Comments

Comments are short papers which comment on papers of other authors previously published in the **Physical Review**. *Each Comment should state clearly to which paper it refers and must be accompanied by a brief abstract. The same publication schedule as for regular articles is followed, and page proofs are sent to authors.*

Monopole Coulomb-deflection factor for heavy-particle inner-shell-ionization cross sections

Grzegorz Lapicki,* Max Goldstein,† and Werner Brandt‡
New York University, New York, New York 10003
(Received 5 May 1980)

The repulsion between positively charged projectiles and the nucleus of target atoms gives rise to a Coulomb-deflection factor that reduces the inner-shell-ionization cross sections calculated for straight-line particle trajectories. In the monopole approximation to the repulsion, this factor depends on the function $G_0(x) = [x\, dK_{ix}(y)/dy|_{y=x}]^2$, where K_{ix} is the Bessel function of imaginary order. Through identities between Bessel functions of complex order and argument we have, in this addendum to an earlier paper [W. Brandt and G. Lapicki, Phys. Rev. A **20**, 465 (1979)], reduced the evaluation of $G_0(x)$ to computed functions. Values of $G_0(x)$ and its integrals as they appear in the theory of K- and L-shell ionizations are tabulated. The monopole approximation is compared with results based on the standard approximation $G(x) = 1$ which describes the experimental data.

The Coulomb-deflection factor, $C(x)$, in the theory of differential cross sections for the ionization of an atomic shell S by slow heavy charged particles[1] can be written in the form

$$C(x) = \exp(-\pi x) G(x) , \tag{1}$$

where $x = \tau\, dq_{0S}$ is the product of the Coulomb-deflection variable[2] dq_{0S} and of $\tau = 1 + \mathcal{E}_f/\omega_{2S}$ in terms of the final energy, $\mathcal{E}_f$, of the ejected electron and its binding energy, ω_{2S}, in S. After integration over $\mathcal{E}_f$, the Coulomb-deflection factor, $C_S(dq_{0S})$, for the total ionization cross section is given by[3]

$$C_S(dq_{0S}) = (9 + 2l_2) \int_1^\infty \frac{e^{-\pi\tau dq_{0S}}}{\tau^{10+2l_2}} G(\tau\, dq_{0S})\, d\tau , \tag{2}$$

where $l_2 = 0$ for the atomic shells $S = K$, L_1, and $l_2 = 1$ for $S = L_2$, L_3. We have used Amundsen's approach[4] to calculate the Coulomb-deflection factor in the monopole approximation (subscript zero) to the repulsion between the projectile and the nucleus of the target atom. The result [Ref. 1, Eqs. (25) and (A3)] is

$$G_0(x) = \left(x \left. \frac{dK_{ix}(y)}{dy} \right|_{y=x} \right)^2 \tag{3}$$

in terms of the derivative of the modified Bessel function, $K_{ix}(y)$, of the second kind and of imaginary order. This is to be compared with the standard approximation[5] $G(x) = 1$ in which $C(x) = \exp(-\pi x)$ and

$$C_S(dq_{0S}) = (9 + 2l_2) E_{10+2l_2}(\pi\, dq_{0S}) , \tag{4}$$

where $E_n(\pi\, dq_0)$ is the exponential integral of order n.[6]

In light of the importance of the Coulomb-deflection effect in inner-shell excitations, this addendum to Ref. 1 makes Eq. (3) accessible to numerical scrutiny by transforming $dK_{ix}(y)/dy$ into functions that are computed with available programs. The recurrence relation for $K_\nu(z)$ of complex order ν and argument z,[6]

$$dK_\nu(z)/dz \equiv K'_\nu(z) = -K_{\nu+1}(z) + \frac{\nu}{z} K_\nu(z) , \tag{5}$$

makes contact, through the identity

$$K_\nu(z) \equiv \frac{\pi i}{2} e^{\nu\pi i/2} [J_\nu(iz) + iY_\nu(iz)] , \tag{6}$$

with J_ν and Y_ν, the Bessel functions of the first and second kind, respectively. The Bessel functions $J_\nu(z)$ are evaluated according to Goldstein.[7] The method[8] produces $J_\nu(z)$ in the form $\mathrm{Re}J_\nu(z)$ and $\mathrm{Im}J_\nu(z)$ for given argument z and all orders ν by using appropriate recursion relations and normalization factors. The functions $Y_\nu(z)$ are calculated by summations of $J_\nu(z)$.

