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Some approaches to the calculation of the normalized Mott cross section, displacement cross section, and the Mott correction to the Bethe formula

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A new exact representation for the normalized Mott cross section is obtained. Some earlier exact and approximate methods for its calculation are compared with the method proposed in this work. It is demonstrated that applying the suggested rigorous method, along with the approximate method of Lijian et al., is most preferable for the above calculations. Some modifications of Lijian's method are proposed. Based on these modifications and the Lijian method itself, new analytical expressions are obtained for the Mott corrections to the Bethe stopping formula and the primary displacement cross section by fast electrons. It is shown that the highest fitting accuracy of the displacement cross sections is provided by the twice modified Lijian method.

1. Introduction

Theoretical and experimental studies of the penetration of charged particles in matter and their stopping play an important role in the development of modern physics and represent an active field of research (Sigmund and Schinner, 2020; Kats et al., 2021; Sunko et al., 2020; Abd Ali and Kadhim, 2020; Forcellini and Artacho, 2019; Banko and Kats, 2019; Gumus et al., 2018; Kadhim and Hussien, 2016). Research in astrophysics, nuclear physics, atomic and molecular physics, biophysics, and many other areas is based on experimental techniques utilizing high-energy radiation and theoretical knowledge of the interaction between radiation and matter. Various aspects of this problem have been explored by leading physicists of the 20th century([Rutherford, 1911; Bohr, 1915; Mott, 1929, 1932; Bethe, 1930, 1932; Bloch, 1933; Fermi, 1940; and others). Many review articles, textbooks and monographs have been written on the subject of charged-particle penetration in matter and particle stopping (Bethe and Ashkin, 1953; Überall, 1971; Ahlen, 1980; Geissel et al., 2002; Weaver and Westphal, 2002; Sigmund, 2006; Sigmund and Schinner, 2016; Bichsel et al., 2020).

For studies on mean free paths of electrons it is necessary to have precise differential cross sections for these particles. Among such differential cross-section is one relating to elastic scattering of electrons and positrons by nuclei, first studied by Mott (Mott, 1929, 1932). Mott expressed an 'exact cross section' in terms of two conditionally convergent series that are defined as an expansion in Legendre polynomials. These resulting series were not summed up analytically, and numerical methods were required to obtain exact results. The numerical calculation of Mott's cross section (or the ratio of Mott's cross section to Rutherford's cross section) has attracted the attention of many authors (Yennie et al., 1954; Doggett and Spencer 1956; Sherman, 1956; Bühring, 1965; Idoeta and Legarda, 1992). However, since these calculations are time-consuming, numerous approximate expressions and their modifications have also been proposed for it (Mott, 1932; McKinley and Feshbach, 1948; Johnson et al., 1961; Lijian et al., 1995; Boschini et al., 2013).

For electrons bound in atoms, Bethe used the 'Born theory' (Bethe, 1930) to obtain his theory of charged-particle passage through matter and particle stopping. At high energies, the Born differential cross section $(d\sigma/dE)_B$ of this theory (E is energy loss) must be additionally modified by polarization of the medium. The other corrections to the Born cross section will be discussed below. The relativistic version of stopping power formula was obtained by Bethe in (Bethe, 1932). Taking into account the density-effect, the average ionization energy loss by moderately relativistic charged heavy particles can be described in the first Born approximation as follows:

$$-\frac{d\overline{E}}{dx} = \zeta L,\ L = L_0 = \ln\left(\frac{E_m}{I}\right) - \beta^2 - \frac{\delta}{2},$$

$$\zeta = 4\pi r^2 mc^2 \cdot N_e \cdot \left(\frac{Z}{\beta}\right)^2 = 4\pi r^2 mc^2 \cdot N_A \rho \frac{Z}{A} \cdot \left(\frac{Z}{\beta}\right)^2,\ E_m = \frac{2mc^2\beta^2}{1-\beta^2}. \quad (1)$$

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The function L_0 of this form is derived originally from quantum perturbation theory (Weaver and Westphal, 2002). The first two of its terms are typically called the Bethe result and the third term is the familiar density effect correction of Fermi (Fermi, 1940). In these equations, x denotes the distance traveled by a particle; 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; I is the effective ionization potential of the absorber atoms, Z is the charge number of incident nucleus, and N_e is the electron density of the material. The electron density is measured either in electrons/g ($\widetilde{N}_e = N_A Z'/A$) or in electrons/ cm^3 ($N_e = N_A \rho Z'/A$), where ρ is density of a material in g cm^{-3}, N_A denotes the Avogadro number, Z' and A refer to the atomic number and weight of the absorber. In the latter case, we can rewrite (1) as

$$-\frac{d\overline{E}}{\rho dx} = \widetilde{\zeta} L,\ \widetilde{\zeta} = 4\pi r^2 mc^2 \cdot \widetilde{N}_e \cdot \left(\frac{Z}{\beta}\right)^2 = 0.307075 \frac{Z'}{A}\left(\frac{Z}{\beta}\right)^2.$$

This is the 'mass stopping power' in units MeV g^{-1}cm^2 (Bichsel et al., 2020).

The above expressions are applicable if $Z\alpha/\beta << 1$, where α is the fine-structure constant. If this condition is not satisfied, the Bloch corrections ΔL_B (Bloch, 1933; Sigmund and Schinner, 2020) and the Mott corrections ΔL_M (Mott, 1929, 1932) are also introduced:

$$\Delta L_B = \psi(1) - \mathrm{Re}\psi(1 + iZ\alpha/\beta)$$

with the digamma function ψ and

$$\Delta L_M = \frac{\widetilde{N}_e}{\widetilde{\zeta}} \int_{\varepsilon}^{E_m} E\left[\left(\frac{d\sigma}{dE}\right)_M - \left(\frac{d\sigma}{dE}\right)_B\right] dE. \tag{2}$$

Here, ε is some energy above which the atomic electron binding energy may be neglected, and $(d\sigma/dE)_{M(B)}$ 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

$$\Delta L_M = 2\pi \frac{\widetilde{N}_e E_m}{\widetilde{\zeta}} \int_{\theta_0}^{\pi} \left[\left(\frac{d\sigma(\theta)}{d\Omega}\right)_M - \left(\frac{d\sigma(\theta)}{d\Omega}\right)_B\right] \sin^2\left(\frac{\theta}{2}\right) \sin\theta d\theta, \tag{3}$$

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 (Eby and Morgan, 1972; Morgan and Eby, 1973) by numerical integration of (2) for several values of Z and β. These calculations demonstrated the importance of taking account of Mott's corrections to the Bethe–Bloch formula for incident nuclei with $Z \geq 20$. Since the expressions (2), (3) for ΔL_M are extremely inconvenient to evaluate the Mott correction, the analytical expressions for ΔL_M in the second and third order Born approximations were also proposed in (Morgan and Eby, 1973). Significant simplification of computing the Mott corrections is provided by a method of (Voskresenskaya et al., 1996) that reduces the problem to the numerical summation of an infinite series.

This paper presents an adaptation of the method (Voskresenskaya et al., 1996) for calculating the Mott differential cross section (MDCS) normalized with respect to the Rutherford differential cross section (NMCS), 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 2 considers various approaches to the MDCS descriptions, namely: a standard description of the (normalized) MDCS (Section 2.1), the different approximations to the normalized Mott cross section (Section 2.2), another exact representation for the normalized MDCS (Section 2.3), and an intercomparison of applying all the mentioned methods (Section 2.3). Section 3 presents some possible applications of the Lijian–Qing–Zhengming (LQZ) method. First we obtain an analytical expression for the Mott correction using this method (Lijian et al., 1995) and its modification, and also compare the obtained results with the corresponding result of Matveev (Matveev, 2002) (Section 3.1). Then we calculate the atomic displacement cross sections (ADCS) using the modified and twice modified LQZ expressions, as well as the LQZ method itself, and compare its values with the ADCS value estimated by the McKinley–Feshbach method (McKinley and Feshbach, 1948) and with Oen's electron displacement cross section (Oen, 1973, 1988) (Section 3.2). Section 4 contains a summary of our results and conclusions. Appendix A shows the derivation of the formula for the normalized Mott cross section. Appendix B presents a twice modified LQZ method.

2. Mott's differential cross section

2.1. Basic formulae

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

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

Within the framework of nonrelativistic quantum mechanics, a solution to this problem was found independently by Gordon (Gordon, 1928) and Mott (Mott, 1928). For the scattering cross section of relativistic electrons through the Coulomb potential (5) an expression was provided by Mott in 1929–1932 (Mott, 1929, 1932). The last expression cannot be given in analytical form and contains slowly converging infinite series of Legendre polynomials (P_k):

$$\sigma_M \equiv \left(\frac{d\sigma}{d\Omega}\right)_M = \left(\frac{\hbar}{mv}\right)^2 (1-\beta^2)\left(\frac{\xi^2 |F_M|^2}{\sin^2(\theta/2)} + \frac{|G_M|^2}{\cos^2(\theta/2)}\right), \tag{5}$$

where

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

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

with

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

The Mott series $F_M(\theta)$ and $G_M(\theta)$ converge only conditionally and are defined as

$$F_M(\theta) = F_0(\theta) + F_1(\theta),\ G_M(\theta) = G_0(\theta) + G_1(\theta), \tag{6}$$

with

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

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

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

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

The functions $C_Z^{(k)}$ and $D^{(k)}$ are given by:

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

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

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

The series $F_1(\theta)$ and $G_1(\theta)$ are only conditionally convergent and converge very slovly (the series G_1

is more slovly convergent than F_1). The formula (5) is 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 the above series was performed by Mott himself (Mott, 1932) for scattering of electrons with relative velocity β from 0.1 to 1.0 by gold nuclei (Z = 79) at 90°. Starting from this work, such calculations began to include a quantity equal to the ratio of the MDCS (σ_M) to the modified RDCS ($\widetilde{\sigma}_R$),

$$R(\theta)=\sigma_M/\widetilde{\sigma}_R,\quad \widetilde{\sigma}_R=\sigma_R\left(1-\beta^2\right), \quad (8)$$

that is, the normalized Mott cross section (NMCS). In the original paper, the indicated quantity has the form:

$$R_M(\theta)=\frac{4\sin^2(\theta/2)}{\eta^2}\left[\xi^2|F_M|^2+\tan^2\left(\frac{\theta}{2}\right)|G_M|^2\right]. \quad (9)$$

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, it becomes important to use analytical approximations to them and to obtain their other representations.

