Relativistic atomic photoelectric effect from the K shell near the threshold in the screened nuclear field: analytic calculation

A. I. Mikhaĭlov

B. P. Konstantinov Leningrad Institute of Nuclear Physics, Academy of Sciences of the USSR
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A simple analytic method is proposed for finding the continuum electron wave function and the amplitude of the photoelectric effect in a screened Coulomb field. A compact expression is derived for the total cross section for the relativistic K-shell photoelectric effect near the threshold, where the cross section is at its maximum. The results agree well with existing numerical calculations.

1. INTRODUCTION

The relativistic photoelectric effect from the K shell (the "K photoelectric effect") near the threshold in the nuclear Coulomb field was studied in Ref. 1. Analytic expressions were derived for the total cross section, the angular distribution, and the polarization correlations through an expansion in the small parameters αZ ($\alpha = 1/137$, and Z is the atomic number) and p/η, where p is the momentum of the photoelectron, and $\eta = m\alpha Z$ is the average momentum of the K electron (m is the mass of an electron). The total and differential cross sections were found within terms $\sim (\alpha Z)^4$ inclusively, so the equations derived can be used to study large-Z atoms, up to uranium.

Although the corrections to the screening in heavy atoms are small, they cause a substantial downward shift of the photoionization threshold (about 12% for the uranium K shell). In intermediate-weight and light atoms, the screening corrections are larger. Numerical calculations of the total cross sections for the screened photoelectric effect have been carried out by Racavy and Ron[2] with the help of a modified Fermi-Amaldi potential. Pratt *et al.*[3,4] have derived expressions for the nonrelativistic photoelectric effect in a screened field in the dipole approximation and for the first correction to the dipole approximation, which stems from the term in the expansion of the photon wave function which is linear in $(\mathbf{k}\cdot\mathbf{r})$ ($\mathbf{k}$ is the momentum of the photon). This "retardation correction" is on the order of v/c, where v is the velocity of the electron, and c the velocity of light, while the relativistic corrections are $\sim (v/c)^2$ or $\sim (\alpha Z)^2$. For small Z, the first correction for retardation near the threshold can thus be calculated with the nonrelativistic wave functions.[4] This correction disappears, however, upon an integration over the electron emission angle. Retardation should be incorporated along with relativistic effects in the total cross section.

Below we analytically derive the total cross section for the K photoelectric effect near the threshold in a screened Coulomb field. As in Ref. 1, the higher multipoles (retardation) and relativistic effects are taken into account to within terms on the order of $(\alpha Z)^4$ inclusively. Since the relativistic corrections are small (about 20% for heavy atoms[1]) near the threshold, screening is considered only in the leading terms of the expressions for the amplitude and the cross section which constitute the nonrelativistic limit of the corresponding quantities.

2. ELECTRON WAVE FUNCTIONS IN A SCREENED NUCLEAR FIELD

The literature[5–8] contains numerous analytic approximations of the atomic potential as a finite sum of Yukawa potentials. In calculations of the photoelectric effect, one needs wave functions for an electron moving in the field created by a nucleus with a charge Z and with $Z-1$ electrons. Such a field can be written in the form

$$V(r)=V_c(r)\Big[1+(1-Z^{-1})\sum_{i=1}^{n} a_i \exp(-\lambda_i r)\Big], \quad V_c=-\frac{\alpha Z}{r}, \tag{1}$$

where

$$a_n=-1, \quad \lambda_n=0, \quad \sum_{i=1}^{n} a_i=0. \tag{1a}$$

The other a_i and λ_i are chosen individually for each atom. Condition (1a) ensures the correct behavior of the potential at short and long range:

$$V \xrightarrow{r\to 0} -\frac{\alpha Z}{r}, \quad V \xrightarrow{r\to\infty} -\frac{\alpha}{r}. \tag{1b}$$

