Asymptotic behavior of photoionization cross section in a central field. Ionization of the $p$ states

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Abstract. We continue our studies of the high energy nonrelativistic asymptotics for the photoionization cross section of the systems bound by a central field $V(r)$. We consider the bound states with the orbital momentum $\ell = 1$. We show, that as well as for the $s$ states the asymptotics can be obtained without solving of the wave equations for the bound and outgoing electrons. The asymptotics of the cross sections is expressed in terms of the asymptotics of the Fourier transform $V(p)$ of the potential and its derivative $V'(p)$ by employing the Lippmann–Schwinger equation. The shape of the energy dependence of the cross sections is determined by the analytical properties of the potential $V(r)$. The cross sections exhibit power drop with the increase of the photon energy for the potentials $V(r)$ which have singularities on the real axis. They experience exponential drop if $V(r)$ has poles in the complex plane. We trace the energy dependence of the ratios of the photoionization cross sections for $s$ and $p$ electrons from the states with the same principle quantum number. We apply the results to the physics of fullerenes.

1 Introduction

In our recent paper [1] we studied the high energy photoionization of $s$ states. We presented a more detailed analysis in Drukarev and Mikhailov [2,3]. Now we turn to the photoionization of the single-particle states with the orbital momentum $\ell = 1$.

We consider the photon energies $\omega$ which are much larger than the ionization potential $I_B$ and find the leading term of expansion of the cross section $\sigma(\omega)$ in terms of $1/\omega$. We assume that the photon energy is much smaller than the electron rest energy $m_e$ (we employ the system of units with $\hbar = 1$, $c = 1$). Thus we consider the photon energies limited by the conditions

$$I_B \ll \omega \ll m_e,$$

analyzing the high energy nonrelativistic asymptotics.

The photoelectron can be treated in nonrelativistic approximation. Its energy is

$$\varepsilon = \omega - I_B = \frac{p^2}{2m_e},$$

with $p$ the photoelectron momentum. Due to equation (1)

$$p \gg \mu,$$

where $\mu = (2mI_B)^{1/2}$ is the characteristic momentum of the bound state. Large momentum $q \approx p \gg \mu$ (the “recoil momentum”) is transferred to the recoil ion.

We assume the electrons to be bound by a local central field $V(r) < 0$. Large recoil momentum $q$ is transferred to the bound electron or to the photoelectron by the source of the field. We show that the relative role of the two mechanisms depends on the behavior of the Fourier transform of the potential $V(r)$ which is $V(p) = \int d^3r V(r)e^{-ipr}$. We omit the tilde sign below. Employing the velocity form of the photon-electron interaction we find that if for large $p \gg \mu$

$$|V'(p)| \gg -\frac{V(p)}{p},$$

(4)

with $V'(p) = \partial V(p)/\partial p$, the recoil momentum is transferred mostly by the bound electron. However for

$$|V'(p)| \sim -\frac{V(p)}{p},$$

(5)

transfer of momentum $q$ by both bound and continuum electrons should be included. For example, in the case of the well potential equation (4) is true, while equation (5) is true for the Coulomb and exponential potentials.

The potential $V(p)$ should drop at least as $1/p$ at $p \to \infty$. Otherwise the corresponding potential in the position space $V(r)$ drops faster than $1/r^2$ causing the “fall to the center” [4]. Thus it cannot form a bound state. In
Sections 2, 3 we analyze the potentials for which
\[ pV(p) \to 0, \]  
(6) 
at \( p \to \infty \). We consider a potential for which \( V(p) \sim 1/p \) in Section 4.1.

We demonstrate that the asymptotics of the photoionization cross section can be obtained without solving the wave equations for the electrons. The shape of the cross section is determined by the analytical properties of the potential \( V(r) \). It is expressed in terms of the potential \( V(p) \) and its derivative \( V'(p) \).

We start with the potentials with singularities at \( r = 0 \). In this case cross sections are directly related to the potential \( V(p) \). We consider first the potentials with the Coulomb short range behavior \( V(r) \to \infty \) if \( r \to 0 \). Such potentials approximate the fields of many-electron atoms. The pure Coulomb field is the most studies case. The expressions for the cross section of photoionization of atoms. The pure Coulomb field is the most studies case.

We also obtained the asymptotic photoionization cross section in exponential potential. The latter found its applications for photoionization in such potentials are expressed among those containing discontinuities on the real axis. It is often used as a simplified model for a short range potential. A potential with sharp edges and flat bottom is often used for description of the electromagnetic field of a fullerene [6]. The cross sections for photoionization in such potentials are expressed in terms of the jumps experienced by the potential \( V(r) \).

It was found recently that in the case of the best studied fullerene \( C_{60} \) a potential with flat bottom is unlikely to be consistent with the data on distribution of the electrons of the fullerene shell. Potential with a sharp minimum would fit better [15]. Such shape can be provided by a potential with a pole in the complex plane-see, e.g. equation (60) below. For the potentials with poles in the complex plane the cross sections experience exponential drop with the power of the exponent determined by the imaginary part of the pole.

Besides the expressions for the cross sections we trace the energy dependence of the ratios
\[ r(\omega) = \frac{\sigma_{ns}(\omega)}{\sigma_{np}(\omega)}, \]  
(7) 
of the photoionization cross sections for \( s \) and \( p \) electrons from the states with the same principle quantum number \( n \).

We present the general equations for the amplitude and the cross sections in Section 2. We consider the particular cases in Section 3. In Section 4 we apply the results for analysis of photoionization of fullerenes. We summarize in Section 5.

