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K-SHELL IONIZATION OF ATOMS AND IONS BY RELATIVISTIC PROJECTILES

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We evaluate the total cross section for the single K-shell ionization of atoms and ions by the impact of relativistic electrons. The study is performed to leading orders of the QED perturbation theory with respect to the parameters αZ and $1/Z$. The results obtained are in good agreement with experimental data for different atomic targets. In the case of moderate values of the nuclear charge Z, the total cross section is described by a simple analytic formula. The K-shell ionization by relativistic heavy particles is also considered.

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1. INTRODUCTION

The single ionization of inner-shell electrons by the impact of relativistic particles is one of the fundamental processes that is being persistently investigated during last decades (see, e.g., papers [1–10] and the references there). Sophisticated numerical approaches or empirical and semiempirical formulas are typically used to predict the ionization cross sections. In Refs. [4–8], simple formulas for the ionization cross sections have been found. However, a consistent theoretical treatment of the problem, which would allow describing the inner-shell ionization for different atomic targets and projectiles at arbitrary collision energy, appears to be still absent in the literature.

In our recent works [11, 12], we have deduced the universal scaling behavior for cross sections of the single K-shell ionization by an electron or positron impact in the entire nonrelativistic energy domain. The results obtained are applicable to a wide family of atomic targets with moderate values of nuclear charge numbers Z. In this paper, we extend the previous formulas to the case of relativistic projectiles. The study is performed to leading orders of the QED perturbation theory with respect to the small parameters $1/Z$ and αZ, where α is the fine-structure constant. Accordingly, we assume that $\alpha Z \ll 1$, but $Z \gg 1$. Relativistic units are used throughout the paper ($\hbar = 1$, $c = 1$).

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2. THEORY

We first consider the inelastic electron scattering on a hydrogen-like ion, which results in the ionization of a K-shell bound electron. The nucleus of the ion can be treated as an external source of the Coulomb field. Accordingly, the problem is reduced to the electron–electron scattering in the external nuclear field (Furry picture). The multicharged ion in the ground state is characterized by the Coulomb ionization potential $I = \eta^2/2m$, where $\eta = m\alpha Z$ is the average momentum of the bound electron and m is the electron mass. An incident electron can be characterized by the energy E and the asymptotic momentum $\mathbf{p}$, which are related via $E^2 = p^2 + m^2$. We focus on the relativistic domain $p \gtrsim m$.

To the leading order of the perturbation theory with respect to the interelectron interaction, the amplitude

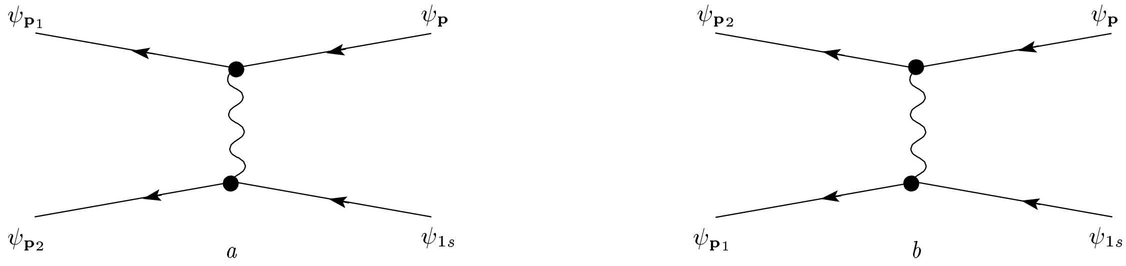

Fig. 1. Feynman diagrams for ionization of a K-shell electron by an electron impact. Solid lines denote electrons in the Coulomb field of the nucleus, and wavy line denotes the electron–electron interaction

of an ionization process is described by the Feynman diagrams depicted in Fig. 1. In the final continuum state, the electron wave functions are denoted as $\psi_{\mathbf{p}_1}$ and $\psi_{\mathbf{p}_2}$. We label the fast (scattered) and slow (ejected) electrons by the respective indices "1" and "2". The asymptotic momenta of the outgoing electrons are estimated as $p_1 \sim p \gg p_2 \sim \eta$. The energy of the scattered electron is given by

$$E_1^2 = p_1^2 + m^2.$$

The energy conservation law implies

$$E + E_{1s} = E_1 + E_2,$$

where

$$E_{1s} \approx m - I$$

and

$$E_2 \approx m + p_2^2/2m.$$

The leading contribution to the total cross section arises from the domain of small momentum transfer $k \lesssim \eta$, where $\mathbf{k} = \mathbf{p} - \mathbf{p}_1$. In this case, the wave functions of the initial and final states overlap most considerably. Accordingly, only the Feynman diagram in Fig. 1a must be taken into account. The contribution of the exchange diagram turns out to be suppressed by a factor of about $(\eta/p)^2$ and can therefore be neglected.

