Photodetachment of the Ps^- ion by high-energy photons: Model potential approach

Alexei M. Frolov
Department of Chemistry, Queen's University, Kingston, Ontario, Canada K7L 3N6
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Photodetachment of the Ps^- ($e^-e^+e^-$) ion by high-energy photons ($\hbar\omega \approx m_e c^2$) is considered. Our present approach is essentially based on the analytical solution of the first-order perturbation equation with the Dirac-type Hamiltonian. The main goal is to produce the universal formulas for the photodetachment cross sections which can be used for photons with arbitrarily high energies. Also, we wanted to study the angular distribution of the emitted photoelectrons and consider correlations between the incident photon and emitted photoelectron. The obtained formulas for the photodetachment cross sections can also be used to describe relativistic photodetachment of arbitrary few-body systems with unit charges. In particular, it can be applied to the H^- ion and to the muonic molecules.

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I. INTRODUCTION

In our previous study [1] the nonrelativistic photodetachment of the Ps^- ion was considered. Presently, our analysis is generalized to the case of high-energy photons ($\hbar\omega \approx m_e c^2$) when the emitted photoelectron has to be considered as a relativistic particle with the bispinor wave function. In fact, this case corresponds to the situation when $\hbar\omega \gg I$, where ω is the frequency of the incident photon and I is the electron affinity of the Ps^- ion ($I \approx 0.012$ a.u. $= 0.3266$ eV). In general, however, the nonrelativistic consideration can also be applied to the cases when $\hbar\omega \gg I$ [1]. So, it is important to note that relativistic approach is really needed when the energy of incident photon ($\hbar\omega$) is comparable with the rest mass of an electron ($m_e c^2 \approx 512$ keV). In other words, if the photon energy is larger than 100–150 keV, then only the relativistic approach can represent quite accurately the photodetachment of the Ps^- ion. Our main goal in this study is to develop such an approach. In fact, it is shown below that the same approach can be used to describe relativistic photodetachment in arbitrary Coulomb three-body system with unit charges, including the hydrogen negative ion H^-. Note that the photodetachment of the Ps^- and H^- ions by low-energy photons has been considered in [1–3]. Such problems are of great interest in astrophysics [4–7]. For instance, the visible spectrum of our Sun and other Stars can be understood only by considering the photodetachment (and photorecombination) of the H^- ion [6]. In some cases, however, it is important to determine the photodetachment cross-sections for high-energy photons, e.g., for the annihilation γ quanta which propagate into the macroscopic electron-positron mixtures. This explains our present interest to the relativistic photodetachment of the negatively charged ions.

We begin with a few words about some notation and some basic approximations. First, in our present study only relativistic units are used. In these units $c = 1, \hbar = 1$, and therefore, $e^2 = \alpha$, $m_e = \alpha^{-1}$, and $a_0 = (m_e e^2)^{-1} = 1$. Here and below, c is the velocity of light, e is the charge of a proton, a_0 is the Bohr radius, m_e is the electron mass and α is the fine structure constant. Below, we shall designate the electron mass by m. In these units, we have $\hbar\omega = \omega \gg I$, and hence, $\mathcal{E} - m = (\gamma - 1)m = \omega - I \approx \omega \gg I$, where γ is the Lorentz γ factor and $\mathcal{E}$ is the kinetic energy of the final (i.e., free) photoelectron. This means that the kinetic energy $\mathcal{E}$ of the emitted photoelectron is significantly larger than the maximal amplitude of interparticle interactions in the Ps^- ion. Therefore, the influence of the final two-body (neutral) system Ps on the emitted photoelectron can be considered as a small perturbation. In fact, in our present study all our formulas are restricted to the first-order perturbation theory upon the fine-structure constant α.

Note that the approximation $\omega \gg I$ is quite common for the photodetachment of arbitrary atomic and molecular systems by high-energy photons. However, for the negative ions one can introduce another general approximation which is based on the fact that the binding energies of such systems are small in comparison to the atomic (ionization) energies of the final (neutral) atoms. This means that the ratio τ of binding energy ϵ of such an ion to the ionization energy E of the remaining (neutral) atom is relatively small. For instance, for the Ps^- and H^- ions the parameters τ are ≈ 0.048 and ≈ 0.055, respectively, i.e., they are significantly smaller than 1. Furthermore, it is easy to find that for an arbitrary negative atomic ion the parameter τ is bounded between 0.048 and 0.075. This means that all negative ions are relatively weakly bound structures. In other words, the outer electron can be considered as almost free particle which moves in the filed of some effective (or model) potential $V(\mathbf{r})$. In fact, such an effective potential $V(\mathbf{r})$ is a weak potential with non-Coulomb asymptotic at large distances r. In the first approximation we can assume that this potential $V(\mathbf{r})$ is a central potential $V(r)$. In actual negative ions, including the Ps^- ion, the spin-spin and spin-orbit components also contribute, but, in general, such contributions are relatively small.

Below, this one-particle approximation is called the weak-field approximation. Note that the weak-field approximation can be applied to describe photodetachment of arbitrary negatively charged ions, including the Ps^- and H^- ions. However, in the case of negative ions with large nuclear charge Z, the probability of photoionization P_i of internal atomic shells increases rapidly with Z [in general, $P_i \sim Z^5$

(see, e.g., Refs. [8,9])]. In fact, already for $Z=4$ (i.e., for the Be^- ion) the considered relativistic photodetachment of the outer electron is negligible in comparison to the photodetachment of the internal $1s^2$-electron shell. Presently, however, our main attention will be given to the photodetachment of the Ps^- and H^- ions, where $Z=1$. Note that in each of these ions with $Z=1$ only the ground $S(L=0)$ state is stable. The photodetachment of these two ions is considered below by using the weak-field approximation mentioned above. This approximation plays a central role in our present study, since it is used to develop the model potential approach. The model potential approach is discussed in detail in Sec. III. The ultrarelativistic and nonrelativistic cases are considered in Sec. IV. Concluding remarks can be found in the last section.