2 Asymptotic forms of the amplitude and the cross section

The general expression for the differential photoionization cross section can be written as
\[ d\sigma = 2\pi n_c \delta(\omega - I_B - p^2/2m_e) \sum_m |F_m|^2 \frac{d^3p}{(2\pi)^3}; \quad p = \sqrt{2m_e\omega}, \]  
(8) 
with \( m = 0, \pm 1 \) the projection of the angular momentum \( \ell = 1 \) of the bound electron. The averaging over the directions of the photon polarization should be carried out. Presenting \( d^3p = p^2dpd\Omega = m_cpe\omega d\Omega \) with \( \Omega - \) the solid angle of the photoelectron, we find that
\[ d\sigma = n_c \frac{m_c}{3\pi} \sum_m |F_m|^2 \frac{df}{4\pi}, \]  
(9) 
The amplitude is
\[ F_m = N(\omega) \int \frac{d^3f}{(2\pi)^3} \psi_p^*(f) \frac{e^* \cdot f}{m_e} \psi_m(f); \quad N(\omega) = \left(\frac{4\pi a}{2m}\right)^{1/2}, \]  
(10) 
with \( \psi_p(f) - \) the wave function of the photoelectron caring the asymptotic momentum \( p \). These expressions can be found e.g. in the books [6] or [16].

Consider first the mechanism in which the large recoil momentum is transferred by the bound electron. The photoelectron can be described by the plane wave i.e.
\[ \psi_p(f) = \psi_p^{(0)}(f) = (2\pi)^{3/2} \delta(f - p), \]  
and the amplitude is
\[ F_m^a = N(\omega) \frac{e^* \cdot p}{m_e} \psi_m(p), \]  
(11) 
with \( \psi_m \) the single particle wave function of the bound electron.

Now we must calculate the function \( \psi_m(p) \) for \( p \gg \mu \). This can be done by employing the Lippmann–Schwinger equation
\[ \psi_m = \psi_m^{(0)} + G(\varepsilon_B)V\psi_m, \]  
(12) 
in momentum space. Here \( \psi_m^{(0)} \) is the wave function at \( V = 0 \), \( G \) is the propagator of the free motion, \( \varepsilon_B = -I_B < 0 \) is the electron energy in the bound state. For the bound states \( \psi_m^{(0)} = 0 \). The matrix element of the free propagator is
\[ \langle p|G(\varepsilon_B)|p_1\rangle = g(\varepsilon_B,p)\delta(p - p_1); \quad g(\varepsilon_B,p) = \frac{1}{\varepsilon_B - p^2/2m_e}. \]

Introducing
\[ J_m(p) = \int \frac{d^3f}{(2\pi)^3} V(p - f) \psi_m(f), \]  
(13)
(of course, $V(p - f)$ depends only on $|p - f|$) we find that for any $p$

$$\psi_m(p) = \langle p | G V | \psi_m \rangle = g(\varepsilon_B, p) J_m(p). \quad (14)$$

In the asymptotics $g(\varepsilon_B, p) = -2m_e / p^2$, and thus

$$\psi_m(p) = -\frac{1}{\omega} J_m(p). \quad (15)$$

Now we analyze the contributions of the three regions of the values of momentum $f$ to the integral $J_m(p)$. In the region $f \sim \mu \ll p$ one can estimate $V(p - f) = V(p)$. Thus this region provides a contribution of the order $V(p)/p^2$ to the function $\psi_m(p)$. The large momenta $f \sim p$ for which $|p - f| \ll p$ provide the contribution of the order $\psi_m(p)/p^2$ to the right hand side of equation (15). It is beyond the asymptotics. As to the region of large momenta $f \sim p$; $|p - f| \sim p$, its contribution to the right-hand side of equation (15) is of the order $mpV(p)\psi_m(p)$. It is also beyond the asymptotics due to equation (6).

Hence the integral $J_m(p)$ is determined by the region of small momenta $f \sim \mu \ll p$ for the potentials $V(p)$, which drop faster than $1/p$ at large $p$. Thus equation (15) ties the values of $\psi_m$ at $f \gg \mu$ with those at $f \sim \mu$.

To separate the angular variables in equation (15) we present the wave function of the bound state with projection $m = 0, \pm 1$ of the orbital momentum $\ell = 1$ as

$$\psi_m(r) = \sqrt{\frac{3}{4\pi}} r m \varphi(r); \quad \varphi(0) \neq 0,$$

$r_m$ is the projection of the position vector $r$. The radial part of the function is $R(r) = r \varphi(r)$. It is normalized by the condition $\int_0^\infty dr r^2 R^2(r) = 1$. In the momentum presentation

$$\psi_m(f) = i \sqrt{\frac{3}{4\pi}} (\nabla_f)_m \varphi(f); \quad \varphi(f) = \int d^3r e^{-if \cdot r} \varphi(r). \quad (16)$$

Employing this expression and integrating by parts we write equation (15) as

$$\psi_m(p) = i \sqrt{\frac{3}{4\pi}} (\nabla_p)_m \varphi(p),$$

with

$$\varphi(p) = -\frac{2m_e}{p^2} f^{(r)}(p); \quad J^{(r)}(p) = \int \frac{d^3f}{(2\pi)^3} V(p - f) \varphi(f). \quad (17)$$

The upper index $(r)$ reminds that $J^{(r)}$ is connected to the radial part of the wave function.

