Photodetachment of the outer-most electrons in few- and many-electron atomic systems

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(Dated: May 8, 2020)

Abstract

Photodetachment of the outer-most electrons in few- and many-electron atomic systems is studied in the non-relativistic dipole approximation. Such a photodetachment is analyzed for the neutral atoms and positively charged atomic ions. We also investigate photodetachment of the outer-most electrons in the negatively charged atomic ions, including the negatively charged hydrogen ion. In all these cases we have derived the closed analytical formulas for the photodetachment cross-section(s) of the outer-most electrons.

PACS number(s): 32.80.Fb, 32.80.Gc and 32.90.+a

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I. INTRODUCTION

In this communication we investigate photodetachment of the outer-most electrons in various atomic systems which include some few- and many-electron atoms and ions. Different solutions of this problem are of great interest in a large number of actual situations which can be found in many stellar and laboratory plasmas. In stellar astrophysics photodetachment of the outer-most electrons in the neutral atoms and ions is very important to understand and describe opacities of stellar photospheres which crucially depend upon surface temperatures, pressures and other factors. For instance, for very hot $O-$stars, where the surface temperatures exceed 75,000 $K$ - 90,000 $K$ (and even 125,000 $K$ for some stars), we have to deal with photoionization of the neutral He atoms and positively charged, one-electron He$^+$ ions. Opacities of photospheres of less hotter $B$ stars (e.g., Rigel), where the surface temperatures $\approx$ 18,000 $K$ - 27,000 $K$, are determined by photodetachments of the neutral hydrogen atoms. There is a separate group of interesting $Be-$stats, which are the stars with rapidly rotating rings of hydrogen atoms and molecules, e.g., $\gamma-$Cassiopeiae. In such systems the hot central star illuminates all surrounding hydrogen rings. Stellar radiation is absorbed by atoms of hydrogen, which move in the ring, and then re-emitted (with smaller frequencies) in all directions. An observer from the distance in a few hundreds of light years can see the regular (or thermal) spectrum of the central star which is combined with one (or a few) sharp and very intense spectral lines, e.g., the red hydrogen line(s) in the spectrum of $\gamma-$Cassiopeiae. Photodetachment of the negatively charged hydrogen $H^-$ ions plays a great role in the actual optical and infrared spectra of many late $F$- and for all $G-$star (see discussion and references in [1]). Our Sun is a star which belongs to the $G2$ spectral class and its average surface temperature is $\approx 5,773 K$. If photodetachment of the negatively charged ions in Solar photosphere is ignored, then it is impossible to explain the actual spectrum of our Sun located between $\approx 6500 \, \text{Å}$ and 20,000 $\text{Å}$, i.e., the both optical and infrared spectra \[2 - 5\].

Photodetachment of atomic systems is defined as absorption of a photon by some bound atomic electron which produces an instant transition of this electron into unbound state. The arising unbound (or 'free') electron moves away from the parental atom/ion in the Coulomb field of the final atomic ion. In the case of negatively charged $H^-$ ion the unbound photoelectron moves in the field of the neutral hydrogen atom. The main goal of this
study is to analyze photodetachment of the outer-most electrons in different atomic systems and derive closed analytical formulas for the photodetachment cross-sections (differential and total). First, we consider photodetachment of the outer-most electrons in the few- and many-electron atoms and positively charged ions. Then, we discuss photodetachment of one-electron atoms and ions. The third problem considered in this study is photodetachment of the outer-most electrons in negatively charged ions. Our main goal is to derive explicitly all analytical formulas for differential and total cross-sections of photodetachment. Also, we want to discuss applications of these formulas to some actual systems.

Note that the general theory of photodetachment is a well developed chapter of modern Quantum Electrodynamics (see, e.g., [6] - [8]). Formulas for the differential and total cross-sections of photodetachment were derived and discussed in [6] - [8]. This fact allows us to reduce the introductory part and proceed directly to derivation of important formulas and discussion of our original results.

II. PHOTODETACHMENT CROSS-SECTION

The differential cross-section of the non-relativistic photodetachment of an arbitrary atomic system is written in the following form

\[
d\sigma = \frac{e^2 m}{2\pi \omega} \left| \frac{e}{p} \cdot \mathbf{v}_{fi} \right|^2 \, d\omega = \frac{p}{2\pi \omega a_0} \left| \frac{e}{p} \cdot \mathbf{v}_{fi} \right|^2 \, d\omega
\]

where \( m \) is the rest mass of electron, \( a_0 \) is the Bohr radius, while \( -e \) is its electric charge and \( e \) is the vector which describes the actual polarization of initial photon. Also, in this formula \( p = |\mathbf{p}| \) is the momentum of the final (or free) photoelectron, \( \omega \) is the cyclic frequency of the incident light quanta, while \( \mathbf{v}_{fi} \) is the matrix element of the ‘transition’ velocity \( \mathbf{v}_{fi} \). For this matrix element we can write \( \mathbf{v}_{fi} = -\frac{i}{\hbar} \langle \psi_f | \nabla | \psi_i \rangle \). The indexes \( f \) and \( i \) in this equation and in all formulas below stand for the final and initial sates, respectively. The formula, Eq. (1), is written in the relativistic units where \( \hbar = 1, c = 1, e^2 = \alpha \) and \( \alpha \) is the fine-structure constant. These relativistic units are convenient to perform analytical calculations in Quantum Electrodynamics. However, in order to determine the non-relativistic cross-sections it is better to apply either the usual units, or atomic units in which \( \hbar = 1, m_e = 1 \) and \( e = 1 \). The formula, Eq. (1), can be re-written in the usual units

\[
d\sigma = \frac{\alpha a_0^2 \mu}{2\pi \omega} \left| \psi_f \langle \psi_f | \nabla | \psi_i \rangle \right|^2 \, d\omega
\]
where \( a_0 = \frac{\hbar^2}{mc} \) is the Bohr radius and \( \alpha = \frac{e^2}{\hbar c} \) is the fine-structure constant. In atomic units \( a_0 = 1 \) and \( \alpha = \frac{1}{\epsilon} (\approx \frac{1}{137}) \). Let us assume that initial electron was bound to some atomic system, i.e., to a neutral atom, negatively and/or positively charged ion. The energy of this bound state (or discrete level) is \( \varepsilon = -I \), where \( I \) is the atomic ionization potential. It is clear that the following relations \( \omega = I + \frac{1}{2}p^2 \) and \( \omega \geq I \) must always be obeyed during photodetachment, where \( p \) is the momentum of the final photoelectron.