II. PHOTODETACHMENT CROSS SECTION

Formally, our present problem is to compute the differential photodetachment cross section $d\sigma$ which is written in the form (see, e.g., Ref. [10])

$$d\sigma = e^2 \frac{\mathcal{E}|\mathbf{p}|}{2\pi\omega} |M_{if}|^2 d\Omega, \tag{1}$$

where $\mathbf{p}=\mathcal{E}\mathbf{v}/c^2$ is the momentum of the emitted photoelectron, $\mathcal{E}$ and $\mathbf{v}$ are the kinetic energy and velocity of the photoelectron, respectively. Presently, we shall assume that the kinetic energy $\mathcal{E}$ includes the rest energy of electron, i.e., $\mathcal{E}=\gamma m$. Also, in this equation M_{if} is the corresponding probability amplitude

$$M_{if} = \int\int \overline{\psi_f}(1,2)(\hat{\alpha}_2\cdot\mathbf{e})\exp(\imath\mathbf{k}\cdot\mathbf{r}_2)\psi_i(1,2)d^3\mathbf{r}_1 d^3\mathbf{r}_2, \tag{2}$$

where $\hat{\alpha}=\gamma_0\hat{\gamma}$ and γ_0 and $\hat{\gamma}=(\gamma_x,\gamma_y,\gamma_z)$ are the Dirac $\hat{\gamma}$ matrices. In contrast with our previous study [1] in the last equation the initial $\psi_i(1,2)$ and final $\psi_f(1,2)$ electron wave functions are the doubled bispinor functions. Also, in this equation $\mathbf{k}$ is the momentum of incident photon (or propagation vector [11], $\mathbf{k}^2=\omega^2$) and $\mathbf{e}$ is the polarization vector of the incident photon. Presently, for the incident photons we shall use only the radiation (or Coulomb) gauge, in which $\mathbf{k}\perp\mathbf{e}$. Moreover, only photons with linear polarization are considered. This means that $\mathbf{e}=(e_x,e_y,e_z)$ is a real vector, i.e., all e_i $(i=x,y,z)$ are real (in fact, in Coulomb gauge $e_z=0$ always).

Now, let us discuss the explicit forms of the initial and final wave functions. Below, we shall assume that for any considered three-particle system the particles 1 and 2 are electrons. The particle 3 is the positron e^+ for the Ps^- ion and proton p^+ for the hydrogen H^- ion. The electron wave function of the final state ψ_f (below, the final wave function, for short) in the case of Ps^- ion takes the form

$$\psi_f = \frac{1}{2\sqrt{2}}(1+\kappa\hat{P}_{12})\frac{1}{\sqrt{\mathcal{E}m}}\tilde{u}(1)\tilde{\Psi}_f(1)[w(2)\exp(\imath\mathbf{p}\cdot\mathbf{r}_2) + \delta\psi_f(2)], \tag{3}$$

where $\hat{P}_{12}$ is the electron-electron permutation, $\kappa=-1$ in the case of the Ps^- and H^- ions, $w(j)$ (below $j=1,2$) is the bispinor amplitude of the photoelectron $[w^*(j)\gamma_0 w(j)=2m]$ and $u(i)$ is the bispinor amplitude of the electron at rest $[u^*(j)\gamma_0 u(j)=2m]$. The explicit forms of these bispinors are not important for our present consideration. Also, in this equation $\Psi_f(1)$ is the final (bound) two-body system (Ps or e^+e^-) and $\delta\psi_f(2)$ is the small relativistic correction $(\sim\alpha)$ to the wave function (i.e., to the plane wave) of the emitted photoelectron. The bispinor wave function $\tilde{u}(1)\tilde{\Psi}_f(1)$ of the two-body (final) system Ps also includes the first-order relativistic correction (see below).

The initial wave function ψ_i is essentially the nonrelativistic three-body function $\Psi(1,2)$ of the Ps^- ion which must be multiplied by the two bispinor amplitudes $u(1)$ and $u(2)$. However, it can be shown that such a wave function cannot produce the correct expression for the probability amplitude M_{if}. The corrected wave function must include the first-order correction upon α which corresponds to the Lorenzt boost of the nonrelativistic wave function $[\sim(\hat{\alpha}_2\cdot\boldsymbol{\nabla}_2)u(2)\Psi_i(1,2)]$. Finally, the correct initial wave function ψ_i is written in the form

$$\psi_i = \frac{1}{2\sqrt{2}}(1+\kappa\hat{h}_{12})\frac{1}{m}u(1)\left(1-\frac{\imath}{2m}(\hat{\alpha}_2\cdot\boldsymbol{\nabla}_2)\right)u(2)\Psi_i(1,2), \tag{4}$$

where $\kappa=-1$ for the Ps^- ion and the function $\Psi_i(1,2)$ is the three-body bound-state wave function of the Ps^- ion (or the H^- ion, respectively). As mentioned above in the Ps^- and H^- ions only the ground $S(L=0)$ states are bound (i.e., stable). Now, the bispinor wave function of the hydrogenlike system $\tilde{u}(1)\tilde{\Psi}_f(1)$ from Eq. (3) can be written in analogous form

$$\tilde{u}(1)\tilde{\Psi}_f(1) = \left(1-\frac{\imath}{2m}(\hat{\alpha}_1\cdot\boldsymbol{\nabla}_1)\right)u(1)\Psi_f(1),$$

where $\Psi_f(1)$ is the exact nonrelativistic wave function of the hydrogenlike Ps (or e^+e^-) system.

The formulas presented above are sufficient to produce the analytical expressions for the Ps^- photodetachment probability amplitude M_{if} and cross section $d\sigma$. The detailed analytical computations can be found in our next study [12]. However, in this study out main attention is given to the weak-field approximation which is essentially the one-particle approximation. Obviously, in this case the formulas for the bispinor functions ψ_f and ψ_i presented above have to be modified. In this case the final wave function is

$$\psi_f = \frac{1}{\sqrt{2\mathcal{E}}}[w\ \exp(\imath\mathbf{p}\cdot\mathbf{r}) + \delta\psi_f], \tag{5}$$

where now only one coordinate $\mathbf{r}$ is presented. The initial wave function takes the form

$$\psi_i=\frac{1}{\sqrt{2m}}\left(1-\frac{\imath}{2m}(\hat{\alpha}\cdot\boldsymbol{\nabla})\right)u\Psi_i. \tag{6}$$

In this equation w and u are the constant bispinors, while $\delta\psi_f$ is an $\mathbf{r}$-dependent bispinor function. In the last equation Ψ_i is the wave function of the original bound state in the Ps^- ion determined in the weak-field approximation. These formulas are used in the following section.

