ISSN 1547-4771, Physics of Particles and Nuclei Letters, 2021, Vol. 18, No. 3, pp. 277–283. © Pleiades Publishing, Ltd., 2021.

PHYSICS OF ELEMENTARY PARTICLES AND ATOMIC NUCLEI. THEORY

Normalized Mott Cross Section in Different Approaches

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Received October 9, 2020; revised November 12, 2020; accepted November 17, 2020

Abstract—An intercomparison is carried out for some earlier approaches to the calculation of the normalized Mott cross section, as well as the approach proposed by the authors of the present work. It is demonstrated that applying the proposed method, along with the method of Lijian et al., is preferable for relevant calculations.

Keywords: energy loss, stopping power, heavy ions

DOI: 10.1134/S1547477121030080

INTRODUCTION

Knowledge of the energy loss of ions in matter, commonly described as stopping power (the ion mean energy loss per unit travelled path length), is fundamental to many applications dependent on the transport of ions in matter, particularly ion implantation, ion-beam modification of materials, ion beam-analysis, and ion-beam therapy [1–3].

The electronic stopping power of a material is described by the Bethe formula (the so-called Bethe's stopping power formula) [4, 5]. It is applicable if $Z\alpha/\beta \ll 1$, where α is the fine-structure constant. If this condition is not satisfied, the Bloch corrections ΔL_{B} [6] and the Mott corrections ΔL_{M} [7, 8] are also introduced:

$$\Delta L_{\mathrm{B}} = \psi(1) - \operatorname{Re}\psi(1 + iZ\alpha/\beta) \tag{1}$$

with the digamma function ψ and

$$\Delta L_{\mathrm{M}} = \frac{\tilde{N}_e}{\tilde{\zeta}}\int_{\varepsilon}^{E_m} E\left[\left(\frac{d\sigma}{dE}\right)_{\mathrm{M}} - \left(\frac{d\sigma}{dE}\right)_{\mathrm{B}}\right]dE,$$
$$\tilde{N}_e = N_{\mathrm{A}}Z'/A,\quad \tilde{\zeta} = 4\pi r^2 mc^2\tilde{N}_e\left(\frac{Z}{\beta}\right)^2 \tag{2}$$
$$= 0.307075\frac{Z'}{A}\left(\frac{Z}{\beta}\right)^2.$$

Here, Z is the charge number of incident nucleus, $\tilde{N}_e$ is the electron density of a material in electrons/g, N_{A} denotes the Avogadro number, Z' and A refer to the atomic number and weight of the absorber, ε is some energy above which the atomic electron binding energy may be neglected, E_m is the maximum transferrable energy to an electron of mass m and classical radius r in a collision with the particle of velocity βc, and $(d\sigma/dE)_{\mathrm{M(B)}}$ are, respectively, the Mott and Born expressions for the scattering cross section of electrons on nuclei.

Switching in the expression (2) from integration over the energy E transferred to an electron to integration over the center-of-mass scattering angle θ, we can rewrite (2) in the form

$$\Delta L_{\mathrm{M}} = 2\pi\frac{\tilde{N}_e E_m}{\tilde{\zeta}} \times \int_{\theta_0}^{\pi}\left[\left(\frac{d\sigma(\theta)}{d\Omega}\right)_{\mathrm{M}} - \left(\frac{d\sigma(\theta)}{d\Omega}\right)_{\mathrm{B}}\right]\sin^2\left(\frac{\theta}{2}\right)\sin\theta d\theta, \tag{3}$$

where θ_0 denotes the scattering angle corresponding to ε and Ω is the usual scattering cross section solid angle.

The Mott correction was first calculated by Eby and Morgan [9, 10] by numerical integration of (2) for several values of Z and β. These calculations demonstrated the importance of taking account of Mott's correction to the Bethe–Bloch formula for incident nuclei with $Z \geq 20$. Since the expressions (2), (3) for ΔL_{M} are extremely inconvenient for practical application, the analytical expressions for ΔL_{M} in the second and third order Born approximations were also proposed in [10]. Significant simplification of computing the Mott corrections is provided by a method of [11] that reduces the problem to the numerical summation of an infinite series.