### A. Wave functions of the final and initial states

Now, we need to develop a logically closed procedure to calculate the matrix element (or transition amplitude) \( \langle \psi_f | \nabla | \psi_i \rangle \) which is included in the formulas, Eq.\( (2) \). Everywhere below, we shall assume that the original (or incident) system was in its lowest-energy (or ground) singlet (or doublet) \( S(L = 0) \)–state. For one-electron atomic system this state is always designated as the doublet \( 1^2s(\ell = 0) \)–state. In the lowest order dipole approximation the outgoing (or final) photoelectron moves in the \( p(\ell = 1) \)–wave. By using this fact we can write the following expression for the wave function of this final electron

\[
\psi_f(r) = \frac{2\ell + 1}{2p} P_{\ell}(nn_1) \psi_{\ell,p}(r) = (nn_1) \frac{3}{2p} \psi_{1,p}(r) = (nn_1) R_{1,p}(r) \tag{3}
\]

where \( \ell = 1, P_{\ell}(x) \) is the Legendre polynomial (see, e.g., [11]) and \( R_{\ell=1,p}(r) = R_{1,p}(r) \) is the corresponding radial function which depends upon the explicit expression for the interaction potential between the outgoing photoelectron and remaining atomic system. Also, in this formula the unit vectors \( n \) and \( n_1 \) are: \( n = \frac{p}{r} \) and \( n_1 = \frac{\xi}{r} \). The unit vector \( n \) determines the direction of outgoing (or final) photoelectron.

If the interaction potential between the outgoing electron and remaining atomic system is a Coulomb potential, then the radial function is the normalized Coulomb function of the first kind (see, e.g., [12]). With the additional factor \( \frac{3}{2p} \) from Eq.\( (3) \) we can write for \( \ell = 1 \) (in atomic units)

\[
R_{1,p}(r) = \sqrt{\frac{2\pi\nu(1 + \nu^2)}{1 - \exp(-2\pi\nu)}} \frac{(pr) \exp(-i\nu r)}{1F_1(2 + \nu; 4; 2ir)} \tag{4}
\]

where the parameter \( \nu \) equals \( \nu = \frac{Z}{p} \) and \( Z \) is the effective electric charge of the remaining (or central) atomic system. In general, the effective electric charge \( Z \) is an increasing function of the nuclear charge \( Q \), but it also depends upon the total number of bound electrons \( N_e \). All
phases and normalization factors in this formula are chosen exactly as in [9]. For the non-Coulomb interaction potential the normalized radial wave function of the continuous spectra is represented as the spherical Bessel function $j_\ell(pr) = j_1(pr)$ which is regular at $r = 0$. In this case final wave function takes the form

$$R_{1,p}(r) = \frac{3}{2p} j_{\ell=1}(pr) = \frac{3}{2p} \sqrt{\frac{\pi}{2pr}} J_{\frac{3}{2}}(pr)$$

(5)

where $j_1(x) = \frac{\sin x}{x} - \frac{\cos x}{x^2}$ and $J_{\frac{3}{2}}(x)$ is the regular at $r = 0$ Bessel function defined in [11].

As mentioned above our goal in this study is to derive the explicit formulas for the photodetachment cross-sections in a number actual cases which differ from each other by the choice of the initial and final wave functions. The two possible wave functions of the final unbound state(s) are mentioned above. Now, let us discuss the wave functions of the incident atomic states in atomic one-center system which has one nucleus with the electric charge $Q$ (or $Qe$) and $N_e$ bound electrons. By analyzing the current experimental data it is easy to understand that non-relativistic photodetachment of the outer-most electrons in a few- and many-electron atomic systems is produced by photons, which have very large wavelengths $\lambda$. In reality, wavelengths of incident light quanta substantially exceed the actual sizes of atoms and ions. For instance, the wavelengths $\lambda$ of photons that produce photodetachment of a negatively charged hydrogen ions in Solar photosphere exceed 7,000 Å, or 11,000 a.u., while the spatial radius $R$ of this ion is only $\approx 2.710\ldots$ a.u. (see e.g., [21]), i.e., $R \ll \lambda$. In other words, photodetachment of the outer-most electron in the $\mathrm{H}^-$ ion is produced at large and very large distances from atomic nucleus, i.e., in asymptotic areas (areas at very large $r$) of the wave function of this ion ($\mathrm{H}^-$). Only in these spatial areas there is a relatively large overlap of the electron and photon wave functions. Similar situations can be found for other neutral atoms and positively charged ions. For each of these Coulomb systems photodetachment of the outer-most electrons occurs in the asymptotic areas of their wave functions. Therefore, we can restrict ourselves to these spatial areas and consider below only the long-range asymptotics of these wave functions. Briefly, this means that we can consider the long-range radial asymptotics of the wave functions as the actual wave functions for each of these atomic systems. In other words, to a very good accuracy we can neglect by the 'correlated' part of atomic wave functions, which is located in the volume of initial atom/ion, and deal with the long-range radial asymptotics of this wave function only. The overall accuracy of such a re-definition of the wave function has been tested many times for
different atomic systems by comparing the photodetachment cross-sections computed in the both ways.