III. NEGATIVE IONS IN THE WEAK-FIELD APPROXIMATION

As mentioned above, in the weak-field approximation the original three- and many-body problems are replaced by some effective one-particle problem. Indeed, in the weak-field approximation it is assumed that the electron moves in some effective potential field $V(\mathbf{r})$. The corresponding nonrelativistic Schrödinger equation for the bound-state wave function $\Psi(\mathbf{r})$ is

$$\left(\frac{1}{m}\Delta+2e^2V(\mathbf{r})-2E\right)\Psi(\mathbf{r})=0, \tag{7}$$

where E is the total bound-state energy and the fine structure $\alpha(=e^2)$ is shown explicitly in front of the effective potential $V(\mathbf{r})$. Note that in our present case the total energy E coincides exactly with the corresponding ionization potential I. Our goal below, is to show that the photodetachment cross section in the case of Eq. (1) can be obtained with the use of only Fourier transforms of the wave function $\Psi(\mathbf{r})$ and potential $V(\mathbf{r})$. In addition to these functions one also has to know the numerical value of the radial δ function [i.e., $\Psi(r=0)$] for the considered system. In other words, if the two following functions

$$\Phi(\mathbf{k})=\int\Psi(\mathbf{r})\exp(-\imath\mathbf{k}\cdot\mathbf{r})d^3\mathbf{r} \quad \text{and}$$

$$W(\mathbf{k})=\int V(\mathbf{r})\exp(-\imath\mathbf{k}\cdot\mathbf{r})d^3\mathbf{r}, \tag{8}$$

and value $\Psi(r=0)$ are known, then one can easily determine the differential $(d\sigma)$ and total (σ) photodetachment cross sections. Note that, in the general case, the potential $V(\mathbf{r})$ and wave function $\Psi(\mathbf{r})$ are not necessarily spherically symmetric functions.

Now for the probability amplitude M_{if} we can write

$$\begin{aligned}M_{if}&=\frac{1}{2\sqrt{\mathcal{E}m}}\int\overline{w}(\hat{\gamma}\cdot\mathbf{e})\exp[\imath(\mathbf{k}-\mathbf{p})\cdot\mathbf{r}]\\&\times\left[\left(1-\frac{\imath}{2m}(\hat{\alpha}\cdot\boldsymbol{\nabla})\right)u\cdot\Psi(\mathbf{r})\right]d^3\mathbf{r}\\&+\frac{1}{2\sqrt{\mathcal{E}m}}\int\overline{\delta\psi_f}(\hat{\gamma}\cdot\mathbf{e})u\cdot\Psi(\mathbf{r})\exp(\imath\mathbf{k}\cdot\mathbf{r})d^3\mathbf{r}\\&=M_{if,1}+M_{if,2}.\end{aligned} \tag{9}$$

The first term in this equation can be written in the form

$$\begin{aligned}M_{if,1}&=\frac{1}{2\sqrt{\mathcal{E}m}}\overline{w}(\hat{\gamma}\cdot\mathbf{e})u\cdot\Phi(\mathbf{p}-\mathbf{k})\\&-\frac{\imath}{4\sqrt{\mathcal{E}m^2}}\overline{w}(\hat{\gamma}\cdot\mathbf{e})\int\exp[\imath(\mathbf{k}-\mathbf{p})\cdot\mathbf{r}]\\&\times(\hat{\alpha}\cdot\boldsymbol{\nabla})u\cdot\Psi(\mathbf{r})d^3\mathbf{r}.\end{aligned} \tag{10}$$

By integrating in this equation the second term by parts, one can transfer the operator $\boldsymbol{\nabla}$ to the exponential factor. Finally, the partial probability amplitude $M_{if,1}$ takes the form

$$\begin{aligned}M_{if,1}&=\frac{1}{2\sqrt{\mathcal{E}m}}\overline{w}(\hat{\gamma}\cdot\mathbf{e})u\cdot\Phi(\mathbf{p}-\mathbf{k})+\frac{1}{4m\sqrt{\mathcal{E}m}}\overline{w}(\hat{\gamma}\cdot\mathbf{e})\\&\times[\hat{\alpha}\cdot(\mathbf{k}-\mathbf{p})]u\cdot\Phi(\mathbf{p}-\mathbf{k})\\&=\frac{1}{2\sqrt{\mathcal{E}m}}\overline{w}\left[(\hat{\gamma}\cdot\mathbf{e})+\frac{1}{2m}(\hat{\gamma}\cdot\mathbf{e})\gamma_0(\hat{\gamma}\cdot(\mathbf{k}-\mathbf{p}))\right]\\&\times u\cdot\Phi(\mathbf{p}-\mathbf{k}).\end{aligned} \tag{11}$$

The second partial amplitude $M_{if,2}$ is written in the form

$$M_{if,2}=\frac{1}{2\sqrt{\mathcal{E}m}}\int\overline{\delta\psi_f}(\mathbf{r})(\hat{\gamma}\cdot\mathbf{e})u\cdot\Psi(\mathbf{r})\exp(\imath\mathbf{k}\cdot\mathbf{r})d^3\mathbf{r}. \tag{12}$$

The physical meaning of the bispinor function $\delta\psi_f(\mathbf{r})$ is obvious. Indeed, this is a small perturbation $(\sim\alpha)$ to the final plane wave. The nonrelativistic ground-state wave function $\Psi(\mathbf{r})$ of the Ps^- ion corresponds to the spherically symmetric $S(L=0)$ state, i.e., in this case $\Psi(\mathbf{r})=\Psi(r)$. Moreover, this radial function is a monotonic function which is slowly varying (decaying) with radius r. Therefore, we can expect that its Taylor series expansion around $r=0$ (or $\mathbf{r}=0$) point

$$\begin{aligned}\Psi(r)&=\Psi(r=0)+r\frac{d\Psi(r)}{dr}+\frac{1}{2}r^2\frac{d^2\Psi(r)}{dr^2}+\cdots\\&=\Psi(0)+\sum_{n=1}\frac{\imath^n}{n!}r^n[p_r^n\Psi(r)]\end{aligned} \tag{13}$$