2.2. Some approximations to the normalized Mott 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 (Mott, 1932), the so-called Mott–-Born result:

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

Further approximations were obtained by McKinley and Feshbach,

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

as well as Johnson, Weber, and Mullin (McKinley and Feshbach, 1948; Johnson et al., 1961)

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

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 (Lijian et al., 1995), where the exact NMCS is approximated by the following expression:

$$R_{LQZ}\left(\theta;Z,E\right)=\sum_{j=0}^{4}a_j(Z,E)(1-\cos\theta)^{j/2},a_j\left(Z,E\right)=\sum_{k=1}^{6}d_Z(j,k)(\beta-\overline{\beta})^{k-1},$$
$$\overline{\beta}=0.7181287. \quad (13)$$

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 (Boschini et al., 2013), where the coefficients $d_Z(j,k)$ were obtained for 118 elements of the Periodic Table of Elements both for electrons and positrons.

2.3. Another representation for the normalized Mott cross section

In (Voskresenskaya et al., 1996) we obtained the following representation for the exact Mott differential cross section:

$$\begin{aligned}\sigma_{VSTT}&\equiv\left(\frac{d\sigma}{d\Omega}\right)_{VSTT}=\left(\frac{\hbar}{mv}\right)^2\left(1-\beta^2\right)\left(\frac{\xi^2|F_M|^2-|F_M^{'}|^2}{\sin^2(\theta/2)}\right)\\&\equiv\left(\frac{\hbar}{mv}\right)^2\left(1-\beta^2\right)\omega_{VSTT},\end{aligned}$$

$$\omega_{VSTT}(\theta)=\omega_Z(\theta)+\lambda(\theta)\Big/\sin^2\left(\frac{\theta}{2}\right),$$

$$\lambda(\theta)\Big/4=\xi^2\left[2\mathrm{Re}\left(\Delta FF_Z^*\right)+|\Delta F|^2\right]+2\mathrm{Re}\left(\Delta F^{'}F_Z^{*'}\right)+|\Delta F^{'}|^2,$$

$$\omega_Z(\theta)=\left[\xi^2+\eta^2\cos^2\left(\frac{\theta}{2}\right)\right]\Big/\sin^2\left(\frac{\theta}{2}\right)\equiv\omega_B(\theta),\Delta F\equiv F_M-F_Z,$$

$$F_Z(\theta)=\frac{i}{2}\sum_{l=0}^{\infty}(-1)^kF_Z^{(k)}P_k(\cos\theta)=\frac{i}{2}\frac{\Gamma(1-i\eta)}{\Gamma(1+i\eta)}\sin^{2i\eta}\left(\frac{\theta}{2}\right),$$
$$F_Z^{(k)}=kC_Z^{(k)}+(k+1)C_Z^{(k+1)},$$

$$F_M^{'}\equiv dF_M(\theta)/d\theta=-\tan(\theta/2)G_M. \quad (14)$$

This representation reduces computing the integrals (2), (3) to a summing of 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 (see Appendix A):

$$R_{KHV}(\theta)=R_B(\theta)+\widetilde{\lambda}(\theta)\sin^2\left(\frac{\theta}{2}\right),$$

$$\widetilde{\lambda}(\theta)\Big/4=\eta^{-2}\left\{\xi^2\left[2\mathrm{Re}\left(\Delta FF_Z^*\right)+|\Delta F|^2\right]+2\mathrm{Re}\left(\Delta F^{'}F_Z^{*'}\right)+|\Delta F^{'}|^2\right\}. \quad (15)$$

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

$$\widetilde{\lambda}(\theta)\Big/4=\eta^{-2}\left\{\xi^2\left[2\mathrm{Re}\left(F_1F_0^*\right)+|F_1|^2\right]+2\mathrm{Re}\left(F_1^{'}F_0^{*'}\right)+|F_1^{'}|^2\right\},$$

and then calculate the ratio $R_{KHV}(\theta)$, for instance, by the method of 'reduced series' (Yennie et al., 1954). However, our calculations show

Table 1
Comparison of the $R(\theta)$ values obtained by different methods for the scattering of electrons by nuclei of charge number $Z = 80$. $R_{M:}$ the summation up to $N = 200$; R_{KHV}: the summation up to $N = 80$; $R_M{}^{(2)}$: the summation up to $N = 150$, the series were 'reduced' with $m = 2$.

θ/β	0.2	0.4	0.5	0.6	0.7	0.8	0.9
30°	$R_M = 1.02$	$R_M = 0.991$	$R_M = 1.04$	$R_M = 1.09$	$R_M = 1.14$	$R_M = 1.19$	$R_M = 1.26$
	R_{KHV} =1.01	$R_{KHV} = 1.00$	$R_{KHV} = 1.03$	$R_{KHV} = 1.08$	$R_{KHV} = 1.15$	$R_{KHV} = 1.22$	$R_{KHV} = 1.29$
	$R_M{}^{(2)} = 1.01$	$R_M{}^{(2)} = 1.00$	$R_M{}^{(2)} = 1.03$	$R_M{}^{(2)} = 1.08$	$R_M{}^{(2)} = 1.15$	$R_M{}^{(2)} = 1.22$	$R_M{}^{(2)} = 1.29$
60°	$R_M = 0.986$	$R_M = 1.12$	$R_M = 1.28$	$R_M = 1.39$	$R_M = 1.52$	$R_M = 1.68$	$R_M = 1.82$
	$R_{KHV} = 0.979$	$R_{KHV} = 1.12$	$R_{KHV} = 1.27$	$R_{KHV} = 1.42$	$R_{KHV} = 1.55$	$R_{KHV} = 1.67$	$R_{KHV} = 1.78$
	$R_M{}^{(2)} = 0.979$	$R_M{}^{(2)} = 1.12$	$R_M{}^{(2)} = 1.27$	$R_M{}^{(2)} = 1.41$	$R_M{}^{(2)} = 1.55$	$R_M{}^{(2)} = 1.67$	$R_M{}^{(2)} = 1.78$
90°	$R_M = 0.956$	$R_M = 1.38$	$R_M = 1.62$	$R_M = 1.69$	$R_M = 1.74$	$R_M = 1.83$	$R_M = 1.93$
	$R_{KHV} = 0.963$	$R_{KHV} = 1.41$	$R_{KHV} = 1.58$	$R_{KHV} = 1.71$	$R_{KHV} = 1.80$	$R_{KHV} = 1.86$	$R_{KHV} = 1.89$
	$R_M{}^{(2)} = 0.963$	$R_M{}^{(2)} = 1.41$	$R_M{}^{(2)} = 1.58$	$R_M{}^{(2)} = 1.71$	$R_M{}^{(2)} = 1.80$	$R_M{}^{(2)} = 1.86$	$R_M{}^{(2)} = 1.89$
120°	$R_M = 1.35$	$R_M = 1.79$	$R_M = 1.75$	$R_M = 1.79$	$R_M = 1.82$	$R_M = 1.67$	$R_M = 1.42$
	$R_{KHV} = 1.33$	$R_{KHV} = 1.75$	$R_{KHV} = 1.81$	$R_{KHV} = 1.79$	$R_{KHV} = 1.72$	$R_{KHV} = 1.60$	$R_{KHV} = 1.44$
	$R_M{}^{(2)} = 1.33$	$R_M{}^{(2)} = 1.75$	$R_M{}^{(2)} = 1.80$	$R_M{}^{(2)} = 1.79$	$R_M{}^{(2)} = 1.72$	$R_M{}^{(2)} = 1.60$	$R_M{}^{(2)} = 1.44$
150°	$R_M = 1.95$	$R_M = 2.13$	$R_M = 1.89$	$R_M = 1.75$	$R_M = 1.66$	$R_M = 1.33$	$R_M = 0.817$
	$R_{KHV} = 1.93$	$R_{KHV} = 2.06$	$R_{KHV} = 1.95$	$R_{KHV} = 1.76$	$R_{KHV} = 1.50$	$R_{KHV} = 1.18$	$R_{KHV} = 0.810$
	$R_M{}^{(2)} = 1.93$	$R_M{}^{(2)} = 2.06$	$R_M{}^{(2)} = 1.95$	$R_M{}^{(2)} = 1.76$	$R_M{}^{(2)} = 1.50$	$R_M{}^{(2)} = 1.18$	$R_M{}^{(2)} = 0.810$

that the elimination from (5) of the slowest converging function $G_1(\theta)$ alone provides even faster convergence of this series compared to that given by the above 'reduction method' (Table 1).

2.4. Comparison of methods

Table 2 lists the results of calculating the normalized Mott cross section $R(\theta)$ by the above methods. It 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).

Fig. 1 compares the results obtained on the basis of Eq. (10)−(13), (15) for scattering of electrons with energies of 0.005 MeV, 1 MeV, and 10 MeV by nuclei of charge number $Z = 13,\ 47$, and 92.

From Fig. 1 it can be seen that the results of Lijian et al. and Boschini et al. (Lijian et al., 1995; Boschini et al., 2013) 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 Eq. (10)−(12) are not applicable.

Additionally we evaluated relative difference between the ratios R_{LQZ} and R_{KHV} obtained by the methods of (Lijian et al., 1995; Boschini et al., 2013) and (Voskresenskaya et al., 1996) as a function of the scattering angle for electrons with energies from 0.005 MeV to 10 MeV scattered by nuclei with charge number from 13 to 92 (Fig. 2):

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

Fig. 2 shows that at low energies (e.g. 0.005 MeV), the maximum value of the relative difference modulus $|\ \delta R(\theta; Z, E)\ |$ increases from 0.036 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 and 3.5 percent for nuclei with Z values 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°, where the values of the ratios R_{LQZ} and R_{KHV} are very small, while over the θ range from 0 to 150°, the relative difference between R_{LQZ} and R_{KHV} is almost zero.

[1] At energies higher than 10 MeV, the results are very close to those of 10 MeV, according to (Lijian et al., 1995), since β in this case is close to 1.

3. Applications of the Lijian−Qing−Zhengming method

3.1. Mott's corrections

In this section, we give an analytical expression for the Mott correction ΔL_M (3), based on the NMCS approximation (13) from [Lijian et al., 1995], and compare it with some other expressions for ΔL_M. A modification of the LQZ method is also considered.