As mentioned above in this study we consider the three following atomic systems: (a) atom/ion which initially contains $N_e$ bound electrons, (b) one-electron atom/ion, where $N_e = 1$, and (c) negatively charged ion where $Q = N_e + 1$. As is well known (see, e.g., [10]) in any atomic $(Q, N_e)$-system the radial wave function of the ground $S(L = 0)$-states has the following long-distance asymptotics

$$R_s(r) = C(b; I)r^{b-1} \exp(-\sqrt{2I}r) = \frac{(2\sqrt{2I})^{b+\frac{1}{2}}}{2\sqrt{\pi\Gamma(2b+1)}} r^{b-1} \exp(-\sqrt{2I}r) = \frac{(2\sqrt{2I})^{b+\frac{1}{2}}}{2\sqrt{\pi\Gamma(2b+1)}} r^{\frac{Q-N_e+1}{\sqrt{2I}}-1} \exp(-\sqrt{2I}r)$$

(6)

where $b = \frac{Q-N_e+1}{\sqrt{2I}} = \frac{Z}{\sqrt{2I}}$ and $Z = Q - N_e + 1$ (or $Z = (Q - N_e + 1)e$) is the electric charge of the remaining atom/ion. In this equation and everywhere below in this study the notation $\Gamma(x)$ denotes the Euler’s gamma-function $\Gamma(1 + x) = x\Gamma(x)$ (also called Euler’s integral of the second kind [11]). The factor $C(b; I)$ is the normalization constant of the radial $R_s(r)$ function, which is supposed to be continued on the whole real axis and includes the radial origin, i.e., the point $r = 0$ (applicability of such a continuation and overall accuracy of this procedure is discussed below). The normalization constant for this radial $R_s(r)$ function, Eq. (6), is

$$C(b; I) = \frac{(2\sqrt{2I})^{b+\frac{1}{2}}}{2\sqrt{\pi\Gamma(2b+1)}}$$

(7)

where the atomic ionization potential $I$ and ‘power parameter’ $b$ are the two real, non-negative numbers. In some places below the $\sqrt{2I}$ value is also designated as $B$.

Now, note that for neutral few-electron atoms we have $Q = N_e$ and $b = \frac{1}{\sqrt{2I}}$, while for the negatively charged (atomic) ion we can write $b = \frac{Q-N_e+1}{\sqrt{2I}} = 0$. This means that the long-distance asymptotic of the radial wave function of an arbitrary negatively charged ion is $R(r) \sim \frac{C}{r} \exp(-\sqrt{2I}r)$, where $C$ is some numerical constant (below we choose $C = \left(\frac{4}{\pi}\right)^{\frac{3}{2}}$), which is often called the normalization constant. For one-electron atom we have $N_e = 1$ and $2I = Q^2$. Therefore, in this case $b = 1$ and we can write the exact wave function of an arbitrary one-electron atom/ion in the form $R(r; Q) = A \exp(-\sqrt{2I}r)$, where $2I = Q^2$, and $A = \frac{Q\sqrt{\pi}}{\pi}$ is the normalization constant. This case is important in applications to some actual one-electron atoms and positively charged ions.
B. Gradient operator and its matrix elements

Let us derive the formulas for the \( \langle \psi_f | \nabla | \psi_i \rangle \) matrix element. It is clear that we need to determine the vector-derivative of the initial wave function. In general, for the interparticle (or relative) \( r_{ij} = r_j - r_i \) vector the corresponding gradient operator in spherical coordinates takes the form (see, e.g., [13] and [14])

\[
\nabla_{ij} = \frac{d}{dr_{ij}} = \frac{r_{ij}}{r_{ij} \partial r_{ij}} + \frac{1}{r_{ij}} \nabla_{ij}(\Omega) = e_{r_{ij}} \frac{\partial}{\partial r_{ij}} + e_{\theta_{ij}} \frac{1}{r_{ij}} \frac{\partial}{\partial \theta_{ij}} + e_{\phi_{ij}} \frac{1}{r_{ij} \sin \theta_{ij}} \frac{\partial}{\partial \phi_{ij}}
\]

where \( \nabla_{ij}(\Omega) \) is the angular part of the gradient vector which depends upon angular variables \((\theta, \phi)\) only, while \( e_{r_{ij}} = \frac{r_{ij}}{r_{ij}} = n_{ij}, e_{\theta_{ij}} \) and \( e_{\phi_{ij}} \) are the three unit vectors in spherical coordinates which are defined by the \( r_j \) and \( r_i \) vectors, where \( r_j \neq r_i \). More details and more useful formulas for the gradient operator(s), written in spherical coordinates, can be found, e.g., in § 5.7 of the excellent book by Edmonds [15].

If the radial parts of the both initial and final wave functions depend upon the radial variable only, then all derivatives in respect to the angular variables \( \theta \) and \( \phi \) equal zero identically and we can write

\[
\nabla_{ij} R(r; Q) = \frac{r_{ij}}{r_{ij}} \frac{\partial R(r_{ij}; Q)}{\partial r_{ij}} = \frac{r_{ij}}{r_{ij}} \frac{dR(r_{ij}; Q)}{dr_{ij}} = n_{ij} \frac{dR(r_{ij}; Q)}{dr_{ij}}
\]

where \( n_{ij} \) is the unit vector in the direction of the inter-particle \( r_{ij} \) variable. For one-center atomic systems we can determine \( r_{ij} = r_j \), and for one-electron systems \( r_{ij} = r_1 = r \). In this case, the formula, Eq. (9), for the inter-particle gradient is written in the form:

\[
\nabla R(r; Q) = n_1 \frac{dR(r)}{dr}
\]

(11)

where \( R_1(p; r) \) and \( R_i(r; Q) \) are the radial functions (or radial parts of the total wave functions) of the final and initial states, respectively. Sometimes these wave functions are considered and the wave functions of the initial and final electrons. The notation \( I_{rd} \) in this formula, Eq. (10), stands for the auxiliary radial integral

\[
I_{rd} = \int_0^{+\infty} \left( R_1(p; r) \frac{dR_1(r; Q)}{dr} \right) r^2 dr = - \int_0^{-\infty} \left( R_i(r; Q) \frac{dR_1(p; r)}{dr} \right) r^2 dr
\]

(11)
where we used the so-called 'transfer of the derivative' which is often helps to simplify analytical calculations of this radial integral.