Using equation (16) and integrating by parts we write equation (11) as

$$F^a_m = -i \sqrt{\frac{3}{4\pi}} \frac{N(\omega)}{\omega} \frac{e \cdot p}{m_e} (\nabla_p)_m J^{(r)}(p), \quad (18)$$

or

$$F^a_m = -i \sqrt{\frac{3}{4\pi}} \frac{N(\omega)}{\omega} \frac{e \cdot p}{m_e} n_m J^{(r)}(p); \quad n = \frac{p}{p}, \quad (19)$$

with $J^{(r)}(p) = \partial J^{(r)}(p) / \partial p$.

Now we include the possibility that the large recoil momentum is transferred by the photoelectron. The corresponding amplitude is $F^b_m$, and the total amplitude is

$$F_m = F^a_m + F^b_m. \quad (20)$$

The photoelectron function in the field of the recoil ion satisfies the Lippmann–Schwinger equation

$$\psi_p = \psi_p^{(0)} + G(\omega + \varepsilon_B) V \psi_p, \quad \text{with } G \text{ the propagator of free motion.}$$

Transfer of the large momentum $p$ is expressed in asymptotics by the first iteration

$$\psi_p^{(1)} = G(\omega + \varepsilon_B) V \psi_p^{(0)}.$$

This can be written as

$$\psi_p^{(1)}(f) = \langle f | G(\omega + \varepsilon_B) V | p \rangle = g(\omega + \varepsilon_B)p - f, \quad g(\omega + \varepsilon_B) = \frac{1}{\omega + \varepsilon_B - f^2 / 2m_e}.$$

We must put $g(\omega + \varepsilon_B) = 1 / \omega$ in the asymptotics. This provides

$$F^b_m = \frac{N(\omega)}{\omega} \int \frac{d^3f}{(2\pi)^3} V(p - f) \frac{e \cdot f}{m_e} \psi_m(f). \quad (21)$$

Employing equation (16) and integrating by parts we find

$$F^b_m = F^b_m^{(1)} + F^b_m^{(2)}, \quad (22)$$

with

$$F^b_m^{(1)} = -i \sqrt{\frac{3}{4\pi}} \frac{N(\omega)}{\omega} m J^{(r)}(p), \quad (23)$$

with $J^{(r)}$ defined by the second equality of equation (17).

The second term on the right hand side of equation (22)is

$$F^b_m^{(2)} = i \sqrt{\frac{3}{4\pi}} \frac{N(\omega)}{\omega} \frac{e \cdot f}{m_e} \omega n_m B'(p); \quad B'(p) = \frac{d^3f}{(2\pi)^3} V(p - f) \frac{e \cdot f}{m_e} \varphi(f), \quad B'(p) = \partial B(p) / \partial p.$$ Comparing this expression with equation (19) for $F^a_m$ one can see that $F^b_m^{(2)}/F^a_m \sim \mu / p \ll 1$ since the integral is saturated by small $f \sim \mu$. This enables us to neglect $F^b_m^{(2)}$, presenting $F_m = F^a_m + F^b_m$. Hence

$$F_m = -i \sqrt{\frac{3}{4\pi}} \frac{N(\omega)}{\omega} \frac{e \cdot n_p}{m_e} J^{(r)}(p) + e_m J^{(r)}(p); \quad n = \frac{p}{p}. \quad (24)$$

Recall that the two terms in the parenthesis on the right hand side describe the transfer of large recoil momentum by the bound electron and by the photoelectron correspondingly.

If the logarithmic derivative of the potential is large enough, i.e. if equation (4) is true, transfer of the recoil momentum by the photoelectron can be neglected, and

$$F_m = -i \sqrt{\frac{3}{4\pi}} \frac{N(\omega)}{\omega} \frac{e \cdot n_p}{m_e} J^{(r)}.$$ (25)

If equation (5) is true, both terms on the right hand side of equation (24) should be included. In this case further
evaluation of the expression for the amplitude is possible since the integral on the right hand side of the second equality of equation (17) is saturated by small \( f \sim \mu \). The integrand can be expanded in powers of \( f \). Once equation (5) holds, we find \( \mu V'(p) \ll V(p) \), and we can put \( V(p - \mathbf{f}) = V(p) \). Thus
\[
J^{(r)}(p) = V(p)\varphi(r = 0),
\]
and
\[
F_m = -i \sqrt{\frac{3}{4\pi \hbar^2}} N(\omega) \left( e \cdot m_m p V'(p) + e_{mV}(p) \right) \varphi(r = 0); \quad n = \frac{p}{\hbar}. \tag{27}
\]

Note that the third situation with \( |pV'(p)| \ll -V(p) \) is not possible for the potentials which satisfy the condition presented by equation (6). For \( p \gg \mu \) we can write \( V(p) = -f(p)/\mu \), with \( f(p) > 0 \) and \( f'(p) < 0 \). Calculating the derivative we find that \( |pV'(p)| \geq V(p) \).