This paper presents an adaptation of the approach [11] to the calculation of the Mott differential cross section (MDCS) normalized with respect to the Rutherford differential cross section (RDCS), as well as a comparison of this adopted method with some other rigorous and approximate methods for relevant calculations. The communication is organized as follows. Section 1 considers some preliminaries that used later in Section 2, i.e. a standard description of the (normalized) MDCS (Section 1.1) and the different approximations to the normalized Mott cross section (Section 1.2). Section 2 presents an another exact representation for the normalized MDCS (Section 2.1) and an intercomparison of applying all the mentioned methods (Section 2.2). Section 3 contains a summary of our results and conclusions.

1. PRELIMINARIES

1.1. Mott's Differential Cross Section

In 1911 Rutherford calculated the differential cross section for scattering of electrons by the Coulomb potential in the framework of classical mechanics [12], obtaining the well-known Rutherford formula:

$$\sigma_{\rm R} \equiv \left(\frac{d\sigma}{d\Omega}\right)_{\rm R} = \left(\frac{Ze^2}{2mv^2}\right)^2 \frac{1}{\sin^4(\theta/2)}. \tag{4}$$

Within the framework of nonrelativistic quantum mechanics, a solution to this problem was found independently by Gordon [13] and Mott [14] in 1928. Six months later, a simpler solution was proposed by Temple [15].

An expression for the scattering cross section of relativistic electrons through the Coulomb potential (Eq. (5)) was provided by Mott in 1929–1932 [7, 8]. This expression cannot be given in analytical form and contains slowly converging infinite series of Legendre polynomials (P_k):

$$\begin{aligned}\sigma_{\rm M} \equiv \left(\frac{d\sigma}{d\Omega}\right)_{\rm M} &= \left(\frac{\hbar}{mv}\right)^2 (1-\beta^2)\\ &\times \left(\frac{\xi^2|F_{\rm M}|^2}{\sin^2(\theta/2)} + \frac{|G_{\rm M}|^2}{\cos^2(\theta/2)}\right),\end{aligned} \tag{5}$$

where

$$F_{\rm M}(\theta) = \frac{1}{2} i \sum_{k=0}^{\infty} (-1)^k [k C_{\rm M}^{(k)} + (k+1) C_{\rm M}^{(k+1)}] P_k(\cos\theta) = \sum_{k=0}^{\infty} F_{\rm M}^{(k)} P_k(\cos\theta),$$

$$G_{\rm M}(\theta) = \frac{1}{2} i \sum_{k=0}^{\infty} (-1)^k [k^2 C_{\rm M}^{(k)} - (k+1)^2 C_{\rm M}^{(k+1)}] P_k(\cos\theta) = \sum_{k=0}^{\infty} G_{\rm M}^{(k)} P_k(\cos\theta),$$

with

$$C_{\rm M}^{(k)} = -e^{-i\pi\rho_k} \frac{\Gamma(\rho_k - i\eta)}{\Gamma(\rho_k + 1 + i\eta)}, \quad \eta = \frac{Z\alpha}{\beta},$$

$$\xi = \eta\sqrt{1-\beta^2}, \quad \rho_k = \sqrt{k^2 - (Z\alpha)^2}, \quad \alpha = \frac{e^2}{\hbar c}.$$

Here, $F_{\rm M}(\theta)$ and $G_{\rm M}(\theta)$ are two complex functions,

$$F_{\rm M}(\theta) = F_0(\theta) + F_1(\theta), \quad G_{\rm M}(\theta) = G_0(\theta) + G_1(\theta), \tag{6}$$

with

$$F_0(\theta) = \frac{1}{2} i \sum_{k=0}^{\infty} (-1)^k [k C_{\rm Z}^{(k)} + (k+1) C_{\rm Z}^{(k+1)}] P_k(\cos\theta),$$

$$G_0(\theta) = \frac{1}{2} i \sum_{k=0}^{\infty} (-1)^k [k^2 C_{\rm Z}^{(k)} - (k+1)^2 C_{\rm Z}^{(k+1)}] P_k(\cos\theta),$$

$$F_1(\theta) = \frac{1}{2} i \sum_{k=0}^{\infty} (-1)^k [k D^{(k)} + (k+1) D^{(k+1)}] P_k(\cos\theta),$$

$$G_1(\theta) = \frac{1}{2} i \sum_{k=0}^{\infty} (-1)^k [k^2 D^{(k)} - (k+1)^2 D^{(k+1)}] P_k(\cos\theta),$$

where the functions $C_{\rm Z}^{(k)}$ and $D^{(k)}$ are as follows:

$$C_{\rm Z}^{(k)} = -e^{-i\pi k} \frac{\Gamma(k - i\eta)}{\Gamma(k + 1 + i\eta)}, \quad D^{(k)} = C_M^{(k)} - C_{\rm Z}^{(k)}.$$