By substituting the expression, Eq.\((\text{10})\), into the formula, Eq.\((\text{2})\), one finds the following 'final' formula for the differential cross-section of the non-relativistic photodetachment of an arbitrary atomic system

\[
d\sigma = \frac{16\pi^2\alpha a_0^2 p}{18\pi \omega} (e \cdot n)^2 |I_{rd}|^2 \, do = \frac{8\pi \alpha a_0^2 p}{9\omega} (e \cdot n)^2 |I_{rd}|^2 \, do
\]

As follows from this formula the angular distribution of photoelectrons is determined by the 'angular' factor \((e \cdot n)^2\). This expression corresponds is the cross-section of photodetachment which corresponds to the truly (i.e., 100 %) polarized light. However, in many actual applications the incident beam of photons is unpolarized (so-called 'natural', or 'white' light). If the incident beam of photons was unpolarized, then we need to apply the formula \((e \cdot n)^2 = \frac{1}{2} (n_l \times n)^2\), where \(n_l\) is the unit vector which describes the direction of incident light propagation and \(n\) is the unit vector which determines the direction of final photoelectron propagation. The notation \((a \times b)\) designates the vector product of the two vectors \(a\) and \(b\). Finally, the differential cross-section of photodetachment takes the form

\[
d\sigma = \left(\frac{8\pi \alpha a_0^2 p}{9\omega}\right) (n_l \times n)^2 |I_{rd}|^2 \, do = \left(\frac{8\pi \alpha a_0^2}{9\omega}\right) \left(\frac{p}{\omega}\right) \sin^2 \Theta |I_{rd}|^2 \, do
\]

where \(\Theta\) is the angle between two unit vectors \(n_l\) and \(n\). The presence of vector product \((n_l \times n)^2\) in Eq.\((\text{13})\) is typical for the dipole approximation. As follows from the formula, Eq.\((\text{13})\), analytical and numerical calculations of the differential cross-section of photodetachment is reduced to analytical computation of the auxiliary radial integral \(I_{rd}\), Eq.\((\text{11})\). By using different expressions for the initial and final wave functions we can solve the problem of photodetachment of the outer most electrons in a few- and many-electron atomic systems. This problem is considered below.

### III. PHOTODETACHMENT OF THE FEW-ELECTRON NEUTRAL ATOMS AND POSITIVELY CHARGED IONS

First, let us consider photodetachment of the outer-most electron(s) in neutral atoms, where \(Q = N_e\), and in positively charged ions, where \(Q > N_e\). In both these cases in the final sub-systems, i.e., outgoing photo-electron and remaining positively charged ion,
interact with each other by an attractive Coulomb potential. In this case the wave function of outgoing photoelectron must be taken in the form of Eq. (1), while the wave function of the initial atomic state is chosen in the form of Eq. (6). The radial derivative of this initial wave function is

\[ \frac{d}{dr} [r^{b-1} \exp(-Br)] = (b - 1)r^{b-2} \exp(-Br) - Br^{b-1} \exp(-Br) \]  

(14)

where \( b = \frac{Q - N_e + 1}{\sqrt{2I}} = \frac{Z}{p} \) and \( B = \sqrt{2I} \). Therefore, the formula for our auxiliary radial integral \( I_{rd} \), Eq. (11), includes two terms, i.e., \( I_{rd} = I_{rd}^{(1)} + I_{rd}^{(2)} \), where

\[ I_{rd}^{(1)} = p \sqrt{\frac{2\pi \nu (1 + \nu^2)}{1 - \exp(-2\pi \nu)}} C(b; B)(b - 1) \int_0^{+\infty} r^{(b+2)-1} \exp(-Br - ipr)_{1} F_{1}(2 + \nu; 4; \) \]

\[ 2ipr)dr = p \sqrt{\frac{2\pi \nu (1 + \nu^2)}{1 - \exp(-2\pi \nu)}} C(b; B) (b - 1) \Gamma(b + 2) \frac{(b + 2)}{(B + ip)^{b+2}} 2F_{1}(2 + \nu; b + 2; 4; \frac{2ip}{B + ip}) \]  

(15)

\[ = p \sqrt{\frac{2\pi \nu (1 + \nu^2)}{1 - \exp(-2\pi \nu)}} C(b; B) (b - 1) \Gamma(b + 3) \frac{B \Gamma(b + 3)}{(B + ip)^{b+3}} 2F_{1}(2 + \nu; b + 3; 4; \frac{2ip}{B + ip}) \]  

(16)

where \( \nu = \frac{Z}{p} \), where \( Z = Q - N_e + 1 \), while \( C(b; B) \) is the normalization constant of the bound state radial function (see below). The explicit formula for the second radial integral \( I_{rd}^{(2)} \) is

\[ I_{rd}^{(2)} = -p \sqrt{\frac{2\pi \nu (1 + \nu^2)}{1 - \exp(-2\pi \nu)}} C(b; B) (b + ip)^{b+2} \int_0^{+\infty} r^{(b+3)-1} \exp(-Br - ipr)_{1} F_{1}(2 + \nu; 4; \) \]

\[ 2ipr)dr = -p \sqrt{\frac{2\pi \nu (1 + \nu^2)}{1 - \exp(-2\pi \nu)}} C(b; B) (b + ip)^{b+3} \frac{B \Gamma(b + 3)}{(B + ip)^{b+3}} 2F_{1}(2 + \nu; 1 - b; 4; \frac{B - ip}{B + ip}) \]