In Table I we collate some values of $G_0(x)$, Eq. (3), and of $C_0(x) = \exp(-\pi x) G_0(x)$.[9] Anholt *et al.*[10] have recently calculated eight numerical values of $C_0(x)$ which agree with Table I, and of the dipole Coulomb-deflection factor. Numerical integration according to Eq. (2) by Simpson's rule yields the tabulated values $C_{0S}(dq_{0S})$ in the monopole approximation for $l_2 = 0 (S = K, L_1)$ and $l_2 = 2 (S = L_2, L_3)$. For comparison we list also $C(x)$ and $C_S(dq_{0S})$, Eq. (4), in the standard approximation $G(x) = 1$. The binding

TABLE I. Coulomb-deflection functions $C(x)$, Eq. (1), and $C_S(dq_{0S})$, Eq. (2), for $S=K$, L_1 shells and $S=L_2$, L_3 shells, as computed in the monopole approximation $G_0(x)$, Eq. (3), and in the approximation $G(x)=1$, Eq. (4). The parentheses (n) stand for factors 10^n. Note that when binding and energy-loss effects are included, the Coulomb-deflection functions should be taken at the increased argument $2dq_{0S}\zeta_S/z_S(1+z_S)$ as defined in the text.

x or dq_{0S}	πx or πdq_{0S}	$G(x)=G_0(x)$: $G_0(x)$	$C_0(x)$ $e^{-\pi x}G_0(x)$	$C_{0S}(dq_{0S})$ $S=K,L_1$	$C_{0S}(dq_{0S})$ L_2,L_3	$G(x)=1$: $C(x)$ $e^{-\pi x}$	$C_S(dq_{0S})$ $S=K,L_1$	$C_S(dq_{0S})$ L_2,L_3
0.00	0.00	1.00(0)	1.00(0)	1.00(0)	1.00(0)	1.00(0)	1.00(0)	1.00(0)
0.01	0.03	9.97(−1)	9.66(−1)	9.62(−1)	9.63(−1)	9.69(−1)	9.65(−1)	9.66(−1)
0.02	0.06	9.91(−1)	9.31(−1)	9.22(−1)	9.24(−1)	9.39(−1)	9.32(−1)	9.33(−1)
0.03	0.09	9.83(−1)	8.95(−1)	8.81(−1)	8.84(−1)	9.10(−1)	8.99(−1)	9.02(−1)
0.04	0.13	9.74(−1)	8.59(−1)	8.41(−1)	8.45(−1)	8.82(−1)	8.68(−1)	8.71(−1)
0.05	0.16	9.63(−1)	8.23(−1)	8.01(−1)	8.06(−1)	8.55(−1)	8.38(−1)	8.41(−1)
0.06	0.19	9.52(−1)	7.88(−1)	7.63(−1)	7.68(−1)	8.28(−1)	8.09(−1)	8.13(−1)
0.07	0.22	9.40(−1)	7.54(−1)	7.25(−1)	7.31(−1)	8.03(−1)	7.81(−1)	7.85(−1)
0.08	0.25	9.27(−1)	7.21(−1)	6.89(−1)	6.95(−1)	7.78(−1)	7.54(−1)	7.59(−1)
0.09	0.28	9.14(−1)	6.89(−1)	6.54(−1)	6.61(−1)	7.54(−1)	7.28(−1)	7.33(−1)
0.10	0.31	9.00(−1)	6.57(−1)	6.21(−1)	6.28(−1)	7.30(−1)	7.03(−1)	7.08(−1)
0.20	0.63	7.54(−1)	4.02(−1)	3.57(−1)	3.65(−1)	5.33(−1)	4.95(−1)	5.02(−1)