The amplitude of the K-shell electron ionization is given by [13]

$$\mathcal{A} = 4\pi\alpha \int d\mathbf{r}_1 \overline{\psi}_{\mathbf{p}_1}(\mathbf{r}_1)\gamma_\mu \psi_{\mathbf{p}}(\mathbf{r}_1) \times \\ \times \int d\mathbf{r}\, \frac{e^{i\omega R}}{4\pi R}\, \overline{\psi}_{\mathbf{p}_2}(\mathbf{r})\gamma^\mu \psi_{1s}(\mathbf{r}), \quad (1)$$

where $R = |\mathbf{r}_1 - \mathbf{r}|$, $\overline{\psi} = \psi^+\gamma_0$, $\gamma^\mu = (\gamma_0, \boldsymbol{\gamma})$ denotes the Dirac matrices, and $\omega = E - E_1$ is the energy acquired by the atomic electron.

Since $p \sim p_1 \gg \eta$, the wave functions of both incident and scattered high-energy electrons can be approximated by plane waves (the first Born approximation), which are given by

$$\psi_{\mathbf{p}}(\mathbf{r}) = u_p \exp(i\mathbf{p}\cdot\mathbf{r}), \quad \overline{u}_p u_p = \frac{m}{E}, \qquad (2)$$

$$\overline{\psi}_{\mathbf{p}_1}(\mathbf{r}) = \overline{u}_{p_1} \exp(-i\mathbf{p}_1\cdot\mathbf{r}), \quad \overline{u}_{p_1} u_{p_1} = \frac{m}{E_1}. \qquad (3)$$

The bispinors u_p and u_{p_1} are normalized to one particle per unit volume. Substitution of Eqs. (2) and (3) in Eq. (1) allows integrating over the variable $\mathbf{r}_1$ and yields

$$\int d\mathbf{r}_1 \frac{e^{i\omega R}}{4\pi R} \exp(i(\mathbf{p} - \mathbf{p}_1)\cdot\mathbf{r}_1) = \frac{\exp(i\mathbf{k}\cdot\mathbf{r})}{k^2 - \omega^2}, \qquad (4)$$

where $\mathbf{k} = \mathbf{p} - \mathbf{p}_1$ is the momentum transfer. Then amplitude (1) can be rewritten as

$$\mathcal{A} = \frac{4\pi\alpha}{k^2 - \omega^2} j_\mu J^\mu, \qquad (5)$$

where

$$j_\mu = \overline{u}_{p_1}\gamma_\mu u_p, \qquad (6)$$

$$J^\mu = \int d\mathbf{r}\, \overline{\psi}_{\mathbf{p}_2}(\mathbf{r})\gamma^\mu \psi_{1s}(\mathbf{r}) \exp(i\mathbf{k}\cdot\mathbf{r}) \qquad (7)$$

are the incident electron and atomic current densities, respectively. The electron–electron interaction is mediated by the exchange of a virtual photon, for which $k^2 \neq \omega^2$. Both 4-vectors $j^\mu = (j_0, \mathbf{j})$ and $J^\mu = (J_0, \mathbf{J})$ satisfy the current conservation law, that is, $\omega j_0 = \mathbf{k}\cdot\mathbf{j}$ and $\omega J_0 = \mathbf{k}\cdot\mathbf{J}$. For small transferred momenta $\mathbf{k}$, we can set $\mathbf{p} = \mathbf{p}_1$ in the electron current. Then with an accuracy up to terms $\mathcal{O}(k/p)$, we have $j^\mu = (1, \mathbf{v})$, where $\mathbf{v} = \mathbf{p}/E$ is the velocity of the incident electron.

In the limit $k \to 0$, the zeroth component of the atomic current J_0 tends to zero due to the orthogonality of the wave functions involved, while the 3-vector $\mathbf{J}$ remains finite. Therefore, for small transferred momenta $k \sim \omega \sim I$, all the components of J^μ are of the same order of magnitude and should be taken into account. To the leading order with respect to the parameter αZ, the component J_0 can be evaluated by using the nonrelativistic Coulomb wave functions (see, e.g., Ref. [11]). The corresponding expression is

$$J_0 = N_{1s} N_{p_2} \frac{4\eta}{ab} \times \times \left[k^2 - (1 + i\xi_2)(\mathbf{p}_2 \cdot \mathbf{k})\right] \Phi_{\mathbf{p}_2}(\mathbf{k}) w_2^+ w_0 \,, \quad (8)$$

where

$$|N_{p_2}|^2 = \frac{2\pi\xi_2}{1 - \exp(-2\pi\xi_2)} \,, \quad N_{1s}^2 = \frac{\eta^3}{\pi} \,, \quad (9)$$

$$\Phi_{\mathbf{p}_2}(\mathbf{k}) = \frac{4\pi}{a} \left(\frac{a}{b}\right)^{i\xi_2} \,, \quad (10)$$

$$a = (\mathbf{k} - \mathbf{p}_2)^2 + \eta^2 \,, \quad (11)$$

$$b = k^2 - (p_2 + i\eta)^2 \,, \quad (12)$$

and $\xi_2 = \eta/p_2$. The two-component spinors w_0 and w_2, which respectively describe the polarization states of the bound and ejected electrons, are normalized as $w_0^+ w_0 = 1$ and $w_2^+ w_2 = 1$.

