Corrections to the higher moments of the heavy ion energy-loss distribution beyond the Born approximation: Dependence of Mott's corrections on the heavy ion velocities

Olga Voskresenskaya

Joint Institute for Nuclear Research, Dubna, Moscow region, 141980 Russia

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Introduction

The average energy loss of a relativistic particle per unit path length is described by the relativistic version of the Bethe formula[1]

$$-\frac{d\bar{E}}{dx} = 2\zeta\left[\ln\left(\frac{E_m}{I}\right) - \beta^2\right]$$

with

$$\zeta = K\left(\frac{Z}{\beta}\right)^2\frac{Z'}{A}, \quad K = 2\pi N_A\frac{e^4}{mc^2}, \quad E_m \approx \frac{2mc^2\beta^2}{1-\beta^2}\,. \tag{1}$$

Here, x is the distance traveled by a particle, E_m denotes the maximum transferrable energy to an electron in a collision with the particle of velocity βc, m is the electron mass, Z is the particle charge number, Z' and A are the atomic number and the weight of an absorber, respectively, N_A is the Avogadro number, and I is its mean excitation potential.

[1] H. Bethe. 1930 Ann. Phys. (Leipz.). **5**, 325; 1932 Z. Phys. **76**, 293
H. A. Bethe and J. Ashkin. 1953 *Experimental Nuclear Physics*, ed. E. Segre (Wiley, New York)

The importance of the Mott higher-order-correction term[2] $\Phi_M/2$ to the formula (1),

$$-\frac{d\bar{E}}{dx} = 2\zeta\left[\ln\left(\frac{E_m}{I}\right) - \beta^2 + \frac{\Phi_M}{2}\right],$$

$$\Phi_M = \frac{1}{\zeta}\Delta_M\left(\frac{d\bar{E}}{dx}\right), \quad \Delta_M\left(\frac{d\bar{E}}{dx}\right) = N\int\left(\frac{d\sigma_M}{d\varepsilon} - \frac{d\sigma_B}{d\varepsilon}\right)\varepsilon d\varepsilon, \tag{2}$$

was noted in various works (see, e.q.,[3]). In the above formula Δ_M denotes the Mott correction (MC), σ_M is the Mott exact cross section, $N = N_A Z'/A$ is the number of target electrons per unit volume, and σ_B represents the first-order Born approximation to the σ_M.

The expression for the MCs from (2) is extremely inconvenient for practical application. In this regard, obtaining convenient and accurate representations for the MCs become significant.

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[2] N. F. Mott. 1929 Proc. Roy. Soc. **A 124**, 425; http://rspa.royalsocietypublishing.org/ content/royprsa/124/794/425.full.pdf

[3] C. Scheidenberger, H. Geissel, H. H. Mikkelsen et al. 1994 Phys. Rev. Lett. **73**, No. 1, 51

Evaluation of the Mott exact phase-shift formula

In[4], devoted to analysis of the contribution of close collisions to the average energy loss of relativistic ions in matter, it was shown that the exact MC expression can be represented in the form of a quite rapidly converging series of quantities, which are bilinear in the Mott partial amplitudes. In such a representation, it can be easily calculated. More precisely, the Mott exact phase-shift formula can be represented as:

$$\frac{d\sigma_M}{d\Omega} = \frac{\hbar^2}{4p^2 \sin^2(\vartheta/2)} \left[\xi^2 |F(\vartheta)|^2 + |G(\vartheta)|^2\right],$$

$$F(\vartheta) = \sum_{l=0}^{\infty} F_l P_l(x), \; x = \cos\vartheta, \quad G(\vartheta) = -cos(\vartheta/2) dF(\vartheta)/d\vartheta\,,$$

$$F_l = lC_l - (l+1)C_{l+1}, \quad C_l = \frac{\Gamma(\rho_l - i\nu)}{\Gamma(\rho_l + 1 + i\nu)} e^{i\pi(l-\rho_l)},$$

$$p = mc\frac{\beta}{\sqrt{1-\beta^2}}, \quad \xi = \nu\sqrt{1-\beta^2}, \quad \rho_l = \sqrt{l^2 - (Z\alpha)^2}, \quad \nu = \frac{Z\alpha}{\beta} \qquad (3)$$

with the Legendre polynomial P_l of order l, and the Euler gamma function Γ.

[4] O. Voskresenskaya, A. Sissakyan, A. Tarasov et al. 1996 JETP Lett. **64**(9), 648

Analytical expressions for the higher moments of energy-loss distribution

Below we apply representation (3) for calculation of the relative Mott corrections to the first-order Born central moments and the normalized central moments of the relativistic ion energy-loss distribution.