In terms of the NMCSs (8)−(10), the expression (3) can be rewritten as follows:

$$\Delta L_M = 2\pi \frac{\widetilde{N}_e E_m}{\widetilde{\zeta}} \left(\frac{Ze^2}{2mv^2}\right)^2 (1-\beta^2) \int_{\theta_0}^{\pi} \frac{R_M(\theta) - R_B(\theta)}{\sin^2(\theta/2)} \sin\theta d\theta.$$

Thus, we obtain:

$$\Delta L_M = \frac{1}{4} \int_{\theta_0}^{\pi} \frac{R_M(\theta) - R_B(\theta)}{\sin^2(\theta/2)} \sin\theta d\theta.$$

The authors of (Banko and Kats, 2019) have shown that to obtain the reference ΔL_M value when comparing different methods for the calculation of ΔL_M, it is convenient to use the precise representation of this correction obtained by (Voskresenskaya et al., 1996) in the limit $\theta_0 \to 0$ in the form of the following absolutely converging series:

$$\Delta L_{MVSTT} = \frac{2}{\eta^2} \sum_{k=0}^{\infty} \frac{k(k+1) + \xi^2}{2k+1} \left(\left| F_M^{(k)} \right|^2 - \left| F_Z^{(k)} \right|^2 \right),$$

$$F_M^{(k)} = \frac{i}{2}(-1)^k \left[k C_M^{(k)} + (k+1) C_M^{(k+1)} \right],\ F_Z^{(k)} = \frac{i}{2}(-1)^k \left[k C_Z^{(k)} + (k+1) C_Z^{(k+1)} \right],$$

$$C_Z^{(k)} = e^{-i\pi k} \frac{\Gamma(k - i\eta)}{\Gamma(k+1+i\eta)},\ C_M^{(k)} = e^{-i\pi\rho_k} \frac{\Gamma(\rho_k - i\eta)}{\Gamma(\rho_k + 1 + i\eta)},\ \eta = \frac{Z\alpha}{\beta},\ \xi = \frac{\eta}{\gamma},$$

$$\rho_k = \sqrt{k^2 - Z^2\alpha^2}.$$

Let us find the Mott correction using expressions (13) and (10) in the limit $\theta_0 \to 0$:

$$\Delta L_{MLQZ} = \frac{1}{4} \lim_{\theta_0 \to 0} \int_{\theta_0}^{\pi} \frac{R_{MLQZ}(\theta) - R_B(\theta)}{\sin^2(\theta/2)} \sin\theta d\theta \equiv \frac{1}{4} \lim_{\theta_0 \to 0} I(\theta).$$

This way we get:

$$I(\theta)=\int_{\theta_0}^{\pi}\frac{a_0+a_1(1-\cos\theta)^{1/2}+a_2(1-\cos\theta)+a_3(1-\cos\theta)^{3/2}+a_4(1-\cos\theta)^2-\left[1-\beta^2\sin^2(\theta/2)\right]}{\sin^2(\theta/2)}\sin\theta d\theta$$

$$=\left\{-\left(2a_2+2a_4+\beta^2\right)\cos\theta-\frac{4}{3}\sqrt{1-\cos\theta}\left[-3a_1-a_3(1-\cos\theta)\right]+\frac{1}{2}a_4\cos(2\theta)+4(a_0-1)\ln[\sin(\theta/2)]\right\}\Big|_{\theta_0}^{\pi}.$$

Since $\theta\to 0$ leads to $R_M(\theta)\to 1$ (Doggett and Spencer, 1956), we have $a_0 = 1$, and the last term in the above expression for $I(\theta)$ vanishes. This leads to the following approximate expression for the Mott correction in the LQZ formalism:

$$\Delta L_{MLQZ}=\frac{\beta^2}{2}+\sqrt{2}a_1+a_2+\frac{2\sqrt{2}a_3}{3}+a_4. \quad (16)$$

Let us compare this result with another convenient approximate expression for ΔL_M proposed by Matveev (Matveev, 2002):

$$\Delta L_{MMT}=\ln[f(Z,\beta)],$$

Table 2
Comparison of the $R(\theta)$ values obtained by different methods for the scattering of electrons with an energy of 10 MeV by 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	1.226	1.122	0.958	0.753	0.533	0.324	0.154	0.042	0.0032
R_{KHV}	1.116	1.215	1.256	1.226	1.122	0.958	0.753	0.533	0.324	0.154	0.042	0.0032
	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_{LQZ}	1.143	1.228	1.240	1.171	1.042	0.867	0.667	0.463	0.278	0.131	0.036	0.0032
R_{JWM}	1.105	1.140	1.108	1.020	0.886	0.724	0.549	0.377	0.224	0.105	0.029	0.0026
R_{MF}	0.983	0.933	0.854	0.751	0.630	0.501	0.372	0.252	0.149	0.069	0.019	0.0026
R_B												

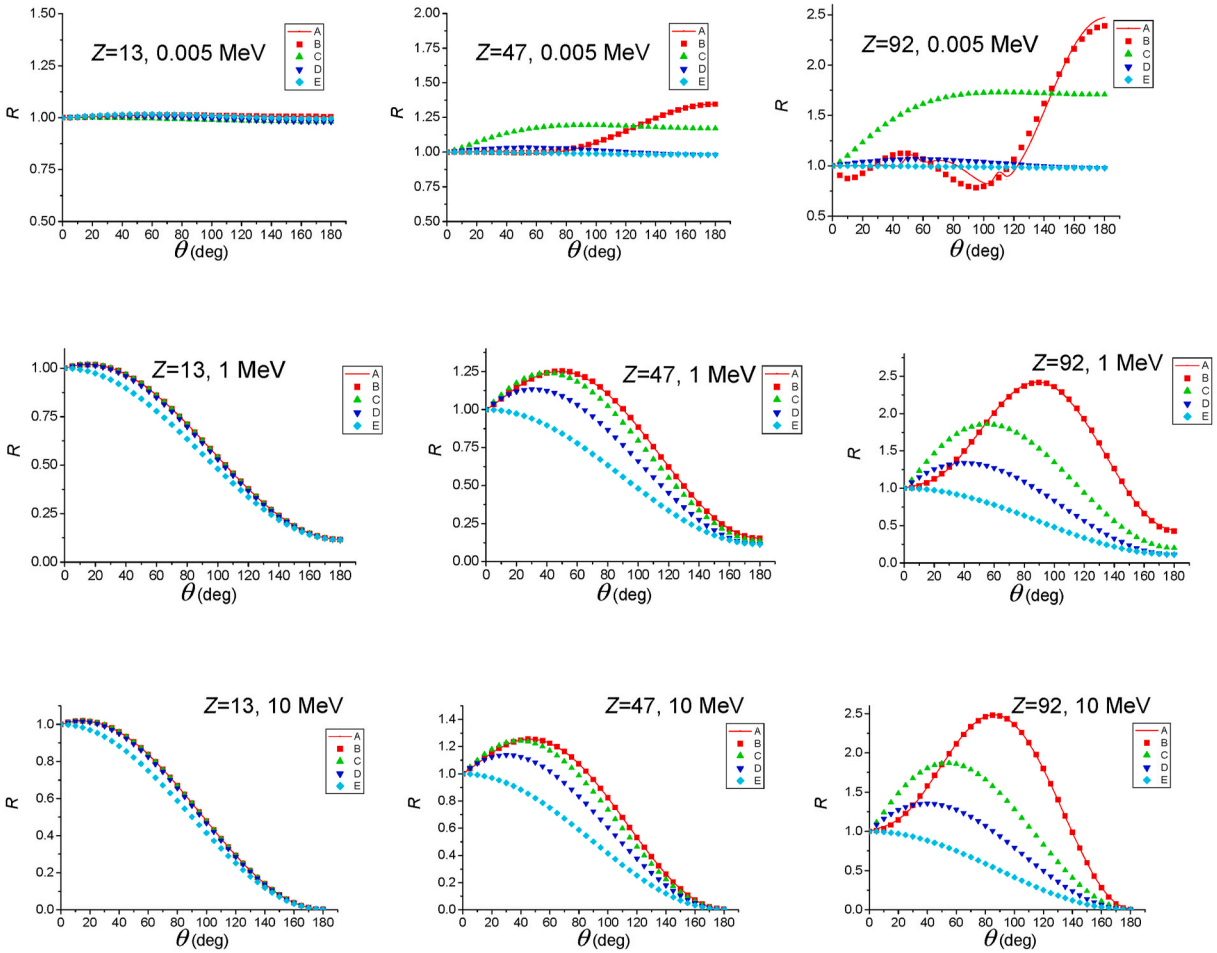

Fig. 1. Cross section ratio, $R(\theta)$, as function of scattering angle obtained from Eq. (15) (A), 13 (B), 12 (C), 11 (D), 10 (E) for scattering of electrons with energies of 0.005 MeV, 1 MeV, and 10 MeV on nuclei of charge number Z equal to 13, 47, and 92.