Hence, the functions $F_0(\theta)$ and $G_0(\theta)$ may be written as

$$\begin{aligned}F_0(\theta) &= \frac{i}{2} \frac{\Gamma(1-i\eta)}{\Gamma(1+i\eta)} \exp\left\{ i\eta \ln\left[\sin^2\left(\frac{\theta}{2}\right)\right]\right\},\\ G_0(\theta) &= -i\eta \frac{F_0(\theta)}{\tan^2(\theta/2)}.\end{aligned} \tag{7}$$

Formula (5) is also referred to as an exact formula for the differential cross section, because no Born approximation of any order is used in its derivation.

The first numerical summation of above series was performed by Mott himself [8] for scattering of electrons with relative velocity β from 0.1 to 1.0 by gold nuclei ($Z = 79$) at 90 degrees. Starting from this work, in such calculations began to introduce a quantity equal to the ratio of the MDCS ($\sigma_{\rm M}$) to the modified RDCS ($\tilde\sigma_{\rm R}$),

$$R(\theta) = \sigma_{\rm M}/\tilde\sigma_{\rm R}, \quad \tilde\sigma_{\rm R} = \sigma_{\rm R}(1-\beta^2), \tag{8}$$

i.e., the normalized Mott cross section (NMCS). In [8], the indicated quantity has the form:

$$R_{\rm M}(\theta) = \frac{4\sin^2(\theta/2)}{\eta^2}\left[\xi^2|F_{\rm M}|^2 + \tan^2\left(\frac{\theta}{2}\right)|G_{\rm M}|^2\right]. \tag{9}$$

Since the "exact" MDCS (5) and NMCS (9) are expressed in terms of slowly converging Legendre polynomial series, their application to calculate integrals (2), (3) is a difficult problem. In this regard, the use of analytical approximations to them and getting other their representations becomes important.

1.2. Some Approximations to the Normalized Mott Differential Cross Section

One way to obtain such approximations is to expand the exact NMCS in terms of power series in αZ. We will present below such results for the above function $R(\theta)$.

The first such expansion was obtained by the author of the exact solution to the scattering problem [8]:

$$R_{\mathrm{B}}(\theta) = 1 - \beta^2 \sin^2\left(\frac{\theta}{2}\right). \quad (10)$$

Further approximations were obtained by McKinley and Feshbach,

$$R_{\mathrm{MF}}(\theta) = R_{\mathrm{B}} + \alpha Z \pi \beta \sin\left(\frac{\theta}{2}\right)\left[1 - \sin\left(\frac{\theta}{2}\right)\right], \quad (11)$$

as well as Johnson, Weber, and Mullin [16, 17],

$$\begin{aligned} R_{\mathrm{JWM}} = {} & R_{\mathrm{MF}} + (\alpha Z)^2 \sin\left(\frac{\theta}{2}\right)\left\{L_2\left[1 - \sin^2\left(\frac{\theta}{2}\right)\right]\right. \\ & - 4L_2\left[1 - \sin\left(\frac{\theta}{2}\right)\right] + 2\sin\left(\frac{\theta}{2}\right)\ln^2\left[\sin\left(\frac{\theta}{2}\right)\right] \\ & + \frac{\pi^2}{2}\left[1 - \sin\left(\frac{\theta}{2}\right)\right] + \frac{\pi^2}{6}\sin\left(\frac{\theta}{2}\right) + \beta^2 \sin\left(\frac{\theta}{2}\right) \\ & \times \left(L_2\left[1 - \sin^2\left(\frac{\theta}{2}\right)\right] + \frac{\sin^2(\theta/2)\ln^2[\sin(\theta/2)]}{1 - \sin^2(\theta/2)}\right. \\ & \left.\left. + \frac{\pi^2}{4}\frac{1 - \sin(\theta/2)}{1 + \sin(\theta/2)} - \frac{\pi^2}{6}\right)\right\}, \end{aligned} \quad (12)$$