0.30	0.94	6.13(−1)	2.39(−1)	2.00(−1)	2.06(−1)	3.90(−1)	3.49(−1)	3.56(−1)
0.40	1.26	4.90(−1)	1.39(−1)	1.10(−1)	1.15(−1)	2.85(−1)	2.47(−1)	2.53(−1)
0.50	1.57	3.86(−1)	8.03(−2)	6.00(−2)	6.30(−2)	2.08(−1)	1.74(−1)	1.80(−1)
0.60	1.88	3.02(−1)	4.58(−2)	3.25(−2)	3.44(−2)	1.52(−1)	1.23(−1)	1.28(−1)
0.70	2.20	2.34(−1)	2.59(−2)	1.75(−2)	1.87(−2)	1.11(−1)	8.75(−2)	9.12(−2)
0.80	2.51	1.80(−1)	1.46(−2)	9.41(−3)	1.01(−2)	8.10(−2)	6.21(−2)	6.50(−2)
0.90	2.83	1.39(−1)	8.20(−3)	5.05(−3)	5.44(−3)	5.92(−2)	4.41(−2)	4.64(−2)
1.0	3.14	1.06(−1)	4.58(−3)	2.70(−3)	2.93(−3)	4.32(−2)	3.13(−2)	3.31(−2)
1.1	3.46	8.07(−2)	2.55(−3)	1.44(−3)	1.57(−3)	3.16(−2)	2.23(−2)	2.36(−2)
1.2	3.77	6.14(−2)	1.41(−3)	7.70(−4)	8.42(−4)	2.31(−2)	1.59(−2)	1.69(−2)
1.3	4.08	4.65(−2)	7.83(−4)	4.10(−4)	4.50(−4)	1.68(−2)	1.13(−2)	1.21(−2)
1.4	4.40	3.52(−2)	4.33(−4)	2.19(−4)	2.41(−4)	1.23(−2)	8.06(−3)	8.62(−3)
1.5	4.71	2.66(−2)	2.39(−4)	1.16(−4)	1.29(−4)	8.98(−3)	5.75(−3)	6.17(−3)
1.6	5.03	2.00(−2)	1.31(−4)	6.19(−5)	6.87(−5)	6.56(−3)	4.10(−3)	4.42(−3)
1.7	5.34	1.51(−2)	7.22(−5)	3.29(−5)	3.66(−5)	4.79(−3)	2.93(−3)	3.16(−3)
1.8	5.65	1.13(−2)	3.96(−5)	1.75(−5)	1.95(−5)	3.50(−3)	2.09(−3)	2.26(−3)
1.9	5.97	8.50(−3)	2.17(−5)	9.31(−6)	1.04(−5)	2.56(−3)	1.50(−3)	1.62(−3)
2.0	6.28	6.37(−3)	1.19(−5)	4.95(−6)	5.55(−6)	1.87(−3)	1.07(−3)	1.16(−3)
2.2	6.91	3.57(−3)	3.56(−6)	1.40(−6)	1.57(−6)	9.96(−4)	5.48(−4)	5.99(−4)
2.4	7.54	1.99(−3)	1.06(−6)	3.94(−7)	4.46(−7)	5.31(−4)	2.81(−4)	3.09(−4)
2.6	8.17	1.11(−3)	3.14(−7)	1.11(−7)	1.26(−7)	2.84(−4)	1.45(−4)	1.59(−4)
2.8	8.80	6.16(−4)	9.31(−8)	3.14(−8)	3.58(−8)	1.51(−4)	7.44(−5)	8.22(−5)
3.0	9.42	3.41(−4)	2.75(−8)	8.86(−9)	1.01(−8)	8.07(−5)	3.84(−5)	4.25(−5)

and energy-loss (E) effects lower $C_S(dq_{0S})$ further[11] to $C_S^E = C_S(2\,dq_{0S}\zeta_S/z_S(1+z_S))$, where $z_S^2 = (1-\omega_{2S}\zeta_S M_1/ME_1)$ is the fraction of the kinetic energy retained by the projectile after the ionizing collision, ζ_S being the binding coefficient[1] and $M=(M_1^{-1}+M_2^{-1})^{-1}$ the reduced mass of the projectile (M_1) and the target nucleus (M_2).