To evaluate the vector component of the current $\mathbf{J}$, we need to use the relativistic functions, which involve corrections of the order αZ to the nonrelativistic wave functions. Formally, it is associated with the structure of the vector $\mathbf{J}$, which contains the Dirac $\boldsymbol{\alpha}$-matrix ($\boldsymbol{\alpha} = \gamma_0 \boldsymbol{\gamma}$). This matrix leads to a mutual interchange of the large and small components of bispinors. However, the product of two Dirac $\boldsymbol{\alpha}$-matrices, which occurs due to corrections to the nonrelativistic wave functions, does not transpose the components of bispinor. Therefore, the corresponding contribution to the atomic current should be taken into account. Physically, it means that at relativistic velocities of the projectile $v \sim 1$, the account for the magnetic part of the electron–electron interaction becomes as important as the electric one.

We evaluate the integral

$$\mathbf{J} = \int d\mathbf{r}\, \psi_{\mathbf{p}_2}^+(\mathbf{r}) \boldsymbol{\alpha} \psi_{1s}(\mathbf{r}) \exp(i\mathbf{k} \cdot \mathbf{r}) \,, \quad (13)$$

neglecting terms of the order $(\alpha Z)^2$. The wave function of the K-shell electron, which coincides with the exact solution of the Dirac equation up to the first order in the parameter αZ, is [14]

$$\psi_{1s}(\mathbf{r}) = \left(1 - \frac{i}{2m} \boldsymbol{\alpha} \cdot \nabla\right) \varphi_{1s}(r) u_0 \,, \quad u_0 = \begin{pmatrix} w_0 \\ 0 \end{pmatrix} , \quad (14)$$

where

$$\varphi_{1s}(r) = N_{1s} e^{-\eta r}$$

is the nonrelativistic wave function and ∇ denotes the gradient. Accordingly, as a wave function of the ejected electron, we need to take the Furry–Sommerfeld–Maue function [14]

$$\psi_{\mathbf{p}_2}^+(\mathbf{r}) = N_{p_2} \exp(-i\mathbf{p}_2 \cdot \mathbf{r}) u_{p_2}^+ \left(1 + \frac{i}{2m} \boldsymbol{\alpha} \cdot \nabla\right) \times \times F(i\xi_2, 1, i(p_2 r + \mathbf{p}_2 \cdot \mathbf{r})), \quad (15)$$

where $\xi_2 = \eta/p_2$ and $F(x, y, z)$ is the confluent hypergeometric function. The bispinor $u_{p_2}^+$ is related to the spinor w_2^+ as

$$u_{p_2}^+ = \left(w_2^+, w_2^+ \frac{\boldsymbol{\sigma} \cdot \mathbf{p}_2}{2m}\right) , \quad (16)$$

where the components of the vector $\boldsymbol{\sigma}$ are the Pauli spin matrices. At asymptotically large distances, $\psi_{\mathbf{p}_2}^+$ behaves like a plane wave plus an outgoing spherical wave.

Substituting Eqs. (14) and (15) in Eq. (13) yields

$$\mathbf{J} = \frac{1}{2m} N_{1s} N_{p_2} w_2^+ \times \times \left[L_0 (\boldsymbol{\sigma} \cdot \mathbf{p}_2) \boldsymbol{\sigma} + i\eta \boldsymbol{\sigma} (\boldsymbol{\sigma} \cdot \mathbf{L}_1) + i (\boldsymbol{\sigma} \cdot \mathbf{L}_2) \boldsymbol{\sigma}\right] w_0, \quad (17)$$

here

$$L_0 = \int d\mathbf{r} \exp(i\mathbf{q} \cdot \mathbf{r} - \eta r) F(i\xi_2, 1, i(p_2 r + \mathbf{p}_2 \cdot \mathbf{r})) = = -\frac{\partial}{\partial \eta} \Phi_{\mathbf{p}_2}(\mathbf{k}) \,, \quad (18)$$

$$\mathbf{L}_1 = \int d\mathbf{r} \exp(i\mathbf{q} \cdot \mathbf{r} - \eta r) \mathbf{n} F(i\xi_2, 1, i(p_2 r + \mathbf{p}_2 \cdot \mathbf{r})) = = -i \nabla_k \Phi_{\mathbf{p}_2}(\mathbf{k}) \,, \quad (19)$$

