

Ultrarelativistic limit for the two-electron photoionization cross sectionM. Ya. Amusia,^{1,2} E. G. Drukarev,³ R. Krivec,⁴ and V. B. Mandelzweig¹¹*Racah Institute of Physics, The Hebrew University, Jerusalem 91904, Israel*²*Ioffe Physico-Technical Institute, St. Petersburg, 194021, Russia*³*Petersburg Institute of Nuclear Physics, Gatchina 188300, Russia*⁴*Department of Theoretical Physics, Jožef Stefan Institute, P.O. Box 3000, 1001 Ljubljana, Slovenia*

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The ratio of double- to single-electron photoionization cross section is calculated in the ultrarelativistic photon frequency region, namely where the photon energy is much larger than the electron rest mass. This ratio can be presented as a sum of the shake-off term and the quasifree term. They are expressed via essentially different integrals of the initial-state two-electron wave function. The shake-off term is calculated in the dipole approximation. The quasifree contribution is nondipole and is determined by the probability of finding both ionizing electrons at the same point in the initial state. The calculations are performed for the negative hydrogen ion, the helium atom, and the heliumlike ions in the ground and excited states using high-precision nonvariational wave functions. The nuclear charge dependence of this correction for heliumlike ions in the ground and the four lowest 1S excited states is calculated. The possibility to detect the quasifree contribution experimentally is discussed.

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I. INTRODUCTION

The ionization of two electrons by a single photon is of great interest since this is the simplest process totally determined by the interelectron interaction. The manifestation of the latter is essentially determined by the photon frequency. It appears that the main mechanism that determines this process changes when the frequency ω increases from values at which the outgoing electrons are fast but nonrelativistic [1–3], to ω so high that it leads to relativistically fast photoelectrons [4,5].

Recently several papers were published, which present results of the calculations of the lowest-order retardation corrections to the two-electron photoionization cross section at high but nonrelativistic photon energies ω . These papers made the first step on the way from ω determined by the inequality $I^{++} \ll \omega \ll c^2$ to $\omega \gg c^2$, where I^{++} is the two-electron ionization potential [24]. In Refs. [4,6,7] the corrections of the first order in ω/c^2 were derived and then expressed [6,7] via the initial-state atomic wave functions. The derivation of the formulas was then repeated and confirmed in Ref. [8]. The numerical results for the coefficients in front of ω/c^2 were obtained [7] using the variational wave functions of different accuracy. In Ref. [9] the correction $\sim \omega/c^2$ was studied for a number of two-electron objects, namely, H^- , the helium atom, and the heliumlike ions in their ground and excited states using the recently obtained very accurate nonvariational initial-state wave function [10].

The aim of this paper is to perform high accuracy calculations similar to that in Ref. [9] but for highly relativistic values of ω , $\omega \gg c^2$ and to compare the contributions of two fundamentally different mechanisms, namely, the one that dominates at $\omega \gg c^2$ and the second one, which is most important at $I^{++} \ll \omega \ll c^2$. As concrete objects, the ground state of H^- and the ground and excited states of the helium atom and the heliumlike ions will be studied. We will use the same wave function as in the nonrelativistic case [10], since, as it

will be demonstrated below, they turn out to be very accurate for the ratios of double- to single-electron ionization cross sections in both frequency regions, namely, not only at $I \ll \omega \ll c^2$ but also at $\omega \gg c^2$.