converge quite rapidly. In this equation $p_r=(-\imath)d/dr$. Now, note that in our present case, $\Psi(r)$ is the nonrelativistic atomic wave function, and therefore, $\langle r\rangle\approx a_0=1$ and $\langle p_r\rangle\approx\alpha$, i.e., $v_e\approx\alpha c$. In general, the electron and positron momenta in the Ps^- ion (as well as the electron momenta in the H^- ions) are $\sim me^2/\hbar$, i.e., small $(\sim\alpha)$ in comparison with mc. In the limit $\alpha\to0$ only the $n=0$ term [i.e., $\Psi(r=0)$] in this series survives. Also, note that higher-order terms from Eq. (13) cannot contribute to the matrix element Eq. (12) computed in the first order upon α, since the bispinor func-

tion $\delta\psi_f$ is already a small value ($\sim\alpha$). Finally, the partial probability amplitude $M_{if,2}$ in our present approximation takes the form

$$M_{if,2}=\frac{\Psi(0)}{4\sqrt{\pi\mathcal{E}m}}\int \overline{\delta\psi_f}(\mathbf{r})(\hat{\gamma}\cdot\mathbf{e})u\exp(\imath\mathbf{k}\cdot\mathbf{r})d^3\mathbf{r}, \quad (14)$$

where $\Psi(0)$ is the value of the nonrelativistic radial wave function at short distances $r\approx\Lambda=\alpha a_0$, where Λ is the Compton radius.

The function $\delta\psi_f$ can be found from the following equation [10,13]

$$(\gamma_0\mathcal{E}+\imath\hat{\gamma}\cdot\boldsymbol{\nabla}-m)\delta\psi_f(\mathbf{r})=e^2(\gamma_0 w)V(\mathbf{r})\exp(\imath\mathbf{p}\cdot\mathbf{r}). \quad (15)$$

Or, in other words

$$(\Delta+\mathbf{p}^2)\delta\psi_f(\mathbf{r})=e^2(\gamma_0\mathcal{E}+\imath\hat{\gamma}\cdot\boldsymbol{\nabla}+m)(\gamma_0 w)V(\mathbf{r})\exp(\imath\mathbf{p}\cdot\mathbf{r}). \quad (16)$$

Now, multiplying both sides of this equation by $\exp(-\imath\mathbf{k}\cdot\mathbf{r})$ and integrating over $d^3\mathbf{r}$ one can reduce the last equation to the form [13]

$$(\mathbf{p}^2-\mathbf{k}^2)\delta\phi_f(\mathbf{k})=e^2(\gamma_0\mathcal{E}-\hat{\gamma}\cdot\mathbf{k}+m)(\gamma_0 w)W(\mathbf{k}-\mathbf{p}), \quad (17)$$

where the following notations

$$\delta\phi(\mathbf{b})=\int \delta\psi_f(\mathbf{r})\exp(-\imath\mathbf{b}\cdot\mathbf{r})d^3\mathbf{r} \quad \text{and}$$

$$W(\mathbf{b})=\int V(\mathbf{r})\exp(-\imath\mathbf{b}\cdot\mathbf{r})d^3\mathbf{r} \quad (18)$$

are used. Now, note that the bispinor amplitude w satisfies the following equation $(\mathcal{E}\gamma_0-\boldsymbol{\gamma}\mathbf{p}-m)w=0$. From here one finds

$$(\mathcal{E}\gamma_0+\boldsymbol{\gamma}\cdot\mathbf{p}-m)\gamma_0 w=0, \quad \text{or} \quad m\gamma_0 w=(\mathcal{E}\gamma_0+\boldsymbol{\gamma}\cdot\mathbf{p})\gamma_0 w. \quad (19)$$

Now, the partial amplitude $M_{if,2}$ is written in the form

$$M_{if,2}=\frac{e^2\Psi(0)}{4\sqrt{\pi\mathcal{E}m}}\frac{W(\mathbf{k}-\mathbf{p})}{(\mathbf{p}^2-\mathbf{k}^2)}\cdot\overline{w}(2\gamma_0\mathcal{E}+\hat{\gamma}\cdot(\mathbf{k}-\mathbf{p}))\gamma_0(\hat{\gamma}\cdot\mathbf{e})u. \quad (20)$$

Note that this expression can also be represented in the form

$$M_{if,2}=a_2\overline{w}(\hat{\gamma}\cdot\mathbf{e})u+\overline{w}(\hat{\gamma}\cdot\mathbf{c})\gamma_0(\hat{\gamma}\cdot\mathbf{e})u, \quad (21)$$

where the explicit expressions for the scalar a_2 and vector $\mathbf{c}$ can easily be found from Eq. (20),

$$a_2=\frac{e^2\Psi(0)W(\mathbf{p}-\mathbf{k})}{2\sqrt{\pi\mathcal{E}m}(\mathbf{p}^2-\mathbf{k}^2)}, \quad \mathbf{c}=\frac{e^2\Psi(0)W(\mathbf{p}-\mathbf{k})}{4m\sqrt{\pi\mathcal{E}m}(\mathbf{p}^2-\mathbf{k}^2)}(\mathbf{p}-\mathbf{k}). \quad (22)$$

The formula for the $M_{if,1}$ can also be rewritten in analogous (but slightly different) form

$$M_{if,1}=a_1\overline{w}(\hat{\gamma}\cdot\mathbf{e})u+\overline{w}(\hat{\gamma}\cdot\mathbf{e})\gamma_0(\hat{\gamma}\cdot\mathbf{b})u, \quad (23)$$

where the scalar a_1 and vector $\mathbf{b}$ can now be determined from Eq. (11). Their values are

$$a_1=\frac{\Phi(\mathbf{p}-\mathbf{k})}{2\sqrt{\mathcal{E}m}}, \quad \mathbf{b}=\frac{\Phi(\mathbf{p}-\mathbf{k})}{4m\sqrt{\mathcal{E}m}}(\mathbf{p}-\mathbf{k}). \quad (24)$$

Note that $\mathbf{b}=\lambda_1(\mathbf{p}-\mathbf{k})$ and $\mathbf{c}=\lambda_2(\mathbf{p}-\mathbf{k})$, where the numerical factors λ_1 and λ_2 are

$$\lambda_1=\frac{\Phi(\mathbf{p}-\mathbf{k})}{4m\sqrt{\mathcal{E}m}}, \quad \lambda_2=\frac{e^2\Psi(0)W(\mathbf{p}-\mathbf{k})}{4m\sqrt{\pi\mathcal{E}m}(\mathbf{p}^2-\mathbf{k}^2)}. \quad (25)$$