$$\mathbf{L}_2 = \int d\mathbf{r} \exp(i\mathbf{q} \cdot \mathbf{r} - \eta r) \nabla F(i\xi_2, 1, i(p_2 r + \mathbf{p}_2 \cdot \mathbf{r})) = = -i\mathbf{q} L_0 + \eta \mathbf{L}_1 \,, \quad (20)$$

where $\mathbf{q} = \mathbf{k} - \mathbf{p}_2$, $\mathbf{n} = \mathbf{r}/r$, and ∇_k is the gradient with respect to the variable k. In Eq. (20), the integration is performed by parts. The integrals in Eqs. (18) and (19) are evaluated explicitly in textbook [13]. Using these results, Eq. (17) can be rewritten as

$$\mathbf{J} = N_{1s}N_{p_2}\frac{2\eta}{mab}(1-i\xi_2)\times \times\left\{b\mathbf{p}_2+\mathbf{k}\left[p_2^2(1+i\xi_2)-(\mathbf{p}_2\cdot\mathbf{k})\right]\right\}\Phi_{\mathbf{p}_2}(\mathbf{k})w_2^+w_0+ + N_{1s}N_{p_2}\frac{i2\eta}{mab}\left[k^2-(1+i\xi_2)(\mathbf{p}_2\cdot\mathbf{k})\right]\times \times\Phi_{\mathbf{p}_2}(\mathbf{k})w_2^+[\boldsymbol{\sigma}\times\mathbf{k}]w_0\,. \quad (21)$$

In Eq. (21), the spin part of the current given by the second term is of the order of $kJ_0/2m$ and it can therefore be neglected for $k \lesssim \eta$. Accordingly, the spin functions are suppressed in what follows. From the current and energy conservation laws, it follows that

$$\mathbf{k}\cdot\mathbf{v} = \omega,$$

while

$$\omega = E_2 - E_{1s} = \frac{p_2^2+\eta^2}{2m}.$$

Then the product of the currents in Eq. (5) is given by

$$j_\mu J^\mu = J_0 - \mathbf{v}\cdot\mathbf{J} = N_{1s}N_{p_2}\frac{4\eta}{ab}\times \times\left\{k^2-\omega^2+(1+i\xi_2)\left[\omega(\mathbf{p}_2\cdot\mathbf{v})-(\mathbf{p}_2\cdot\mathbf{k})\right]\right\}\times \times\Phi_{\mathbf{p}_2}(\mathbf{k}), \quad (22)$$

where we omit small terms of the order of k/m with respect to the leading one.

The differential cross section for ionization of a K-shell electron is related to the amplitude $\mathcal{A}$ as

$$d\sigma_{\mathrm{K}}^+ = \frac{2\pi}{v}|\mathcal{A}|^2\frac{d\mathbf{p}_1}{(2\pi)^3}\frac{d\mathbf{p}_2}{(2\pi)^3}\delta(E_1+E_2-E-E_{1s}). \quad (23)$$

Equation (23) defines the distributions over energy and ejection angles of the fast and slow electrons. The elements of phase space volumes for the electrons scattered and ejected into the respective solid angles $d\Omega_1$ and $d\Omega_2$ can be written as

$$d\mathbf{p}_1 = p_1E_1\,dE_1\,d\Omega_1 \approx \frac{\pi}{v}\,dE_1\,dk^2\,, \quad (24)$$

$$d\mathbf{p}_2 = \frac{p_2}{2}\,dp_2^2\,d\Omega_2\,. \quad (25)$$

Integrating Eq. (23) over the energy E_1 and the angles of ejection of slow electrons yields

$$d\sigma_{\mathrm{K}}^+ = \frac{2^9}{3}\frac{\pi\alpha^2\eta^6 u\exp(2\xi_2\delta)}{[1-\exp(-2\pi\xi_2)]}\frac{dk^2dp_2^2}{v^2\chi^3}\,, \quad (26)$$

where

$$\delta = \arg(b) = \arg(k^2+\eta^2-p_2^2-i2\eta p_2)\,, \quad (27)$$

$$\chi = |b|^2 = (k^2+\eta^2-p_2^2)^2+4\eta^2p_2^2\,, \quad (28)$$

$$u = 3+\frac{2m\omega}{k^2-\omega^2}\left[1-\frac{(1-v^2)\omega^2}{k^2-\omega^2}\right]. \quad (29)$$

We note that the distribution over the ejection angles of fast electrons is reduced to the dependence on the square of the transferred momentum, k^2.

