Compton scattering from positronium and validity of the impulse approximation

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The cross sections for Compton scattering from positronium are calculated in the range from 1 to 100 keV incident photon energy. The calculations are based on the A^2 term of the photon-electron or photon-positron interaction. Unlike in hydrogen, the scattering occurs from two centers and the interference effect plays an important role for energies below 8 keV. Because of the interference, the criterion for validity of the impulse approximation for positronium is more restrictive compared to that for hydrogen.

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I. INTRODUCTION

Recently, interference effects of Young-type have been reported in photoionization of the H_2 molecule [1] and in dissociative electron-transfer collision between H_2^+ and helium [2]. In photoionization of H_2, the interference effects are due to photoelectron scattering from two nuclear centers, while in the case of H_2^+ collision with He these effects are due to two-center electron capture.

Here we report on the interference effects in Compton scattering from the positronium atom (Ps), where the final state of the process consists of a scattered photon and a free electron and positron. Although positronium is a hydrogen-like system, the inelastic photon scattering from positronium occurs from two centers, unlike in the scattering from hydrogen (taking the proton mass as infinite), and the scattering is described by two amplitudes. The interference effects are due to the interference of these amplitudes and the effects become negligible at sufficiently high incident energies.

In the standard calculations of Compton scattering from atoms, electrons are usually described as independent in an effective potential dominated by the electron-nucleus interaction. This independent particle approximation (IPA) is generally quite good, except at low energies. It leads to there being no interference between the different amplitudes corresponding to the individual atomic electrons, even when a proper antisymmetrization is carried out. The electron correlations, neglected in IPA, will cause interference terms, even with proper antisymmetrization, and they are included in full many-body calculations with small effects on total cross sections. However, in the positronium case, there is no dominant effective potential and only the electron-positron interaction, not separable in the two particles, matters. Thus, unlike in scattering from helium, where there are no interference terms at the dominant IPA level, in scattering from positronium we have a coherent sum of the two amplitudes, with interference, in the first order of calculation.

We focus our consideration on the peak region of the Compton spectrum, where the A^2 term of the photon-electron or photon-positron interaction is expected to be sufficient for cross-section calculations for scattering in the peak region of the spectrum from hydrogen or low Z atoms for incident photon energies above 1 keV [3,4].

Using the A^2 term, we derive a general expression for the doubly differential cross section (DDCS) for Compton scattering from a two-particle bound system (of not necessarily equal mass particles), which breaks up after scattering takes place, and when only the scattered photon is observed. The evaluation of the matrix elements and the summation over the final particle states are performed using the internal variables and the internal states in the center-of-mass (c.m.) frame of the two-particle system. When this is applied to the positronium ground state we obtain an analytic expression for the DDCS, with an explicit separation of direct and interference terms in the scattering. For energies above 10 keV, the positronium total cross section approaches twice the hydrogenic atom cross section. However, for energies below 10 keV, there is an interference in the cross section between the direct scattering amplitudes, and the positronium cross section deviates significantly from twice the hydrogenic result at these lower energies.

Compton scattering is a useful experimental method for determining momentum density in atomic, molecular, and condensed-matter systems [5], in situations for which the measured DDCS may be interpreted in terms of the impulse approximation (IA). The generally accepted criterion for the validity of the IA is that the photon momentum transfer, k, must be much larger than the average momentum p_{avg} of the bound electron, $p_{\mathrm{avg}}/k \ll 1$. However, in the case of the hydrogen atom, as well as heavier atoms, the IA is known to be adequate for the DDCS as long as $p_{\mathrm{avg}}/k \lesssim 1$ [4,6]. Because positronium is a hydrogen-like system, but the scattering takes place from two centers and interference effects are present, it is interesting to investigate the adequacy of the IA in this case.

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Assuming A^2 approximation, we have derived the DDCS in the IA for the positronium ground state in analytic form. We find that the interference effects present in the scattering at lower energies are not adequately given in the IA calculation unless $p_{\rm avg}/k \ll 1$, so that the extended validity of the IA that is observed in hydrogen is not observed in positronium. Advances in technology are making it possible to manipulate pulses of positronium atoms [7], suggesting that it may become possible to study scattering from positronium, as discussed here.

Our paper is organized as follows. In Sec. II, we give general expressions for the DDCS for Compton scattering from a bound state of two particles of opposite charges and different masses. In Sec. III, we specialize to the DDCS in A^2 approximation for the scattering from the positronium ground state (equal mass case), evaluating the general expressions, and in Sec. IV we present the results of its calculation. The IA approach is developed in Sec. V and our conclusions are summarized in Sec. VI. We employ the units $\hbar = c = 1$.

II. CROSS SECTION IN A^2 APPROXIMATION

For the calculation of the DDCS for Compton scattering from two particles of opposite charges $e^{\pm}$ and respective masses $m_{\pm}$, which form an initial bound state $|i\rangle$, we employ a nonrelativistic perturbation theory with the A^2 term of the charged particle-photon interaction. The corresponding DDCS is

$$\frac{d^2\sigma}{d\omega_2 d\Omega_2} = \frac{1}{2}\alpha^2\frac{\omega_2}{\omega_1}\sum_{\rm pol}\sum_f \left|(\vec{\epsilon}_1\cdot\vec{\epsilon}_2)\left\langle f\left|\frac{1}{m_+}e^{i\vec{k}\cdot\vec{r}_+}+\frac{1}{m_-}e^{i\vec{k}\cdot\vec{r}_-}\right|i\right\rangle\right|^2 \times \delta(\omega_1 + E_B - \omega_2 - E_+ - E_-), \quad (1)$$

where the energy, momentum, and polarization of the incoming and scattered photon are $\omega_{1,2}$, $\vec{k}_{1,2}$, and $\vec{\epsilon}_{1,2}$, respectively, and $d\Omega_2$ is the scattered photon solid angle, while $\sum_{\rm pol}$ denotes a summation over photon polarizations. The coordinates and momenta of the charged particles are $\vec{r}_{\pm}$ and $\vec{p}_{\pm}$, respectively, while their respective energies in the final continuum energy state $|f\rangle$ are $E_{\pm}$. The symbol $\sum_f$ denotes a summation over all particle final states. We denote by α the fine-structure constant and by E_B the binding energy of the initial $e^{\pm}$ state. In Eq. (1), we have also introduced the momentum transfer $\vec{k}$,

$$\vec{k} = \vec{k}_1 - \vec{k}_2. \quad (2)$$

In order to simplify evaluation of the matrix elements in Eq. (1) and the summation over the final two-particle states, we introduce instead of coordinates $\vec{r}_{\pm}$ and momenta $\vec{p}_{\pm}$ the coordinate $\vec{R}$ and the momentum $\vec{P}$ of the c.m. of the $e^{\pm}$ system, and correspondingly the internal coordinate $\vec{r}$ and momentum $\vec{p}$, by the standard transformation.