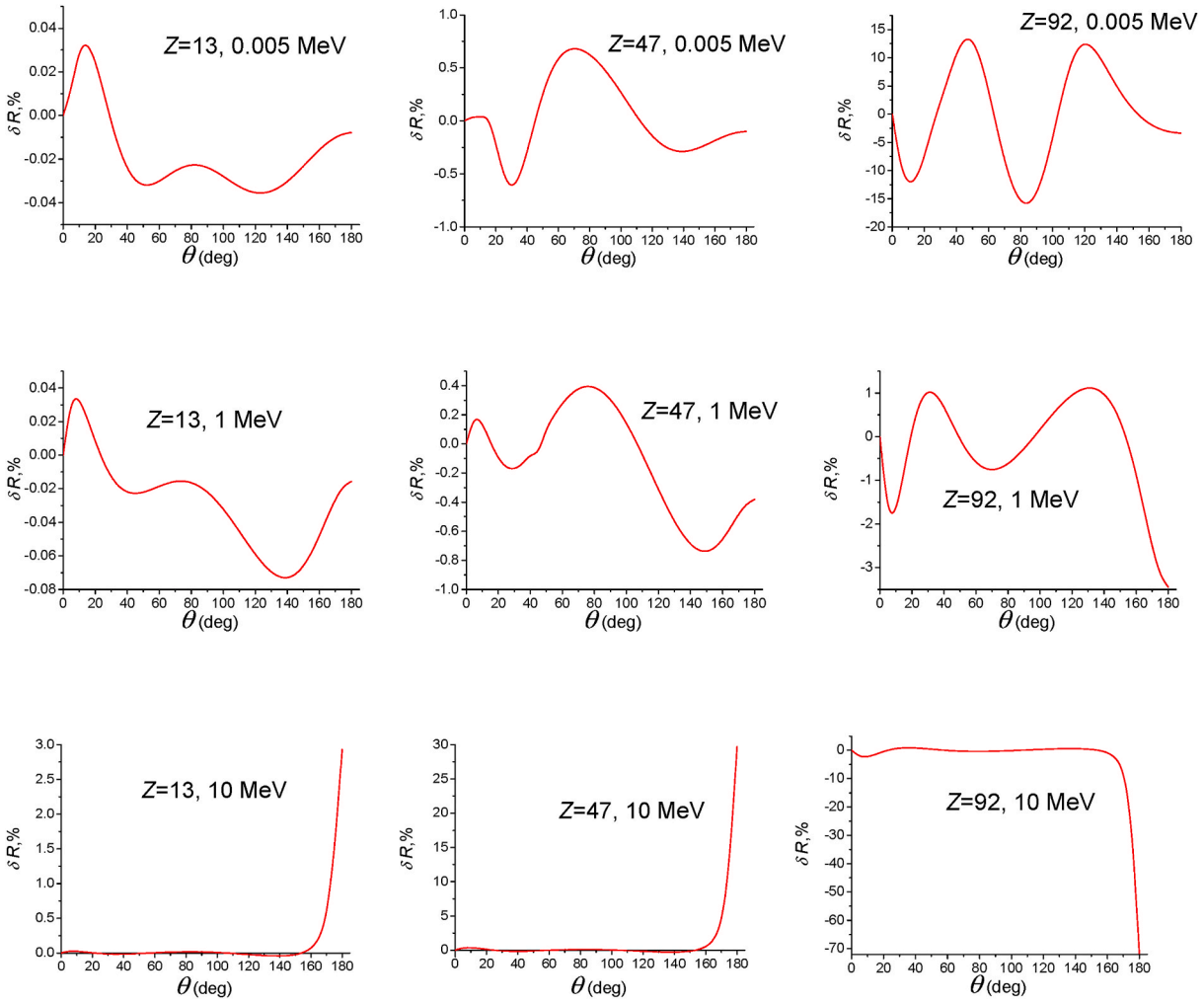

Fig. 2. Relative difference between the ratios R_{LQZ} and R_{KHV} obtained from Eqs. (13) and (15) as function of scattering angle (in degrees) for electrons with energies of 0.005 MeV, 1 MeV, and 10 MeV scattered by nuclei of charge number $Z = 13$, 47, and 92.

$$f(Z,\beta)=1+\left\{0.222592\beta-0.042948\beta^2+\left(0.6016+5.15289\beta-3.73293\beta^2\right)Z\alpha -\left(0.52308+5.71287\beta-8.11358\beta^2\right)(Z\alpha)^2\right\}^2.$$

To do this, we use the relative difference

$$\delta=\frac{|\Delta L_M-\Delta L_{MVSTT}|}{\Delta L_{MVSTT}}\cdot 100\ \%$$

that is presented in Table 3. In this Table the δ values in excess of 10% are highlighted. It is obvious that the difference of ΔL_{MLQZ} correction substantially exceeds the ΔL_{MMT} difference for small and medium-Z values. For $Z \geq 80$ and some β, the relative difference of ΔL_{MLQZ} is large enough. It can be assumed that this is due to the fact that the authors of papers (Lijian et al., 1995) and (Boschini et al., 2013) did not use the asymptotics $\lim_{\theta\to 0} R_M(\theta) = 1$. A consequence of which may be, in particular, the proximity, but not exact equality to unity of the coefficient a_0 from (13). To test this assumption, we will consider a modification of the LQZ method.

Let us represent the normalized Mott cross section as

$$R_{MLQZm}\left(\theta;Z,\beta\right)=1+\sum_{j=1}^{4}a_j(Z,\beta)(1-\cos\theta)^{j/2},\ a_j\left(Z,\beta\right)=\sum_{k=1}^{6}d_Z(j,k)(\beta-\overline{\beta}\,)^{k-1},\ \overline{\beta}=0.668269. \tag{17}$$

In this case, the indicated asymptotics is performed automatically. To find new coefficients $d_z(j,k)$, we will use the method described in (Lijian et al., 1995), but with some modifications. Since R_{MLQZm} is expressed directly through β, we will immediately consider the interval of the relative velocity β from 0.1 to 0.999 (the upper limit corresponds to the electron energy of 10.92 MeV), and not the energy range. In (Lijian et al., 1995) and (Boschini et al., 2013), energies up to 900 MeV were considered, but, firstly, at energies above 10 MeV, the results differ very little from the results at 10 MeV, since β changes very insignificantly near 1 (Lijian et al., 1995), and, secondly, we leave the region of applicability of the point-nucleus approximation considered here at these energies. For the considered interval of β, the average β value is $\overline{\beta}$

Table 3
Relative difference between the corrections ΔL_M ($\Delta L_M = \Delta L_{MLQZ}$, ΔL_{MMT}) and ΔL_{MVSTT} over the Z and β ranges $10 \le Z \le 100$ and $0.3 \le \beta \le 0.999$.

β/Z	10	20	30	40	50
0.3	$\boldsymbol{\delta_{MT} = 22.2}$ $\delta_{LQZ} = 2.56$	$\boldsymbol{\delta_{MT} = 15.3}$ $\delta_{LQZ} = 1.12$	$\delta_{MT} = 6.83$ $\delta_{LQZ} = 2.28$	$\delta_{MT} = 0.975$ $\delta_{LQZ} = 4.00$	$\delta_{MT} = 6.89$ $\delta_{LQZ} = 3.42$
0.4	$\boldsymbol{\delta_{MT} = 12.3}$ $\delta_{LQZ} = 1.41$	$\delta_{MT} = 8.34$ $\delta_{LQZ} = 2.76$	$\delta_{MT} = 3.99$ $\delta_{LQZ} = 1.49$	$\delta_{MT} = 0.514$ $\delta_{LQZ} = 2.15$	$\delta_{MT} = 1.91$ $\delta_{LQZ} = 6.45$
0.5	$\delta_{MT} = 5.71$ $\delta_{LQZ} = 0.899$	$\delta_{MT} = 3.34$ $\delta_{LQZ} = 2.50$	$\delta_{MT} = 0.844$ $\delta_{LQZ} = 2.71$	$\delta_{MT} = 0.407$ $\delta_{LQZ} = 0.507$	$\delta_{MT} = 0.837$ $\delta_{LQZ} = 3.46$
0.6	$\delta_{MT} = 2.40$ $\delta_{LQZ} = 0.903$	$\delta_{MT} = 0.929$ $\delta_{LQZ} = 1.49$	$\delta_{MT} = 1.086$ $\delta_{LQZ} = 2.33$	$\delta_{MT} = 1.582$ $\delta_{LQZ} = 2.53$	$\delta_{MT} = 1.17$ $\delta_{LQZ} = 0.883$
0.7	$\delta_{MT} = 1.96$ $\delta_{LQZ} = 0.979$	$\delta_{MT} = 1.05$ $\delta_{LQZ} = 0.787$	$\delta_{MT} = 1.39$ $\delta_{LQZ} = 1.61$	$\delta_{MT} = 2.20$ $\delta_{LQZ} = 3.21$	$\delta_{MT} = 1.85$ $\delta_{LQZ} = 3.40$
0.8	$\delta_{MT} = 4.00$ $\delta_{LQZ} = 0.820$	$\delta_{MT} = 3.42$ $\delta_{LQZ} = 0.831$	$\delta_{MT} = 0.0757$ $\delta_{LQZ} = 1.41$	$\delta_{MT} = 1.99$ $\delta_{LQZ} = 2.61$	$\delta_{MT} = 2.42$ $\delta_{LQZ} = 2.98$
0.9	$\delta_{MT} = 8.14$ $\delta_{LQZ} = 0.479$	$\delta_{MT} = 7.71$ $\delta_{LQZ} = 1.29$	$\delta_{MT} = 2.72$ $\delta_{LQZ} = 1.73$	$\delta_{MT} = 0.891$ $\delta_{LQ\,Z} = 1.58$	$\delta_{MT} = 2.66$ $\delta_{LQZ} = 0.970$
0.99	$\boldsymbol{\delta_{MT} = 13.4}$ $\delta_{LQZ} = 0.436$	$\boldsymbol{\delta_{MT} = 13.0}$ $\delta_{LQZ} = 1.11$	$\delta_{MT} = 6.35$ $\delta_{LQZ} = 1.56$	$\delta_{MT} = 0.816$ $\delta_{LQZ} = 1.59$	$\delta_{MT} = 2.53$ $\delta_{LQZ} = 1.19$
0.999	$\boldsymbol{\delta_{MT} = 14.0}$ $\delta_{LQZ} = 0.472$	$\boldsymbol{\delta_{MT} = 13.5}$ $\delta_{LQZ} = 1.01$	$\delta_{MT} = 6.77$ $\delta_{LQZ} = 1.47$	$\delta_{MT} = 1.02$ $\delta_{LQZ} = 1.71$	$\delta_{MT} = 2.50$ $\delta_{LQZ} = 1.51$
β/Z	60	70	80	90	100
0.3	$\boldsymbol{\delta_{MT} = 10.3}$ $\delta_{LQZ} = 1.94$	$\boldsymbol{\delta_{MT} = 15.3}$ $\delta_{LQZ} = 1.12$	$\delta_{MT} = 9.51$ $\delta_{LQZ} = 5.54$	$\delta_{MT} = 5.66$ $\boldsymbol{\delta_{LQZ} = 19.8}$	$\delta_{MT} = 0.00667$ $\boldsymbol{\delta_{LQZ.} = 34.3}$
0.4	$\delta_{MT} = 3.11$ $\delta_{LQZ} = 9.50$	$\delta_{MT} = 3.08$ $\delta_{LQZ} = 6.19$	$\delta_{MT} = 1.95$ $\delta_{LQZ} = 6.32$	$\delta_{MT} = 0.00124$ $\delta_{LQZ} = 0.58$	$\delta_{MT} = 2.26$ $\delta_{LQZ} = 3.76$
0.5	$\delta_{MT} = 0.691$ $\delta_{LQZ} = 7.76$	$\delta_{MT} = 0.114$ $\delta_{LQZ} = 7.18$	$\delta_{MT} = 0.715$ $\boldsymbol{\delta_{LQZ} = 10.34}$	$\delta_{MT} = 1.49$ $\delta_{LQZ} = 5.44$	$\delta_{MT} = 1.66$ $\delta_{LQZ} = 4.65$
0.6	$\delta_{MT} = 0.352$ $\delta_{LQZ} = 2.83$	$\delta_{MT} = 0.556$ $\delta_{LQZ} = 5.65$	$\delta_{MT} = 1.299$ $\boldsymbol{\delta_{LQZ} = 11.46}$	$\delta_{MT} = 1.542$ $\boldsymbol{\delta_{LQZ} = 11.76}$	$\delta_{MT} = 0.702$ $\delta_{LQZ} = 2.06$
0.7	$\delta_{MT} = 0.952$ $\delta_{LQZ} = 0.875$	$\delta_{MT} = 0.0716$ $\delta_{LQZ} = 3.47$	$\delta_{MT} = 0.872$ $\delta_{LQZ} = 9.66$	$\delta_{MT} = 1.07$ $\boldsymbol{\delta_{LQZ} = 13.23}$	$\delta_{MT} = 0.0822$ $\delta_{LQZ} = 6.17$
0.8	$\delta_{MT} = 1.92$ $\delta_{LQZ} = 1.46$	$\delta_{MT} = 1.00$ $\delta_{LQZ} = 1.86$	$\delta_{MT} = 0.0764$ $\delta_{LQZ} = 6.29$	$\delta_{MT} = 0.414$ $\delta_{LQZ} = 9.65$	$\delta_{MT} = 0.141$ $\delta_{LQZ} = 5.44$
0.9	$\delta_{MT} = 2.96$ $\delta_{LQZ} = 0.0492$	$\delta_{MT} = 2.34$ $\delta_{LQZ} = 1.16$	$\delta_{MT} = 1.28$ $\delta_{LQZ} = 3.21$	$\delta_{MT} = 0.314$ $\delta_{LQZ} = 4.43$	$\delta_{MT} = 0.0846$ $\delta_{LQZ} = 2.18$
0.99	$\delta_{MT} = 3.84$ $\delta_{LQZ} = 0.354$	$\delta_{MT} = 3.62$ $\delta_{LQZ} = 0.739$	$\delta_{MT} = 2.47$ $\delta_{LQZ} = 2.48$	$\delta_{MT} = 0.988$ $\delta_{LQZ} = 3.60$	$\delta_{MT} = 0.0957$ $\delta_{LQZ} = 1.81$
0.999	$\delta_{MT} = 3.92$ $\delta_{LQZ} = 0.694$	$\delta_{MT} = 3.75$ $\delta_{LQZ} = 0.663$	$\delta_{MT} = 2.59$ $\delta_{LQZ} = 2.58$	$\delta_{MT} = 1.06$ $\delta_{LQZ} = 3.98$	$\delta_{MT} = 0.117$ $\delta_{LQZ} = 2.15$