where L_2 denotes Euler's dilogarithm defined by

$$L_2(x) = -\int_0^x \frac{\ln(1 - y)}{y} dy.$$

Another approach was proposed by Lijian, Qing, and Zhengming [18], where the exact NMCS is approximated by the following expression:

$$\begin{aligned} R_{\mathrm{LQZ}}(\theta; Z, E) &= \sum_{j=0}^{4} a_j(Z, E)(1 - \cos\theta)^{j/2}, \\ a_j(Z, E) &= \sum_{k=1}^{6} d_Z(j, k)(\beta - \bar{\beta})^{k-1}, \\ \bar{\beta} &= 0.7181287. \end{aligned} \quad (13)$$

The authors calculated 30 coefficients $d_Z(j,k)$ for 90 elements of the Periodic System with target atomic number Z from 1 to 90 in a wide range of energy. Investigations in this direction were continued by Boschini, Consolandi, Gervasi et al. in the work [19], where the coefficients $d_Z(j,k)$ were obtained for 118 elements of the Periodic Table of Elements both for electrons and positrons.

2. RESULTS AND DISCUSSIONS

2.1. Another Representation for the Normalized Mott Cross Section

In [11] we got the following representation for the exact Mott differential cross section:

$$\begin{aligned} \sigma_{\mathrm{VSST}} &\equiv \left(\frac{d\sigma}{d\Omega}\right)_{\mathrm{VSTT}} = \left(\frac{\hbar}{mv}\right)^2 (1 - \beta^2) \\ &\times \left(\frac{\xi^2 |F_{\mathrm{M}}|^2 - |F'_{\mathrm{M}}|^2}{\sin^2(\theta/2)}\right) \equiv \left(\frac{\hbar}{mv}\right)^2 (1 - \beta^2)\omega_{\mathrm{VSST}}, \\ \omega_{\mathrm{VSTT}}(\theta) &= \omega_{\mathrm{Z}}(\theta) + \lambda(\theta)\Big/\sin^2\left(\frac{\theta}{2}\right), \\ \lambda(\theta)/4 &= \xi^2[2\,\mathrm{Re}(\Delta F F_{\mathrm{Z}}^*) + |\Delta F|^2] \\ &\quad + 2\,\mathrm{Re}(\Delta F' F_{\mathrm{Z}}^{*}{}') + |\Delta F'|^2, \\ \omega_{\mathrm{Z}}(\theta) &= \left[\xi^2 + \eta^2 \cos^2\left(\frac{\theta}{2}\right)\right]\Big/\sin^2\left(\frac{\theta}{2}\right) \equiv \omega_{\mathrm{B}}(\theta), \\ \Delta F &\equiv F_{\mathrm{M}} - F_{\mathrm{Z}},\ F_{\mathrm{Z}}(\theta) = \frac{i}{2}\sum_{l=0}^{\infty}(-1)^k F_{\mathrm{Z}}^{(k)} P_k(\cos\theta) \\ &= \frac{i}{2}\frac{\Gamma(1 - i\eta)}{\Gamma(1 + i\eta)}\sin^{2i\eta}\left(\frac{\theta}{2}\right),\quad F_{\mathrm{Z}}^{(k)} = kC_{\mathrm{Z}}^{(k)} + (k+1)C_{\mathrm{Z}}^{(k+1)}, \\ F'_{\mathrm{M}} &\equiv dF_{\mathrm{M}}(\theta)/d\theta = -\tan^2(\theta/2)G_{\mathrm{M}}. \end{aligned} \quad (14)$$

This representation reduces computing the integrals (2), (3) to a summing the fast converging infinite series whose terms are bilinear in the Mott partial amplitudes and can be simply implemented using the numerical summation methods of converging series for a given level of precision.

