim \Gamma$, the threshold laws have been altered. The cross sections are now finite at $\varepsilon = \varepsilon_{\rm thr}$. It is also easy to check that the annihilation cross section (21) and the para-Ps formation cross section (23) are in fact identical. This means that for an unstable particle there is no clear-cut difference between its virtual and real formation. In other words, the smearing of the Ps formation cross section near threshold and the enhancement of annihilation below threshold have the same origin. This is illustrated by Fig. 3 using the hydrogen values of $A_{\rm Ps}$ and k.

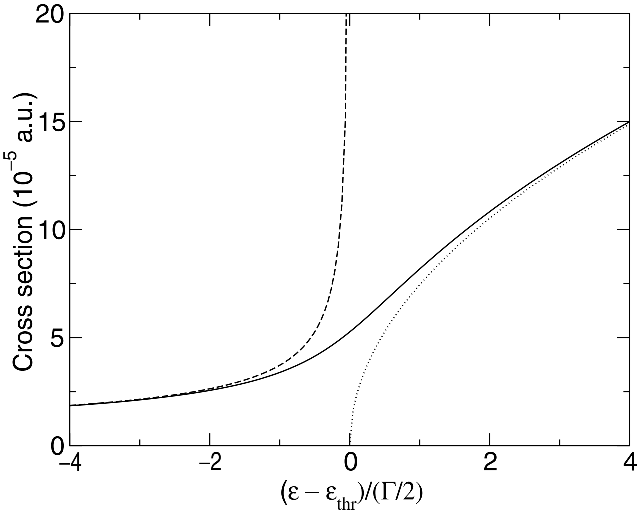

FIG. 3. The solid line shows the identical annihilation and para-Ps formation cross section [Eqs. (21) and (23)]. When the effect of the Ps width is neglected, the para-Ps formation cross section is given by Eq. (11) times $\frac{1}{4}$ (dotted line), and the annihilation cross section is given by Eq. (9) (dashed line).

We have shown that $Z_{\rm eff}$ grows as $(\varepsilon_{\rm thr} - \varepsilon)^{-1/2}$ below the Ps formation threshold. The singularity in $Z_{\rm eff}$ is removed when the finite lifetime of para-Ps is considered. The virtual Ps contributions to the two-photon annihilation cross section and the para-Ps cross section are found to be identical. A similar relation can be derived for the three-photon annihilation and ortho-Ps formation.

In hydrogen the predicted threshold law gives a good description of $Z_{\rm eff}$ from the numerical calculations [3]. For other atoms, e.g., heavier noble-gas atoms, the s-wave Ps formation cross sections can be much larger than that for hydrogen [15]. For example, we estimate that for Xe $|A_{\rm Ps}|^2$ is about 10^2 times that for hydrogen. This means that 0.1 eV below threshold the threshold enhancement of $Z_{\rm eff}$ [Eq. (8)] is about 10.

Previously there was little hope that the above effects could be observed experimentally. The recent development of a cold positron beam [16] looks promising. However, the finite-energy spread of the beam ($\sim$20 meV) poses a problem. If the high-energy tail of the positron energy distribution overlaps with the large Ps formation cross sections above threshold, the "real" Ps annihilation will drown the enhanced (but still small) subthreshold annihilation signal.

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