To obtain the energy distribution of the ejected electrons, expression (26) should be integrated over k^2 within the range from

$$k^2_{min} = (p-p_1)^2 \approx (\omega/v)^2$$

to

$$k^2_{max} = (p+p_1)^2 \approx 4p^2.$$

In what follows, it is convenient to use dimensionless quantities such as

$$x = (k/\eta)^2, \quad \varepsilon = (p/\eta)^2,$$

$$\varepsilon_2 = (p_2/\eta)^2, \quad \Delta = (\omega/\eta)^2.$$

Then we obtain

$$\frac{d\sigma_{\mathrm{K}}^+}{d\varepsilon_2} = \frac{2^8\alpha^2\sigma_0}{3Z^2v^2\,\mathrm{sh}(\pi\xi_2)}\times \times\int_{x_1}^{x_2}\left\{3+\frac{\varkappa}{x-\Delta}\left[1-\frac{(1-v^2)\Delta}{x-\Delta}\right]\right\}f(x)\,dx\,, \quad (30)$$

where

$$f(x) = \frac{\exp(2\xi_2\,\mathrm{arctg}\,\phi)}{[(x+\nu)^2+4\varepsilon_2]^3}\,, \quad \Delta = \frac{\varkappa^2}{4}(\alpha Z)^2\,, \quad (31)$$

$$\nu = 1-\varepsilon_2\,, \quad \varkappa = 1+\varepsilon_2\,, \quad (32)$$

$$\phi = \frac{x+\nu}{2\sqrt{\varepsilon_2}}\,, \quad \xi_2 = \frac{1}{\sqrt{\varepsilon_2}}\,, \quad (33)$$

$$x_1 = \frac{k^2_{min}}{\eta^2} = \frac{\Delta}{v^2}\,, \quad x_2 = \frac{k^2_{max}}{\eta^2} = 4\varepsilon\,. \quad (34)$$

In Eq. (30), $\sigma_0 = \pi a_0^2 = 87.974$ Mb, where $a_0 = 1/m\alpha$ is the Bohr radius. For completeness, we also note that $v = p/E$ and $E^2 = p^2+m^2$. The range of the principal value of $\mathrm{arctg}\,\phi$ lies between $-\pi/2$ and $\pi/2$. To obtain the K-shell ionization cross section σ_K^+, the energy distribution (30) should be integrated over the variable ε_2 from 0 to $\varepsilon_{2max} = (E_{kin}/I - 1)/2$, where $E_{kin} = E - m$ is the kinetic energy of the incident electron. As can be seen, in the relativistic case, the dependence of the cross section on the nuclear charge Z differs from that in the nonrelativistic limit. But in the energy range $I \ll E_{kin} \ll m$, Eq. (30) is consistent with the nonrelativistic formula obtained in Ref. [11].

In Eq. (30), the integral over x is saturated near the lower bound x_1. For convenience of numerical integration, one can integrate by parts. This yields

$$\int_{x_1}^{x_2} \frac{f(x)\,dx}{x-\Delta} \approx -f(x_1)\ln(x_1-\Delta) - \int_{x_1}^{x_2} f'(x)\ln(x-\Delta)\,dx\,, \quad (35)$$

$$\int_{x_1}^{x_2} \frac{f(x)\,dx}{(x-\Delta)^2} \approx \frac{f(x_1)}{x_1-\Delta} - f'(x_1)\ln(x_1-\Delta) - \int_{x_1}^{x_2} f''(x)\ln(x-\Delta)\,dx\,, \quad (36)$$

where the prime denotes the derivative with respect to x. The first terms in approximations (35) and (36) are dominant. In Eq. (30), the contribution of integral (36) is suppressed by a small factor. Therefore, in calculations of the ionization cross sections, this integral can be approximated by the leading term only.

If the nuclear charge number Z is not too large, formula (30) can be simplified further. Taking two terms of the Taylor expansion for the exponential function and setting the integration limits as $x_1 = 0$, $x_2 = \infty$, and $\varepsilon_{2max} = \infty$ allow evaluating both integrals over x and ε_2 analytically. In integrals (35) and (36), we keep the dominant contributions only. Then the total cross section is given by

$$\sigma_K^+ = \frac{2^7\alpha^2\sigma_0}{Z^2v^2e^4}\,\frac{13}{27}\left(\ln\varepsilon - v^2 + C\right), \quad (37)$$

$$C = \frac{511}{192} + \frac{(81e^4 - 3136)\ln 2}{624} \approx 4.091\,, \quad (38)$$

where $e \approx 2.718$ is the Napier–Euler number.

Equations (30) and (37) describe the single ionization of hydrogen-like ions in the ground state. However, these formulas can be easily generalized to the case of atomic targets in which the K-shell is completely occupied. First, the cross section should be multiplied by the factor 2 taking the number of K-shell electrons into account. Second, we need to simulate the screening effect of the passive electrons on the active K-shell electron participating in the ionization process. This can be achieved by replacing the true nuclear charge Z with the effective value Z_{eff}, which is defined via [15]

$$I_{exp} = \frac{m}{2}(\alpha Z_{eff})^2\,, \quad (39)$$

where I_{exp} is the experimental ionization threshold. Accordingly, the average momentum $\eta = m\alpha Z$ is replaced with $\eta_{eff} = m\alpha Z_{eff}$.