$= 0.668269$. In this case, the number of parameters $d_z(j,k)$ turns out to be equal to 24, and not 30 for each Z, since the coefficient a_0 from (13) is equal to one, but is not expressed in terms of the parameters $d_z(j,k)$.

To estimate the accuracy of the approximations (13) and (17), the value of the relative error ER (Lijian et al., 1995) was calculated (Table 4):

$$ER = \sqrt{\frac{\sum_{i=0}^{36}\left[R_{MLQZ(m)}(\theta_i;Z,\beta) - R_{MVSTT}(\theta_i;Z,\beta).\right]^2}{\sum_{i=0}^{36} R_{MVSTT}(\theta_i;Z,\beta)^2}} \cdot 100\ \%.$$

Table 4 shows that the reduction in the number of parameters did not lead to a noticeable deterioration in the accuracy of the NMCS calculations. Table 5 presents the relative difference between the Mott correction calculated by the approximate LQZ, LQZm methods and the precise VSTT method.

It can be seen that in all cases, except for $Z = 100$ and $\beta = 0.3$, the relative deviation of the Mott correction obtained using the LQZm method does not exceed 10%. In cases where the Mott correction obtained by the LQZm method turns out to be less accurate than that found by the LQZ method, the δ_{LQZm} value does not exceed 6%.

Table 4
Relative error ER in the calculations of the normalized Mott cross section according to (13) and (17).

β/Z	90	100
0.2	$ER_{LQZ} = 1.60$ $ER_{LQZm} = 1.65$	$ER_{LQZ} = 4.36$ $ER_{LQZm} = 4.38$
0.5	$ER_{LQZ} = 0.946$ $ER_{LQZm} = 0.949$	$ER_{LQZ} = 0.893$ $ER_{LQZm} = 0.892$
0.9	$ER_{LQZ} = 0.629$ $ER_{LQZm} = 0.678$	$ER_{LQZ} = 0.659$ $ER_{LQZm} = 0.679$

3.2. Analytical expression for primary displacement cross sections by fast electrons on the basis of the modified and twice modified LQZ methods

To study the damaging effect of high-energy electrons on materials, the calculation of the atomic displacement cross section (ADCS) is used (Sherman et al., 1966; Sunko et al., 2020). In particular, the cross section for producing primary atomic displacements is (Oen, 1973)

$$\sigma_p(E,T_d) = \int_{T_d}^{T_m} \frac{d\sigma}{dT} dT, \tag{18}$$

where E is the energy of an electron; T_m is the maximum energy that can be transferred to the nucleus of an atom of mass M in a collision with an electron of mass m; T_d is the threshold energy, that is, the minimum transferred energy at which an atom can be displaced from its equilibrium position; and $d\sigma/dT$ is the differential scattering cross section for transferring an energy T to an atom by an electron of energy E. Switching

Table 5
Relative difference between the values of approximate Mott's corrections ΔL_{MLQZ}, ΔL_{MLQZm} and the exact ΔL_{MVSTT} value.

β/Z	90	100
0.3	$\boldsymbol{\delta_{LQZ} = 19.8}$ $\delta_{LQZm} = 4.00$	$\boldsymbol{\delta_{LQZ} = 34.3}$ $\boldsymbol{\delta_{LQZm} = 25.0}$
0.4	$\delta_{LQZ} = 0.58$ $\delta_{LQZm} = 1.04$	$\delta_{LQZ} = 3.76$ $\delta_{LQZm} = 4.11$
0.5	$\delta_{LQZ} = 5.44$ $\delta_{LQZm} = 2.68$	$\delta_{LQZ} = 4.65$ $\delta_{LQZm} = 4.41$
0.6	$\boldsymbol{\delta_{LQZ} = 11.8}$ $\delta_{LQZm} = 5.57$	$\delta_{LQZ} = 2.06$ $\delta_{LQZm} = 0.64$
0.7	$\boldsymbol{\delta_{LQZ} = 13.2}$ $\delta_{LQZm} = 6.13$	$\delta_{LQZ} = 6.17$ $\delta_{LQZm} = 3.82$
0.8	$\delta_{LQZ} = 9.65$ $\delta_{LQZm} = 4.88$	$\delta_{LQZ} = 5.44$ $\delta_{LQZm} = 3.72$
0.9	$\delta_{LQZ} = 4.43$ $\delta_{LQZm} = 3.18$	$\delta_{LQZ} = 2.18$ $\delta_{LQZm} = 1.96$
0.99	$\delta_{LQZ} = 3.60$ $\delta_{LQZm} = 2.83$	$\delta_{LQZ} = 1.81$ $\delta_{LQZm} = 2.07$
0.999	$\delta_{LQZ} = 3.98$ $\delta_{LQZm} = 2.93$	$\delta_{LQZ} = 2.15$ $\delta_{LQZm} = 2.32$
0.9999	$\delta_{LQZ} = 4.03$ $\delta_{LQZm} = 2.94$	$\delta_{LQZ} = 2.19$ $\delta_{LQZm} = 2.35$

Table 6
Comparison of the displacement cross sections (20), (23)–(25), and (21) for platinum atoms as functions of electron energy.

E, MeV	σ_{pMF}	σ_{pLQZ}	σ_{pLQZm}	σ_{pLQZm2}	σ_{pO}
1.38	0.14	0.37	0.37	0.38	0.39
1.39	0.27	0.77	0.77	0.79	0.80
1.42	0.72	2.38	2.37	2.40	2.43
1.46	1.45	5.33	5.32	5.32	5.38
1.51	2.54	10.01	10.01	9.96	10.04
1.58	4.33	17.86	17.85	17.73	17.83
1.66	6.64	27.90	27.90	27.71	27.82
1.77	10.12	42.44	42.43	42.21	42.30
1.91	14.82	60.72	60.70	60.49	60.55
2.12	21.97	85.63	85.59	85.50	85.51
2.39	30.77	111.87	111.78	111.85	111.85
2.73	40.76	136.20	136.08	136.26	136.32
3.14	51.08	155.61	155.46	155.68	155.82
3.69	62.26	170.42	170.27	170.43	170.63
4.37	72.83	178.51	178.39	178.45	178.63
5.19	82.19	180.79	180.74	180.69	180.77
6.15	90.03	178.96	179.00	178.88	178.83
7.11	95.69	175.36	175.48	175.31	175.17
8.20	100.40	170.75	170.96	170.77	170.55
9.57	104.64	165.21	165.51	165.32	165.09
11.60	108.85	158.22	158.60	158.43	158.26
13.60	111.57	152.75	153.19	153.04	152.94
20.50	116.27	141.07	141.55	141.50	141.97
27.30	118.16	135.19	135.63	135.63	136.53
41.00	119.71	129.51	129.86	129.91	130.70
68.40	120.61	125.47	125.67	125.74	126.21
136.00	121.03	123.00	123.04	123.10	123.44
273.00	121.14	122.03	121.96	122.00	120.93

Table 7
Comparison of the displacement cross sections (20), (23)–(25), and (21) for gold atoms as functions of electron energy.

E,MeV	σ_{pMF}	σ_{pLQZ}	σ_{pLQZm}	σ_{pLQZm2}	σ_{pO}
1.39	0.16	0.44	0.44	0.45	0.46
1.40	0.29	0.86	0.87	0.88	0.90
1.43	0.75	2.56	2.56	2.58	2.61
1.47	1.49	5.65	5.65	5.64	5.69
1.52	2.59	10.54	10.52	10.48	10.56
1.59	4.39	18.70	18.67	18.57	18.67
1.67	6.72	29.15	29.08	28.94	29.05
1.78	10.24	44.24	44.13	43.98	44.08
1.92	14.99	63.17	63.04	62.93	62.98
2.13	22.21	88.92	88.78	88.77	88.79
2.40	31.11	115.95	115.83	115.94	115.95
2.75	41.52	141.53	141.44	141.61	141.67
3.16	51.93	161.10	161.05	161.19	161.34
3.71	63.23	175.87	175.85	175.89	176.10
4.40	74.06	183.78	183.80	183.72	183.90
5.23	83.60	185.62	185.67	185.50	185.57
6.19	91.51	183.31	183.40	183.19	183.14
7.15	97.22	179.31	179.43	179.24	179.08
8.26	102.06	174.26	174.42	174.27	174.03
9.63	106.33	168.39	168.57	168.50	168.25
11.70	110.64	160.93	161.13	161.16	160.99
13.70	113.38	155.26	155.47	155.59	155.49
20.60	118.11	143.24	143.42	143.73	144.23
27.50	120.05	137.14	137.28	137.67	138.63
41.30	121.61	131.37	131.45	131.85	132.70
68.80	122.52	127.32	127.31	127.66	128.16
137.00	122.95	124.88	124.77	125.01	125.36
275.00	123.06	123.94	123.77	123.91	122.74

in (18) from integration over the transferred energy T to integration over the center-of-mass scattering angle θ, we can rewrite (18) in the form (Sunko et al., 2020):

$$\sigma_p(E,T_d)=2\pi\int\limits_{\theta(T_d)}^{\pi}\frac{d\sigma}{d\Omega}\sin\theta d\theta, \tag{19}$$

where the relationship between the scattering angle and the transferred energy can be written as follows:

$$\sin^2\frac{\theta}{2}=\frac{T}{T_m},\ T_m=\frac{2E(E+2mc^2)}{Mc^2}.$$

Only relativistic electrons can cause the displacement of atoms, so (19) includes the Mott differential scattering cross section (5). But since the MDCS is expressed in terms of slowly converging series and the calculation of integrals using this cross-section is very difficult, one of the common methods for the ADCS calculations is to use the analytical McKinley–Feshbach approximation for the MDCS (McKinley and Feshbach, 1948), which leads to the following analytical ADCS expression (Khandelwal and Merzbacher, 1963):

$$\sigma_{pMF}=\frac{\pi Z^2e^4}{m^2c^4\beta^4}\left(1-\beta^2\right)\left\{\frac{1}{y}-1+\beta^2\ln(y)+\pi\alpha\beta\left[\frac{2}{\sqrt{y}}-2+\ln(y)\right]\right\},\ y=\frac{T_d}{T_m}. \tag{20}$$