The two-particle states in Eq. (1) are now specified by the motion of their c.m. and their internal wave functions, such that

$$|i\rangle = |I\rangle|\phi\rangle, \qquad |f\rangle = |F\rangle|\vec{p}\rangle, \quad (3)$$

where $|I\rangle$ and $|F\rangle$ are the c.m. plane waves corresponding to the initial and final c.m. state with respective momenta $\vec{P}_I$ and $\vec{P}_F$. The internal wave functions $|\phi\rangle$ and $|\vec{p}\rangle$ represent the initial bound state and the final state with momentum $\vec{p}$, respectively. The summation over two-particle final states $\sum_f$ now becomes an integration over $d\vec{P}\,d\vec{p}$.

When the new variables, together with the representation of the states given by Eq. (3), are introduced in Eq. (1), we derive, after some calculation and integration over the c.m. degrees of freedom, the expression for the DDCS in the form

$$\frac{d^2\sigma}{d\omega_2 d\Omega_2} = \frac{\alpha^2}{2}\frac{\omega_2}{\omega_1}\sum_{\rm pol}\int\frac{d\vec{p}}{(2\pi)^3}\left|\left\langle\vec{p}\left|(\vec{\varepsilon}_1\cdot\vec{\varepsilon}_2)\left(\frac{1}{m_-}e^{i(m_+/M)\vec{k}\cdot\vec{r}} + \frac{1}{m_+}e^{-i(m_-/M)\vec{k}\cdot\vec{r}}\right)\right|\phi\right\rangle\right|^2 \delta\left(\omega_1 - E_B - \omega_2 - E_{\rm c.m.} - \frac{\vec{p}^2}{2\mu}\right), \quad (4)$$

where we have assumed without loss of generality that $\vec{P}_I \equiv 0$. In Eq. (4), we have introduced the reduced mass

$$\mu = \frac{m_+ m_-}{M}, \quad (5)$$

where $M = m_+ + m_-$ is the total mass of the system.

From energy-momentum conservation, we have in Eq. (4) for the c.m. energy

$$E_{\rm c.m.} = \frac{\vec{k}^2}{2M}. \quad (6)$$

When using Eq. (4) for hydrogen, the cross section reduces to the known expression, where only the photon-electron interaction contributes, due to the large proton mass, and the c.m. energy $E_{\rm c.m.}$ is negligible. In the case of positronium, both the photon-electron and the photon-positron interaction terms contribute.

III. HIGH-ENERGY SCATTERING FROM POSITRONIUM

For Compton scattering from positronium (the ground-state energy E_0 is 6.8 eV) we expect that, for incident photon energies above 1 keV, calculation of cross sections using only the A^2 term of the electron-photon or positron-photon interaction, as in the preceding section, is sufficient for the peak region. We performed calculations also including the $p\cdot A$ term, which showed that even at low incident energy such as 1 keV the contribution of this term is completely negligible in the peak region. However, a correct calculation for the low-energy region of the spectrum must include the $p\cdot A$ term, because within A^2 approximation the cross section is vanishing for $\omega_2 \to 0$, while in fact low-energy Compton spectra exhibit an infrared divergence in the limit $\omega_2 \to 0$ [3,8]. Our analysis for low ω_1 and for the low-energy region of spectra will be presented separately.

For the equal mass case, denoting by m the electron (positron) mass, we obtain from Eq. (4) the DDCS as

$$\frac{d^2\sigma}{d\omega_2 d\Omega_2} = \frac{1}{2}\frac{r_e^2}{m}\frac{\omega_2}{\omega_1}\sum_{\text{pol}}(\vec{\varepsilon}_1\cdot\vec{\varepsilon}_2)^2\int\frac{d\vec{p}}{(2\pi)^3} \times\left|\left\langle\vec{p}\left|e^{(1/2)i\vec{k}\cdot\vec{r}}+e^{-(1/2)i\vec{k}\cdot\vec{r}}\right|\phi_0\right\rangle\right|^2 \times\delta\left(\omega_1-\omega_2-E_0-\frac{\vec{k}^2}{4m}+\frac{\vec{p}^2}{2m}\right), \quad (7)$$

where $|\phi_0\rangle$ is the wave function of the positronium ground state with energy E_0 and $|\vec{p}\rangle$ is the Coulombic wave function of the electron and positron continuum state of internal momentum $\vec{p}$. The electron classical radius is denoted by r_e.

The cross section given by Eq. (7) is determined by the superposition of two amplitudes $a_\pm$, which correspond to scattering from the electron or positron separately. When the polarization of the photons and the final electron and positron states are not observed, we obtain from Eq. (7), after integration over the δ function, the cross section

$$\frac{d^2\sigma}{d\omega_2\,d\Omega_2} = \left(\frac{d^2\sigma}{d\omega_2\,d\Omega_2}\right)_+ + \left(\frac{d^2\sigma}{d\omega_2\,d\Omega_2}\right)_- + \mathbb{I}, \quad (8a)$$

where

$$\left(\frac{d^2\sigma}{d\omega_2\,d\Omega_2}\right)_\pm = \frac{1}{2\pi}\frac{\omega_2}{\omega_1}\frac{\sigma_T}{m}\frac{\eta^6}{1-e^{-2\pi\zeta}}\int|a_\pm|^2\,d\Omega \quad (8b)$$

are the cross sections for direct scattering from the positron or electron separately, while

$$\mathbb{I} = \frac{1}{2\pi}\frac{\omega_2}{\omega_1}\frac{\sigma_T}{m}\frac{\eta^6}{1-e^{-2\pi\zeta}}\int 2\,\text{Re}\,(a_+a_-^*)d\Omega \quad (8c)$$

is the interference term in the scattering (Re indicates the real part of a complex number).