Also it follows from these equations that $a_1=2m\lambda_1$, $a_2=2m\lambda_2$, and therefore, $a=2m(\lambda_1+\lambda_2)$. Finally, the expression for the M_{if} $(=M_{if,1}+M_{if,2})$ amplitude is

$$M_{if}=\overline{w}\hat{A}u=a\overline{w}(\hat{\gamma}\cdot\mathbf{e})u+\overline{w}(\hat{\gamma}\cdot\mathbf{e})\gamma_0(\hat{\gamma}\cdot\mathbf{b})u+\overline{w}(\hat{\gamma}\cdot\mathbf{c})\gamma_0(\hat{\gamma}\cdot\mathbf{e})u, \quad (26)$$

where now $a=a_1+a_2$ and 4×4 matrix $\hat{A}$ is

$$\hat{A}=a(\hat{\gamma}\cdot\mathbf{e})+(\hat{\gamma}\cdot\mathbf{e})\gamma_0(\hat{\gamma}\cdot\mathbf{b})+(\hat{\gamma}\cdot\mathbf{c})\gamma_0(\hat{\gamma}\cdot\mathbf{e}). \quad (27)$$

The cross section $d\sigma$ is written in the form

$$d\sigma=e^2\frac{\mathcal{E}|\mathbf{p}|}{2\pi\omega}(\overline{w}\hat{A}u)(\overline{u}\gamma_0\hat{A}^+\gamma_0 w)d\Omega. \quad (28)$$

In our present case, this expression must be summed over all (initial and final) directions of the electron spin. This gives the common factor 4. Then, the answer has to be multiplied by $\frac{1}{2}$ (this corresponds to the averaging over the initial direction of the electron spin). The computation of the $(\overline{w}\hat{A}u)(\overline{u}\gamma_0\hat{A}^\dagger\gamma_0 w)$ matrix element is performed by using the formal rules from Ref. [10] (see also Ref. [13]). First, the product of the bispinor amplitude components must be changed in the following way $u_i\overline{u}_k\rightarrow\rho_{ik}$ and $w_i\overline{w}_k\rightarrow\rho'_{ik}$, where

$$\rho=\frac{m}{2}(\gamma_0+1) \quad \text{and} \quad \rho'=\frac{1}{2}(\gamma_0\mathcal{E}-\boldsymbol{\gamma}\cdot\mathbf{p}+m),$$

where ρ and ρ' are the density 4×4 matrices. Now, to determine the matrix element one has to calculate the trace of the following 4×4 matrix

$$(\overline{w}\hat{A}u)(\overline{u}\gamma_0\hat{A}^\dagger\gamma_0 w)=\frac{m}{4}Sp[(\gamma_0\mathcal{E}-\boldsymbol{\gamma}\cdot\mathbf{p}+1)\times\hat{A}(\gamma_0+1)\hat{A}^\dagger\gamma_0], \quad (29)$$

where the 4×4 matrix $\hat{A}$ is given by Eq. (27) and $Sp(\hat{B})$ is the trace of the 4×4 matrix $\hat{B}$. The computation of this trace is straightforward and final general expression takes the form

$$(\overline{w}\hat{A}u)(\overline{u}\gamma_0\hat{A}^\dagger\gamma_0 w)=m(\mathcal{E}-m)a^2+m(\mathcal{E}+m)(\mathbf{b}-\mathbf{c})^2 -2ma\mathbf{p}\cdot(\mathbf{b}-\mathbf{c})+4m(\mathcal{E}+m)(\mathbf{b}\cdot\mathbf{e}) \times(\mathbf{c}\cdot\mathbf{e})+4ma(\mathbf{b}\cdot\mathbf{e})(\mathbf{p}\cdot\mathbf{e}), \quad (30)$$

where all notations are exactly the same as in Eq. (27). In fact, in our present case $\mathbf{p}^2=\mathcal{E}^2-m^2$ and $(\mathbf{p}-\mathbf{k})\cdot\mathbf{e}=\mathbf{p}\cdot\mathbf{e}$, since $\mathbf{k}\perp\mathbf{e}$.

The formula for the photodetachment cross section is now written in the following form

$$d\sigma=\frac{e^2m\mathcal{E}}{\pi}\sqrt{\frac{\mathcal{E}+m}{\mathcal{E}-m}}[(\mathcal{E}-m)a^2+(\mathcal{E}+m)(\mathbf{b}-\mathbf{c})^2-2a\mathbf{p}\cdot(\mathbf{b}-\mathbf{c})+4(\mathcal{E}+m)(\mathbf{b}\cdot\mathbf{e})(\mathbf{c}\cdot\mathbf{e})+4a(\mathbf{b}\cdot\mathbf{e})(\mathbf{p}\cdot\mathbf{e})]d\Omega, \quad (31)$$

or, in other words [since $a=2m(\lambda_1+\lambda_2)$]

$$d\sigma=\frac{e^2m\mathcal{E}}{\pi}\sqrt{\frac{\mathcal{E}+m}{\mathcal{E}-m}}[4m^2(\mathcal{E}-m)(\lambda_1+\lambda_2)^2+(\mathcal{E}+m)(\lambda_1-\lambda_2)^2(\mathbf{p}-\mathbf{k})^2-4m(\lambda_1^2-\lambda_2^2)\mathbf{p}\cdot(\mathbf{p}-\mathbf{k})+4(\mathcal{E}+m)\lambda_1\lambda_2(\mathbf{p}\cdot\mathbf{e})^2+8m(\lambda_1^2+\lambda_1\lambda_2)(\mathbf{p}\cdot\mathbf{e})^2]d\Omega. \quad (32)$$

This formula can be rewritten to a slightly different form by introducing the polar angle θ between the directions of $\mathbf{p}$ and $\mathbf{k}$, i.e., $\cos\theta=(\mathbf{p}/|\mathbf{p}|)\cdot(\mathbf{k}/\omega)=\mathbf{p}\cdot\mathbf{k}/\omega\sqrt{\omega(E+m)}$. The azimuthal angle ϕ can be determined from the relation $\mathbf{p}\cdot\mathbf{e}=|\mathbf{p}|\sin\theta\cos\phi$. Moreover, it is straightforward to obtain that in our present case the following relations

$$\mathbf{p}^2-\mathbf{k}^2=2m(\mathcal{E}-m), \quad (\mathbf{p}-\mathbf{k})^2=2\mathcal{E}(\mathcal{E}-m)(1-v\cos\theta), \quad (33)$$

$$\mathbf{p}\cdot(\mathbf{p}-\mathbf{k})=(\mathcal{E}-m)(\mathcal{E}+m-\mathcal{E}v\cos\theta)$$

are obeyed. Here and below $v=|\mathbf{v}|$ is the velocity of the emitted photoelectron. In fact, in our present case $v=\sqrt{1-m^2/\mathcal{E}^2}=\sqrt{1-1/\gamma^2}$, where γ is the Lorentz γ factor, i.e., $\gamma=\mathcal{E}/m$.