Table. For various multicharged ions, the Coulomb ionization potentials $I = m(\alpha Z)^2/2$, the kinetic energies E_{kin} of incident electrons, and the theoretical and experimental cross sections σ_K^+ are tabulated. For uranium ions, the measurements are performed in Ref. [16]. The other experimental data are adopted from Ref. [17]

Target	I, keV	E_{kin}, keV	σ_K^+, b	
			This work	Experiment
Mo^{41+}	24.0	64.8	34.4	30.8 ± 2.6
		95.6	35.7	34.7 ± 7.2
Dy^{65+}	59.3	95.1	3.90	4.17 ± 0.58
		153.1	6.19	6.29 ± 0.83
Au^{78+}	84.9	153.1	2.32	2.33 ± 0.33
Bi^{82+}	93.7	191.6	2.23	2.37 ± 0.19
U^{91+}	115	198	1.22	1.55 ± 0.27
U^{90+}	115	198	2.44	2.82 ± 0.35

3. RESULTS AND DISCUSSION

In the Table and Fig. 2, we present numerical evaluations of the ionization cross sections σ_K^+ for multicharged ions and neutral atoms. Although Eq. (30) is not expected to be applicable to heavy targets, the agreement of our predictions with the experimental data appears to be remarkably good. This occurs due to mutual cancelations of some contributions arising from the relativistic and correlation terms. For example, for neutral uranium, the measurements yield $\sigma_K^+ = 18.1 \pm 1.8$ b at the incident electron kinetic energy $E_{kin} = 90$ MeV [22, 31]. Using the experimental ionization potential $I_{exp} = 115.6$ keV [32], we obtain the