Now we can obtain the asymptotic expressions for the cross sections. If \( |pV'(p)| \gg -V(p) \) we find employing equations (25) and (9)
\[
\sigma(\omega) = n_e \frac{\alpha}{3\pi \omega^2} |J^{(r)}(p)|^2; \quad p = \sqrt{2m_e \omega}, \tag{28}
\]
with \( n_e \) the number of electrons bound in the \( p \) state. If \( |pV'(p)| \sim -V(p) \), equations (27) and (9) provide
\[
\sigma(\omega) = n_e \frac{\alpha}{3\pi \omega^2} \left( p^2 V'(p) + 2pV(p) V'(p) + 3V^2(p) \right) \varphi^2(r = 0). \tag{29}
\]

### 3 Analytical properties of potential and the asymptotic behavior of the cross section

#### 3.1 Potentials with singularities at the origin

Start with the Coulomb potential created by the point nucleus with the charge \( Z \). It is \( V_C(r) = -\alpha Z/r \), with a pole at \( r = 0 \). Its Fourier transform is
\[
V_C(p) = -\frac{4\pi \alpha Z}{p^2}. \tag{30}
\]

In this case \( pV'(p) = -2V(p) \), and equation (5) is true. The large recoil momentum can be transferred by both the bound electron and the photoelectron. The cross section is described by equation (29). Note that the first and second terms in parenthesis on the right hand side of equation (29) cancel. Thus only transfer of large recoil momentum by the photoelectron becomes important. We find
\[
\sigma_{2p}(\omega) = n_e 16 \alpha^2 \frac{Z^2}{\omega^4} \varphi_{2p}^2(r = 0). \tag{31}
\]

The expression for the cross section at \( n = 2 \) is presented in the book [5]. Later in this Section we demonstrate that for \( n = 2, \ell = 1 \) equation (31) reproduces the result given in [5]. The cross section \( \sigma_{np} \) drops as \( \omega^{-b/2} \). Recall that the asymptotics for photoionization cross section \( \sigma_{ns} \) of \( s \) states is \( \omega^{-7/2} \). Thus the ratio \( r(\omega) \) defined by equation (7) is proportional to \( \omega \).

The Fourier transform of the Yukawa potential \( V_\lambda(r) = -ge^{-\lambda r}/r(\omega > 0) \) is
\[
V_\lambda(p) = \frac{-4\pi g}{p^2 + \lambda^2}. \tag{32}
\]

One can see that \( V_\lambda(p) = -4\pi g/p^2 \) at large \( p \gg \lambda \), and the asymptotics of the cross section in the Yukawa field coincides with that in the Coulomb field with the charge of the nucleus \( Z = g/\alpha \). The shape of the cross section is determined by equation (31). The difference of the cross section values in the fields \( V_C(r) \) and \( V_\lambda(r) \) manifests itself through the difference of the values of \( \varphi_{2p}^2(r = 0) \).

Note that the cross section for photoionization of 2p subshell in the Coulomb field for all energies \( \omega \ll m_e \) can be expressed by combining equations (71.15) and (69.3) of the book [5]
\[
\sigma_{2p}(\omega) = \frac{2^{11}\pi \alpha}{3m} \frac{I_2}{\omega^2} \left( 3 + \frac{I_2}{\omega} \right) F(p). \tag{33}
\]

Here
\[
F(p) = \frac{p}{2\pi \eta} \Phi(p),
\]

presents the last factor on the right hand side of equation (71.15) of [5]: \( \Phi(p) \to 1 \) at \( p \to \infty \), \( \eta = maZ \). We employed the energies \( \omega = 2\pi \nu \), \( I_2 = 2\pi \nu_2 \) instead of the frequencies \( \nu \) and \( \nu_2 \) used in (71.15), \( I_2 = \eta^2/(8m) \) is the Coulomb binding energy of the states with \( n = 2 \). Also,
\[
\Phi(p) = D(\pi \xi) \exp(4\xi \arctan \xi); \quad D(\pi \xi) = \frac{2\pi \exp(-2\pi \xi)}{1 - \exp(-2\pi \xi)}, \quad \xi = \eta/p.
\]

To describe the asymptotics we must put \( p \to \infty \), \( \xi = 0 \), and thus \( \Phi = 1 \) and \( F(p) = \frac{p}{2\pi \eta} \) on the right hand side of equation (33). We should also neglect the second term in the parenthesis since \( 8I_2/\omega = 2\xi^2 \to 0 \). Since \( \varphi_{2p}^2(0) = \eta^3/24 \) [5], equations (31) and (33) provide identical results for asymptotics of photoionization of totally occupied 2p subshell in the Coulomb field
\[
\sigma_{2p}(\omega) = 4\pi \alpha (\alpha Z)^2 \frac{\eta^5}{\omega^4 p^3}; \quad \eta = maZ.
\]

Now we analyze the deviations from the asymptotic law for the potentials with the short range behavior \( V(r) \to \infty \) for \( r \to 0 \). We do it in the same way as we did for photoionization of \( s \) states [3]. As we mentioned in Introduction, such potentials approximate the fields of many-electron atoms.

Start with the case of the Coulomb field. The cross section is expressed by equation (33). Note that the function \( \Phi(p) \) depends on parameters \( \xi^2 \) and \( \xi^2 \) separately, i.e. \( \Phi(p) = \Phi(\pi \xi, \xi^2) \). Neglecting the terms of the order \( \xi^2 \) and without assuming the parameter \( \pi \xi \) to be small
\[1\] Of course, this remarkable cancelation can be obtained by using the explicit expressions for photoionization cross sections of the 2p states in the Coulomb field obtained long ago (see, e.g. [5]). However, as far as we know, it was discussed for the first time in Drukarev and Mikhailov [6].
we find that the main deviations from the asymptotic law are described in the Coulomb case by the Stobbe factor [5],

$$ S(\omega) = \Phi(\pi \xi, \xi^2 = 0) = \frac{\pi \xi}{\sin(\pi \xi)} \exp(-\pi \xi) \approx \exp(-\pi \xi). $$

(34)