(see, e.g. (Nagase et al., 2012)). However, as noted in (Khandelwal and Merzbacher, 1963), the expression (20) is not applicable for large charge numbers Z, since the McKinley–Feshbach approximation is obtained for small Z. In this regard, an another possible approach to finding the ADCS using the analytical LQZ approximation (Lijian et al., 1995) is advisable (Sunko et al., 2020).

According to (Oen, 1973), the cross section for the formation of the primary displacement of an atom can be represented as

$$\sigma_p(E,T_d)=\frac{\pi Z^2e^4}{m^2c^4\beta^4}\left(1-\beta^2\right)\int\limits_{T_d/T_m}^{1}\frac{R(x,E)}{x^2}dx,\ x=\sin^2\frac{\theta}{2}=\frac{T}{T_m}. \tag{21}$$

After substituting (13) into (17), we get

$$\sigma_p(E,T_d)=\frac{\pi Z^2e^4}{m^2c^4\beta^4}\left(1-\beta^2\right)\int\limits_{y}^{1}\frac{\sum_{j=0}^{4}a_j(Z,E)(2x)^{j/2}}{x^2}dx. \tag{22}$$

Integration of expression (22) leads to the analytical expression

$$\sigma_{pLQZ}=\frac{\pi Z^2e^4}{m^2c^4\beta^4}\frac{\left(1-\beta^2\right)}{y}\left\{\left(1-\sqrt{y}\right)\left(a_0(Z,\beta)+\left(a_0(Z,\beta)+2\sqrt{2}a_1(Z,\beta)\right)\sqrt{y}+4\left(\sqrt{2}a_3(Z,\beta)+a_4(Z,\beta)\right)y+4a_4(Z,\beta)y^{3/2}\right)-2a_2(Z,\beta)y\ln y\right\}. \tag{23}$$

In Section 3.1, a modified LQZ method (17) was proposed that provides the correct asymptotic NMCS behavior in the limit $\theta\to0$. In the twice modified LQZ method (see Appendix B), the expression for NMCS can be represented as follows:

$$R_{LQZm2}(\theta,Z,E)=1+\sum_{j=1}^{5}a_j(Z,E)(1-\cos\theta)^{j/2}.$$

Using these methods, the following analytical σ_p expressions can be obtained:

$$\sigma_{pLQZm}=\frac{\pi Z^2e^4}{m^2c^4\beta^4}\left(1-\beta^2\right)\left\{-1-2\sqrt{2}a_1(Z,\beta)+4\left(\sqrt{2}a_3(Z,\beta)+a_4(Z,\beta)\right)+\frac{1}{y}+2\sqrt{2}a_1(Z,\beta)\Big/\sqrt{y}-4\sqrt{2}a_3(Z,\beta)\sqrt{y}-4a_4(Z,\beta)y-2a_2(Z,\beta)\ln y\right\}, \tag{24}$$

$$\sigma_{pLQZm2}=\frac{\pi Z^2 e^4}{m^2c^4\beta^4}(1-\beta^2)\Big\{-1-2\sqrt{2}a_1(Z,\beta)+4\Big(\sqrt{2}\,a_3(Z,\beta)+a_4(Z,\beta)\Big)+\frac{1}{y}+2\sqrt{2}a_1(Z,\beta)\Big/\sqrt{y}-$$

$$-4\sqrt{2}\,a_3(Z,\beta)\sqrt{y}-4a_4(Z,\beta)y-2a_2(Z,\beta)\ln y+\frac{8}{3}\sqrt{2}\,a_5(Z,\beta)\left(1-y^{3/2}\right)\Big\}. \quad (25)$$

Tables 6 and 7 show the results of σ_{pLQZ}, σ_{pLQZm}, and σ_{pLQZm2} calculations for platinum ($Z = 78$, $M = 195.09$ amu) and gold ($Z = 79$, $M = 197.00$ amu) at $T_d = 36.0$ eV. For comparison, the data of the numerical σ_{pO} calculations from (Oen, 1973) using exact MDCS, as well as the σ_{pMF} calculations in the McKinley–Feshbach approximation (McKinley and Feshbach, 1948) are also presented. Cross sections are given in barns.

It follows that the expression (20) is not applicable to the ADCS calculations for atoms of heavy elements, except for cases of very high electron energies, where it gives a result close to that obtained by the numerical MDCS integration. Note, however, that at such high energies, the size of the nucleus already plays a role, which is not taken into account in the MDCS calculations. As for the other methods, the results of applying the modified and twice modified methods, as well as the LQZ method itself, are in very good agreement with the results of precise calculations.

To compare the accuracy of these methods, the average relative error was calculated:

$$\delta=\frac{1}{28}\sum_{i=1}^{28}\frac{\left|\sigma_p(E_i)-\sigma_{pO}(E_i)\right|}{\sigma_{pO}(E_i)}.$$

As a result, we got: $\delta_{LQZm} = 0.68$ %, $\delta_{LQZm2} = 0.44$ %, $\delta_{LQZ} = 0.67$ % for platinum and $\delta_{LQZm} = 0.61$%, $\delta_{LQZm2} = 0.45$ %, $\delta_{LQZ} = 0.67$ % for gold.

Thus, we can conclude that all three methods provide an average error of less than 1%. The highest accuracy for the considered elements on average in energies is provided by the twice modified LQZ method.

4. 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 approximate expressions for the normalized Mott cross section: i) the conventional Mott-exact 'phase-shift' formula (point-charge nucleus, no screening) (Mott, 1932), ii) the approximate Lijian–Qing–Zhengming expression (Lijian et al., 1995), iii) the Johnson–Weber–Mullin formula (Johnson et al., 1961), iv) the McKinley–Feshbach expression (McKinley and Feshbach, 1948), and v) the Mott–Born result (Mott, 1932).
- 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°.
  - It is shown that while all the methods 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 method 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 (Lijian et al., 1995), but only over the θ range from 0 to 150° at high energies.
  - 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° 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 $\theta = 180°$).
- Thus, we can conclude that both the rigorous method suggested in this work and the approximate Lijian–Qing–Zhengming method 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 methods is preferred in its application area for relevant calculations of the NMCS.
- Possible applications of the LQZ method for fitting Mott's corrections and the
  atomic displacement cross sections by fast electrons are also considered.
  - The derivation of the analytical expression for the Mott correction in the LQZ technique (ΔL_{MLQZ}) is given.
  - A comparison of ΔL_{MLQZ} with some other representations of Mott's correction is carried out. It is shown that the accuracy of ΔL_{MLQZ} correction substantially exceeds the accuracy of the Mott correction in the Matveev approximation (ΔL_{MMT}) for small and medium-Z values.
  - A modification of the LQZ method (the LQZm method) is also proposed. The relative differences between the Mott correction calculated by the approximate LQZ, LQZm methods and the precise VSTT method are evaluated.
  - A twice modified LQZ method (the LQZm2 method) has also been developed.
  - In addition, analytical expressions for the primary displacement cross sections by fast electrons are obtained on the basis of the modified, twice modified LQZ methods, and the LQZ method itself.
  - It is shown that the results of applying these three methods to the calculations of ADCSs are very well consistent with the results of their precise calculations. In the electron energy range considered for platinum and gold atoms, they provide an average error of less than 1%. The twice modified LQZ method has the highest accuracy.

CRediT authorship contribution statement

P.B. Kats: Conceptualization. **K.V. Halenka:** Investigation, Visualization. **I.D. Halenka:** Investigation, Visualization. **O.O. Voskresenskaya:** Conceptualization, Methodology, Writing – original draft.

Declaration of competing interest

The authors declare that they have no known competing financial interests or personal relationships that could have appeared to influence the work reported in this paper.

Appendix A. Derivation of the formula for the normalized Mott cross section

The derivation of the formula (15) in terms of $F_0(\theta)$ and $F_1(\theta)$ can be represented as follows.

Substituting the expression for G_M from (14) into (9) and taking into account (6), we have

$$R_M(\theta)=\frac{4\sin^2(\theta/2)}{\eta^2}\left[\xi^2\left|F_M\right|^2+\left|F_M{}'\right|^2\right]=\frac{4\sin^2(\theta/2)}{\eta^2}\left[\xi^2\left|F_0+F_1\right|^2+\left|F_0{}'+F_1{}'\right|^2\right]. \tag{A1}$$

After carrying out a number of transformations in (A.1), we can write it as

$$R_M(\theta)=\frac{4\sin^2(\theta/2)}{\eta^2}\left[\xi^2(F_0+F_1)(F_0{}^*+F_1{}^*)+\left(F_0'+F_1\right)(F_0{}'^*+F_1{}'^*)\right]=$$

$$=\frac{4\sin^2(\theta/2)}{\eta^2}\left\{\xi^2\left|F_0\right|^2+\left|F_0{}'\right|^2+\xi^2\left[2\mathrm{Re}\left(F_1F_0^*\right)+|F_1|^2\right]+2\mathrm{Re}\left(F_1{}'F_0^{*'}\right)+|F_1{}'|^2\right\},$$

$$\left|F_0\right|^2=\frac{1}{4},\ \left|F_0{}'\right|^2=\frac{\eta^2}{4\tan^2(\theta/2)}.$$

Thus, we get as a result the following expression for the normalized Mott cross section:

$$R_{KHV}(\theta)=R_B(\theta)+\widetilde{\lambda}(\theta)\sin^2\left(\frac{\theta}{2}\right),$$

$$\widetilde{\lambda}(\theta)=\frac{4}{\eta^2}\left\{\xi^2\left[2\mathrm{Re}\left(F_1F_0^*\right)+|F_1|^2\right]+2\mathrm{Re}\left(F_1{}'F_0^{*'}\right)+|F_1{}'|^2\right\},$$

$$R_Z(\theta)=\frac{4\sin^2(\theta/2)}{\eta^2}\left[\frac{\xi^2}{4}+\frac{\eta^2}{4\tan^2(\theta/2)}\right]=1-\beta^2\sin^2(\theta/2)\equiv R_B(\theta). \tag{A2}$$

This normalized Mott cross section (A.2) can be calculated for instance by the Sherman method (Sherman, 1956).