It leads to the following exact expression for the normalized Mott cross section:

$$\begin{aligned} R_{\mathrm{KHV}}(\theta) &= R_{\mathrm{B}}(\theta) + \tilde{\lambda}(\theta)\sin^2\left(\frac{\theta}{2}\right), \\ \tilde{\lambda}(\theta)/4 &= \eta^{-2}\{\xi^2[2\,\mathrm{Re}(\Delta F F_{\mathrm{Z}}^*) \\ &\quad + |\Delta F|^2] + 2\,\mathrm{Re}(\Delta F' F_{\mathrm{Z}}^{*}{}') + |\Delta F'|^2\}. \end{aligned} \quad (15)$$

Taking into account (6), (7), we can rewrite $\tilde{\lambda}(\theta)$ in terms of functions $F_0(\theta)$ and $F_1(\theta)$,

$$\begin{aligned} \tilde{\lambda}(\theta)/4 &= \eta^{-2}\{\xi^2[2\,\mathrm{Re}(F_1 F_0^*) + |F_1|^2] \\ &\quad + 2\,\mathrm{Re}(F_1' F_0^{*}{}') + |F_1'|^2\}. \end{aligned}$$

Our calculations show that elimination from (5) of the slowest converging function $G_1(\theta)$ provides a convergence of these series comparable to that obtained by the so-called "reduction method" [20].

Table 1. Comparison of the $R(\theta)$ values obtained by different methods for the scattering of electrons with an energy of 10 MeV on nuclei of charge number $Z = 47$

R/θ	15	30	45	60	75	90	105	120	135	150	165	180
R_M	1.116	1.215	1.256	1.225	1.122	0.958	0.753	0.533	0.324	0.154	0.042	0.0032
R_{KHV}	1.116	1.215	1.256	1.225	1.122	0.958	0.753	0.533	0.324	0.154	0.042	0.0032
R_{LQZ}	1.118	1.214	1.255	1.225	1.123	0.959	0.753	0.532	0.323	0.153	0.043	0.0041
R_{JWM}	1.143	1.228	1.240	1.171	1.042	0.867	0.667	0.463	0.278	0.131	0.036	0.0028
R_{MF}	1.105	1.140	1.108	1.020	0.887	0.724	0.549	0.377	0.224	0.105	0.029	0.0024
R_B	0.983	0.933	0.854	0.751	0.630	0.501	0.372	0.252	0.148	0.069	0.019	0.0024

2.2. Comparison of Methods

In this section we present the results of calculating the normalized Mott cross section $R(\theta)$ by the above methods using the Wolfram Mathematica computer algebra system. The expression (9) was calculated by the "method of reduced series" [20] that can be represented in the following way.

Let us represent a function $f(\theta)$ by

$$f(\theta) = \sum_{l=0}^{\infty} A_l P_l(\cos\theta). \tag{16}$$

Then the mth 'reduced' series is defined as

$$(1 - \cos\theta)^m f(\theta) = \sum_{l=0}^{\infty} A_l^{(m)} P_l(\cos\theta). \tag{17}$$

Using the recurrence relations for Legendre polynomials, we find:

$$A_l^{(m)} = A_l^{(m-1)} - \frac{l+1}{2l+3} A_{l+1}^{(m-1)} + \frac{l}{2l-1} A_{l+1}^{(m-1)}. \tag{18}$$

For large l, it turns out that

$$\left|A_l^{(m)}\right| = O\left(\left|A_l^{(m-1)}\right|/l^2\right), \tag{19}$$

so that after a few reductions the series converges quite rapidly.

Table 1 lists the results of calculations performed and shows an excellent agreement between the results obtained from Eqs. (15) and (9) as well as an increasing deviation from these results in the transition from (13) to (10). This allows us to carry out further comparison with respect to the results obtained on the basis of (15).

Figure 1 compares the results obtained on the basis of Eqs. (10)–(13), (15) for scattering of electrons with energies of 0.005, 1, and 10 MeV on nuclei of charge number $Z = 13$, 47, and 92.

From this Figure it can be seen that the results of Lijian et al. and Boschini et al. [18, 19] obtained from Eq. (13) significantly differ from the exact ones only in the area of low energies and high charge numbers (e.g. for $Z = 92$, 0.005 MeV). In other cases, they are close to rigorous results. For light elements, all approximations give fairly accurate results. For elements with moderately high values of Z at medium and high energies, the approximation (12) gives higher accuracy than (11) and (10). For heavy elements, the approximate methods based on Eqs. (10)–(12) are not applicable.