This can be done for any $p$ state bound by the Coulomb field in the same way. The ratio of photoionization cross section of any $p$ state at large photon energies $\omega_1$ and $\omega_2$ is

$$ \frac{\sigma(\omega_1)}{\sigma(\omega_2)} = \left( \frac{\omega_2}{\omega_1} \right)^{3/2} S(\omega_1)/S(\omega_2), $$

(35)

It was demonstrated in Avdonina et al. [10] (see also Ch. 7 of [6]) that the experimental data on photoionization of many-electron atoms as well as the results of calculations in framework of Hartree-Fock approximation are well described by inclusion of the Stobbe factor. This happens because the Stobbe factor is formed at small distances of the order 1/p from the nucleus. It is not influenced much by the electron interaction. For photoionization cross section in any field with the Coulomb short range behavior $V(r) \to \infty$ for $r \to 0$ the high energy cross sections ratio is expressed by equation (35). This makes possible the asymptotic analysis. The accuracy of calculations can be still improved by calculation of the contributions of the terms of $\xi^2$ series as described in McEnnan et al. [11] and Oh et al. [12].

Potential $V(r)$ can have a singularity at $r = 0$ even if $V(r = 0)$ does not turn to infinity. The exponential potential

$$ V_{\exp}(r) = -V_0 e^{-\lambda r}; \quad V_0 > 0, $$

(36)

provides an example. Being treated as a function of $x$ in the interval $-\infty < x < \infty$ it can be written as $V_{\exp}(x) = -V_0 e^{-\lambda |x|}$, with a cusp at $x = 0$. We can present

$$ V_{\exp}(r) = -\frac{V_0 \partial V_\lambda}{g} \frac{\partial \lambda}{\partial \lambda}, $$

and thus

$$ V_{\exp}(p) = -\frac{8\pi V_0 \lambda}{p^4}. $$

(37)

In this case $pV'(p) = -4V(p)$. The asymptotics of the photoionization cross section is given by equation (29) with all three terms in the parenthesis on the right hand side being important. The large recoil momentum can be transferred by both recoil electron and the photoelectron. We find

$$ \sigma(\omega) = n_e \frac{11 \cdot 64}{3} \alpha \pi V_0^2 \lambda^2 \omega^2/r = 0/\omega^2 p^3, $$

(38)

The cross section drops as $\omega^{-13/2}$. Note that similar analysis for photoionization of $s$ states provides $\sigma_s \sim \omega^{-11/2}$. Thus as well as in previous cases $r(\omega) \sim \omega$.

In the examples presented above the shapes of the cross sections are determined directly by the shape of the potential $V(p)$. The cross sections contain the squared wave function $\varphi^2(r = 0)$ at the singular point of the potential $V(r)$.

### 3.2 Potentials with singularities on the real axis

For such potentials it is instructive to write expression for $J^{(r)'}(p)$ provided by second equality of equation (17) in the position presentation

$$ J^{(r)}(p) = \int d^3 r V(r) \varphi(r) e^{-ipr} = \frac{4\pi}{p} \int_0^\infty dr V(r) \varphi(r) \sin(pr). $$

(39)

In the asymptotics

$$ J^{(r)'}(p) = \frac{4\pi}{p} \int_0^\infty dr V(r) \chi(r) \cos(pr); \quad \chi(r) = r^2 \varphi(r). $$

(40)

Consider first the rectangular well potential for which $V(r) = -V_0 < 0$ for $0 \leq r \leq R$ while $V(r) = 0$ for $r > R$. It has a singularity on the real axis at $r = R$, where the function $V(r)$ experience a jump.

The asymptotics of the Fourier transform for this potential is

$$ V(p) = \frac{4\pi V_0 R}{p^2} \cos pR, $$

(41)

and $pV'(p) \gg -V$ at $p \to \infty$. Thus the large recoil momentum is transferred by the bound state electron, and the amplitude is determined by equation (25).

To calculate the asymptotics of the integral $J^{(r)'}(p)$ we integrate by parts the integral on the right hand side of equation (40). This provides

$$ J^{(r)'}(p) = -\frac{4\pi V_0}{p^2} \left[ \sin(pr) \chi(R) - \int_0^R dr \sin(pr) \chi'(r) \right]. $$

(42)

The asymptotics is determined by the first term in the parenthesis on the right hand side. Further integration by parts of the second term provides additional factors $1/p$, leading to the terms which contribute beyond the asymptotics. Thus for the rectangular well potential

$$ J^{(r)'}(p) = -\frac{4\pi V_0 \chi(R)}{p^2} \sin(pR). $$

(43)

Employing equation (28) we find

$$ \sigma(\omega) = n_e \frac{16 \pi}{3} \alpha \pi V_0^2 \chi^2(R) / \omega^2 p^3 \sin^2 pR. $$

(44)

In a more general case the potential $V(r)$ experience a jump on the real axis at certain $r = R$.

$$ V(r) = V_1(r) \quad 0 \leq r \leq R; \quad V(r) = V_2(r) \quad R < r < \infty, $$

(45)

with $V_1(R) \neq V_2(R)$. Similar to equation (40) we write

$$ J^{(r)'}(p) = \frac{4\pi}{p} \int_0^R dr V_1(r) \chi(r) \cos(pr) + \frac{4\pi}{p} \int_R^\infty dr V_2(r) \chi(r) \cos(pr). $$

(46)
The function \( \varphi(r) \) is continuous on the real axis. Thus integration by parts provides
\[
J^{(r)}(p) = -\frac{4\pi \chi(R) \sin(pR)\delta(R)}{p^2}; \quad \delta(R) = V_2(R) - V_1(R),
\]
leading to the cross section
\[
\sigma(\omega) = n_e \frac{16}{3} \alpha \pi \frac{(\delta(R))^2 \chi^2(R)}{\omega^2 p^2} \sin^2(pR).
\]

Carrying out similar calculation for \( s \) states we find that equation (7) provides the oscillating cross sections ratio \( r(\omega) \sim \cos^2(pR)/\sin^2(pR) \).