Predictions based on the standard approximation $G(x)=1$ appear to agree with the preponderance of experimental evidence.[1,11-13] It is not as yet understood, however, in which way monopole, dipole, and higher-pole contributions combine to yield the experimental results. Still, as Anholt *et al.*[10] summarize, the data decline as predicted exponentially with dq_{0S} and, when so scaled, show no definite Z_2 fluctuations from this trend. The evaluation of $G(x)$ beyond the monopole approximation remains a pressing problem.

ACKNOWLEDGMENT

This work was supported by the United States Department of Energy.

*Present address: Department of Chemistry and Physics, Northwestern State University of Louisiana, Natchitoches, Louisiana 71457.

†Courant Institute of Mathematical Sciences.

‡Radiation and Solid State Laboratory.

[1]W. Brandt and G. Lapicki, Phys. Rev. A 20, 465 (1979).

[2]The factor $d = Z_1 Z_2 e^2 / M v_1^2$ is the half-distance of the closest approach between the projectile of charge $Z_1 e$, mass M_1, and velocity v_1, and the target nucleus of charge $Z_2 e$ and M_2, in terms of the reduced mass $M = (M_1^{-1} + M_2^{-1})^{-1}$; the factor $q_{0S} = \omega_{2S}/v_1$ relates to the minimum momentum transfer $\hbar q_{0S}$ for the ionization of shell S with electron binding energy $\hbar\omega_{2S}$.

[3]The normalization factor $(9 + 2l_2)$ was inadvertently omitted in the printing of the right-hand side of Eq. (27) in Ref. 1.

[4]P. A. Amundsen, J. Phys. B 10, 2177 (1977).

[5]W. Brandt, R. Laubert, and I. Sellin, Phys. Lett. 21, 518 (1966); Phys. Rev. 151, 56 (1966).

[6]M. Abramowitz and I. A. Stegun, *Handbook of Mathematical Functions* (Dover, New York, 1965).

[7]M. Goldstein, *Bessel functions for complex argument and order, FORTRAN coded*, NYU CIMS BES4 (1965) (unpublished), available from the Computing and Applied Mathematics Center, Courant Institute of Mathematical Sciences, New York University, New York, New York 10012.

[8]M. Goldstein and R. Thaler, *Recurrence Techniques for the Calculation of Bessel Functions*, *Math. Tables and Other Aids to Computations 13* (National Academy of Sciences-National Research Council, Washington, D. C., 1959), No. 66, pp. 102–108.

[9]This amounts to an evaluation in the monopole approximation of the correction $(1 - G_0)$ labeled f in Eq. (3.41) of J. Bang and J. M. Hansteen, K. Dan. Vidensk. Selsk. Mat. Fys. Medd. 31, 13 (1959), and labeled Δ in Eq. (31) of G. Basbas, W. Brandt, and R. Laubert, Phys. Rev. A 7, 983 (1973). Other numerical evaluations of these corrections are quoted in Footnotes 60–62 of Ref. 1.

[10]R. Anholt, D. P. Wang, and Y. C. Liu, J. Phys. Soc. Jpn. 47, 1260 (1979). Note that the heading of the first column of their Table I should read πx, not x.

[11]W. Brandt and G. Lapicki, Phys. Rev. A 23, 1717 (1981).

[12]G. Lapicki, R. Laubert, and W. Brandt, Phys. Rev. A 22, 1889 (1980).

[13]For recent contributions, cf. *Proceedings of the Workshop on Theories of Inner-Shell Ionization by Heavy Particles, Linz, Austria, 1979*, edited by H. Paul [Nucl. Instrum. Methods 169, 249 (1980)].