To simplify the equations below, we introduce the notation:

$$(1-Z^{-1})\sum_{i=1}^{n} a_i f(\lambda_i)=S_\lambda f(\lambda). \tag{2}$$

By virtue of property (1a), the result of applying S_λ to a function which is independent of λ is zero:

$$S_\lambda \cdot 1=0. \tag{2a}$$

The wave function Ψ_K and energy ε of a bound electron can be found by perturbation theory if $V-V_c$ in (1) is adopted as the perturbation. Using the expressions derived in Ref. 9, we have, in first-order perturbation theory,

$$\Psi_K \approx \Psi_{\kappa^c}\{1+{}^1/_4 S_\lambda \nu^2[-3+\rho^2+{}^1/_3\nu(11-2\rho^2-{}^2/_3\rho^3)]\}, \quad \rho=\eta r, \quad \nu=\frac{\lambda}{\eta}, \tag{3}$$

$$\varepsilon=\varepsilon_c+\varepsilon_1, \quad \varepsilon_1 \simeq \alpha Z \eta S_\lambda \nu(1-{}^3/_4\nu+{}^1/_2\nu^2). \tag{4}$$

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Here Ψ_K^c and ε_c are the wave function and energy of a K electron in the nuclear Coulomb field. In deriving (3) and (4) we used a series expansion in the parameter $\nu \sim r_K/r_A$, where r_K and r_A are the average radii of the K shell and of the atom. It is necessary to restrict the discussion to terms $\sim \nu^3$ here because the screening correction in second-order perturbation theory is[9] $\sim (S_\lambda \nu^2)^2$.

We expand the wave function Ψ_p of the final state of an electron with a momentum p, in partial waves:

$$\Psi_p = \frac{1}{pr} \sum_{l=0}^{\infty} (2l+1) i^l R_{pl}(r) P_l(\cos\theta). \tag{5}$$

To derive Ψ_p with the appropriate asymptotic behavior (a plane wave plus a converging spherical wave), we need a radial function R_{pl} which has the behavior

$$R_{pl}(r) \overset{r\to\infty}{\sim} e^{-i\delta_l} \sin(pr - l\pi/2 + \xi \ln 2pr + \delta_l), \tag{6}$$

where $\xi = \eta/p$, and δ_l is the scattering phase shift. We write δ_l as the sum

$$\delta_l = \sigma_l + \vartheta_l, \tag{7}$$

where $\sigma_l = \arg\Gamma(l+1+i\xi)$ is the Coulomb phase shift, and ϑ_l is the additional phase shift which stems from the difference between the atomic field and a Coulomb field. Choosing a regular solution $u_l(r)$ and an irregular solution $v_l(r)$ of the Schrödinger equation for the Coulomb field, in such a way that the condition

$$u_l v_l' - u_l' v_l = 1 \tag{8}$$

holds (the prime means a derivative with respect to r), we can construct a radial wave function for the screened field in the following form:

$$R_{pl} = e^{-i\sigma_l} f_{pl}(r), \tag{9}$$

$$f_{pl}(r) = u_l(r) + v_l(r) \int_0^r u_l(r') W f_l(r')\, dr' + u_l(r) \int_r^{\infty} v_l(r') W f_l(r')\, dr', \tag{10}$$

where

$$W = 2m(V - V_c) = -2\eta S_\lambda e^{-\lambda r}/r \xrightarrow[\lambda\to 0]{} 0, \tag{10a}$$

$$u_l(r) = e^{\pi\xi/2} \frac{|\Gamma(l+1+i\xi)|}{2\Gamma(2l+2)} (2pr)^{l+1} \times e^{-ipr} F(l+1+i\xi,\ 2l+2;\ 2ipr), \tag{10b}$$

$$v_l(r) = \frac{i}{p} e^{-\pi\xi/2} \frac{|\Gamma(l+1+i\xi)|}{\Gamma(l+1-i\xi)} (-2pr)^{l+1} \times e^{-ipr} \Psi(l+1+i\xi,\ 2l+2;\ 2ipr). \tag{10c}$$

Here $F(a, b, z)$ and $\Psi(a, b; z)$ are, respectively, the regular and irregular confluent hypergeometric functions.