(15)

where \( C(b; B) \) is the normalization constant, Eq. (17), and \( B = \sqrt{2I} \), where \( I \) is the ionization potential. To simplify the two last formulas we note that

\[ \left( \frac{B + ip}{B - ip} \right)^{\nu} = \left( \frac{\nu + 1}{\frac{B}{b} - \nu} \right)^{\nu} = \exp[-2\nu \arctan\left(\frac{\nu}{b}\right)] \]  

(17)

where \( \nu = \frac{Z}{p} = \frac{Q - N_e + 1}{p} \) and \( b = \frac{Q - N_e + 1}{\sqrt{2I}} \) (here \( Z = Q - N_e + 1 \), see above) and \( \frac{B}{p} = \frac{\nu}{b} \), or \( \nu = \frac{bB}{p} \).

After a few additional, relatively simple steps of transformations we can write the following expression for the total radial integral \( I_{rd} = I_{rd}^{(1)} + I_{rd}^{(2)} \):

\[ I_{rd} = p \sqrt{\frac{2\pi \nu (1 + \nu^2)}{1 - \exp(-2\pi \nu)}} C(b; B) \frac{\Gamma(b + 2)(B - ip)^{1-b}}{(B^2 + p^2)^2} \exp[-2\nu \arctan\left(\frac{\nu}{b}\right)](b - 1) \times \]
\[(B - ip) \ 2F_1(2 - \nu; 2 - b; 4; \frac{B - ip}{B + ip}) - B (b + 2) \ 2F_1(2 - \nu, 1 - b; 4; \frac{B - ip}{B + ip}) \]\]

From this expression one easily finds the following formula for the \(|I_{rd}|^2\) value

\[|I_{rd}|^2 = \frac{4^b (Q - N_e + 1)^2 (1 + \nu^2) B^{2b+1}}{\nu (1 - \exp(-2\pi\nu))} \frac{\Gamma^2(b + 2)}{\Gamma(2b + 1)} \frac{B^2 + p^2)^{2-b}}{\Gamma(2b^2 + 1)} \frac{1}{1 - b} \frac{d}{dz} 2F_1(2 - \nu, 1 - b; 4; z) (20)\]

By multiplying this expression by the \((\frac{8\pi a^2 \mu p}{9\nu}) (n_l \times n)^2\) factor one finds the final formula for the differential photodetachment cross-section, Eq.(13), of the few- and many-electron neutral atoms and/or positively charged ions each of which contains \(N_e\) bound electrons, while the electric charge of the central nucleus equals \(Q\).

Now, by using the formula, Eq.(19), derived above it is straightforward to obtain the explicit formulas for the both differential and total cross-sections of photodetachment of the few-electron neutral atoms and positively charged ions. The parameter \(b\) in these formulas is an arbitrary real number bounded between 0 and 2 \((0 \leq b < 2)\). This means that the hypergeometric functions in Eqs.(15) and (16) can be determined only numerically (two exceptional cases when \(b = 1\) and \(b = 0\) are considered in the next Sections). Recently, a number of very fast and numerically stable algorithms have been developed and used for accurate calculations of the hypergeometric functions. Our final formula can be simplified even further, if one applies the following relation (see, e.g., Eq.15.2.3 in [12]) between two hypergeometric functions which are included in our Eq.(19):

\[2F_1(2 - \nu, 2 - b; 4; \frac{B - ip}{B + ip}) = 2F_1(2 - \nu, 1 - b; 4; \frac{B - ip}{B + ip}) + \frac{1}{1 - b} \frac{d}{dz} 2F_1(2 - \nu, 1 - b; 4; z)\]

where \(z = \frac{\nu - i}{\frac{b}{b} + i}\). This formula allows one to operate with one hypergeometric function only. All formulas derived and presented in this Section can directly be used to determine the both differential and total cross-sections of photodetachment of the few-electron neutral atoms and positively charged ions. It is clear that for one-electron atoms and positively charged ions analogous problem simplifies significantly. This problem is considered in the next Section.
Photodetachment of one-electron atomic systems is significantly simpler than photodetachment of few-electron atomic systems considered above. Indeed, in this case we have the atomic ionization potential $I$ depends upon the nuclear charge $Q$ only, i.e., $I = I(Q)$ (for few- and many-electron atomic system such a potential $I$ also depends upon $N_e$). Furthermore, for one-electron atoms and ions we always have $2I = Q^2$, and therefore, in the both formulas, Eqs.(15) and Eq.(16) the parameter $b = 1$ and the first term in Eq.(14) equals zero identically. The normalization constant of the incident wave function equals $C(b; B) = C(1; Q) = \frac{Q \sqrt{Q}}{\sqrt{\pi}}$. Now, the formula for the auxiliary radial integral $I_{rd} = I_{rd}^{(2)}$ term in Eq.(14) takes the form

$$I_{rd} = -pQ^2 \sqrt{\frac{Q2\nu(1+\nu^2)}{2(1-\exp(-2\pi\nu))}} C(1; Q) \int_0^{+\infty} r^{(4-1)} \exp(-Qr - ipr) \mathbb{F}_1(2 + \nu; 4; 2ipr) dr$$

$$= -pQ^2 \sqrt{\frac{Q2\nu(1+\nu^2)}{2(1-\exp(-2\pi\nu))}} \frac{\Gamma(4)}{(Q+ip)^4} 2\mathbb{F}_1(2 + \nu; 4; 2ip; Q+ip)$$

where $\nu = \frac{Q}{p}$ and $\Gamma(4) = 3 \cdot 2 = 6$. The hypergeometric function can be transformed to the form