Until recently, most of the publications dealing with two-electron photoionization were considering it in the dipole approximation. Thus they were neglecting completely the incoming photon momentum and therefore neglecting the effects of retardation of the electromagnetic field as well. In the frame of the dipole approximation it was demonstrated that the main contribution to the two-electron photoionization cross section $\sigma^{++}(\omega)$ at high ω comes from the so-called shake-off mechanism [1–3]. According to this mechanism, one of the electrons, namely, that which absorbs the incoming photon, leaves the ionized atom very fast. This instantly changes the field that acts upon the second electron and causes its elimination from the atom. The fast electron carries away almost all photon energy, $\epsilon_1 \approx \omega \gg I^{++}$, while the energy of the second electron, ϵ_2 , is of the order of I^{++} , $\epsilon_2 \sim I^{++}$. The shake-off mechanism predicted that the ω dependences of $\sigma^{++}(\omega)$ and the one-electron photoionization cross section $\sigma^+(\omega)$ are the same, namely, $\sigma^+(\omega) \sim \sigma^{++}(\omega) \sim \omega^{-7/2}$ at high ω , $\omega \gg I^{++}$. The ω dependence of the cross section of ionization with excitation $\sigma^{+*}(\omega)$ is also the same. All the cross sections in this high but nonrelativistic ω region, $c^2 \gg \omega \gg I^{++}$, are expressed via the initial-state wave function (see, e.g., Ref. [11]). This is why in this ω region the ratio $R(\omega) = \sigma^{++}(\omega) / [\sigma^+(\omega) + \sigma^{+*}(\omega)]$ is ω independent. For He the corresponding value is $R_d \approx 0.0165$ [3], where the index d emphasizes that R is calculated in the dipole approximation. The most recent value is $R_d \approx 0.01644$ (see Ref. [12] and discussion therein). The ω dependence of the cross section $\sigma^{++}(\omega)$ and the value of R at $c^2 \gg \omega \gg I^{++}$ that follows from the shake-off approach seems to be in good agreement with the experimental data [13], starting from 1 keV for He. The shake-off calculations

of the double ionization of the excited 2^1S and 2^3S helium states were carried out in Ref. [14].

It is essential to have in mind that while $\sigma^{++}(\omega)$ decreases rapidly with ω growth, the cross section of ionization of two electrons in Compton scattering $\sigma_C^{++}(\omega)$ is almost ω independent. For He, $\sigma^{++}(\omega)$ and $\sigma_C^{++}(\omega)$ become equal already at $\omega = 6$ keV. However, the contribution of $\sigma^{++}(\omega)$ and $\sigma_C^{++}(\omega)$ at nonrelativistically high ω can be separated experimentally (see Ref. [13], and references therein). This separation is based on the analysis of the recoil momentum of the residual ion He^{++} : in the shake-off double photoionization the whole recoil goes to the ion while in the Compton photoionization the ion remains almost at rest.

In the framework of the shake-off mechanism, the cross sections $\sigma^{++}(\omega)$ and $\sigma^+(\omega)$ are expressed via the integrals over the initial n^1S state nonrelativistic wave function $\bar{\Psi}_n(\mathbf{r}_1, 0)$, where one electron is at the nucleus (at $r_2 \approx 0$), which corresponds to high photoelectron linear momentum, while the other is at the position $|\mathbf{r}_1|$ somewhere inside the atom. We shall use the notation $\bar{\Psi}_n(\mathbf{r}_1, \mathbf{r}_2) = \Psi_n(\mathbf{r}_{12}, \mathbf{s}_{12})$, where \mathbf{r}_1 , \mathbf{r}_2 denote the electron coordinates relative to the nucleus, and \mathbf{r}_{12} and \mathbf{s}_{12} denote the Jacobi vectors, \mathbf{r}_{12} connecting the electrons, and \mathbf{s}_{12} connecting the center of mass of the electrons and the nucleus.

The shake-off approach seems to be so well established that other alternative mechanisms were until recently usually not discussed at all [15]. However, it was demonstrated already in 1975 that there exists the so-called quasifree (QF) mechanism [4,11] that is becoming more and more important with ω growth. The main idea that forms the foundation of this mechanism is the following: two free electrons can absorb a single photon in contrast to one electron. As a result of photon absorption, the electrons acquire almost equal energies $\epsilon_1 \approx \epsilon_2 \approx \omega/2$ and move in approximately opposite directions, thus not transferring, just as in the case of Compton ionization, momentum to the residual ion. Note that the QF mechanism requires going beyond the dipole approximation of the electron-photon interaction.