The Coulomb wave functions are normalized in accordance with

$$u_l(r)|_{r\to\infty} \sim \sin(pr - l\pi/2 + \xi \ln 2pr + \sigma_l),$$
$$v_l(r)|_{r\to\infty} \sim -\frac{1}{p} \exp\{-i(pr - l\pi/2 + \xi \ln 2pr + \sigma_l)\}. \tag{11}$$

This choice of $u_l(r)$ and $v_l(r)$ leads to the asymptotic behavior in (6) for $R_{pl}(r)$. In addition, $u_l(r)$ is a real function, while $v_l(r)$ can be written in the form

$$v_l(r) = \frac{1}{p}[\chi_l(r) + i u_l(r)], \tag{12}$$

where $\chi_l(r)$ is a real function, normalized by the condition

$$\chi_l(r)|_{r\to\infty} \sim -\cos(pr - l\pi/2 + \xi \ln 2pr + \sigma_l). \tag{13}$$

We introduce the function[10] $y_l(r)$:

$$y_l(r) = u_l(r) + v_l(r) \int_0^r u_l(r') W y_l(r')\, dr' - u_l(r) \int_0^r v_l(r') W y_l(r')\, dr'. \tag{14}$$

It is related to $f_l(r)$ by

$$y_l(r) = L_l f_l(r), \tag{15}$$

$$L_l = 1 - \int_0^{\infty} v_l W y_l\, dr. \tag{16}$$

It is convenient to express the function f_l in terms of y_l ($f_l = L_l^{-1} y_l$) when the process occurs in the inner region of the atom. In this case, $y_l(r)$ is determined by the behavior of the potential $W(r)$ in the atom, and the potential over the entire range of r need be known only to find the normalization factor L_l.

Taking iterations in (14), we find a perturbation-theory series in the additional potential W in (10a). The use of this series to calculate L_l leads to the appearance of integrals of the following sort, which diverge as $\lambda \to 0$:

$$\int_0^{\infty} u_l^2 W\, dr.$$

However, one can construct an expression for L_l in which the terms which diverge as $\lambda \to 0$ are present only in the phase factor and do not affect the cross section of the process. For this purpose we introduce the functions

$$\Lambda_1(r) = 1 - \frac{1}{p} \int_0^r \chi W y\, dr, \qquad \Lambda_2(r) = -\frac{1}{p} \int_0^r u W y\, dr \tag{17}$$

(here and below, we are omitting the subscript l from the functions and the phase shifts which depend on l). Substituting (12) into (14) and (16), we find

$$y(r) = u(r)\Lambda_1(r) - \chi(r)\Lambda_2(r), \tag{18}$$

$$L = \Lambda_1(\infty) + i\Lambda_2(\infty). \tag{19}$$

Differentiating (17) with respect to r, and using (18), we find

$$\Lambda_1' = S\Lambda_2 - F\Lambda_1,$$
$$\Lambda_2' = F\Lambda_2 - \Phi\Lambda_1, \tag{20}$$

where

$$S = \frac{1}{p}\chi^2 W, \quad F = \frac{1}{p}\chi u W, \quad \Phi = \frac{1}{p}u^2 W. \tag{21}$$

The system of coupled equations in (20) is to be solved under the boundary conditions

$$\Lambda_1(0) = 1, \quad \Lambda_2(0) = 0, \tag{22}$$

which follow from definition (17). These equations can be uncoupled by making use of the substitutions

$$\Lambda_1 = g(r)\cos\vartheta(r), \quad \Lambda_2 = g(r)\sin\vartheta(r). \tag{23}$$

Then

$$g(r) = \exp\left\{\int_0^r [-F + {}^1/_2(S-\Phi)\sin 2\vartheta + 2F\sin^2\vartheta]\,dr\right\}, \tag{24}$$

$$\vartheta' = -\Phi + F\sin 2\vartheta + (\Phi - S)\sin^2\vartheta, \quad \vartheta(0) = 0. \tag{25}$$

The normalization factor L in (19) becomes

$$L = g(\infty)\exp\{i\vartheta(\infty)\}. \tag{26}$$

The integral which determines $g(\infty)$ remains finite in the limit $\lambda \to 0$ because of the oscillatory behavior of the functions F and $S - \Phi$. This result means that the integral converges at distances $r < \lambda^{-1}$. At such r, the phase function vanishes [$\vartheta(r) \to 0$] as $\lambda \to 0$ and can be found by perturbation theory. This circumstance leads in turn to a perturbation-theory series for $g(\infty)$. The only term which diverges as $\lambda \to 0$ is in the phase $\vartheta(\infty)$ and is given by

$$\vartheta(\infty) \approx -\int_0^\infty \Phi\,dr = -\frac{1}{p}\int_0^\infty u^2 W\,dr = -\xi S_\lambda \ln\frac{2p}{\lambda} + O(\lambda). \tag{27}$$

Since the result in (27) does not depend on the angular momentum l, the part of the solution which is singular in terms of λ can be separated out as a common phase factor in front of the overall wave function of the continuum. This fact was pointed out in Refs. 11, 12, and 8.