Finally, one finds for the photodetachment cross section

$$d\sigma=\frac{2e^2m\mathcal{E}}{\pi}\sqrt{\mathcal{E}^2-m^2}[2m^2(\lambda_1+\lambda_2)^2+(\mathcal{E}+m)(\lambda_1-\lambda_2)^2(\mathcal{E}-\sqrt{\mathcal{E}^2-m^2}\cos\theta)-2m(\lambda_1^2-\lambda_2^2)(\mathcal{E}+m-\sqrt{\mathcal{E}^2-m^2}\cos\theta)+2(\mathcal{E}+m)^2\lambda_1\lambda_2\sin^2\theta\cos^2\phi+4m(\mathcal{E}+m)(\lambda_1^2+\lambda_1\lambda_2)\sin^2\theta\cos^2\phi]\sin\theta d\theta d\phi. \quad (34)$$

This form corresponds to the $\sigma(\mathcal{E})$ dependence. By substituting $\mathcal{E}=\omega+m$ one can obtain the explicit formula for the $\sigma(\omega)$ function. Another useful formula for the photodetachment cross section can be easily produced from the last equation by using the Lorentz γ factor.

In all formulas for the photodetachment cross sections presented above we assumed that the incident photons have a linear polarization $\mathbf{e}$. For unpolarized photons all these formulas must be averaged over the directions of $\mathbf{e}$. For the systems with central potential $V(r)$ in the last expression one has to replace $\overline{\cos^2\phi}$ by its averaged value $\frac{1}{2}(2\pi)=\pi$ and multiply all other terms by 2π. Indeed, according to Eqs. (33) for an arbitrary central potential $V(r)$ the constants λ_1 and λ_2 in the last equation can depend only on polar angle $\cos\theta$. Finally, one finds for the photodetachment cross section in the case of unpolarized photons and for a central potential $V(r)$,

$$d\sigma=4e^2m\mathcal{E}\sqrt{\mathcal{E}^2-m^2}[2m^2(\lambda_1+\lambda_2)^2+(\mathcal{E}+m)(\lambda_1-\lambda_2)^2\times(\mathcal{E}-\sqrt{\mathcal{E}^2-m^2}\cos\theta)-2m(\lambda_1^2-\lambda_2^2)(\mathcal{E}+m-\sqrt{\mathcal{E}^2-m^2}\cos\theta)+(\mathcal{E}+m)^2\lambda_1\lambda_2\sin^2\theta+2m(\mathcal{E}+m)\times(\lambda_1^2+\lambda_1\lambda_2)\cdot\sin^2\theta]\sin\theta d\theta. \quad (35)$$

In this case the differential cross section σ depends only upon the polar angle θ. In the general case of noncentral potential $V(\mathbf{r})$, the averaging of Eq. (34) over azimuthal angle ϕ is more complicated.

IV. DISCUSSION

The angular distribution of the emitted photoelectrons and correlations between $\mathbf{k}$ and $\mathbf{p}$ vectors are of specific interest in a number of applications. In general, to study the angular dependence for the photodetachment cross section one has to consider the explicit expressions for the factors λ_1 and λ_2 from the last equation. However, a few important conclusions can be deduced from the consideration of Eqs. (34) and (35). For instance, the main difference between our present case and nonrelativistic results from Ref. [1] can be formulated as follows. The right hand sides of Eqs. (34) and (35) include the linear and quadratic powers of $\cos\theta$, while in the nonrelativistic case [1], analogous expression contains only the quadratic powers of $\cos\theta$ [14]. This is mainly related to the fact that the dipole approximation is very accurate in the nonrelativistic case i.e., all corrections to the dipole approximation are relatively small. Note also, that formulas for the photodetachment cross sections obtained with the use of three-body approach also contain the linear powers of $\cos\theta$.

In the ultrarelativistic case ($\mathcal{E}\gg m$) Eq. (34) takes the form

$$d\sigma=\frac{2e^2m\mathcal{E}^2}{\pi}[2m^2(\lambda_1+\lambda_2)^2+\mathcal{E}^2(\lambda_1-\lambda_2)^2(1-\cos\theta)-2m\mathcal{E}(\lambda_1^2-\lambda_2^2)(1-\cos\theta)+2\mathcal{E}^2\lambda_1\lambda_2\sin^2\theta\cos^2\phi+4m\mathcal{E}(\lambda_1^2+\lambda_1\lambda_2)\sin^2\theta\cos^2\phi]\sin\theta d\theta d\phi. \quad (36)$$

For ultrarelativistic energies ($\mathcal{E}\gg m$) the distribution of the emitted photoelectrons is tipped forward and has a sharp maximum at very small polar angles $\theta=\arcsin(m/\mathcal{E})\approx(m/\mathcal{E})=(1/\gamma)$. For θ which are close to the maximal angle

$\theta_{max} \approx m/\mathcal{E}$ all terms in this expression can be written in the form $\mathcal{E}^2(m/\mathcal{E})^2 \sim m^2$, i.e., they are finite. However, the factor $\sin\theta d\theta \approx (1/\mathcal{E}^2) d\mathcal{E}/\mathcal{E}$ determines the final dependence of the photodetachment cross sections $\sigma(\mathcal{E})$ upon the photoelectron energy $\mathcal{E}$ [$\sigma(\mathcal{E}) \sim \mathcal{E}^{-2} \sim \gamma^{-2}$] in the ultrarelativistic case.