Additionally we evaluated relative difference between the ratios R_{LQZ} and R_{KHV} obtained by the methods of works [18, 19] and [11] as a function of the scattering angle for electrons with energies from 0.005 to 10 MeV on nuclei with charge number from 13 to 92 (Fig. 2):

$$\delta R(\theta; Z, E) = \frac{R_{LQZ}(\theta; Z, E) - R_{KHV}(\theta; Z, E)}{R_{KHV}(\theta; Z, E)}.$$

Figure 2 shows that at low energies (e.g. 0.005 MeV), the maximum value of the relative difference modulus $\left|\delta R(\theta; Z, E)\right|$ increases from 0.04 to 16 percent in the transition from nucleus charge number $Z = 13$ to $Z = 92$. From Fig. 2 also follows that at medium energies (1 MeV), this value varies between 0.07–3.5 percent for nucleus with a Z value of 13 to 92. At high energies[1] (e.g. 10 MeV), the approximation (13) differs significantly (up to 70 percent) from the exact expression (15) only in the range of scattering angles from 160 to 180 deg, where the values of the ratios R_{LQZ} and R_{KHV} are very small, while over the θ range from 0 to 150 deg, where the relative difference between R_{LQZ} and R_{KHV} is almost zero.

3. SUMMARY AND CONCLUSIONS

■ In the present work, an new exact representation for the normalized MDCS is proposed that reduces the calculation of the NMCS in terms of the Mott series $F_M(\theta)$ and $G_M(\theta)$ to its calculation in terms of $F_M(\theta)$ alone, excluding the most slowly converging series in the NMCS computation.

■ Numerical results are obtained on the basis of the obtained formula and the following exact and approx-

[1] At energies higher than 10 MeV, the results are very close to those of 10 MeV, according to [18], since β in this case is close to 1.