Appendix B. Twice modified Lijian–Qing–Zhengming method

Section 3.1 shows that the use of the LQZm method reduces the error in calculating the Mott correction in comparison with the LQZ method in some cases. However, when using the LQZm method, only 24 parameters are calculated for each chemical element. As a result, the error in calculating the Mott cross section by this method can be higher than when using the unmodified LQZ method.

Let us consider a method that can be called the twice modified LQZ method (LQZm2 method). In this case, we will use the NMCS fitting formula of the form:

$$R_{LQZm2}\left(\theta,Z,E\right)=1+\sum_{j=1}^{5}a_j(Z,E)(1-\cos\theta)^{j/2},\ a_j\left(Z,E\right)=\sum_{k=1}^{6}d_Z(j,k)(\beta-\overline{\beta}\,)^{k-1},\ \overline{\beta}=0.6682692. \tag{B1}$$

In this way, the correct asymptotics for $\theta\to 0$ is ensured and 30 fitting coefficients $d_z(j,k)$ are used for each element, as in the LQZ method, instead of 24 coefficients.

To test the LQZm2 method, we calculate parameter values for elements with $Z=70$, 81, 83 and 88. As for the LQZm method, we use a value $\overline{\beta}=0.6682692$ that is different from $\overline{\beta}$ value in (13) due to a different partition of the velocity interval for which the approximation is performed. As a result, the following values are obtained for the parameters in the LQZm method (Table B1) and in the LQZm2 method (Table B2).

Table B1
Coefficiens $d_z(j,k)$ for the modified Lijian–Qing–Zhengming fitting formula.

$Z=70$						
j/k	1	2	3	4	5	6
1	−0.117097	1.590253	2.100864	−17.930588	8.231681	81.723154
2	2.115626	1.045715	−10.010708	52.239196	2.973975	−276.776871
3	−1.613745	−2.089075	10.203722	−42.377089	−29.896816	261.057158
4	0.170306	−0.323641	−3.546846	10.193186	16.852913	−73.634195
$Z=81$						
j/k	1	2	3	4	5	6
1	−0.286297	0.202209	6.715470	−4.527384	−26.697815	28.340698
2	2.049489	6.944500	−23.437792	−17.655068	147.514284	−1.297584
3	−0.642491	−6.211913	22.701869	48.086061	−197.176984	−104.539343
4	−0.333937	−0.042929	−7.635192	−23.627474	75.439762	67.117769
$Z=83$						
j/k	1	2	3	4	5	6
1	−0.295129	−0.149815	7.509213	−0.141828	−34.752023	10.832988
2	1.897427	8.122841	−25.252749	−37.360225	178.242481	77.814789
3	−0.285968	−6.776373	24.107223	71.805643	−230.941099	−202.411330
4	−0.486802	−0.145317	−8.081800	−32.109415	86.830333	103.156404

(*continued on next page*)

Table B1 (*continued*)

$Z = 70$						
j/k	1	2	3	4	5	6
$Z = 88$						
j/k	1	2	3	4	5	6
1	−0.266864	−1.086932	9.066972	13.178267	−55.323832	−41.953018
2	1.252624	10.746192	−27.599468	−94.044275	253.003571	305.867615
3	0.919089	−7.291868	25.076862	137.912154	−310.181533	−476.915000
4	−0.970317	−0.859607	−8.376039	−55.244544	112.805746	202.331290

Table B2
Coefficiens $d_z(j,k)$ for the twice modified Lijian−Qing−Zhengming fitting formula.

$Z = 70$						
j/k	1	2	3	4	5	6
1	−0.007282	−0.330475	7.951533	15.554740	−48.045321	−89.362043
2	1.431259	13.015653	−46.471966	−156.440748	353.691213	789.422924
3	−0.237090	−26.167469	83.548176	377.397686	−735.389863	−1883.680712
4	−0.941892	19.129275	−62.801776	−328.942541	586.820219	1659.097930
5	0.3133138	−5.476952	16.683174	95.483370	−160.473800	−487.849225
$Z = 81$						
j/k	1	2	3	4	5	6
1	0.096814	−2.204374	9.981497	44.211996	−78.485094	−216.454163
2	−0.338052	21.942278	−43.791614	−321.397985	470.251653	1524.259479
3	4.160220	−36.381026	63.645050	659.086869	−846.386505	−3173.307523
4	−4.214043	24.330674	−40.713158	−517.254570	599.935650	2546.373292
5	1.092441	−6.862367	9.313073	138.980280	−147.671362	−698.032239
$Z = 83$						
j/k	1	2	3	4	5	6
1	0.149837	−2.488075	9.539049	48.739025	−79.319061	−234.643058
2	−0.875590	22.694832	−37.902647	−341.984796	455.983441	1607.616983
3	5.292156	−36.088986	49.553407	684.579962	−789.637094	−3279.718900
4	−4.993365	23.536321	−28.639753	−527.169330	538.200411	2589.310894
5	1.268819	−6.667544	5.788074	139.383689	−127.082853	−699.974638
$Z = 88$						
j/k	1	2	3	4	5	6
1	0.336236	−2.958256	6.926453	56.793358	−71.294719	−263.026130
2	−2.505887	22.408245	−14.259792	−365.852719	352.533846	1683.591176
3	8.479606	−30.750931	−1.756857	684.674465	−510.393869	−3248.305419
4	−7.078453	18.092953	13.302903	−496.973407	274.557143	2441.335542
5	1.719740	−5.336077	−6.103687	124.368378	−45.540965	−630.389703

To compare the accuracy of the LQZ, LQZm, LQZm2 methods, we recalculated the coefficients $d_z(j,k)$ from (13) for elements with $Z = 70$, 81, 83, and 88, since these coefficients are given in (Lijian et al., 1995) with typos (see, e.g. (Jun et al., 2009)). First, we found five $a_j(Z,\beta)$ coefficients for each value of the relative velocity β from a certain interval using the least squares method. In contrast to (Lijian et al., 1995), we did not consider the energy interval, but the interval of relative velocities, since exactly this value, and not the energy, is included in the formulas for the NMCS. When considering 26 β values of from the range from 0.1 to 0.999, we calculated 26 values of the $a_j(Z,\beta)$ coefficients. Then we found six $d_z(j,k)$ values for each $a_j(Z,\beta)$ using the least squares method. As a result, we obtain 30 $d_z(j,k)$ values for each given Z, as in (Lijian et al., 1995) and (Boschini et al., 2013) These coefficients are presented in Table B3.

Table B3
Coefficiens $d_z(j,k)$ for the Lijian−Qing−Zhengming fitting formula.

$Z = 70$						
j/k	1	2	3	4	5	6
0	1.010882	−0.090371	0.150291	1.527942	−1.938665	−7.280354
1	−0.202571	2.300050	0.920433	−29.931479	23.458506	138.905128
2	2.313632	−0.598580	−7.276158	80.040084	−32.300008	−409.242835
3	−1.789798	−0.627081	7.772348	−67.095730	1.466389	378.836800
4	0.223441	−0.764889	−2.813028	17.653578	7.387109	−109.181549
$Z = 81$						
j/k	1	2	3	4	5	6
0	1.037813	0.003422	−0.370637	0.536148	0.635975	−3.927775
1	−0.583293	0.175331	9.626561	−8.738443	−31.692940	59.190559

(*continued on next page*)

Table B3 (*continued*)

$Z = 70$						
j/k	1	2	3	4	5	6
2	2.737501	7.006764	−30.181535	−7.899862	159.085834	−72.763401
3	−1.254224	−6.267274	28.697942	39.412401	−207.465612	−40.996844
4	−0.149308	−0.026221	−9.444881	−21.009656	78.544998	47.939856
$Z = 83$						
j/k	1	2	3	4	5	6
0	1.029074	−0.046521	−0.246270	1.189134	0.477234	−5.480766
1	−0.523482	0.215570	9.443489	−9.481625	−38.500352	53.880486
2	2.426423	7.276400	−29.733630	−15.723945	186.925741	−21.907692
3	−0.756315	−6.023777	28.091314	52.568149	−238.661658	−113.744945
4	−0.344846	−0.372460	−9.284248	−26.303301	89.160493	76.395792
$Z = 88$						
j/k	1	2	3	4	5	6
0	1.034780	0.004077	−0.465651	0.484244	2.220917	−2.340048
1	−0.540038	−1.118956	12.724330	9.374875	−72.767548	−23.573612
2	1.885451	10.820377	−36.071988	−85.233457	293.413137	263.290462
3	0.356422	−7.357828	32.610046	130.078180	−346.110945	−439.058319
4	−0.800497	−0.839699	−10.649647	−52.880154	123.649688	190.905675

Let us present the arithmetic mean of the relative error for the considered elements using the LQZ, LQZm, and LQZm2 methods (Table B4). For comparison, we also give the *ER* arithmetic mean obtained by the LQZ method using the parameters from (Boschini et al., 2013) ($\langle ER, \% \rangle$).

Table B4
Arithmetic mean of the relative error *ER* for elements with $Z = 70$, 81, 83, and 88.

Z	70	81	83	88
$\langle ER \rangle, \%$	0.55	0.95	1.04	1.26
$\langle ER \rangle_{LQZ}, \%$	0.40	0.78	0.85	1.08
$\langle ER \rangle_{LQZm}, \%$	0.43	0.84	0.93	1.16
$\langle ER \rangle_{LQZm2}, \%$	0.30	0.42	0.44	0.52

Table B4 shows that the modified LQZ method did not lead to an increase in accuracy compared to the conventional LQZ method for the considered elements, although it gave a higher accuracy than the LQZ method with parameters from (Boschini et al., 2013). The twice modified LQZ method provided the highest accuracy in calculating the NMCS.

The relative deviations of the Mott correction calculated using the twice modified LQZ method from ΔL_M correction calculated by summing the series according to (Voskresenskaya et al., 1996) are also less in most cases than when using the LQZ and LQZm methods (Table B5). In this Table, relative deviations exceeding 10 percent are highlighted.