In the opposite (i.e., nonrelativistic) case, when $\omega \ll m$ (but $\omega \gg I$), the photodetachment cross-section $d\sigma$ can also be obtained from Eqs. (34) and (35). Only in this case one has to use the substitution $\mathcal{E} = m + \omega$, where the incident photon frequency ω is the small parameter. In this case, the explicit expression for the photodetachment cross section $d\sigma$, Eq. (34), takes the form

$$d\sigma = \frac{8e^2m^4}{\pi}\sqrt{2m\omega}\lambda_1^2 \sin^2\theta\cos^2\phi d\Omega$$

$$= \frac{\alpha}{2\pi}\sqrt{2m\omega}\Phi^2(\mathbf{p}-\mathbf{k})\sin^2\theta\cos^2\phi \sin\theta d\theta d\phi. \tag{37}$$

As follows from this formula the nonrelativistic photodetachment cross section $d\sigma$ is invariant under $\theta \to \pi - \theta$ transformation. Moreover, if $\Phi(\mathbf{p}-\mathbf{k})$ is a regular (i.e., analytic) function of $\mathbf{p}-\mathbf{k}$, then such cross sections explicitly depend on semi-integer powers of ω. Also, the non-relativistic photodetachment cross-section contains only the Fourier transform of the bound-state wave function and does not include the Fourier transform of the potential $V(r)$. Furthermore, the factor $\sin^2\theta\cos^2\phi \sim (\mathbf{e}\cdot\mathbf{p})^2$ represents the well-known photon-electron momentum correlation for the low-energy photodetachment of arbitrary two-body systems. In fact, all mentioned properties of the nonrelativistic photodetachment cross sections are supported by the results of numerous experiments and earlier theoretical studies (see, e.g., Refs. [8,15], and references therein).

Let us consider the case of Coulomb potential $V(r) = -Ze^2/r$. In the considered nonrelativistic case ($\omega \ll m$, but $\omega \gg I$) the normalized solution of the appropriate Schrödinger equation (ground state) takes the form (in relativistic units)

$$\Psi(\mathbf{r}) = \frac{Z^{3/2}e^3m^{3/2}}{\sqrt{\pi}}\exp(-Ze^2mr), \tag{38}$$

and therefore,

$$\Phi(\mathbf{p}-\mathbf{k}) = \frac{8\sqrt{\pi}Z^{5/2}e^5m^{5/2}}{(\mathbf{p}-\mathbf{k})^4}. \tag{39}$$

Now, one easily finds

$$d\sigma = \alpha\sqrt{2m\omega}\,\frac{32Z^5e^{10}m^5}{(\mathbf{p}-\mathbf{k})^8}\sin^2\theta\cos^2\phi d\Omega. \tag{40}$$

By using Eq. (33) one finds $(\mathbf{p}-\mathbf{k})^4 = 16\mathcal{E}^4\omega^4(1-v\cos\theta)^4 \approx 16m^4\omega^4(1-v\cos\theta)^4$. Also, the integration over spherical angles gives the factor $(4\pi/3)$. Finally, we have for the total photodetachment cross section

$$\sigma = \alpha(2m)^{1/2}\frac{8\pi Z^5e^{10}m^5}{3m^4\omega^{7/2}} = \alpha\frac{64\pi Z^5}{3m^2e^4}\left(\frac{e^4m}{2\omega}\right)^{7/2}$$

$$= \frac{64\pi Z^5}{3}\alpha a_0^2\left(\frac{I_0}{\omega}\right)^{7/2}, \tag{41}$$

where $I_0 = (e^4m/2\omega)$ is the ionization potential (in this case) and $a_0 = (me^2)^{-1}$ is the Bohr radius. The last result coincides exactly with the known formula for the one electron, multi-charged ions with the nuclear charge Z (see, e.g., Ref. [16]). In this case, the asymptotic behavior of the cross section $\sim (I_0/\omega)^{7/2}$ is correct only if $\omega \ll m$. For higher energies of the incident photon ω all terms from Eq. (34) are also contributed.

The second coefficient λ_2 ($\lambda_2 \approx \alpha\lambda_1$) in Eqs. (34)–(36) contains the factor $W(\mathbf{p}-\mathbf{k})$, which is the Fourier transform of the model interaction potential $V(\mathbf{r})$. In general, the $W(\mathbf{p}-\mathbf{k})$ function essentially coincides with the scattering amplitude $f_B(\mathbf{p}-\mathbf{k})$ computed in the Born approximation (see, e.g., Ref. [17]). By using this scattering (Born) amplitudes one can rewrite our formulas for the photodetachment cross section Eqs. (34) and (35) in a number of different forms. In general, this means that, if the nonrelativistic scattering amplitude $f_B(\mathbf{p}-\mathbf{k})$ is known, then the reconstruction of the relativistic photodetachment cross section simplifies significantly.

Thus, as follows from Eqs. (34)–(36) the relativistic photodetachment cross section can be reconstructed completely, if the radial δ function $\Psi(r=0)$ and Fourier transforms of the wave function $\Psi(\mathbf{r})$ and potential $V(\mathbf{r})$ are known. For some potentials $V(r)$ the corresponding Schrödinger equation can be solved analytically, but in actual applications the bound-state wave function $\Psi(\mathbf{r})$ is usually approximated numerically by using, e.g., the exponential variational expansion. Also, note that for the considered negative ions Ps^- and H^- the model potential $V(r)$ must be reconstructed as a short range, non-Coulomb potential. A very good choice for the model potential $V(r)$ is the regularized polarization potential [18,19] which has the correct asymptotic form $V_A(r)$ at large r and has no singularity at $r=0$. For the considered Ps^- and H^- ions the correct asymptotic form $V_A(r)$ is [19]

$$V_A(r) = -\frac{A_1}{2r^4} - \left(\frac{A_2}{2} + 3B_1\right)\frac{1}{r^6} + O\left(\frac{1}{r^7}\right), \tag{42}$$

where A_1 and A_2 are the dipole and quadruple polarizabilities, respectively, while B_1 is the nonadiabatic term. In general, the regularized polarization potential can be chosen in a few different forms, which include some numerical parameters. Later, such parameters can be varied to make the potential $V(r)$ more realistic. The realistic potentials $V(r)$ must reproduce quite accurately the bound-state energies for the ground $S(L=0)$ states in the Ps^- and H^- ions (all excited states in these systems must be unbound). Moreover, such a potential must also be able to reproduce all known scattering data (phase shifts, or cross sections) for the (e^-,Ps) and (e^-,H) scattering. The results of our numerical study with some model potentials will be published elsewhere.