In Eqs. (8b) and (8c), $d\Omega$ is an infinitesimal solid angle in the direction of the momentum $\vec{p}$ and σ_T is the Thomson cross section. The symbols η and ζ are defined as

$$\eta = \tfrac{1}{2}\alpha m, \quad \zeta = \frac{\eta}{p}, \quad (9)$$

where the magnitude of the momentum $\vec{p}$ is determined from conservation of energy as

$$p = m\sqrt{\omega_1-\omega_2-|E_0|-\vec{k}^2/4m}. \quad (10)$$

The squared amplitudes $|a_\pm|^2$ and $\text{Re}(a_+a_-^*)$ of Eqs. (8b) and (8c) are

$$|a_\pm|^2 = 64\kappa^2\frac{\kappa^2\mp2\kappa p\cos\beta+(p^2+\eta^2)\cos^2\beta}{[\kappa^2+p^2\mp2\kappa p\cos\beta+\eta^2]^4[(p^2+\eta^2+\kappa^2)^2-4p^2\kappa^2]}e^{-2\zeta\psi} \quad (11a)$$

and

$$\text{Re}(a_+a_-^*) = 64\kappa^2\frac{[\kappa^2-(1+\zeta^2)p^2\cos^2\beta]\cos\chi+2\zeta\kappa p\cos\beta\sin\chi}{[(\kappa^2+p^2+\eta^2)^2-4(\kappa p\cos\beta)^2]^2[(p^2+\eta^2+\kappa^2)^2-4p^2\kappa^2]}e^{-2\zeta\psi}. \quad (11b)$$

In Eqs. (11) we have introduced the quantities

$$\vec{\kappa} = \tfrac{1}{2}\vec{k} \quad\text{and}\quad \kappa = |\vec{\kappa}|,$$
$$\psi = \arctan\frac{2\eta p}{\kappa^2-p^2+\eta^2},$$
$$\chi = \zeta\ln\frac{\kappa^2+p^2+\eta^2-2\vec{\kappa}\cdot\vec{p}}{\kappa^2+p^2+\eta^2+2\vec{\kappa}\cdot\vec{p}}, \quad (12)$$
$$\vec{\kappa}\cdot\vec{p} = \kappa p\cos\beta.$$

At this point, we introduce the commonly used variables u and y for Compton scattering cross sections,

$$y = \frac{\eta}{\kappa} \quad\text{and}\quad u = \frac{p_z}{\eta}, \quad (13)$$

where η is given by Eq. (9) and p_z is defined as

$$p_z = \frac{m}{k}(\omega_1-\omega_2)-\frac{k}{2}, \quad (14)$$

where $k = |\vec{k}|$.

The quantities $|a_\pm|^2$ and $\text{Re}(a_+a_-^*)$ given by Eqs. (11) are now written as

$$|a_\pm|^2 = e^{-2\zeta\psi}\frac{y^6}{\eta^8}\frac{1\mp2\gamma t+(1+2uy)t^2}{(1+u^2)(1+uy\mp\gamma t)^4} \quad (15a)$$

and

$$\text{Re}(a_-a_+^*) = e^{-2\zeta\psi}\frac{y^6}{\eta^8}\frac{[1-(1+2uy)t^2]\cos\chi+2yt\sin\chi}{(1+u^2)[(1+uy)^2-\gamma^2t^2]^2}. \quad (15b)$$

In the above equations

$$\chi = \zeta\ln\frac{1+uy-\gamma t}{1+uy+\gamma t},$$
$$\psi = \arccos\frac{y-u}{\sqrt{1+u^2}},$$
$$\gamma = \sqrt{1+2uy-y^2}, \quad (16)$$
$$\zeta = \frac{y}{\gamma},$$

and $t = \cos\beta$ is introduced.

The angular integration in Eq. (8b), for the contribution of the direct terms to the cross section, can be performed analytically and the result expressed in the u and y variables is

$$\left(\frac{d^2\sigma}{d\omega_2\,d\Omega_2}\right)_\pm = \frac{32}{3\alpha^2}\frac{\sigma_T}{m}y^2\frac{\omega_2}{\omega_1}\frac{1+uy/2}{(1+u^2)^3}\frac{e^{-2\zeta\psi}}{1-e^{-2\pi\zeta}}. \quad (17)$$

For comparison, we give the corresponding expression for the DDCS for the hydrogen atom in u and y variables:

$$\left(\frac{d^2\sigma}{d\omega_2\, d\Omega_2}\right)_H = \frac{16}{3\alpha^2}\frac{\sigma_T}{m}y^2\frac{\omega_2}{\omega_1}\frac{1+xy/2}{(1+x^2)^3}\frac{e^{-2\zeta_H\psi_H}}{1-e^{-2\pi\zeta_H}}, \quad (18a)$$

where

$$\psi_H = \arccos\frac{y-x}{\sqrt{1+x^2}},$$
$$\zeta_H = \frac{y}{\gamma_H}, \quad (18b)$$
$$\gamma_H = \sqrt{1+2xy-y^2}.$$

In these equations $x = u/2$, while y and u are defined by Eq. (13).