$$2\mathbb{F}_1(2 + \nu; 4; 2ip; Q+ip) = (1 - \frac{2ip}{Q+ip})^{4-2} 2\mathbb{F}_1(2 - \nu; 4; 2ip; Q+ip) = (\frac{Q+ip}{Q-ip})^{2+\nu}$$

by using the formula $2\mathbb{F}_1(\alpha, \beta; \gamma; z) = (1 - z)^{\gamma-\alpha-\beta} 2\mathbb{F}_1(\gamma - \alpha, \gamma - \beta; \gamma; z)$ (see, Eq.(9.131) in [11]). Another way to obtain the same formula, Eq.(22), is to apply the following formula for the integral in Eq.(21) with the confluent hypergeometric function(s) (see, e.g., [9] and [11])

$$\int_0^{+\infty} \exp(-\lambda z)z^{\gamma-1} \mathbb{F}_1(\alpha; \gamma; bz) dz = \frac{\Gamma(\gamma)}{\lambda^\gamma} \left(\frac{\lambda}{\lambda - b}\right)^\alpha \frac{\Gamma(\gamma)}{\lambda^\gamma} \left(\frac{\lambda}{\lambda - b}\right)^\alpha$$

Now, the formula, Eq.(22), is reduced to the form

$$I_{rd} = -pQ^2 \sqrt{\frac{Q2\nu(1+\nu^2)}{1-\exp(-2\pi\nu)}} \frac{1}{(1+\nu^2)^2} \left(\frac{\nu + i}{\nu - i}\right)^\nu \frac{1}{(1+\nu^2)^2} \exp(-2\nu \arctan \nu)$$

$$= \frac{6}{\sqrt{p}} \sqrt{\frac{2\nu^3(1+\nu^2)}{1-\exp(-2\pi\nu)}} \frac{1}{(1+\nu^2)^2} \exp(-4\nu \arctan \nu)$$

The explicit formula for the $|I_{rd}|^2 = |I_{rd}^{(2)}|^2$ factor takes the form

$$|I_{rd}|^2 = \left(\frac{72\pi}{p}\right)^\nu \frac{\nu^3}{1-\exp(-2\pi\nu)} \frac{1}{(1+\nu^2)^3} \exp(-4\nu \arctan \nu)$$
The final formulas for the differential cross-sections of photodetachment are
\[
d\sigma = \frac{64\pi\alpha^2 a_0^2 (e \cdot n)^2 \left| I_{rd} \right|^2 \nu^3}{\omega (1 - \exp(-2\pi\nu))(1 + \nu^2)^3} \exp(-4\nu \arctan \nu) do \tag{26}
\]
for completely polarized light, and
\[
d\sigma = \left( \frac{32\pi\alpha^2 a_0^2 \mu}{\omega} \right) (n_l \times n)^2 \frac{\nu^3}{(1 - \exp(-2\pi\nu))(1 + \nu^2)^3} \exp(-4\nu \arctan \nu) do \tag{27}
\]
for the natural (unpolarized) light. The total cross-section of photodetachment in this case is
\[
\sigma = \left( \frac{128\pi^2\alpha a_0^2 \mu}{3\omega} \right) \frac{\nu^3}{(1 - \exp(-2\pi\nu))(1 + \nu^2)^3} \exp(-4\nu \arctan \nu) \tag{28}
\]
This result coincides with the formula obtained earlier by Stobbe in 1930 \cite{16}. As mentioned above for one-electron atoms and ions the ionization potential \( I \) is the explicit (and simple) function of the nuclear charge \( Q \) only. By using this fact and additional relation \( \nu = \frac{Q}{p} \) allows one to present this formula in a number of different ways (see, e.g., \cite{17} and references therein). Here we do not want to reproduce all possible forms of these expressions and discuss their limits at \( \nu \to \infty \) and \( \nu = 1 \) (more details, can be found, e.g., in \cite{17}, \cite{18} and \cite{19}).

V. PHOTODETACHMENT OF THE NEGATIVELY CHARGED IONS

Photodetachment of the negatively charged atomic ions are of great interest in numerous applications. In general, there is a fundamental difference in photodetachment of the negatively charged ions and positively charged atomic ions and neutral atoms. In particular, it is clear \textit{a priori} that for the negatively charged ions the effective electrical charge \( Z = Q - N_e + 1 \) equals zero identically. Therefore, in this case we cannot introduce the parameter \( \nu = \frac{Z}{p} \), which was used in the two previous Sections. This means all our formulas, derived for the photodetachment cross-sections (see below), will contain only the momentum of photoelectron \( p \) and ionization potential \( I \) (or parameter \( B = \sqrt{2I} \) used below). These two variables \( p \) and \( B \) are crucial for our analysis of non-relativistic photodetachment of the negatively charged ions. As mentioned above photodetachment of the negatively charged, two-electron \( \text{H}^- \) ion is of great interest for understanding the actual visible and infrared spectra of some stars, including our Sun (see discussion and references in \cite{1}). analogous process for the negatively charged \( \text{Ps}^- \) ion was considered in \cite{20} and \cite{21}. Photodetachment
of the four-electron Li\textsuperscript{−} ion also plays some role in developing of very compact and reliable photoelements and recharged batteries.