3. CALCULATION OF THE AMPLITUDE FOR THE PHOTOELECTRIC EFFECT IN A SCREENED FIELD

The amplitude of the nonrelativistic photoelectric effect, Q, is given in the dipole approximation by

$$Q = \frac{1}{m}\int \Psi_p^*(-i\nabla\mathbf{e})\Psi_K\,d^3r, \tag{28}$$

where $\mathbf{e}$ is the photon polarization vector. We substitute wave functions (3) and (5) into (28). After integrating over the angular variables in the sum over partial waves in (5), we are left with only the $l = 1$ term. Using definitions (9), (10), (14), and (15), we find the following expression for the complex-conjugate amplitude:

$$Q^* = A\int_0^\infty yre^{-\eta r}(1 + R_K^s)\,dr, \tag{29}$$

where

$$A = 4\pi\xi(\mathbf{e}^*\mathbf{n}_p)N_K e^{-i\sigma}L^{-1}, \quad N_K = \left(\frac{\eta^3}{\pi}\right)^{1/2}, \quad \mathbf{n}_p = \mathbf{p}/p, \tag{29a}$$

$$R_K^s = \left(1 - \frac{d}{d\rho}\right)G_K^s(\rho), \quad \rho = \eta r. \tag{29b}$$

The function G_K^s is related to Ψ_K by the equation

$$\Psi_K = \Psi_K^c(1 + G_K^s). \tag{29c}$$

The integral in (29) converges at distances $r \sim \eta^{-1} \sim r_K$, where the perturbation W is small, so the amplitude Q can be found by perturbation theory. In first order in W we have

$$Q^* = A(T^c + T_p^s + T_K^s), \tag{30}$$

$$T^c = \int_0^\infty ure^{-\eta r}\,dr = \mathcal{J}^c(\eta), \tag{30a}$$

$$T^c + T_p^s = \int_0^\infty yre^{-\eta r}\,dr = \mathcal{J}(\eta), \tag{30b}$$

$$T_K^s = \int_0^\infty ure^{-\eta r}R_K^s\,dr. \tag{30c}$$

We will first calculate the Coulomb amplitude T^c and the correction to it, T_K^s. Using the Coulomb function $u_l(r)$ from (10b) with $l = 1$, we find

$$T^c = N_p(\eta^2 + p^2)^{-2}\exp(-2\xi\,\mathrm{arcctg}\,\xi),$$
$$N_p = 2p^2\exp(\pi\xi/2)\,|\Gamma(2 + i\xi)|, \tag{31}$$
$$T_K^s = T^c S_\lambda \nu^2[-{}^3/_4 + {}^{49}/_{36}\nu + O(\nu^2, \xi^{-2})] \tag{32}$$

(the Coulomb parameter is $\xi \gg 1$ near the threshold).

The integral $\mathcal{J}(\eta)$ in (30b) can be calculated through the use of expressions (18) and (23) for $y(r)$, but this is not the simplest approach. We will derive for $\mathcal{J}(\eta)$ an integral equation which can be solved easily in any order of perturbation theory. For this purpose we consider the integral

$$\mathcal{J}(\mu) = \int_0^\infty e^{-\mu r}ry\,dr, \tag{33}$$

as a function of the parameter μ. Differentiating with respect to μ, and using a Schrödinger equation for the function $y_l(r)$ with $l = 1$, we find an equation for $\mathcal{J}(\mu)$:

$$\frac{d\mathcal{J}(\mu)}{d\mu} + \frac{4\mu - 2\eta}{\mu^2 + p^2}\mathcal{J}(\mu) - \frac{2\eta}{\mu^2 + p^2}S_\lambda\mathcal{J}(\mu + \lambda) = 0. \tag{34}$$