The interference contribution $\mathbb{I}$ to the cross section given by Eq. (8c), after insertion of the expression for $\mathrm{Re}(a_+a_-^*)$ given by Eq. (15b) and after performing the azimuth angle integration, in u and y variables is

$$\mathbb{I} = \frac{2\sigma_T}{m}\frac{\omega_2}{\omega_1}\frac{y^6}{\eta^2}\frac{1}{1-e^{-2\pi\zeta}}\frac{e^{-2\zeta\psi}}{1+u^2}\mathbb{I}_0, \quad (19a)$$

where

$$\mathbb{I}_0 = \int_{-1}^{1}\frac{[1-(1+2uy)t^2]\cos\chi + 2yt\sin\chi}{[(1+uy)^2-\gamma^2t^2]^2}dt. \quad (19b)$$

$\mathbb{I}_0$ is singular at $y = 0$. The integration in Eq. (19b) has not been performed in terms of elementary function. However, for the Compton peak region, i.e., when $u \sim 0$, the integration is straightforward for $u = 0$ and the result is

$$\mathbb{I}_0(u=0) = \cos\psi_0 + \frac{2-y^2}{2y}\sin\psi_0, \quad (20)$$

where

$$\psi_0 = \frac{y}{\gamma_0}\ln\frac{1-\gamma_0}{1+\gamma_0}, \quad \gamma_0 = \sqrt{1-y^2}.$$

From Eq. (20), we get the small-y expansion for the peak region

$$\mathbb{I}_0(u=0) = 1 + 2\ln y/2 + O(y^2)\,, \quad (21)$$

which displays the logarithmic nature of the singularity in $\mathbb{I}_0$ at $y = 0$. Because of the factor y^6 which enters in the factor which multiplies $\mathbb{I}_0$ to give the interference term $\mathbb{I}$, given by Eq. (19a), the interference term is unimportant for $y = 0$. For $u = 0$ and small y, we calculate the ratio R_{ID} of interference to direct term contributions in the DDCS, Eqs. (8b) and (8c), as

$$R_{\mathrm{ID}} = \frac{\int_{-1}^{1}2\,\mathrm{Re}(a_-a_+^*)dt}{\int_{-1}^{1}(|a_+|^2+|a_-|^2)dt} = \frac{3}{8}y^4\left[1+2\ln\frac{y}{2}+O(y)^2\right]. \quad (22)$$

This demonstrates that the contribution of direct terms dominates for small y, i.e., for large k.

IV. RESULTS OF CALCULATIONS IN A^2 APPROXIMATION

We have performed calculations of the DDCS in A^2 approximation, both making a numerical evaluation of the angular integrals indicated in Eqs. (8b) and (8c), and also in parallel simply using Eq. (17), together with a numerical evaluation of the integral $\mathbb{I}_0$ given by Eq. (19b). The results obtained from these two integrations showed complete agreement, as they should, since no approximation was made getting Eq. (17). Singly differential cross sections and total cross sections are obtained by additional numerical integration. (We express the cross sections in units of the classical electron radius r_e.)

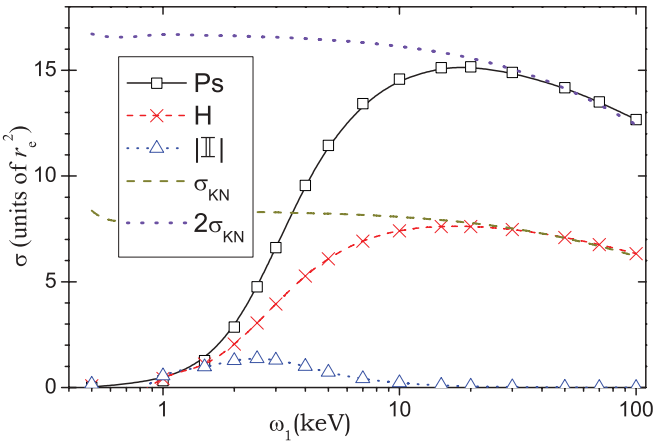

FIG. 1. (Color online) Total cross section for Compton scattering on positronium Ps (squares) and hydrogen H (×) in A^2 approximation. Also shown is the magnitude $|\mathbb{I}|$ of the interference term contribution (triangles) for scattering on positronium, as well as the Klein-Nishina cross sections σ_{KN} (dashes) and $2\sigma_{\mathrm{KN}}$ (dots).

In Fig. 1, we show the values of the total cross section in the range 1–100 keV incident photon energy. We present our results for scattering from positronium, and the results for scattering from hydrogen [calculated from Eq. (18a)], as well as results obtained from the Klein-Nishina formula (scattering from a free electron or positron at rest). We also plot the contribution $|\mathbb{I}|$ of the magnitude of the interference term. One can observe that for higher energies, i.e., above 10 keV, the cross section for positronium matches twice the hydrogenic value and twice the Klein-Nishina value.

In Fig. 2, we show in detail the total cross sections of Fig. 1 for the lower-energy range, from $\omega_1 = 1$ to 10 keV. The interference contribution is always negative, as we see in the peak region for small y, from the $\ln y$ term of Eq. (22), and it becomes less important above 8 keV, when the positronium cross section approaches twice the hydrogenic cross section.

In Fig. 3, we plot the ratios of positronium to hydrogen total cross sections. We present the values of the ratio both with and without interference contribution, as R and R_D, respectively. From this figure, one sees that the positronium cross section at the lower energies is smaller than twice that of hydrogen and that the ratio of cross sections approaches 2 with increasing energy. Large deviations of the ratio R from a factor of 2 in the lower-energy region are a consequence of negative interference. However, the ratio R_D, defined by the direct terms, is about 2 in the entire energy range. For very low energies, R_D becomes greater than 2 due to larger energy phase space (for fixed incident photon energy) in positronium scattering compared to the scattering from hydrogen. This effect is not important for higher incident energies.

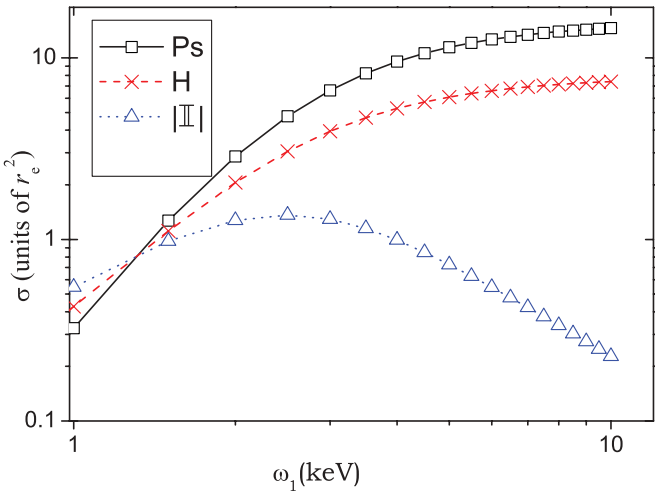

FIG. 2. (Color online) Total cross sections in A^2 approximation for Compton scattering on positronium and hydrogen in the low-energy range. The symbols are the same as in Fig. 1.