For the negatively charged atomic ions the radial derivative of radial wave function of the initial state is written as follows

\[
\frac{d}{dr} \left( \frac{C}{r} \exp(-Br) \right) = -Cr^{-2} \exp(-Br) - CB r^{-1} \exp(-Br)
\]  

(29)

where \( C \) is the normalization constant which equals \( \sqrt{\frac{I}{\pi}} \) (this follows from Eq.(7) for \( b = 0 \)). Therefore, the formula for our auxiliary radial integral \( I_{rd} \), Eq.(11), also includes two terms, i.e., \( I_{rd} = J_{rd}^{(1)} + J_{rd}^{(2)} \), where

\[
J_{rd}^{(1)} = C \sqrt{\frac{\pi}{2p}} \int_0^\infty dr J_{\frac{1}{2}}(pr) r^{\frac{1}{2}} \exp(-Br) = \sqrt{\frac{I}{2p}} \left( \frac{p}{2} \right)^{\frac{3}{2}} \frac{\Gamma(\frac{5}{2})}{\Gamma\left(\frac{5}{2}\right)} (B^2 + p^2) \times
\]

\[
2F1\left(1, 1; \frac{5}{2}; \frac{p^2}{B^2 + p^2}\right) = \sqrt{\frac{I}{\pi}} \frac{p}{3(B^2 + p^2)} 2F1\left(\frac{3}{2}, \frac{3}{2}; \frac{5}{2}; B^2 + p^2\right)
\]  

(30)

The hypergeometric function in the last equation can be reduced to some combination of elementary functions. To show this we apply the following formulas

\[
\frac{d}{dz} 2F1(\alpha, \beta; \gamma; z) = \frac{\alpha \beta}{\gamma} 2F1(\alpha + 1, \beta + 1; \gamma + 1; z)
\]  

(31)

where in our case \( \alpha = \frac{1}{2}, \beta = \frac{1}{2} \) and \( \gamma = \frac{3}{2} \). For these values of \( \alpha, \beta \) and \( \gamma \) the last formula takes the form

\[
\frac{d}{dz} \left[ 2F1\left(\frac{1}{2}, \frac{1}{2}; \frac{3}{2}; z\right) \right] = \frac{1}{6} 2F1\left(\frac{3}{2}, \frac{3}{2}; \frac{5}{2}; z\right)
\]  

(32)

where the argument \( z \) varies between zero and unity, i.e., \( 0 \leq z \leq 1 \). In our case this is true, since \( z = \frac{p^2}{B^2 + p^2} \). Now, we can write

\[
2F1\left(\frac{3}{2}, \frac{3}{2}; \frac{5}{2}; z\right) = \frac{6}{dz} 2F1\left(\frac{1}{2}; \frac{1}{2}; \frac{5}{2}; \frac{p}{B^2 + p^2}\right) = \frac{6}{dz} \left( \frac{\arcsin \sqrt{z}}{\sqrt{z}} \right) = 3 \sqrt{z} - \sqrt{1 - z} \arcsin \sqrt{z}
\]  

(33)

where we used the formula Eq.(15.1.6) from [12] for the \( 2F1(\frac{1}{2}, \frac{1}{2}; \frac{3}{2}; z) \) function.

\[
2F1(\frac{1}{2}, \frac{1}{2}; \frac{3}{2}; z) = \frac{\arcsin \sqrt{z}}{\sqrt{z}}
\]

(34)

The analytical formula, Eq.(33), derived for the \( 2F1(\frac{3}{2}, \frac{3}{2}; \frac{5}{2}; z) \) function is our original result which cannot be found directly neither in [11], nor in [12]. In our case \( z = \frac{p^2}{B^2 + p^2} \) and \( \sqrt{z} = \frac{p}{\sqrt{B^2 + p^2}} \) and the final formula for the \( J_{rd}^{(1)} \) integral takes the form

\[
J_{rd}^{(1)} = \sqrt{\frac{I}{\pi(B^2 + p^2)}} \frac{\sqrt{z} - \sqrt{1 - z} \arcsin \sqrt{z}}{z \sqrt{1 - z}}
\]  

(34)
Note that the expression in the right-hand side of this equation is not singular at $z \to 0$ (or at $p \to 0$), since

$$\lim_{z \to 0} \frac{\sqrt{z} - \sqrt{1 - z} \arcsin \sqrt{z}}{z \sqrt{1 - z}} = \frac{1}{6} \lim_{z \to 0} \sqrt{z} = 0$$

Analogous formula for the radial integral $J_{rd}^{(2)}$ is

$$J_{rd}^{(2)} = C \sqrt{B} \int_0^{\infty} dr J_{\frac{1}{2}}(pr)^{\frac{3}{2} - 1} \exp(-Br) = \sqrt{\frac{I}{2p}} \frac{B \Gamma(3)}{\Gamma(\frac{5}{2})(B^2 + p^2)^{\frac{3}{2}}} \times 2F_1\left(\frac{3}{2}, \frac{1}{2}; \frac{5}{2}; \frac{p^2}{B^2 + p^2}\right)$$

(35)

It is possible to obtain the explicit expression of the $2F_1\left(\frac{3}{2}, \frac{1}{2}; \frac{5}{2}; z\right)$ function in terms of some elementary functions. For this purpose we need to use the known analytical formula for the $2F_1\left(\frac{1}{2}, \frac{1}{2}; \frac{3}{2}; z\right)$ function (which equals $\arcsin \sqrt{z}$, see, Eq.(33)) and apply the following formula Eq.(15.2.7) from [12] for $n = 1$

$$\frac{d}{dz} \left[(1 - z)^a 2F_1(a, b; c; z)\right] = -\frac{a(c - b)}{c}(1 - z)^{a-1} 2F_1(a + 1, b; c + 1; z)$$

(36)

where $a = \frac{1}{2}$, $b = \frac{1}{2}$ and $c = \frac{3}{2}$. Now, for the $2F_1\left(\frac{1}{2}, \frac{1}{2}; \frac{3}{2}; z\right)$ function one finds

$$\frac{d}{dz} \left[(1 - z)^{\frac{1}{2}} 2F_1\left(\frac{1}{2}, \frac{1}{2}; \frac{3}{2}; z\right)\right] = -\frac{1}{3}(1 - z)^{-\frac{1}{2}} 2F_1\left(\frac{3}{2}, \frac{1}{2}; \frac{5}{2}; z\right)$$