It was demonstrated long ago [4,11] that the QF mechanism leads to corrections of the order of $\omega/c^2 \ll 1$ at nonrelativistic photon energies. At $\omega/c^2 \geq 1$, however, the QF mechanism becomes dominant [5]. In the frequency domain $\omega/c^2 \gg 1$ the ratio $R(\omega)$ is again ω independent, tending to the ultrarelativistic limit R^{ur} , which, as we shall show, is considerably larger than the value $R_d \approx 0.0165$ obtained in the dipole approximation.

The results in Refs. [4,11,5] were obtained in the first order of the interelectron interaction. It is clear, however, that numerically such an approach is not accurate enough. Indeed, in this approximation the value $R_d^{(1)}$ is 0.0235, which is considerably larger than the nonperturbative value. Qualitatively, it is clear that the contribution of the QF mechanism depends upon the initial-state wave function with two ionizing electrons at small interelectron distances $r_{12} \approx 1/p \rightarrow 0$, $\bar{\Psi}_n(\mathbf{r}_1, \mathbf{r}_1) = \Psi_n(0, \mathbf{s}_{12})$, with p being the photoelectron linear momentum that increases infinitely with ω growth.

One needs the relativistic initial-state wave function when considering cross sections at $\omega \gg c^2$. For the single ionization

and for the shake-off mechanism of the double photoionization, this becomes quite explicit if one considers the initial two-electron wave functions in momentum space. One of the momenta is of the order mc , thus requiring relativistic treatment. However, with the accuracy $(Z/137)^2 \ll 1$ the relativistic wave function can be expressed through the nonrelativistic one by using the lowest-order iteration of the Bethe-Salpeter equation.

As it is well known (see, e.g., Refs. [16,17]), the cross section $\sigma^+ \omega$ at $\omega \gg c^2$ has completely different ω dependence and angular distribution of photoelectrons than at $I^{++} \ll \omega \ll c^2$. Indeed, one has for hydrogenlike ions with the nuclear charge Z [16,17] at $\omega \gg c^2$ in the lowest order of expansion in powers of $(Z/137)^2$,

$$\sigma^+(\omega) = \frac{2\pi Z^5}{c^6} \frac{1}{\omega} \quad (1)$$

instead of

$$\sigma^+(\omega) = \frac{2^8 \pi Z^5}{3c} \frac{1}{\omega^{7/2}} \quad (2)$$

at $I^{++} \ll \omega \ll c^2$. The relativistic photoelectrons carry away almost all photon momentum, thus being strongly aligned toward the photon direction. This behavior differs qualitatively from the almost isotropic angular distribution of photoelectrons at $I^{++} \ll \omega \ll c^2$. Similar differences between $I^{++} \ll \omega \ll c^2$ and $\omega \gg c^2$ regions exist also for the cross sections of the two-electron ionization $\sigma^{++}(\omega)$ and the ionization with excitation $\sigma^{+*}(\omega)$.

Although the energy dependence of the single-ionization cross sections are quite different in these limiting regions, the asymptotics of the double-to-single ratios is the same in the shake-off approximation. This is because the dynamical origin of the energy dependence is quite similar in both processes being connected with the necessity to transfer large momentum to the nucleus. In the nonrelativistic region the transferred momentum depends on the photon energy as $(\omega/c)^{1/2}$. In the ultrarelativistic region it is of the order of mc and does not depend on the photon energy. Since the shake-off double photoionization can be viewed as the single one followed by ejection of a slow electron, all the energy dependence of the amplitudes of the single and double processes is the same. For $(\alpha Z)^2 \ll 1$, the relativistic wave function can be expressed through the nonrelativistic one [16,17]. With the terms of the order $(\alpha Z)^2$ being neglected, the relativistic effects manifest themselves through the energy-dependent factor that is the same in the amplitudes of the single and double photoionization. Thus the constant value of the double- to single-shake-off ratio, calculated with the nonrelativistic wave function is still true in relativistic region [5].