The formulas obtained above can also be used to produce (evaluate) the photorecombination cross section σ_R, which is of great interest in astrophysics. By using the principle of detailed balancing (see, e.g., Ref. [13]) one finds the following relation between the corresponding cross sections $g_i p_i^2 \sigma_{i\to f} = g_f p_f^2 \sigma_{f\to i}$. Here $g_a (a=i,f)$ are the statistical weights of the incident and final states, $p_a (a=i,f)$ are the momenta of the relative motion of the particles, while $\sigma_{i\to f}$ and $\sigma_{f\to i}$ are the corresponding cross sections (for the direct and inverse processes). In our present case, $g_i = 2$ for the photon. Finally, we find for the photorecombination cross section $\sigma_R(\mathcal{E})$

$$\sigma_R(\mathcal{E}) = \frac{2\omega}{2m+\omega}\sigma_P(\mathcal{E}) = \frac{2\hbar\omega}{2mc^2+\hbar\omega}\sigma_P(\mathcal{E}), \qquad (43)$$

where $\sigma_P(\mathcal{E})$ is the photodetachment cross section determined for the same electron energy [Eqs. (34)–(36)].

In conclusion, it should be mentioned that the approach used in our present study is based on a few approximations. First, the model potential $V(r)$ is relatively weak, i.e., it is small in comparison to the rest mass of the electron m. Furthermore, we have made an assumption that the maximal electron momentum p cannot exceed the value $\alpha(mc)$ [in relativistic units $\alpha(mc)=1$]. This means that our present approach cannot be applied to describe the photodetachment of internal electron shells in heavy atoms and ions. Another restriction of this approach is related with the ignored electron-electron correlations in the Ps^- and H^- ions. However, the electron-electron correlations are extremely important to obtain the correct bound-state spectra in these ions. In fact, the boundness of the ground $S(L=0)$ states in the Ps^- and H^- ions can easily be shown by using the fully correlated trial wave functions written in the relative three-body coordinates r_{32}, r_{31}, and r_{21} [20]. In contrast with this, the Hartree-Fock and other similar (i.e., one particle) methods fail to reproduce the bound states in the Ps^- and H^- ions.

In addition to the electron-electron correlations in the model potential approach developed above we have neglected all effects arising from the electron-electron permutations. In fact, the both Ps^- and H^- ions are the two-electron systems, i.e., their wave functions must be antisymmetric under the simultaneous interchange of the spatial and spin coordinates of the two electrons. This ensures that the Pauli exclusion principle is satisfied. In fact, the photodetachment of the Ps^- and H^- ions by high-energy photons can accurately be described only in terms of the three-body approach. The model potential approach developed above can be considered as the first approximation to actual systems, which, however, gives a correct qualitative account of the relativistic photodetachment of the Ps^- and H^- ions. Likewise, this method has a significant flexibility, since by varying the nonlinear parameters in the model potential $V(r)$ one can easily improve the final agreement with the experimental data. In fact, we expect that the maximal deviation between our present results and results produced by the three-body approach will not exceed $\approx 5-10$ %.

V. CONCLUSION

Thus, in our present study we have considered the photodetachment of the positronium negative ion (Ps^-) by high-energy photons $\hbar\omega \approx m_e c^2$. Our analysis is based essentially on the model potential approximation. Briefly, this means that the original three-body, weakly bound system is replaced by a model two-body system with some effective interaction potential $V(r)$. Finally, the photodetachment cross section is represented by the two parameter formulas [see Eqs. (34)–(36)]. For any given values of these two parameters [λ_1 and λ_2 in Eqs. (34)–(36)] the photodetachment cross section is uniformly determined. In general, the λ_1 and λ_2 parameters are easily determined by using the potential- and bound-state wave functions of the Schrödinger equation. The results of this study can be applied to describe the relativistic photodetachment in various systems, including the negative ions of light elements and arbitrary three- and few-body systems with unit charges.

It is interesting to note a few differences between our present results Eqs. (34)–(36) and nonrelativistic photodetachment of the Ps^- ion considered in Ref. [1]. The main difference can be found for the angular dependence of the relativistic and nonrelativistic photodetachment cross sections. The nonrelativistic photodetachment cross section [1] contains terms that are either constants (upon θ), or include factor $\sim\cos^2\theta$, where $\cos\theta \sim (\mathbf{k}\cdot\mathbf{p})$. In other words, the nonrelativistic photodetachment cross section is invariant under the $\theta \to \pi - \theta$ transformation. In the relativistic case, the photodetachment cross sections for the Ps^- and H^- ions also include terms which are linear upon $\cos\theta$. The general dependence of the relativistic photodetachment cross-section upon $\cos\theta$ takes a very complicated form, since each of the two parameters λ_1 and λ_2 in Eqs. (34)–(36) is also θ dependent. This means that the relativistic photodetachment cross-section is not invariant under the $\theta \to \pi - \theta$ transformation. In the ultrarelativistic case the distribution of the emitted photoelectrons is confined to small angles in the forward direction. The photodetachment cross section $d\sigma$ falls off in photoelectron energy $\mathcal{E}$ approximately as $\mathcal{E}^{-2}$. However, its final asymptotic form depends on the considered potential $V(r)$ and nonrelativistic wave function $\Psi(\mathbf{r})$.

In fact, our present approach allows one to obtain the explicit and relatively simple formulas for the photodetachment cross sections of any weakly bound system, including the Ps^- and H^- ions. Such formulas can be used to determine the photodetachment cross sections for various energies of incident photon, e.g., in the ultrarelativistic, relativistic and semirelativistic cases and also to produce the classical limit. Our present approach is also very useful for the understanding of all important features of the relativistic photodetachment in weakly bound systems. Moreover, we expect that this approach must also be quite accurate quantitavely in actual applications. However, the model potential approach is only an approximate method which ignores all electron-electron correlations in the considered Ps^- and H^- ions as well as the Pauli principle for two- and many-electron systems. In our next study [12] a more accurate three-body ap-

proach is developed which allows one to consider all three-body effects missing in the course of our present analysis. In conclusion, it is important to note that for the considered energies of incident photons ($\hbar\omega \geqslant 100$ keV) the photodetachment of the Ps^- and H^- ions is the dominant photon-ion process, since its cross section significantly exceeds the cross sections of all other photon-ion processes, e.g., the Rayleigh scattering, Compton scattering, and some others (see, e.g., Ref. [21]).

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