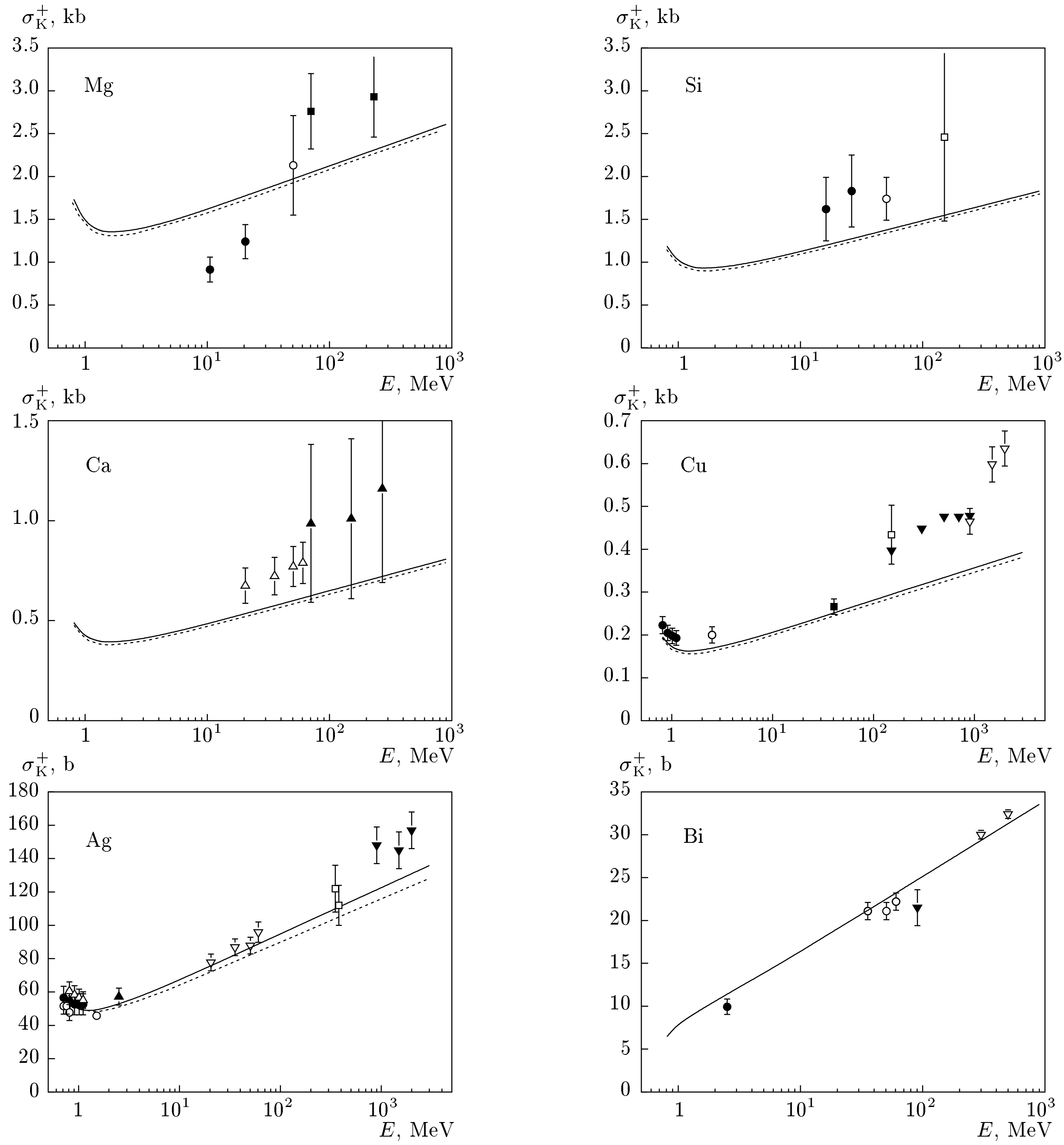

Fig. 2. K-shell ionization of neutral atoms by electron impact. Solid line, numerical calculation; dotted line, analytic approximation. Experimental data: Mg, ● [18], ○ [19], ■ [20]; Si, ○ [19], ● [21], □ [22]; Ca, △ [19], ▲ [22]; Cu, ■ [19], □ [22], ● [23], ○ [24], ▼ [25], ▽ [26]; Ag, ▽ [19], ▲ [24], ▼ [26], ● [27], ○ [28], △ [29], □ [30]; Bi, ○ [19], ▼ [22], ● [24], ▽ [25]. The original experimental data are given according to the last reevaluation made in Ref. [31]. In the numerical calculations, we used the effective values Z_{eff}, defined via the experimental ionization potentials I_{exp} [32]

effective nuclear charge $Z_{eff} = 92.2$ and the theoretical cross section $\sigma_K^+ = 18.3$ b. We note that Z_{eff} almost coincides with the true value of the nuclear charge Z.

The analytic approximation (37) is satisfactory for the K-shell ionization of atomic systems with moderate values $Z \lesssim 50$ (see Fig. 2). A formula similar to Eq. (37) has also been found by Kolbenstvedt [4]. However, our numerical coefficient C differs from that in Ref. [4]. In the case of neutral atoms, we use another procedure for the simulation of the screening effect of

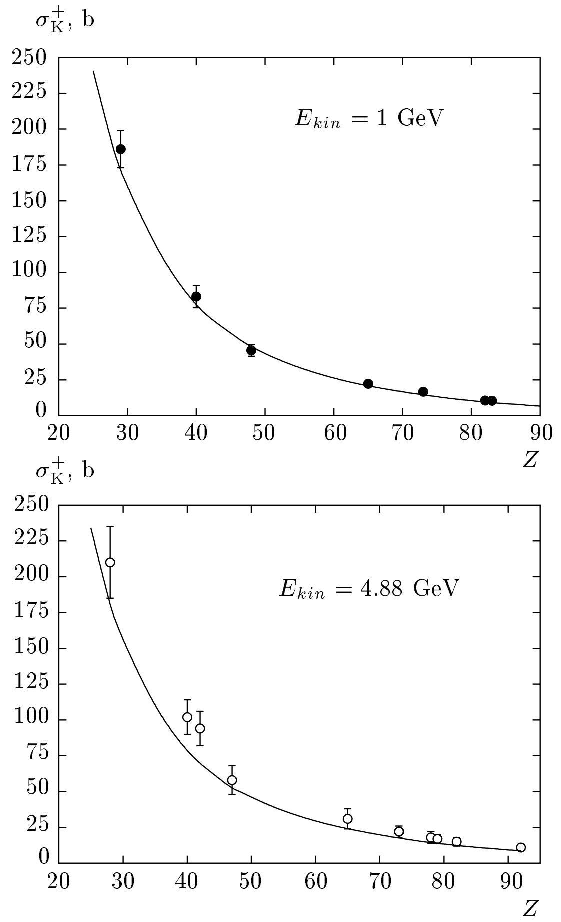

Fig. 3. K-shell ionization of neutral atoms by proton impact. The solid curves represent the results of the numerical calculations. The experimental data: • [33]; ∘ [34]

the outer-shell electrons, in particular, another definition of the effective value Z_{eff}.

The formulas for the differential cross section $d\sigma_K^+$ given by Eqs. (30)–(34) can also be applied to the single ionization of a K-shell electron by charged projectiles with the mass $M \neq m$ and the energy $E_{kin} \gtrsim M$. In this case, the exchange diagram is absent. The incident kinetic energy is given by $E_{kin} = E - M$, where $E^2 = p^2 + M^2$. In Fig. 3, we compare the theoretical and experimental cross sections for the K-shell ionization of neutral atoms by a proton impact at $E_{kin} = 1$ and 4.88 GeV. The numerical calculations are performed with the use of the effective nuclear charges Z_{eff}. These are obtained in accordance with Eq. (39), where the experimental ionization potentials I_{exp} are adopted from Ref. [32].

Concluding, we have deduced the total cross section for the single K-shell ionization of atoms and ions by the impact of relativistic projectiles. The consideration is performed to leading orders of the QED perturbation theory with respect to the parameters αZ and $1/Z$. The results are consistent with the universal scaling formulas that have been previously obtained for the nonrelativistic energy domain. The agreement with experimental data is found to be quite satisfactory for a wide family of atomic targets and different incident particles.