In the QF mechanism the electrons approach each other at the distances $\rho = |\mathbf{r}_1 - \mathbf{r}_2|$, which are much smaller than the size of the atom. This means that the electrons exchange by large momentum. At $\omega \geq mc^2$ this momentum is of the order ω/c . Thus the relative motion of the electrons requires the

relativistic treatment. However, the motion of the electrons with respect to the nucleus before this exchange by large momentum can be treated nonrelativistically since their momenta with respect to the nucleus are still of the order $mc(\alpha Z) \ll mc$. The Bethe-Salpeter equation connects the wave functions with relativistic momentum Q of the order mc and with nonrelativistic one of the order $mc(\alpha Z)$. The latter can be taken in the nonrelativistic approximation. In the leading order, the lowest-order iteration of the Bethe-Salpeter equation is sufficient.

In this paper, we will concentrate on calculating the ultrarelativistic values of the ratio R_n using the very precise nonvariational initial-state two-electron wave functions [10,12,18,19]. We shall compare our results with numerical results obtained there, and with the pure Coulombic limit [5], in order to study how sensitive are the ultrarelativistic ratios to the details of $\Psi_n(\mathbf{r}_1, \mathbf{r}_2)$. The experimental investigation of the QF mechanism contribution at $\omega \gg c^2$ is therefore of interest. However, it cannot be done simply by measuring the recoil momenta of the residual ion [20], since this mechanism, as it was mentioned above, just as the two-electron ionization in Compton scattering, can proceed almost without participation of the nucleus. In order to identify the QF contribution, a coincidence experiment with simultaneous observation of the doubly charged ion and the measurement of one of the outgoing electron's energy is required.

II. MAIN EQUATIONS

At $I^{++} \ll \omega \ll c^2$ the leading contribution to the double- to single-photoionization cross-sections ratio, i.e., the leading term of the expansion in powers of ω^{-1} comes from the shake-off mechanism which can be treated in the dipole approximation. The leading correction of the order ω is provided by QF mechanism that requires going beyond the dipole approximation [4]. In all the region $\omega \gg I^{++}$ can present [6,7] for double ionization of n^1S state

$$R^n(\omega) = R_{s.o.}^n(\omega) + \frac{\sigma_0(\omega)}{\sigma^+(\omega)} \mathcal{I}^n \quad (3)$$

with $\sigma_0(\omega)$ being the cross section of ionization of two free electrons at rest, while

$$J^n = \int d\mathbf{r}_1 |\bar{\Psi}_n(\mathbf{r}_1, \mathbf{r}_1)|^2. \quad (4)$$

At $\omega \ll c^2$, the second term in the right-hand side (rhs) of Eq. (3) provides correction of the order ω/c^2 to the first one [4,6,7]

$$R^n(\omega) = R_{s.o.}^n + \frac{8\sqrt{2}}{5Z^2} \mathcal{I}_n \frac{\omega}{C^2} \quad (5)$$

with

$$\mathcal{I}_n = \frac{J^n}{N_n} \quad (6)$$

and

$$N_n = \sum_{\nu=1}^{\infty} \left| \int d\mathbf{r}_1 \bar{\Psi}_n(\mathbf{r}_1, 0) \psi_{\nu 00}(\mathbf{r}_1) \right|^2. \quad (7)$$

Here $\psi_{\nu lm}(\mathbf{r})$ are the one-electron wave functions in the field of the nucleus; only $l=m=0$ contribute. In this paper, $\bar{\Psi}_n(\mathbf{r}_1, \mathbf{r}_2)$ is the H^- , He, or the heliumlike ion three-body wave function in the ground or in the first few excited (except for H^-) n^1S states. (Additional indices on R_n^{ur} , R_d^n , and \mathcal{I}_n shall be used to denote the physical system or extrapolation in Z .)