We write the solution of this equation in the form

$$\mathcal{J}(\mu) = (\mu^2 + p^2)^{-2}\exp\left(2\xi\,\mathrm{arctg}\,\frac{\mu}{p}\right)$$
$$\times\left\{C - 2\eta S_\lambda\int_\mu^\infty (x^2 + p^2)\exp\left(-2\xi\,\mathrm{arctg}\,\frac{\mu}{p}\right)\mathcal{J}(x + \lambda)\,dx\right\}, \tag{35}$$

where C is an integration constant. In principle, this constant may depend on the screening parameter λ, so we would like to find it without taking the limit $\lambda \to 0$. From (35) we have

$$C = \lim_{\mu\to\infty} e^{-\pi\xi}\mu^4\mathcal{J}(\mu). \tag{36}$$

The integral $\mathcal{J}(\mu)$ converges at $r\sim\mu^{-1}$. Its value at $\mu\to\infty$ can be found since at small r the function $y(r)$ is the same as the Coulomb function $u(r)$:

$$y(r)\approx u(r)+\frac{1}{p}\Big[\chi(r)\int_0^r u^2W\,dr-u(r)\int_0^r \chi uW\,dr\Big]$$

$$\approx u(r)\{1+O(\eta^2r^2\nu)\}. \tag{37}$$

We thus find

$$C=\lim_{\mu\to\infty}e^{-\pi\xi}\mu^4\mathcal{J}^c(\mu)=e^{-\pi\xi}N_p, \tag{38}$$

where N_p is given in (31).

Treating the integral term in (35) as a perturbation, and going through an iterative procedure, we find a perturbation-theory series. The terms of this series can be calculated easily if the integrand is expanded in λ and p. Retaining terms up to λ^3 inclusively, and restricting the discussion to the leading term in the expansion in p, we find, after the first iteration,

$$\mathcal{J}(\eta)=T^c\{1+{}^8/_3S_\lambda\nu(1-{}^{37}/_{40}\nu+{}^{17}/_{28}\nu^2)\}. \tag{39}$$

We are left with calculating the normalization factor of the wave function of the continuum, L in (26), for $l=1$. In first-order perturbation theory we have

$$|L|=g(\infty)\approx 1-\int_0^\infty F\,dr=1-\frac{1}{p}\int_0^\infty \chi Wu\,dr. \tag{40}$$

We use an expansion of the Coulomb functions $u(r)$ and $\chi(r)$ in series in Bessel functions.[13] This expansion is effectively an expansion in powers of pr/ξ, and at $\xi\gg pr$ we need retain only the first term of the series:

$$u(r)\approx(\pi pr)^{1/2}J_3((8\eta r)^{1/2}),\quad \chi(r)\approx(\pi pr)^{1/2}Y_3((8\eta r)^{1/2}), \tag{41}$$

where $J_3(x)$ and $Y_3(x)$ are, respectively, Bessel and Neumann functions.

Evaluating the integral in (40) with the functions in (41), we find

$$|L|=1+S_\lambda\nu[1-{}^1/_4\nu+O(\xi^{-2})] \tag{42}$$

[expression (42) does not contain a term cubic in λ].

Combining (29)–(32), (39), and (42), we can express the nonrelativistic amplitude for the photoelectric effect in the following form:

$$|Q|=|Q^c|\{1+D(\lambda)\}, \tag{43}$$

where

$$|Q^c|=4\pi\xi|\mathbf{e}n_p|m^{-1}N_KT^c, \tag{43a}$$

$$D(\lambda)=\frac{5}{3}S_\lambda\nu\left(1-\frac{89}{50}\nu+\frac{751}{420}\nu^2\right),\quad \nu=\frac{\lambda}{\eta}. \tag{43b}$$

4. CROSS SECTION FOR THE PHOTOELECTRIC EFFECT

The differential cross section ($d\sigma^{nr}/d\Omega$) and the total cross section (σ^{nr}) for the nonrelativistic K photoelectric effect are given by the following expressions when two electrons in the K shell are taken into account ($\hbar=c=1$):

$$\frac{d\sigma^{nr}}{d\Omega}=\frac{\alpha pm}{\pi\omega}|Q|^2=\frac{3}{4\pi}|\mathbf{e}n_p|^2\sigma^{nr}, \tag{44}$$

$$\sigma^{nr}=\sigma_0F(\xi,\lambda),\quad \sigma_0=\frac{2^9\pi^2e^{-4}\alpha}{3m\omega}=336\frac{m}{\omega}\quad\text{(b)} \tag{45}$$