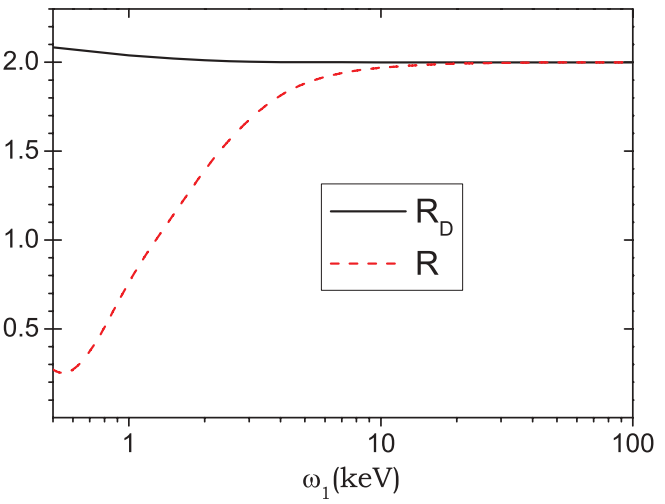

FIG. 3. (Color online) Ratios of positronium to hydrogen total cross sections $R = \sigma_{\rm Ps}/\sigma_{\rm H}$, and $R_D = \sigma_{\rm Ps}^D/\sigma_{\rm H}$, the ratio when the interference term in positronium scattering is omitted (direct terms only).

In Fig. 4, we show the DDCS for scattering of 5 and 10 keV photons from positronium and from hydrogen, as a function of scattered photon energy ω_2, for a scattering angle of 123°. The peak of the positronium curve for 10 keV is four times higher than that of the hydrogen peak, which follows when the expressions for the positronium direct terms, Eq. (17), and for hydrogen, Eq. (18a), are evaluated at the peak position (i.e., $u = x = 0$), and the interference contribution in scattering from positronium is negligible. The hydrogenic curve is broader than that of positronium because of the larger hydrogen average momentum. The area underneath the positronium curve (i.e., the singly differential cross section) is about twice the hydrogenic one. Interference, not visible at 10 keV, is becoming barely visible at 5 keV.

In Fig. 5, we show the DDCS for scattering of 2 keV photons from positronium and hydrogen at the scattering angle of 123°. At this lower energy, the interference contribution to the scattering from positronium is important, as is seen from the figure, and the positronium peak is only approximately three times that of hydrogen. The singly differential cross section (SDCS) for positronium is ∼1.6 times that of hydrogen for this kinematics.

In Fig. 6, we show the SDCS $d\sigma/d\Omega_2$ for scattering of 5 keV photons (upper panel) and 2 keV photons (lower panel) from positronium and hydrogen, as a function of the scattering angle Θ_2. We also plot the contribution $|\mathbb{I}|$ of the magnitude of the interference term, as well as the contribution D of the direct terms in the scattering from positronium. At 2 keV, the interference contribution persists in the entire angular range. However, by 5 keV, the interference contribution is very small for the backscattering angles, as the momentum transfer has sufficiently increased and y is small.

These results demonstrate that the interference term in the cross sections for scattering from positronium in the lower-energy region of 1–8 keV gives an important negative

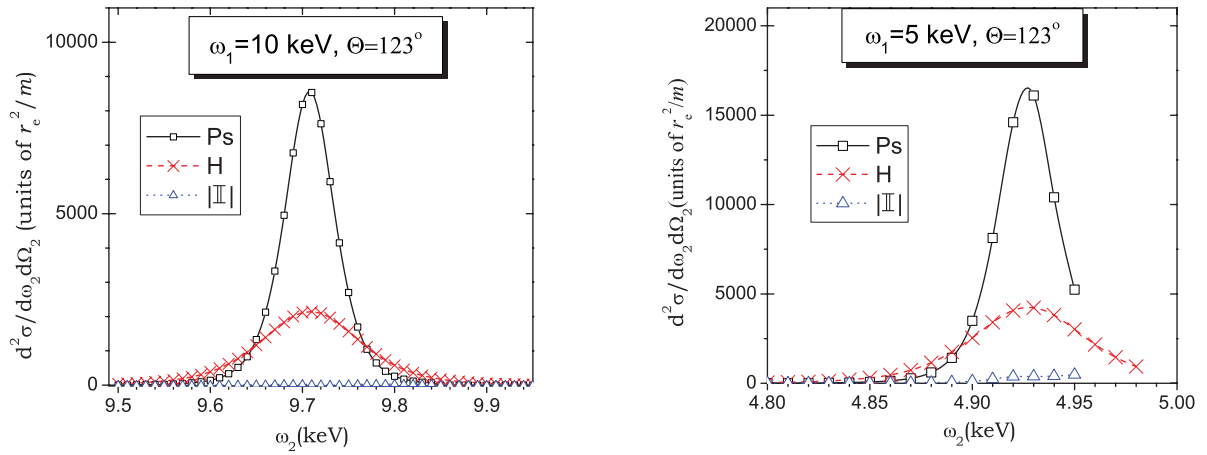

FIG. 4. (Color online) DDCS for Compton scattering of photons with energy $\omega_1 = 10$ keV (left panel) and $\omega_1 = 5$ keV (right panel) from positronium Ps (squares) and from hydrogen H (×) for the scattering angle $\theta = 123°$. Also shown is the absolute value of the interference term $|\mathbb{I}|$ (triangles).