Table B5
Relative deviations of the Mott corrections ΔL_{MLQZ}, ΔL_{MLQZm}, and ΔL_{MLQZm2} from the correction ΔL_{MVSTT}.

β/Z	90	100
0.3	$\boldsymbol{\delta_{LQZ} = 19.8}$ $\delta_{LQZm} = 4.00$ $\delta_{LQZm2} = 1.57$	$\boldsymbol{\delta_{LQZ} = 34.3}$ $\boldsymbol{\delta_{LQZm} = 25.0}$ $\delta_{LQZm2} = 2.72$
0.4	$\delta_{LQZ} = 0.58$ $\delta_{LQZm} = 1.04$ $\delta_{LQZm2} = 7.29$	$\delta_{LQZ} = 3.76$ $\delta_{LQZm} = 4.11$ $\delta_{LQZm2} = 6.71$
0.6	$\boldsymbol{\delta_{LQZ} = 11.8}$ $\delta_{LQZm} = 5.57$ $\delta_{LQZm2} = 2.39$	$\delta_{LQZ} = 2.06$ $\delta_{LQZm} = 0.64$ $\delta_{LQZm2} = 6.34$
0.7	$\boldsymbol{\delta_{LQZ} = 13.2}$ $\delta_{LQZm} = 6.13$ $\delta_{LQZm2} = 0.86$	$\delta_{LQZ} = 6.17$ $\delta_{LQZm} = 3.82$ $\delta_{LQZm2} = 2.91$

References

Abd Ali, S.A.H., Kadhim, R.O., 2020. Calculation of stopping power for protons in biological human parts. Prensa Med. Argent. 106 (6), 245, 1–4.

Ahlen, B.P., 1980. Theoretical and experimental aspects of the energy loss of relativistic heavily ionizing particles. Rev. Mod. Phys. 52 (1), 121–173. https://doi.org/10.1103/RevModPhys.52.121.

Banko, D.N., Kats, P.B., 2019. Methods for calculation of Mott's correction to the Bethe–Bloch formula. In: Kolbas, N.Yu (Ed.), Proc. Repub. Conf. 'Mendeleev Readings 2019'. Brest, BrSU, pp. 8–11.

Bethe, H.A., 1930. Zur Theorie des Durchgangs schneller Korpuskularstrahlen durch Materie. Ann. Phys. 5, 325–400.

Bethe, H., 1932. Bremsformel für Elektronen relativistischer Geschwindigkeit. Z. Physik. 76, 293–299. https://doi.org/10.1007/BF01342532.

Bethe, H.A., Ashkin, J., 1953. In: Segre, E. (Ed.), Experimental Nuclear Physics. Wiley, New York.

Bichsel, H., Groom, D.E., Klein, S.R., 2020. Passage of particles through matter. Ch. 34. In: Zyla, P.A., et al. (Eds.), (PGG), Prog. Theor. Exp. Phys., vols. 1–37, 083C01.

Bloch, F., 1933. Zur Bremsung rasch bewegter Teilchen beim Durchgang durch Materie. Ann. Phys. 16, 285–320. https://doi.org/10.1002/andp.19334080303.

Bohr, N., 1915. On the decrease of velocity of swiftly moving electrified particles in passing through matter. Phil. Mag. 30, 581–612.

Boschini, M.J., Consolandi, C., Gervasi, M., Giani, S., Grandi, D., Ivanchenko, V., Nieminem, P., Pensotti, S., Rancoita, P.G., Tacconi, M., 2013. An expression for the

Mott cross section of electrons and positrons on nuclei with Z up to 118. Radiat. Phys. Chem. 90, 39–66.
Bühring, W., 1965. Computational improvements in phase shift calculations of elastic electron scattering. Z. Physik. 187, 180–196.
Doggett, J.A., Spencer, L.V., 1956. Elastic scattering of electrons and positrons by point nuclei. Phys. Rev. 103, 1597–1601. https://doi.org/10.1103/PhysRev.103.1597.
Eby, P.B., Morgan Jr., S.H., 1972. Charge dependence of ionization energy loss for relativistic heavy nuclei. Phys. Rev. A 6, 2536–2541. https://doi.org/10.1103/PhysRevA.5.2536.
Fermi, E., 1940. The ionization loss of energy in gases and in condensed materials. Phys. Rev. 571, 485–493.
Forcellini, N., Artacho, E., 2019. Floquet Theory for the Electronic Stopping of Projectiles in Solids. arXiv:1908.09783 [cond-mat.Mtrl-Sci], 26 Aug 2019.
Geissel, H., Weick, H., Scheidenberger, C., Bimbot, R., Gardès, D., 2002. Experimental studies of heavy-ion slowing down in matter. GSI Preprint 2002–24, 52.
Gordon, W., 1928. Über den Stoß zweier Punktladungen nach der Wellenmechanik. Z. Physik. 48, 180–191. https://doi.org/10.1007/BF01351302.
Gumus, H., Namdar, T., Bentabet, A., 2018. Positron stopping power in some biological compounds for intermediate energies with generalized oscillator strength model. Int. J. Mol. Biol. 3 (3), 84–92. https://doi.org/10.15406/ijmboa.2018.03.00057.
Idoeta, R., Legarda, F., 1992. Review and calculation of Mott scattering cross section by unscreened point nuclei. Nucl. Instr. Meth. Phys. Res. B 71, 116–125. https://doi.org/10.1016/0168-583X(92)95312-F.
Johnson, W.R., Weber, T.A., Mullin, C.J., 1961. Coulomb scattering of polarized electrons. Phys. Rev. 121, 933–939.
Jun, I., Kim, W., Evans, R., 2009. Electron nonionizing energy loss for device applications. IEEE Trans. Nucl. Sci. 56 (6), 3229–3235. https://doi.org/10.1109/TNS.2009.2033692.
Kadhim, R.O., Hussien, A.H., 2016. Stopping power calculation of protons using Bloch correction and semi empirical relation. Int. J. Sci. Res. 5 (3), 43–48.
Khandelwal, G.S., Merzbacher, M., 1963. Displacement cross sections for fast electrons incident on. Gold Phys. Rev. 130, 1822–1825.
Kats, P.B., Halenka, K.V., Voskresenskaya, O.O., 2021. Comparison of the Lindhard−Sørensen and Mott−Bloch corrections to the Bethe stopping formula at moderately relativistic energies. PEPAN Lett 18 (3), 267–276. https://doi.org/10.1134/S1547477121030079.
Lijian, T., Qing, H., Zhengming, L., 1995. Analytic fitting to the Mott cross section of electrons. Radiat. Phys. Chem. 45, 235–245. https://doi.org/10.1103/PhysRev.74.1759.
Matveev, V.I., 2002. Effective stopping of relativistic composite heavy ions colliding with atoms. Tech. Phys. 47, 523–528. https://doi.org/10.1134/1.1479976.
McKinley, W.A., Feshbach, H., 1948. The Coulomb scattering of relativistic electrons by nuclei. Phys. Rev. 74, 1759–1763. https://doi.org/10.1103/PhysRev.74.1759.
Morgan Jr., S.H., Eby, P.B., 1973. Corrections to the Bethe−Bloch formula for average ionization energy loss of relativistic heavy nucley. Nucl. Instrum. Methods 106, 429–435. https://doi.org/10.1016/0029-554X(73)90303-0.
Mott, N.F., 1928. The solution of the wave equation for the scattering of particles by a coulombian centre of force. Proc. Roy. Soc. A 118, 542–549. https://doi.org/10.1098/rspa.1928.0067.
Mott, N.F., 1929. The scattering of fast electrons by atomic nuclei. Proc. Roy. Soc. A 124, 425–442. https://doi.org/10.1098/rspa.1929.0127.
Mott, N.F., 1932. The polarization of electrons by double scattering. Proc. Roy. Soc. A 135, 429–458. https://doi.org/10.1098/rspa.1932.0044.
Nagase, T., Sanda, T., Nino, A., Quin, W., Yasuda, H., Mori, H., Umakoshi, Y., Szpunar, J. A., 2012. MeV electron irradiation induced crystallization in metallic glasses: atomic structure, crystallization mechanism and stability of an amorphous phase under the irradiation. J. Non-Cryst. Solids 358, 502–518. https://doi.org/10.1016/j.jnoncrysol.2011.11.010. https://www.sciencedirect.com/science/article/pii/S0022309311006843.
Oen, O.S., 1973. Cross Sections for Atomic Displacements in Solids by Fast Electrons. ORNL, p. 4897.
Oen, O.S., 1988. Cross sections for atomic displacements in solids by fast positrons. Nucl. Instrum. Methods B 33, 744–747.
Rutherford, E., 1911. The scattering of α and β particles by matter and the structure of the atom. Phil. Mag. 21, 669–688.
Sherman, N., 1956. Coulomb scattering of relativistic electrons by point nuclei. Phys. Rev. 103, 1601–1607.
Sherman, C.H., Lowe, L.F., Burke, E.A., 1966. Probability of atomic displacement in platinum. Phys. Rev. 145, 568–575.
Sigmund, P., 2006. Particle Penetration and Radiation Effects: General Aspects and Stopping of Swift Point Particles Springer Series in Solid State Sciences, vol. 151. Springer-Verlag, Berlin–Heidelberg.
Sigmund, P., Schinner, A., 2016. Progress in understanding heavy-ion stopping. Nucl. Instrum. Methods B 382, 15–25.
Sigmund, P., Schinner, A., 2020. The Bloch correction, key to heavy-ion stopping. J. Appl. Phys. 128 (1−12), 100903. https://doi.org/10.1016/j.nimb.2015.12.041.
Sunko, V., McGuinness, P., Chang, C.S., Zhakina, E., Khim, S., Dreyer, C., Konczykowski, M., König, M., Muller, D., Mackenzie, A., 2020. Controlled introduction of defects to delafossite metals by electron irradiation. Phys. Rev. X 10 (1–16), 021018. https://doi.org/10.1103/PhysRevX.10.021018.
Überall, P., 1971. Electron Scattering from Complex Nuclei, Part A. Academic Press, New York.
Voskresenskaya, O.O., Sissakyan, A.N., Tarasov, A.V., Torosyan, G.T., 1996. Expression for the Mott corrections to the Bethe−Bloch formula in terms of the Mott partial amplitudes. JETP Lett. (Engl. Transl.) 64, 604–607. https://doi.org/10.1134/1.567276.
Weaver, B.A., Westphal, A.J., 2002. Energy loss of relativistic heavy ions in matter. Nucl. Instrum. Methods B 187, 285–301.
Yennie, D.R., Ravenhall, D.G., Wilson, R.N., 1954. Phase-shift calculation of high-energy electron scattering. Phys. Rev. 95, 500–512.