At larger values of the photon energy $\omega \sim c^2$, the ratio R presented by Eq. (3) depends on ω again due to the energy dependence of the second term in the rhs. At $\omega \gg c^2$, corresponding to ultrarelativistic energies transferred to the atomic electrons, we come to a new limiting value

$$R^{n,ur} = R_d^n + \frac{4}{Z^2} \mathcal{I}_n, \quad (8)$$

with \mathcal{I}_n defined by Eq. (6). Thus, both high-energy nonrelativistic and ultrarelativistic limits are determined by the same initial-state parameter \mathcal{I}_n . The calculations carried out in Refs. [6] and [22] show strong dependence of the parameter \mathcal{I}_n on the choice of the initial-state function $\Psi_n(\mathbf{r}, \mathbf{r})$ at least for the ground state of atomic helium.

From Eq. (3) it follows that \mathcal{I}_n is determined by the initial-state two-electron wave function $\bar{\Psi}_n(\mathbf{r}_1, \mathbf{r}_2)$ in two different space coordinate regions: at $r_k=0$, $k=1,2$ and at $r_{12}=0$. On the other hand, R_d is determined only by the initial-state two-electron wave function with one coordinate \mathbf{r}_2 being equal to zero, $\bar{\Psi}_n(\mathbf{r}_1, 0)$. As a consequence of the nonanalyticity of the nuclear Coulomb potential $-Z/r$ under the change of sign $r \rightarrow -r$, the wave function $\bar{\Psi}_n(\mathbf{r}_1, \mathbf{r}_2)$ has singularities at $r_k \rightarrow 0$, $k=1,2$, called the Kato cusps [21]. A similar singularity exists in $\bar{\Psi}_n(\mathbf{r}_1, \mathbf{r}_2)$ when $r_{12} \rightarrow 0$, which is a consequence of the nonanalyticity of the interelectron interaction $1/r_{12}$ under the change of sign $r_{12} \rightarrow -r_{12}$. The importance of the Kato cusp conditions in the double-photoionization problem was discussed recently in Refs. [22,23]. The peculiarities that characterize the wave function $\bar{\Psi}_n(\mathbf{r}_1, \mathbf{r}_2)$ at $r_k=0$, $k=1,2$ and at $r_{12}=0$ must be reproduced well by the wave function that we use in our calculations in order to give reliable values for R_d^n and \mathcal{I}_n .

In this work, therefore we employ the parameter \mathcal{I}_n that was calculated numerically in Ref. [9] using the recently computed locally correct nonvariational initial-state wave function described in Refs. [9,10,12,18,19] and obtained by the so-called correlation function hyperspherical harmonic method (CFHHM). For the readers' convenience we repeat here the main points of this method. In CFHHM, the wave function Ψ is decomposed as

$$\Psi = e^f \phi, \quad (9)$$

where f is the correlation function describing the singularities of Ψ , and ϕ is a smooth remainder that can be expanded in a fast converging hyperspherical harmonic expansion. The function f depends on interparticle distances and takes into account analytically the two- and three-body Coulomb singularities of the wave function, i.e., it satisfies the Kato cusp conditions exactly. The function Ψ is obtained by a direct solution of the three-body Schrödinger equation, which guarantees local correctness of Ψ because the convergence of Ψ across the configuration space is uniform.

III. RESULTS OF CALCULATIONS AND DISCUSSIONS

In this work we use the values of the parameter \mathcal{I}_n calculated in Ref. [9] for H^- , He, and heliumlike ions for both ground and, except in H^- , for the four lowest $1S$ excited states. By drawing the Z dependence of \mathcal{I}_n , it is possible to extrapolate \mathcal{I}_n to asymptotically high values of Z , $Z \gg 1$ [still keeping $(Z/137)^2 \ll 1$]. In this limit, the pure hydrogenic model must be valid. In its frame the interelectron interaction is treated in the first order, which is correct for $Z \gg 1$. For the ground state of the target ion in the frame of this model, one obtains [6] $\mathcal{I}_1 = 1/8$. This value coincides excellently [9] with the result of our extrapolation of the calculated curve to $Z \gg 1$.