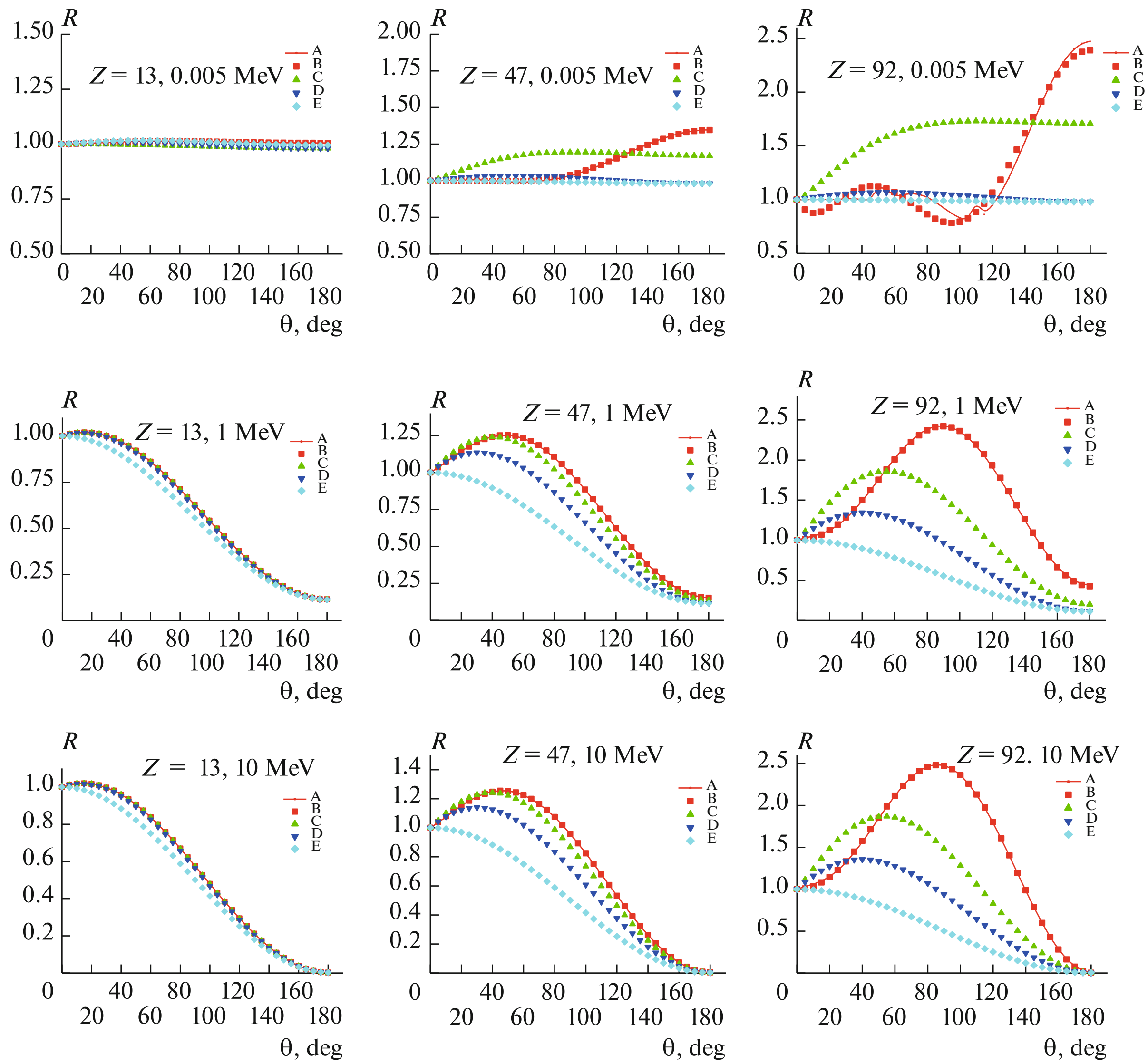

Fig. 1. (Color online) Cross section ratio, $R(\theta)$, as function of scattering angle obtained from Eqs. 15 (A), 13 (B), 12 (C), 11 (D), 10 (E) for scattering of electrons with energies of 0.005, 1, and 10 MeV on nuclei of charge number Z equal to 13, 47, and 92.

imate expressions for the normalized Mott cross section: (i) the conventional Mott-exact ‘phase-shift’ formula (point-charge nucleus, no screening) [8], (ii) the approximate Lijian–Qing–Zhengming expression [18], (iii) the Johnson–Weber–Mullin formula [17], (iv) the McKinley–Feshbach expression [16], and (v) the Mott–Born result [8].

■ An intercomparison of the obtained numerical results is presented in the range of nucleus charge number from $Z = 13$ to $Z = 92$ for electron energies from 0.005 MeV to 10 MeV and scattering angles over the range of 0–180 deg.

• It is shown that while all the approaches discussed give sufficiently accurate results for low-Z nuclei in the entire range of energies, the approximate Mott–Born, McKinley–Feshbach, and Johnson–Weber–Mullin methods are not applicable for high-Z nuclei at the same energies.

• The approximate Lijian–Qing–Zhengming approach gives fairly accurate results in the entire range of charge numbers and electron energies, except for the area of low energies and high charge numbers.

• The results of the rigorous methods considered are remarkably consistent.

• The accuracy was estimated, and the range of applicability was established for the Lijian–Qing–Zhengming method, which gives the best approximation to rigorous results.

• We managed to show that for $Z < 90$, this method can be applied with an error of less than 1%, in accordance with [18], but only over the θ range from 0 to 150 deg at high energies.