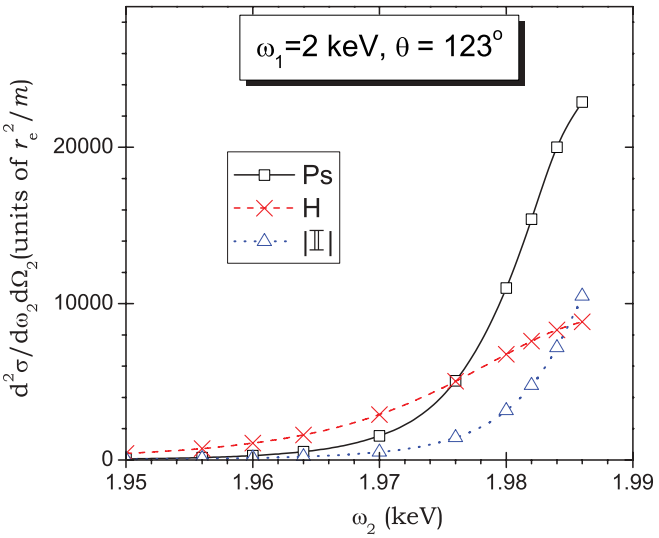

FIG. 5. (Color online) Same as Fig. 4 for incident photon energy $\omega_1 = 2$ keV.

contribution to the cross section from the positive direct terms, which represent the scattering from electron and positron separately. The contribution of interference is negligible above 10 keV incident photon energy.

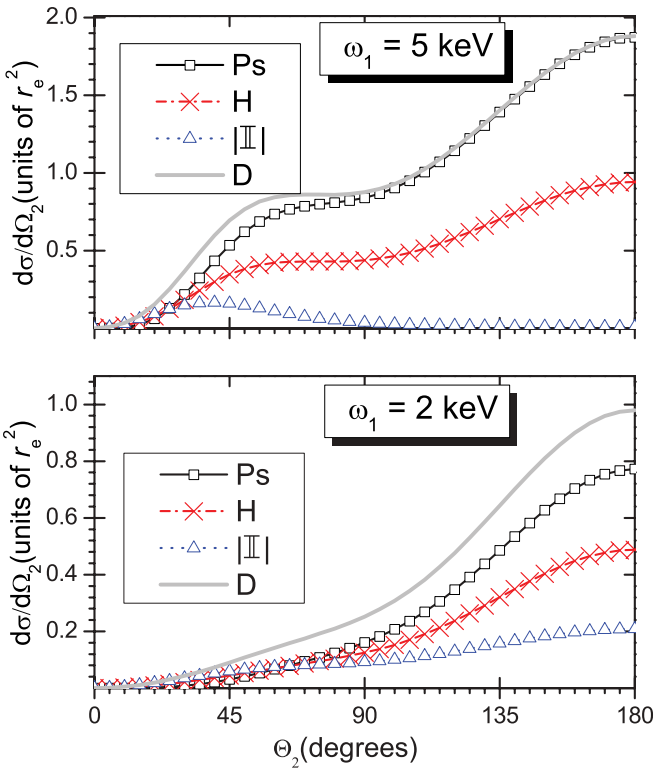

FIG. 6. (Color online) SDCS for scattering of 5 keV photons (upper panel) and 2 keV photons (lower panel) from positronium Ps (squares) and hydrogen H (×) as a function of the scattering angle Θ_2. Also shown is the absolute value of the interference term $|\mathbb{I}|$ (triangles) and the cross section obtained by using only direct terms in the scattering D (line).

V. IMPULSE APPROXIMATION

The impulse approximation (IA), describing scattering as from a momentum distribution of free electrons corresponding to the Fourier decomposition of the bound state, is a very useful method allowing a simple determination of electron momentum density from the experimental results of Compton scattering [5]. The IA is applicable in the Compton peak region and can be derived assuming $p_{\rm avg}/k \ll 1$ ($p_{\rm avg}$ being the average electron momentum and k the photon momentum transfer).

In the case of the hydrogen atom, and also for corresponding higher Z systems, the IA is known to be adequate even for $p_{\rm avg}/k \lesssim 1$. Because the positronium atom is a quantum-mechanical system similar to hydrogen, it is interesting to investigate the adequacy of the IA in the positronium case.

Employing standard operator procedures [9] to the cross section given by Eq. (1), and using the same technique as described in Sec. II for the case of positronium in the ground state $|\phi_0\rangle$, we obtain the IA cross section in A^2 approximation:

$$\left(\frac{d^2\sigma}{d\omega_2\, d\Omega_2}\right)_{\rm IA} = 2\sigma_T \frac{\omega_2}{\omega_1}\int d\vec{q}\,\langle\phi_0|\vec{q}\rangle\Big\{[\langle\vec{q}|\phi_0\rangle + \langle\vec{q}-\vec{k}|\phi_0\rangle] \times \delta\left(\omega_1-\omega_2-\frac{\vec{k}^2}{2m}+\frac{\vec{k}\cdot\vec{q}}{m}\right) \times [\langle\vec{q}|\phi_0\rangle + \langle\vec{q}+\vec{k}|\phi_0\rangle] \times \delta\left(\omega_1-\omega_2-\frac{\vec{k}^2}{2m}-\frac{\vec{k}\cdot\vec{q}}{m}\right)\Big\}, \tag{23}$$

where $|\vec{q}\rangle$ denotes a plane wave of momentum $\vec{q}$ in the electron-positron c.m. frame.

After performing the indicated $\vec{q}$ integrations in Eq. (23), we obtain the IA cross section,

$$\left(\frac{d^2\sigma}{d\omega_2\, d\Omega_2}\right)_{\rm IA} = \frac{32}{\alpha\pi}\frac{y}{m}\sigma_T\frac{\omega_2}{\omega_1}(J_0+J_1). \tag{24}$$

Here

$$J_0 = \frac{1}{3z^3} \tag{25a}$$

and

$$J_1 = \frac{1}{b^2(b+z)} + \frac{1}{b^2 z} - \frac{2}{b^3}\ln\frac{z+b}{z}, \tag{25b}$$

with

$$z = 1+u^2 \quad \text{and} \quad b = \frac{4}{y^2(1+uy)}. \tag{25c}$$

The variables u and y are defined by Eq. (13).