The cross section of photoionization in the field \( V(r) \) which is continuous on the real axis while the derivative \( V'(r) \) of the potential experience a jump at \( r = R \) can be obtained in the same way. One needs two integrations by parts on the right hand side of equation (46). The function \( J^{(r)}(p) \) obtains additional factor \( 1/p \). The cross section drops as \( \omega^{-9/2} \). The case when only higher derivatives experience jumps can be considered in similar way. We shall provide an example in Section 4.2.

3.3 Potentials with singularities in the complex plane

Consider now a simple potential
\[
V(r) = -\frac{U_0}{r} \frac{a}{r^2 + a^2}; \quad a > 0,
\]
\( U_0 > 0 \) is a dimensionless constant. Its Fourier transform is
\[
V(p) = -\frac{2\pi U_0 a}{p} \exp(-pa).
\]

The exponential drop is due to the contributions of the poles \( r = \pm ia \) in integration in the complex plane.

We can proceed further in the same way as we did for the \( s \) states in Drukarev and Mikhailov [3]. The integral
\[
J^{(r)}(p) = -\frac{2\pi U_0}{p} \int \frac{d^3 f}{(2\pi)^3} \frac{e^{-v(f)}a}{v(f)} \varphi(f);
\]
\[
v(f) = |p - f| = (p^2 - 2pf + f^2)^{1/2},
\]
dominated by small \( f \sim 1/a \ll p \). To find the asymptotics one can put \( v = p \) in the denominator of the integrand. However this cannot be done in the power of the exponential factor. To obtain the \( p \) dependence of the right hand side we present equation (51) as
\[
J^{(r)}(p) = -\frac{2\pi U_0}{p} I^{(r)}(p); \quad I^{(r)}(p) = \int \frac{d^3 f}{(2\pi)^3} e^{-v(f)}a \varphi(f),
\]
and
\[
J^{(r)}(p) = -\frac{2\pi U_0}{p} I^{(r)}(p)
\]
in the asymptotics.

To find the shape of the dependence \( I^{(r)}(p) \) we calculate its derivative with respect to \( p \)
\[
I^{(r)}(p) = -a \int \frac{d^3 f}{(2\pi)^3} e^{-v(f)}a \frac{dv}{dp}(f) \varphi(f),
\]
with \( v'_p = \partial v/\partial p \). One can put \( v'_p = 1 \) with the accuracy \( 1/p^2 \). Thus we can write a simple differential equation
\[
I^{(r)}(p) = -a I^{(r)}(p),
\]
with the solution \( I^{(r)}(p) = \kappa_1 e^{-pa} \) where \( \kappa_1 \) is an unknown constant. It can be estimated as \( \kappa_1 \approx \varphi(r = 0) \).

The expression for the cross section
\[
\frac{\sigma(\omega_1)}{\sigma(\omega_2)} = \frac{\omega_2^{5/2}}{\omega_1^{5/2}} e^{-2(p_1 - p_2)/a}; \quad p_i = (2m_e \omega_i)^{1/2}.
\]

The equation for ionization of \( s \) states has the same form [3]. Thus the ratio \( r(\omega) \) does not depend on \( \omega \).

We can proceed in similar way for the Gaussian potential
\[
V(r) = -V_0 e^{-r^2/\lambda^2}; \quad V_0 > 0; \quad \lambda > 0,
\]
\( U_0 > 0 \) with the essential singularity in the complex plane. The Fourier transform is
\[
V(p) = -\pi^{3/2} V_0 a^{5} e^{-p^2 a^2/4}.
\]

Proceeding in the same way as in previous case we find
\[
J^{(r)}(p) = \frac{\pi^{3/2} V_0 a^{5} \kappa_1}{2} e^{-p^2 a^2/4},
\]
\[
\sigma = \frac{\pi^2 a}{2} \frac{V_0 a^{10} m_e p}{\omega} e^{-p^2 a^2/2} \kappa_1^2,
\]
with \( \kappa_1 \approx \varphi^2(r = 0) \). For the cross sections ratio at large values of the photon energies \( \omega_{1,2} \)
\[
\frac{\sigma(\omega_1)}{\sigma(\omega_2)} = \frac{\omega_1^{1/2}}{\omega_2^{1/2}} e^{-m_e a^2(\omega_1 - \omega_2)}.
\]

Comparing with the results for photoionization of \( s \) states one can see that \( r(\omega) \sim 1/\omega \). The cross section for photoionization of \( p \) states drops slower than that for \( s \) states while the photon energy increases.

4 Photoionization of fullerenes

Recall that fullerene is a bound system of several dozens of the carbon atoms. The number of the atoms is usually
denoted by \( N \) and the fullerene is \( C_N \). The \( 2N \) 1s electrons are bound to their nuclei while the other \( 4N \) ones are collectivized. Here we analyze the case when the fullerenes have approximately spherical shape. The fullerene \( C_{60} \) is the most studied one. In such fullerenes the electrons are often assumed to move in the field described by a spherical potential \( V(r) \). The electrons are located in the layer between the spheres of radii \( R - \Delta/2 \) and \( R + \Delta/2 \). Characteristic values of the width of the layer \( \Delta \) are of the order \( r_0 = 1 \) a.u. while the empirical values of the radii are about \( R = 6r_0 = 6 \) a.u. The field \( V(r) \) reaches its largest values in the interval \( R - \Delta/2 \leq r \leq R + \Delta/2 \).