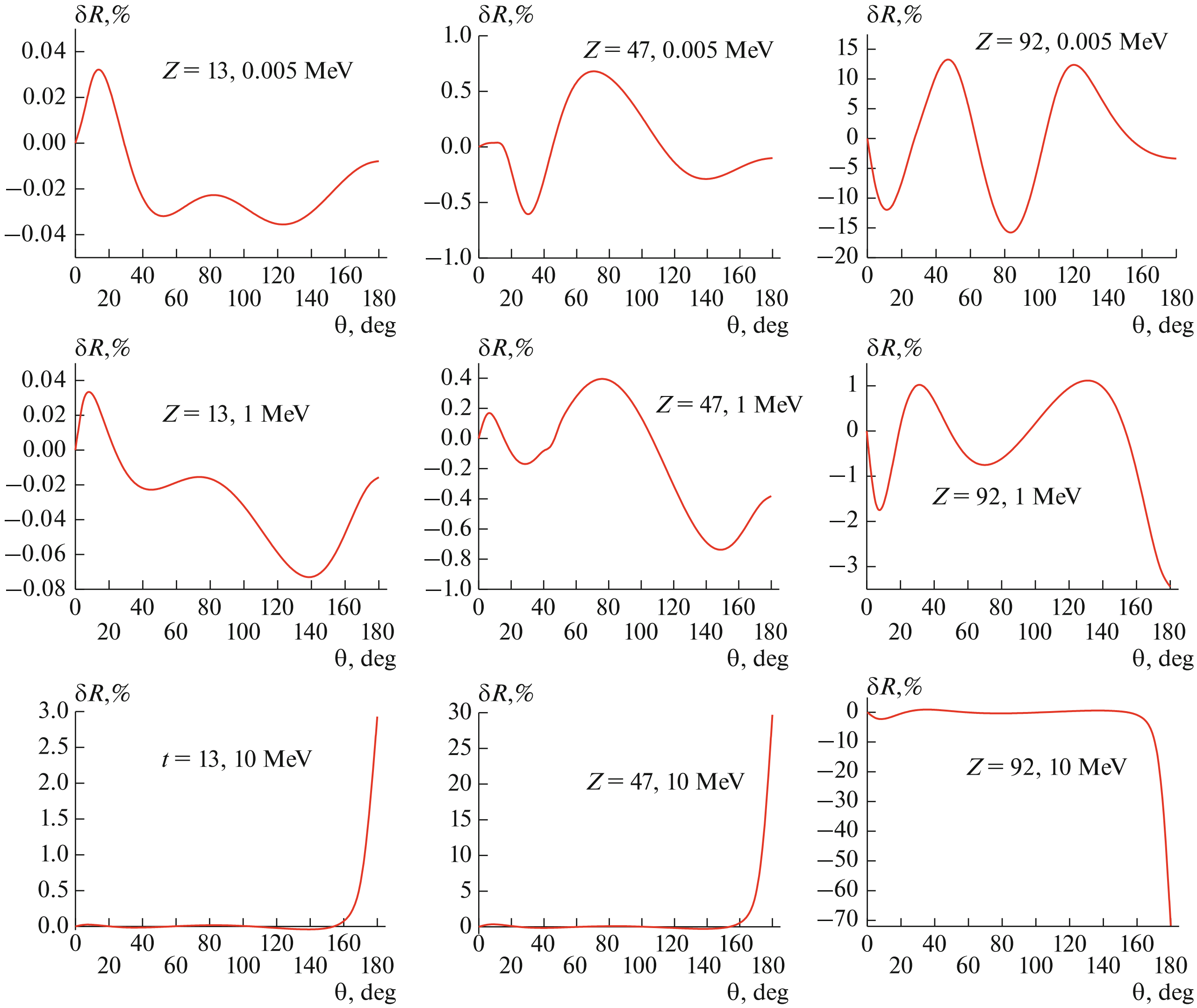

Fig. 2. Relative difference between the ratios R_{LQZ} and R_{KHV} obtained from Eqs. (13) and (15) as function of scattering angle (in degrees) for electrons with energies of 0.005, 1, and 10 MeV scattered on nuclei of charge number $Z = 13$, 47, and 92.

• In the case of $Z \geq 90$, the specified method can also be applied with the same error, however also only in the θ range of 0–150 deg for high and medium energies.

• Outside of the specified ranges, the error can increase up to 16 percent (for $Z = 92$, 0.005 MeV) and even up to 70% (for $Z = 92$, 10 MeV, and $\theta = 180$ deg).

■ Thus, we can conclude that both the rigorous approach suggested in this work and the approximate Lijian–Qing–Zhengming approach can be recommended for practical calculations of the normalized Mott cross section $R(\theta)$.

• Although the second method has somewhat limited accuracy, its advantage compared to first method is the ability to perform integration with a given lower integration limit.

• The advantage of the first method over the second one is its greater accuracy, as well as the possibility of its use beyond the applicability of the approximate method by Lijian, Qing, and Zhengming.

• Therefore, each of these approaches is preferred in its application area for relevant calculations of the NMCS.

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