For comparison, we give the corresponding hydrogenic cross section in IA,

$$\left(\frac{d^2\sigma}{d\omega_2\, d\Omega_2}\right)^{\rm H}_{\rm IA} = \frac{8}{\alpha\pi}\frac{y}{m}\sigma_T\frac{\omega_2}{\omega_1}J_0^{\rm H}, \tag{26a}$$

where

$$J_0^{\rm H} = \frac{1}{3z_{\rm H}^3}, \tag{26b}$$

with

$$z_{\rm H} = 1+\left(\frac{u}{2}\right)^2. \tag{26c}$$

The positronium IA cross section, given by Eq. (24), consists of two terms. The first term J_0, Eq. (25a), originates

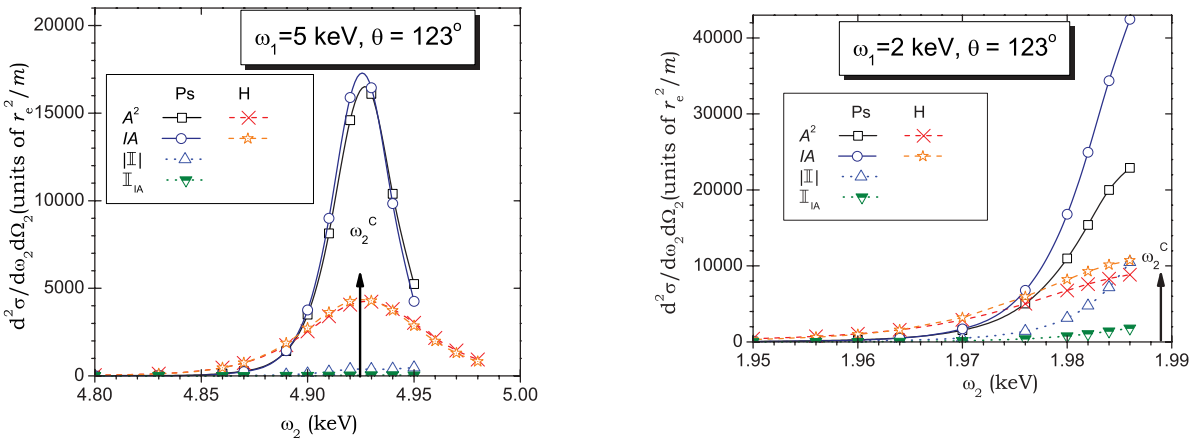

FIG. 7. (Color online) DDCS from positronium Ps and hydrogen H in the A^2 approximation and IA for the scattering angle $\theta = 123^\circ$ and the incident photon energy $\omega_1 = 5$ keV (a) and $\omega_1 = 2$ keV (b). In the legend, $|\mathbb{I}|$ is the absolute value of the interference contribution to the DDCS obtained in A^2 approximation and $\mathbb{I}_{\rm IA}$ is the interference contribution to the DDCS obtained in IA.

from the direct terms of scattering from an electron or a positron separately, while J_1 originates from the interference contribution. For $u = 0$ and small y, we obtain the ratio of the interference contribution to the direct term contributions,

$$R_{\rm ID}^{\rm IA} \equiv J_1/J_0 \approx \frac{y^4}{16} + \frac{y^6}{64}\left(1 + 4\ln\frac{y}{2}\right) + \cdots. \qquad (27)$$

When compared with Eq. (22), which defines the ratio $R_{\rm ID}$ for the A^2 calculation under the same conditions, we observe the same leading power y^4, but with a different coefficient and omitting the $\ln y$ factor, leading to a positive (not negative) value of $R_{\rm ID}^{\rm IA}$, for small y.

The accuracy of IA is usually expressed in terms of the y variable, and its validity is restricted to the Compton peak region. Eisenberger and Platzman [9] asserted, from the analysis of moments in the hydrogen case, that the relative error of IA in comparison to the A^2 calculation was of the order of y^4, which they said implied a criterion of y somewhat less then 1 for its validity. Furthermore, it has been observed that the IA calculation is in very good agreement with both the S-matrix calculation [10], and experiments [11], even for $y \simeq 1$, both for hydrogen and for heavier atoms. However, based on Eqs. (26a) and (18a), Surić [12] derived, for the relative error in the hydrogenic case for $u = 0$, the expansion for small y:

$$\frac{\left(\frac{d^2\sigma}{d\omega_2\,\Omega_2}\right)^{\rm H}_{A^2}}{\left(\frac{d^2\sigma}{d\omega_2\,\Omega_2}\right)^{\rm H}_{\rm IA}} = 1 - 0.144\,934y^2 - 0.009\,936\,17y^4 + 0.000\,729\,726y^6 + \cdots. \qquad (28)$$

Equation (28) demonstrates that the relative error is of the order of y^2 (and for $u \neq 0$ it is even of the order of y, with terms linear in uy [12]), contrary to Eisenberger and Platzman, but that it is rather the smallness of the coefficients that secures the validity of IA even for $y \simeq 1$.

In the positronium case, Eq. (28) holds true only if the interference contributions are dropped in both the IA and A^2 calculations. Keeping the interference contributions, we obtain for $u = 0$ an expansion for the ratio of DDCS in the A^2 approximation to IA based on Eqs. (4), (17), (19), and (24):

$$\frac{\left(\frac{d^2\sigma}{d\omega_2\,d\Omega_2}\right)_{A^2}}{\left(\frac{d^2\sigma}{d\omega_2\,d\Omega_2}\right)_{\rm IA}} = 1 - 0.144\,934y^2 + 0.302\,563\,83y^4 + \frac{3}{4}y^4\ln y/2 + y^6(-0.044\,562\,14 + 0.108\,700\,5\ln y/2) + \cdots. \qquad (29)$$

Note that the coefficients of this expansion are much larger compared to the coefficients in the expansion given by Eq. (28).

From Eq. (29), we find that a value of $y = 0.527$ (or $p_{\rm avg}/k = 0.26$) gives an error of 10%, or $y = 0.915$ (or $p_{\rm avg}/k = 0.46$) gives an error of 30%, which indicates that for positronium the criterion $p_{\rm avg}/k \ll 1$ must be used for the validity of IA. The corresponding errors for hydrogen are 4% and 12%, respectively.

In Fig. 7, we show results for the DDCS from positronium and hydrogen calculated in the A^2 approximation, Eqs. (17), (19), and (18a), as well as in IA, Eqs. (24) and (26a). The cross sections are shown as a function of scattered photon energy ω_2, for a scattering angle of 123° and for the incident photon energies of 5 and 2 keV. We also plot the interference contributions as $|\mathbb{I}|$ for the A^2 calculation and $\mathbb{I}_{\rm IA}$ in IA calculation.