At $Z \gg 1$ the shake-off contribution R_d^1 is given by the expression $R_d^{1,\infty} \approx 0.095/Z^2$ while for the QF term ($\mathcal{I}_1 = 1/8$) one has $\Delta R_1^{ur,\infty} = 0.5/Z^2$. Thus, one obtains

$$R_1^{ur,\infty} \approx 6.25 R_d^{1,\infty} \approx 0.594/Z^2 . \tag{10}$$

It is of interest to note that the QF contribution to the R^{ur} values is almost the same for He and H^- : indeed, the value of \mathcal{I}/Z^2 is 0.011 49 in He and 0.0169 in H^- .

Using our numerical values for He, the following expression for $R_{1,He}(\omega)$ can be given:

$$R_{1,He}^{ur} \approx 4.632 R_d^1 \approx 0.0762 . \tag{11}$$

It is obvious that for $\omega \gg c^2$ the value R_n^{ur} due to the contribution of QF mechanism is altered qualitatively. Comparison of the value that follows from Eq. (10) at $Z=2$ with the value $R_{1,He}^{ur} \approx 0.0762$ shows that the pure Coulomb-like calculation overestimates the value $R_{1,He}^{ur}$ by the factor 1.952.

Our calculations of $R_n^{ur} = [1 + 4\mathcal{I}_n / (Z^2 R_d^n)] R_d^n \equiv \zeta_Z^{(n)} R_d^n$ for all considered cases are summed up in Tables I and II that present the ratios R_n^{ur} and the factors $\zeta_Z^{(n)}$ as functions of Z and n for H^- , He, and for the helium isoelectronic sequence for the ground and the four lowest-excited states. The last rows of Table II show the extrapolations to infinite Z , using the forms $a_n + b_n/Z^2$ ($T=2$) and $a_n + b_n/Z^2 + c_n/Z^3$ ($T=3$) on a subset of $\zeta_Z^{(n)}$ to calculate least-squares fits and the coefficients a_n as the corresponding extrapolated values. For $n=1$, the extrapolated values are most sensitive to discarding the points for small Z , increasing slowly and reaching 6.25 for $T=2$ if the $\zeta_1^{(1)}, \dots, \zeta_7^{(1)}$ values are discarded. The check using $T=3$ stabilizes at a slightly larger value, 6.30; the shift from $T=2-3$ is about the same as if one or two

TABLE I. Ratios R_n^{ur} as functions of Z and n .

n	1	2	3	4	5
Z	R_1^{ur}	R_2^{ur}	R_3^{ur}	R_4^{ur}	R_5^{ur}
1	0.08366				
2	0.07615	0.01569	0.00559	0.00247	0.00127
3	0.04347	0.01844	0.01023	0.00627	0.00402
4	0.02733	0.01492	0.01001	0.00741	0.00563
5	0.01864	0.01148	0.00845	0.00692	0.00579
6	0.01349	0.00890	0.00690	0.00600	0.00532
7	0.01020	0.00703	0.00564	0.00510	0.00469
8	0.00798	0.00567	0.00465	0.00431	0.00408
9	0.00641	0.00466	0.00388	0.00367	0.00354
10	0.00526	0.00389	0.00328	0.00315	0.00308

more Z points are added at $T=2$. For $n > 1$, the $T=3$ extrapolated values do deviate slightly from the $T=2$ values if only the largest Z are taken into account, but approach them if more Z are included.

It is understandable that the role of the QF mechanism is considerably smaller for the excited than for the ground states of the target atom or ion. In the latter case, one of the electrons is much less bound than the second one and so the shake-off contribution becomes considerably more important.