### 4.1 The “bubble” potentials

In the Dirac bubble potential [17] the width of the layer \( \Delta = 0 \), and

\[
V(r) = -U_0 \delta(R - r); \quad U_0 > 0, \tag{60}
\]

where \( U_0 \) is a dimensionless constant. The Fourier transform of this potential

\[
V(p) = -4\pi U_0 R \frac{\sin(pR)}{p}, \tag{61}
\]

does not satisfy the condition expressed by equation (6). Hence all momenta \( f \leq p \) contribute to the integral for the function \( J^{(r)}(p) \) – see equation (17).

Our result for the contribution \( F^s_m \) to the amplitude describing transfer of large recoil momentum by the bound electron presented by equation (19) is true. Our analysis of the contribution \( F^s_m \) describing transfer of large recoil momentum by the photoelectron does not work in this case since it employed the smallness of the momentum \( f \ll p \). However another approach based on the partial waves expansion [18] demonstrates that the photoelectron can be described by the plane wave in the asymptotics. Thus the photoionization cross section is given by equation (28). Since

\[
J^{(r)}(p) = -4\pi U_0 R \frac{\sin(pR)}{p} \varphi(R), \tag{62}
\]

the cross section is

\[
\sigma = n_e \frac{16}{3} \alpha \pi U_0^2 \chi^2(R) \frac{\cos^2(pR)}{\omega^2 p}, \tag{63}
\]
dropping as \( \omega^{-5/2} \). This leads to the oscillating photoionization cross sections ratio \( \tau(\omega) \sim \sin^2(pR)/\cos^2(pR) \).

The Dirac bubble potential can bound one electron with orbital momenta \( \ell = 0, 1, 2 \) if \( R = 6r_0 \), \( \Delta = 1 \) a.u. [17]. Thus it is good for the description of photoionization of extra electron in the ion \( C_N \) with \( n_e = 1 \) in equation (63). For photoionization of the fullerene \( C_N \) it is more reasonable to consider the valence electrons to be moving in the Lorentz bubble potential

\[
V(r) = -\frac{U_0}{\pi} \frac{a}{(r - R)^2 + a^2}, \tag{64}
\]

where \( U_0 > 0 \) is a dimensionless constant, \( a \ll R \). At \( a \to 0 \) this is just the Dirac bubble potential given by equation (60). We can proceed in the same way as we did in Drukarev and Mikhailov [2] for photoionization of \( s \) states. The Fourier transform of the potential determined by equation (64) is

\[
V_A(p) = -4\pi \frac{U_0 R}{p} e^{-pa} \sin(pR),
\]
and

\[
V_B(p) = \frac{16U_0a}{p(pR)^2},
\]

coming from the regions \( |r - R| \ll R \) and \( r \sim 1/p \) correspondingly. The contribution \( V_B \) becomes important in the region of the photoelectron energies of the order of several keV where the cross section becomes unobservably small. Thus we can put \( V(p) = V_A(p) \) in the region of the photon energies which are of physical interest. Now the condition expressed by equation (4) is true and the cross section is given by equation (28). We find

\[
\sigma = n_e \frac{16}{3} \alpha \pi U_0^2 \chi^2(R) \frac{e^{-2pa} \cos^2(pR)}{\omega^2 p}. \tag{65}
\]

As well as in the case of \( s \) states this is just the cross section for photoionization in the field of the Dirac bubble potential multiplied by the exponential factor \( e^{-2pa} \).

### 4.2 Jellium model

Now the positive charge of the core is assumed to be uniformly distributed inside the fullerene layer [19]. Introducing \( R_1 = R - \Delta/2 \), \( R_2 = R + \Delta/2 \) we approximate the electron potential energy in the field of the core by the function \( V(r) = V_1(r) \) at \( 0 \leq r < R_1 \), \( V(r) = V_2(r) \) at \( R_1 \leq r < R_2 \) and \( V(r) = V_3(r) \) at \( r > R_2 \), where

\[
V_1(r) = -U_0 \frac{3R_1^2 - R_2^2}{2(R_2^2 - R_1^2)};
\]

\[
V_2(r) = -\frac{U_0}{2(R_2^2 - R_1^2)} \left( 3R_2^2 - r^2 \left( 1 + \frac{2R_1^2}{r^2} \right) \right);
\]

\[
V_3(r) = -\frac{U_0}{r}; \quad U_0 > 0. \tag{66}
\]

Here \( U_0 \) is the dimensionless constant. This potential is continuous at the real axis. The same refers to its derivatives. The second derivatives \( V^{(2)}(r) \) experience jumps at \( r = R_{1,2} \).