At an energy of 2 keV, in Fig. 7(b), we notice a significant discrepancy between A^2 calculation and IA calculation for positronium, even in the peak region, where $p_{\rm avg}/k \approx 0.6$. The interference contribution is not negligible. At the same energy for hydrogen the agreement between the IA and A^2 calculation is much better, despite the fact that $p_{\rm avg}/k \approx 1.1$.

At an energy of 5 keV, Fig. 7(a), good agreement between A^2 and IA calculation is found for both the positronium and hydrogenic case, but $p_{\rm avg}/k \approx 0.25$ for scattering on positronium.

In Fig. 8, we show the total cross sections for positronium and hydrogen obtained from the A^2 calculation (already shown in Figs. 1 and 2) and the IA calculation. Figure 8(a) shows cross

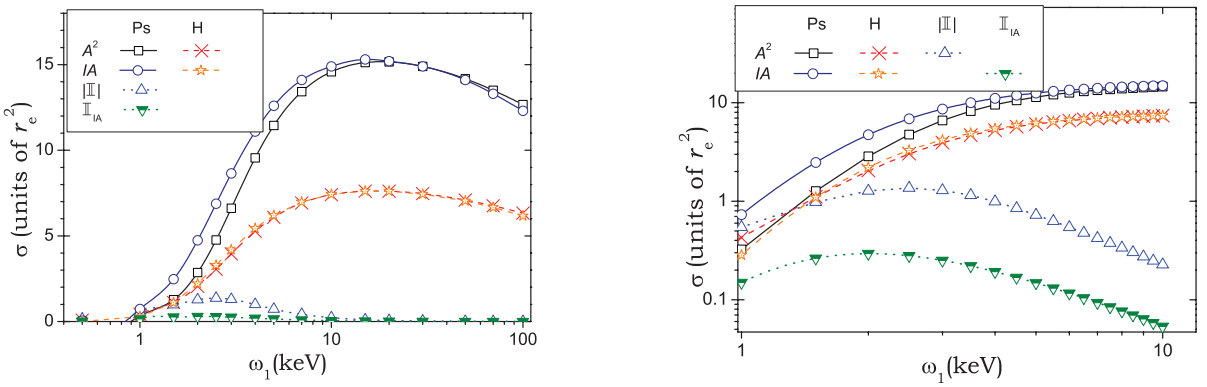

FIG. 8. (Color online) Total cross sections for positronium and hydrogen in the A^2 calculation and the IA calculation (a). In (b), the lower-energy region is displayed in more detail. Symbols are the same as in Fig. 7.

sections for the incident photon energy range 1–100 keV, while Fig. 8(b) shows the lower-energy region 1–8 keV. For energy higher than 10 keV, the A^2 calculation and the IA calculation are in agreement for both positronium and hydrogen. For lower energies, Fig. 8(b), the A^2 calculation and IA calculation are in fair agreement for hydrogen, but we notice significant discrepancy in the positronium case. The negative interference contribution to the scattering is not negligible for these lower energies.

We conclude that the IA calculation for scattering from positronium is reliable for $p_{\rm avg}/k \ll 1$, but not for $p_{\rm avg}/k \approx 1$. In the total cross section, the disagreement between the IA and A^2 calculations occurs over the wide range 1–10 keV, where interference in the DDCS in A^2 approximation is important. The interference is not accurately represented in the IA calculation.

VI. CONCLUSIONS

Above 1 keV, where contribution from the A^2 matrix element dominates, the contributions to the DDCS peak region of Compton scattering from positronium come from direct electron and positron A^2 scattering amplitudes and the interference of these amplitudes. Our results for these DDCS and for the corresponding total cross section for energies below 8 keV show a significant decrease due to the interference effect. In consequence, the positronium total cross sections are smaller than twice the corresponding hydrogen values. However, for energies above 10 keV, and also for DDCS for higher momentum transfer, i.e., $p_{\rm avg}/k \ll 1$, the interference effect is less important. For these higher energies, the positronium total cross section coincides with twice the hydrogenic and Klein-Nishina values, which are the same at such energies.

Our study of the application of IA for positronium demonstrates that the extended validity of IA, $p_{\rm avg}/k \lesssim 1$, observed for hydrogen and heavier atoms DDCS, is not found, and the stronger criterion $p_{\rm avg}/k \ll 1$ should be applied. These findings about the validity of IA for positronium may perhaps apply whenever Compton scattering occurs from more than one center, as in molecules, so that the interference effect can play a role at lower energies.

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[1] J. Fernández, O. Fojón, and F. Martín, Phys. Rev. A **79**, 023420 (2009).
[2] L. Ph. H. Schmidt, S. Schössler, F. Afaneh, M. Schöffler, K. E. Stiebing, H. Schmidt-Böcking, and R. Dörner, Phys. Rev. Lett. **101**, 173202 (2008).
[3] M. Gavrila, Phys. Rev. A **6**, 1348 (1972).
[4] P. M. Bergstrom, T. Surić, K. Pisk, and R. H. Pratt, Nucl. Instrum. Methods Phys. Res., Sect. B **71**, 1 (1992).
[5] M. J. Cooper, Rep. Prog. Phys. **48**, 415 (1985).
[6] Z. Kaliman, T. Surić, K. Pisk, and R. H. Pratt, Fiz. A **9**, 1 (2000).
[7] D. B. Cassidy, P. Crivelli, T. H. Hisakado, L. Liszkay, V. E. Meligne, P. Perez, H. W. K. Tom, and A. P. Mills, Phys. Rev. A **81**, 012715 (2010).
[8] T. Surić, P. M. Bergstrom, K. Pisk, and R. H. Pratt, Phys. Rev. Lett. **67**, 189 (1991).
[9] P. Eisenberger and P. M. Platzman, Phys. Rev. A **2**, 415 (1970).
[10] P. M. Bergstrom, T. Surić, K. Pisk, and R. H. Pratt, Phys. Rev. A **48**, 1134 (1993).
[11] S. Manninen, K. Hämäläinen, and J. Graeffe, Phys. Rev. B **41**, 1224 (1990).
[12] T. Surić (private communication).