(37)

From this equation we derive

$$2F_1\left(\frac{3}{2}, \frac{1}{2}; \frac{5}{2}; z\right) = -3\sqrt{1 - z} \frac{d}{dz} \left[\sqrt{1 - z} \frac{\arcsin \sqrt{z}}{\sqrt{z}}\right]$$

$$= \frac{3}{2} \frac{\arcsin \sqrt{z}}{\sqrt{z}} - \frac{\sqrt{1 - z}}{z} + \frac{1 - z}{z \sqrt{z}} \arcsin \sqrt{z}$$

(38)

where $z = \frac{p^2}{B^2 + p^2} \leq 1$ (it is also clear that $z$ is non-negative). This analytical formula for the $2F_1\left(\frac{3}{2}, \frac{1}{2}; \frac{5}{2}; z\right)$ function is another original result which cannot be found neither in [11], nor in [12]. Note also that analytical formula for this integral can also be derived as a partial derivative of the $J_{rd}^{(1)}$ in respect to the parameter $B$. Thus, the both auxiliary radial integrals $J_{rd}^{(1)}$ and $J_{rd}^{(2)}$ are expressed in terms of the elementary functions. In particular, the final formula for the $J_{rd}^{(2)}$ integral is

$$J_{rd}^{(2)} = \sqrt{\frac{I}{\pi(B^2 + p^2)}} \sqrt{1 - z^2} \left[\frac{\arcsin \sqrt{z}}{z} - \sqrt{\frac{1 - z}{z}}\right]$$

(39)
where \( z = \frac{p^2}{B^2 + p^2} \) and \( \sqrt{z} = \frac{p}{\sqrt{B^2 + p^2}} \). Again, by using the formula, 1.641 from [11] for the \( \arcsin x \) one can easily show that

\[
\lim_{z \to 0} \left( \frac{1 - z}{z} \arcsin \sqrt{z} - \sqrt{\frac{1 - z}{z}} \right) = 0
\]

which means that our formula for the \( J_{rd}^{(2)} \) integral is not singular at \( z \to 0 \) (or at \( p \to 0 \)). The formula Eq. (2) for the differential cross-section of photodetachment contains an additional factor \( p \) in its numerator. Therefore, such a cross-section always approaches zero when \( p \to 0 \). Analogous cross-sections considered in the two previous Sections for neutral atoms and positively charged ions are always finite. The same arguments are applied to the total cross-section of photodetachment of the negatively charged ions. Analytical computations of the total auxiliary \( J_{rd}^{(1)} + J_{rd}^{(2)} \) integral and analogous calculations of the differential and total cross-sections is simple and straightforward. The final formula, Eq. (13), for the differential cross-section of photodetachment for the negatively charged ions takes the form

\[
d\sigma = \left( \frac{8\pi \alpha a_0^2}{9\omega} \right) (\mathbf{n} \times \mathbf{n})^2 |I_{rd}|^2 d\omega = \frac{8}{9} \alpha a_0^2 \left[ \frac{p I}{\omega(2I + p^2)} \right] \sin^2 \Theta \left| J_{rd}^{(1)} - J_{rd}^{(2)} \right|^2 d\omega
\]

\[
= \frac{4}{9} \alpha a_0^2 \left[ \frac{2Ip}{\omega(2I + p^2)} \right] \left[ (\sqrt{1 - z^2} + 1) \frac{\arcsin(\sqrt{z})}{z} - \frac{(1 - z)\sqrt{1 - z^2} + 1}{\sqrt{z(1 - z)}} \right]^2 d\omega
\]

\[
= \frac{8}{9} \alpha a_0^2 \left( \frac{I}{p\omega} \right) \left[ (\sqrt{1 - z^2} + 1) \frac{\arcsin(\sqrt{z})}{\sqrt{z}} - \frac{(1 - z)\sqrt{1 - z^2} + 1}{\sqrt{1 - z}} \right]^2 d\omega
\]

where \( z = \frac{p^2}{2I + p^2} \) and \( \sqrt{z} = \frac{p}{\sqrt{2I + p^2}} \). This formula for the differential cross-section of photodetachment of the negatively charged ions is one of the main results of this study. Derivation of the formula for the corresponding total cross-section from this our formula is simple and straightforward.

**VI. DISCUSSION AND CONCLUSIONS**

We have studied photodetachment of the outer-most electrons in a few- and many-electron atomic systems. Such systems include positively charged atomic ions and neutral atoms. We also investigated photodetachment of neutral atoms, positively charged atomic systems and negatively charged ions in which \( N_e = Q + 1 \). Analytical formulas derived in each of these cases for the differential and total cross-sections provide a complete and accurate description of photodetachment of the outer-most electrons in a few- and many-electron
atomic systems. Another advantage of our formulas follows from the fact that for all physical systems considered in this study the corresponding differential and total cross-sections of photodetachment are written as the explicit and simple functions of a few basic variables of the problem which include the momentum of outgoing photoelectron $p$, atomic ionization potential $I$, electrical charge of atomic nucleus $Q$ and total number of bound electrons $N_e$ in the incident atomic system. The derived formulas and other results of our study are of interest in some problems currently known in stellar astrophysics, physics of high- and low-temperature plasmas, solid state physics, etc.

Note also that our approach developed in this study can easily be generalized to actual few- and many-electron atoms and ions. In this approach all initial and final wave functions are represented as products (or sums of products) of the asymptotic wave function of the outer-most electron and self-correlated wave function of the central atomic core. These wave functions must be properly symmetrized for all possible permutations of identical particles (electrons). If the trial wave functions have been symmetrized, then the corresponding transition operator can be used in its single-particle form exactly as it is described above. Therefore, we can expect that such a ’many-electron’ description of non-relativistic photodetachment in actual atoms and ions will not change (at least qualitatively) the main results of this article.

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