$$F(\xi,\lambda)=R(\xi)[1+2D(\lambda)],\quad \xi=\eta/p, \tag{46}$$

$$R(\xi)=(1+\xi^{-2})^{-3}\exp(4-4\xi\,\mathrm{arcctg}\,\xi)$$

$$\approx 1-\frac{5}{3}\xi^{-2}+\frac{94}{45}\xi^{-4}+O(\xi^{-6}). \tag{47}$$

The electron momentum p is related to the screening parameter λ by energy conservation:

$$E=\omega+\varepsilon=\omega+\varepsilon_c+\varepsilon_1=E_c+\varepsilon_1$$

or

$$p^2=p_c^2+2m\varepsilon_1. \tag{48}$$

Here E_c and p_c are, respectively, the energy and momentum of the electron in the Coulomb field, and ω is the energy of the photon. Considering the correction to the energy only in the term on the order of p^2, we can write (46) in the form

$$F(\xi,\lambda)=R(\xi_c)\left[1+S_\lambda\nu^2\left(-\frac{103}{30}+\frac{541}{126}\nu\right)\right],$$
$$\xi_c=\eta/p_c. \tag{49}$$

This expression has no terms linear in λ, so we have further support for the validity of the result. Our reasoning here is that, if the potential V in (1) is expanded in powers of λr, the term linear in λ in this expression will not depend on r. Its presence shifts the origin of the energy scale in the problem, but it cannot affect the probability for the physical process, since the total energy is always determined within a constant. A result similar to (49) was derived in Ref. 3 by a totally different method, through the addition of a polynomial in λr to the Coulomb potential. This polynomial was chosen in Ref. 8 in such a way that it gives a fairly good description of the inner region of the atom. In the outer region, in contrast, that potential has the wrong behavior. In our approach, an expansion in the screening parameter is carried out only in the final expressions. If this expansion is illegitimate,[1)] the expressions for the cross section should be rederived without an expansion in λ. In that case, however, they lose their attractiveness. It is thus desirable to choose the potential as in (1), with parameters which make it possible to use an expansion in λ and to retain an acceptable accuracy. A potential satisfying these requirements was found in Ref. 8.

If relativistic effects and the contribution of the higher multipoles in the approximation of the Coulomb field are now taken into account, as in Ref. 1, we find the total cross section for the relativistic K photoelectric effect in the energy region $\xi^{-1}\lesssim\alpha Z$ to be

$$\sigma=\sigma_0\{F(\xi,\lambda)-0{,}393(\alpha Z)^2-0{,}144(\alpha Z)^4$$
$$+1{,}023(\alpha Z)^2\xi_c^{-2}+O(\alpha^6Z^6)\}. \tag{50}$$

Table I shows results calculated from this expression. Shown for comparison in this table are the results of numerical relativistic calculations by Racavy and Ron.[2] The quantity $F(\xi,\lambda)$ was calculated for the potential of Ref. 8, which is an analytic approximation of a numerical Hartree-Fock-

TABLE I. Comparison of cross sections for the photoionization of an atomic K shell found from expression (50) (σ) and numerical calculations by Racavy and Ron[2] (σ_{RR}).

Z	13	26	26	50	50
ω, keV	2	7,65	10	30	40
σ,b	9,46(4) *	2,80(4)	1,39(4)	6,76(3)	3,19(3)
σ_{RR},b	9,36(4)	2,76(4)	1,39(4)	6,68(3)	3,17(3)

Z	74	74	92	92
ω, keV	71	81	116,5	130
σ, b	2,57(3)	1,80(3)	1,41(3)	1,04(3)
σ_{RR}, b	2,54(3)	1,80(3)	1,37(3)	1,04(3)

*$A(n)$ means $A\cdot 10^n$.

Slater potential[14] (Racavy and Ron used a modified Fermi-Amaldi atomic potential, for which there is no analytic expression). In the case of uranium, a Molière potential[5] was used to calculate $F(\xi,\lambda)$. That potential is a good model of the Thomas-Fermi potential, which was used for uranium in Ref. 2.

It can be seen from Table I that the agreement between the analytic and numerical calculations is good, particularly in view of the circumstance that the potentials used in the calculations being compared here were only approximately the same, not identical.

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[1)] For the Molière potential,[5,9] the second term ($\sim\lambda^3$) in the expansion in (49) is greater than the first ($\sim\lambda^2$) for $Z<20$.

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