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REFERENCES

1. M. Inokuti, Rev. Mod. Phys. **43**, 297 (1971).
2. M. Inokuti, Y. Itikawa, and J. E. Turner, Rev. Mod. Phys. **50**, 23 (1978).
3. D. M. Davidović and B. L. Moiseiwitsch, J. Phys. B **8**, 947 (1975).
4. H. Kolbenstvedt, J. Appl. Phys. **46**, 2771 (1975).
5. J. H. Scofield, Phys. Rev. A **18**, 963 (1978).
6. R. Anholt, Phys. Rev. A **19**, 1004 (1979).
7. P. Eschwey and P. Manakos, Z. Phys. A **308**, 199 (1982).
8. V. G. Gorshkov, A. I. Mikhailov, and V. I. Fomichev, Yad. Fiz. **44**, 1514 (1986).
9. D. L. Moores and M. S. Pindzola, Phys. Rev. A **41**, 3603 (1990).
10. D. Bote and F. Salvat, Phys. Rev. A **77**, 042701 (2008).
11. A. I. Mikhailov, A. V. Nefiodov, and G. Plunien, Phys. Lett. A **372**, 4451 (2008).
12. A. I. Mikhailov, A. V. Nefiodov, and G. Plunien, Phys. Lett. A **372**, 5171 (2008).
13. A. I. Akhiezer and V. B. Berestetskii, *Quantum Electrodynamics*, Wiley, New York (1974).
14. V. B. Berestetskii, E. M. Lifshits, and L. P. Pitaevskii, *Quantum Electrodynamics*, Pergamon Press, London (1982).

15. A. I. Mikhailov, I. A. Mikhailov, A. V. Nefiodov, G. Plunien, and G. Soff, Pis'ma Zh. Eksp. Teor. Fiz. **78**, 141 (2003) [JETP Lett. **78**, 110 (2003)].

16. R. E. Marrs, S. R. Elliott, and D. A. Knapp, Phys. Rev. Lett. **72**, 4082 (1994).

17. R. E. Marrs, S. R. Elliott, and J. H. Scofield, Phys. Rev. A **56**, 1338 (1997).

18. S. C. McDonald and B. M. Spicer, Phys. Rev. A **37**, 985 (1988).

19. D. H. H. Hoffmann, C. Brendel, H. Genz, W. Löw, S. Müller, and A. Richter, Z. Phys. A **293**, 187 (1979).

20. M. Kamiya, A. Kuwako, K. Ishii, S. Morita, and M. Oyamada, Phys. Rev. A **22**, 413 (1980).

21. A. V. Shchagin, V. I. Pristupa, and N. A. Khizhnyak, Nucl. Instrum. Methods B **84**, 9 (1994).

22. K. Ishii, M. Kamiya, K. Sera, S. Morita, H. Tawara, M. Oyamada, and T. C. Chu, Phys. Rev. A **15**, 906 (1977).

23. D. Berényi, G. Hock, S. Ricz, B. Schlenk, and A. Valek, J. Phys. B **11**, 709 (1978).

24. A. Li-Scholz, R. Collé, I. L. Preiss, and W. Scholz, Phys. Rev. A **7**, 1957 (1973).

25. L. M. Middleman, R. L. Ford, and R. Hofstadter, Phys. Rev. A **2**, 1429 (1970).

26. H. Genz, C. Brendel, P. Eschwey, U. Kuhn, W. Löw, A. Richter, P. Seserko, and R. Sauerwein, Z. Phys. A **305**, 9 (1982).

27. K. Kiss, G. Kalman, J. Palinkas, and B. Schlenk, Acta Phys. Hung. **50**, 97 (1981).

28. D. H. Rester and W. E. Dance, Phys. Rev. **152**, 1 (1966).

29. S. Ricz, B. Schlenk, D. Berényi, G. Hock, and A. Valek, Acta Phys. Hung. **42**, 269 (1977).

30. Y. Watanabe, T. Kubozoe, T. Tomimasu, T. Mikado, and T. Yamazaki, Phys. Rev. A **35**, 1423 (1987).

31. M. Liu, Z. An, C. Tang, Z. Luo, X. Peng, and X. Long, At. Data Nucl. Data Tables **76**, 213 (2000).

32. A. A. Radzig and B. M. Smirnov, *Reference Data on Atoms, Molecules and Ions*, Springer, Berlin (1985).

33. I. B. Vodopyanov, V. V. Pashuk, and M. V. Stabnikov, J. Phys. B **29**, 2543 (1996).

34. R. Anholt, S. Nagamiya, J. O. Rasmussen, H. Bowman, J. G. Ioannou-Yannou, and E. Rauscher, Phys. Rev. A **14**, 2103 (1976).