In our case equation (39) takes the form

\[
J^{(r)}(p) = \frac{4\pi}{p} \left( \int_0^{R_1} dr V_1(r) r \varphi(r) \sin(pr) \right.
\]

\[
+ \int_{R_1}^{R_2} dr V_2(r) r \varphi(r) \sin(pr)
\]

\[
+ \left. \int_{R_2}^{\infty} dr V_3(r) r \varphi(r) \sin(pr) \right).
\]

We need three integrations by parts to obtain the asymptotics.
\[ J^{(r)}(p) = \frac{4\pi}{p^3} (\zeta(R_1) + \zeta(R_2)); \]
\[ \zeta(R_i) = -R_i \varphi(R_i) \cos(pR_i) \delta(R_i); \]
\[ \delta(R_1) = V''_2(R_1) - V''_1(R_1), \quad \delta(R_2) = V''_2(R_2) - V''_1(R_2); \]
\[ \text{the jumps of the second derivatives} \]
\[ \text{of the potential } V(r). \]
\[ \text{In the limit } \Delta \ll R \text{ they are} \]
\[ \delta(R_1) = \frac{U_0}{R^2 \Delta}; \quad \delta(R_2) = -\frac{U_0}{R^2 \Delta}. \]

The asymptotics of the Fourier transform of the jellium model potential can be obtained by putting \( \varphi(r) = 1 \) in expressions for \( J^{(r)}(p) \) provided by equations (39) and (67)
\[ V(p) = -\frac{8\pi U_0}{\Delta R} \frac{\sin(\pi \Delta/2) \sin(pR)}{p^4}. \]

One can see that equation (4) is true. The large recoil momentum is transferred by the bound electron.

The asymptotics of cross section is provided by equation (28). In the lowest order of expansion in powers of \( \Delta/R \)
\[ J^{(r)}(p) = \frac{4\pi U_0}{p^3} \frac{\delta(R_1)}{\Delta} \left( \varphi(R_1) \sin(pR_1) - \varphi(R_2) \sin(pR_2) \right). \]

Note that the function \( \varphi(r) \) changes significantly in the interval \( R_1 \leq r \leq R_2 \). Thus \( \varphi(R_{1,2}) \) cannot be expanded in powers of \( \Delta/R \). The cross section is
\[ \sigma = \frac{16}{3} \alpha \pi \frac{V_0^2}{\Delta^2} \frac{\left( \varphi(R_1) \sin(pR_1) - \varphi(R_2) \sin(pR_2) \right)^2}{\omega^2 p^2}. \]
\[ \text{It drops as } \omega^{-11/2}. \]

5 Summary

We demonstrated that the high energy nonrelativistic asymptotics of photoionization cross section for the single–particle states with \( \ell = 1 \) bound by a central field \( V(r) \) can be obtained without solving the wave equations for the electrons. The asymptotics can be expressed in terms of the Fourier transform \( V(p) \) of the potential and its first derivative \( V'(p) \). The large recoil momentum can be transferred to the nucleus either by the bound electron or by the photoelectron. The role of the two mechanisms depends on the relation between \( V(p) \) and \( V'(p) \). The latter depends on the form (“gauge”) of the electron-photon interaction. We work in the velocity gauge. If the derivative \( V'(p) \) is large enough and equation (4) is true, the recoil momentum is transferred by the bound electron. If equation (5) is true, both mechanisms should be included.

On the other hand relation between \( V(p) \) and \( V'(p) \) depends on the analytical properties of the potential \( V(r) \). For the potentials with a singularity at \( r = 0 \) equation (5) is true and both mechanisms should be included. In the important case of the potentials with Coulomb behavior at \( r = 0 \) with \( pV'(p)/V(p) = -2 \) the squared amplitude describing transfer of recoil momentum by the bound electron is totally canceled by the term describing the interference of the two mechanisms in the expression for the cross section. Thus the latter is determined by transfer of large momentum by the photoelectron.

For potentials with the short range Coulomb behavior \( V(r) \sim 1/r \) at \( r \to 0 \), (e.g. any atomic potential) there are large corrections to the asymptotic law. They can be summed to all orders of perturbative theory forming the Stobbe factor. Inclusion of the Stobbe factor to photoionization cross section makes the asymptotic analysis possible.

In the case of exponential potential with the cusp at \( r = 0 \) and \( pV'(p)/V(p) = -4 \) large recoil momentum can be transferred by the bound electron or by the photoelectron. The cross section of ionization of \( p \) states drops faster than that of \( s \) states for any potential with a singularity at \( r = 0 \). The ratio \( r(\omega) \) determined by equation (7) exhibits a linear rise with \( \omega \).

For the potentials \( V(r) \) with discontinuity on the real axis we presented the cross section in terms of the jump of the potential \( V(r) \) at the discontinuity point. The large recoil momentum is transferred by the bound electron. The same approach can be applied for potentials which are continuous on the real axis while the its derivatives experience jumps. In these cases the ratio \( r(\omega) \) oscillates.

If the binding field is approximated by an analytical function \( V(r) \) with poles in the complex plane, the cross section exhibits exponential drop. The shape of the energy dependence of the cross section is determined by the derivative \( V'(p) \). The ratio \( r(\omega) \) does not depend on the photon energy. For the Gaussian potential with essential singularity in the complex plane the cross section exhibits the Gaussian-type drop. The cross section of photoionization of \( p \) states drops slower than that of \( s \) states, and \( r(\omega) \sim 1/\omega \).

The results can be applied in the studies of photoionization of fullerenes. Here a typical binding energy is about \( 10 \) eV\[6\]. Thus we can expect the asymptotic analysis to be possible for the photon energies exceeding about \( 100 \) eV. The model potentials for the description of interaction between the valence electrons and the core are often used. We provided two examples, calculating the asymptotics of the photoionization cross section in the Dirac bubble model and in the jellium model. In the former case the potential experiences the infinite jump on the rear axis. In the latter case the potential is continuous, while the second derivatives experience jumps. In both cases the ratio \( r(\omega) \) exhibits oscillating behavior. As it stands now, there are not enough experimental data on the high energy photoionization of fullerenes to compare with the theoretical predictions.

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Author contribution statement

Both authors contributed equally to the paper.
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