Note that for the ground states $\zeta_Z^{(1)}$ increases monotonically for $Z > 2$ while the ratio R_1^{ur} monotonically decreases with increasing Z . On the contrary, the function $\zeta_Z^{(2)}$ reaches

TABLE II. Factors $\zeta_Z^{(n)}$ as functions of Z and n . The last entries show the extrapolations to infinite Z . $T=2$ implies the fitting function of the form $a + b/Z^2$ and $T=3$ implies the fitting function of the form $a + b/Z^2 + c/Z^3$. Z_{\min} is the smallest Z taken into account in the extrapolation.

n	1	2	3	4	5
(ZT)	$\zeta_Z^{(1)}$	$\zeta_Z^{(2)}$	$\zeta_Z^{(3)}$	$\zeta_Z^{(4)}$	$\zeta_Z^{(5)}$
1	5.222				
2	4.632	1.737	1.515	1.462	1.444
3	5.081	1.531	1.232	1.148	1.115
4	5.380	1.500	1.180	1.095	1.062
5	5.583	1.495	1.161	1.077	1.046
6	5.727	1.497	1.153	1.069	1.039
7	5.835	1.500	1.148	1.064	1.035
8	5.919	1.503	1.145	1.062	1.032
9	5.986	1.507	1.144	1.060	1.031
10	6.040	1.510	1.142	1.058	1.030
∞ 2	6.25	1.52	1.14	1.05	1.03
Z_{\min}	8	6	6	4	6
∞ 3	6.30	1.52	1.12	1.04	1.02
Z_{\min}	8	8	8	7	8
∞ 3	6.30	1.53	1.14	1.05	1.03
Z_{\min}	8	7	7	6	7

its minimum value at $Z=5$ while $\zeta_Z^{(n)}$ decreases monotonically for $n>2$. The biggest absolute value R_n^{ur} , 8.4%, is reached for H^- , $n=1$. With the increase of both Z and n , R_n^{ur} decreases rapidly.

To illustrate the sensitivity of \mathcal{I}_n values to the quality of the initial-state wave function, let us discuss the results for \mathcal{I}_n that were calculated in Ref. [6] using different wave functions. Using the Hartree-Fock wave function for He, the result $\mathcal{I}_{1,He}=0.11$ was obtained. The Hylleraas three- and six-parameter wave functions generated the \mathcal{I}_{He} values 0.07 and 0.068, respectively. For the Kinoshita wave function the value is 0.055. The details about these wave functions can be found in Table 6 of the book [16]. It is obvious that \mathcal{I} is quite sensitive to the choice of the wave function.

One should also have in mind that the interelectron interaction must be taken into account nonperturbatively. This is demonstrated by the large difference in \mathcal{I} values for both relatively small and infinitely large values of Z and for the high- Z limit: as it is shown in Ref. [9], the difference between \mathcal{I}_{He} and \mathcal{I}^∞ is rapidly increasing with increasing n .

Note that for the triplet excited states 3S , the QF term is zero in the frame of the approximation used in this paper, since the triplet state wave function $\bar{\Psi}_n^{(3)}(\mathbf{r},\mathbf{r})=0$ due to the Pauli principle.

The possibility to reproduce the accurate results for \mathcal{I} within the framework of the lowest-order hydrogenic approximation [4], but using effective charges, is discussed in Ref. [9]. Note that the ratio R must include at least two effective charges, namely, the screening or the Slater effective charges $Z_{\text{eff}}^{\text{He}}=Z-5/16$ and the interelectron interaction one $Z_{\text{eff}}^{\text{in}}$, which takes into account the higher-order corrections.

The results of calculations of the value R^{ur} thus are very sensitive to the accuracy of the initial-state wave function. The experimental determination of it is a challenging experimental problem, but it will contribute enormously to deepen our understanding of the two-electron photoionization process and to the verification of the validity of the wave functions calculated nonvariationally with high accuracy in Refs. [10,12,18,19].

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