Let us consider the central moments of the relativistic ion energy-loss distribution in the Mott approximation:

$$\mu_{n,M} = 2\pi N \Delta x \int_0^{\pi} [\Delta\varepsilon(\vartheta)]^n \frac{d\sigma_M}{d\Omega} \sin\vartheta d\vartheta, \quad \Delta\varepsilon(\vartheta) = \frac{2p^2}{m}(1-\cos\vartheta), \qquad (4)$$

where Δx is the thickness of the target material traversed by an ion and $\Delta\varepsilon(\vartheta)$ is the energy transfer to a target electron in a collision leading to a center-of-mass scattering angle ϑ.

With the use of (3), (4), the expression

$$(2l+1)xP_l^m(\cos\vartheta) = (l+1-|m|)P_{l+1}^m(\cos\vartheta) - (l+|m|)P_{l-1}^m(\cos\vartheta) \qquad (5)$$

and the orthogonality relation

$$\int_{-1}^{1} P_{l_1}^m(\cos\vartheta) P_{l_2}^n(\cos\vartheta) \sin\vartheta d\vartheta = \frac{2}{2l_1+1} \frac{(l_1+|m|)!}{(l_1-|m|)!} \delta_{l_1 l_2}, \qquad (6)$$

we obtain the representation for the central moments of the relativistic ion energy-loss distribution $\mu_{n,M}$ $(n = 2, 3, 4)$

$$\mu_{2,M} = a \sum_{l=0}^{\infty} (l+1) \left[\xi^2 \left| \frac{F_l}{2l+1} - \frac{F_{l-1}}{2l+3} \right|^2 + \left| \frac{l F_l}{2l+1} - \frac{(l+2) F_{l+1}}{2l+3} \right|^2 \right], \tag{7}$$

$$\mu_{3,M} = \frac{a p^2}{m} \sum_{l=0}^{\infty} \frac{1}{(2l+1)} \left[\xi^2 \left| \tilde{F}_l \right|^2 + l(l+1) \left| \tilde{G}_l \right|^2 \right], \tag{8}$$

$$\mu_{4,M} = a \left(\frac{p^2}{m_e} \right)^2 \sum_{l=0}^{\infty} (l+1) \left[\xi^2 \left| \frac{\tilde{F}_l}{2l+1} - \frac{\tilde{F}_{l+1}}{2l+3} \right|^2 + \left| \frac{l \tilde{G}_l}{2l+1} - \frac{(l+2) \tilde{G}_{l+1}}{2l+3} \right|^2 \right] \tag{9}$$

with

$$\tilde{F}_l = F_l - \frac{l}{2l-1} F_{l-1} - \frac{l+1}{2l+3} F_{l+1}, \quad \tilde{G}_l = F_l - \frac{l-1}{2l-1} F_{l-1} - \frac{l+2}{2l+3} F_{l+1}, \tag{10}$$

$$a = \frac{2\pi N \Delta x (\hbar c \beta)^2}{1 - \beta^2} \tag{11}$$

in the form of rapidly converging series. The terms of these series decrease as l^{-2n+1} $(n = \overline{2, 4})$ when $l \to \infty$, and that the series converges absolutely.

Numerical results for the MCs to the central moments of the heavy ion energy-loss distribution

The dominant contribution to the higher moments of the particle energy-loss distribution that determine its shape is made by close collisions. Therefore, we can expect significant deviations from the results of the Born approximation in calculations of these quantities.

Let us introduce the quantities that characterize the relative Mott corrections in the computation of the distribution central moments μ_n ($n = \overline{2-4}$):

$$\delta_n \equiv \delta_n(\mu) = \frac{\mu_{n,M} - \mu_{n,B}}{\mu_{n,B}}, \quad n = \overline{2-4}, \tag{12}$$

where $\mu_{n,M}$ values ($n = \overline{2-4}$) are determined by (7)–(11) and $\mu_{n,B}$ ($n = \overline{2-4}$) are given by

$$\mu_{n,B} = \pi N \Delta x \left(\frac{\nu\hbar}{m}\right)^2 \left(\frac{2p^2}{m}\right)^n \left(\frac{1}{n-1} - \frac{\beta^2}{n}\right). \tag{13}$$

The calculation results for the above corrections $\delta_n(Z, \beta)$ are illustrated in Figure 1 and are also given in Table 1; they give the dependence of δ_n on the relative ion velocity $\beta = v/c$.

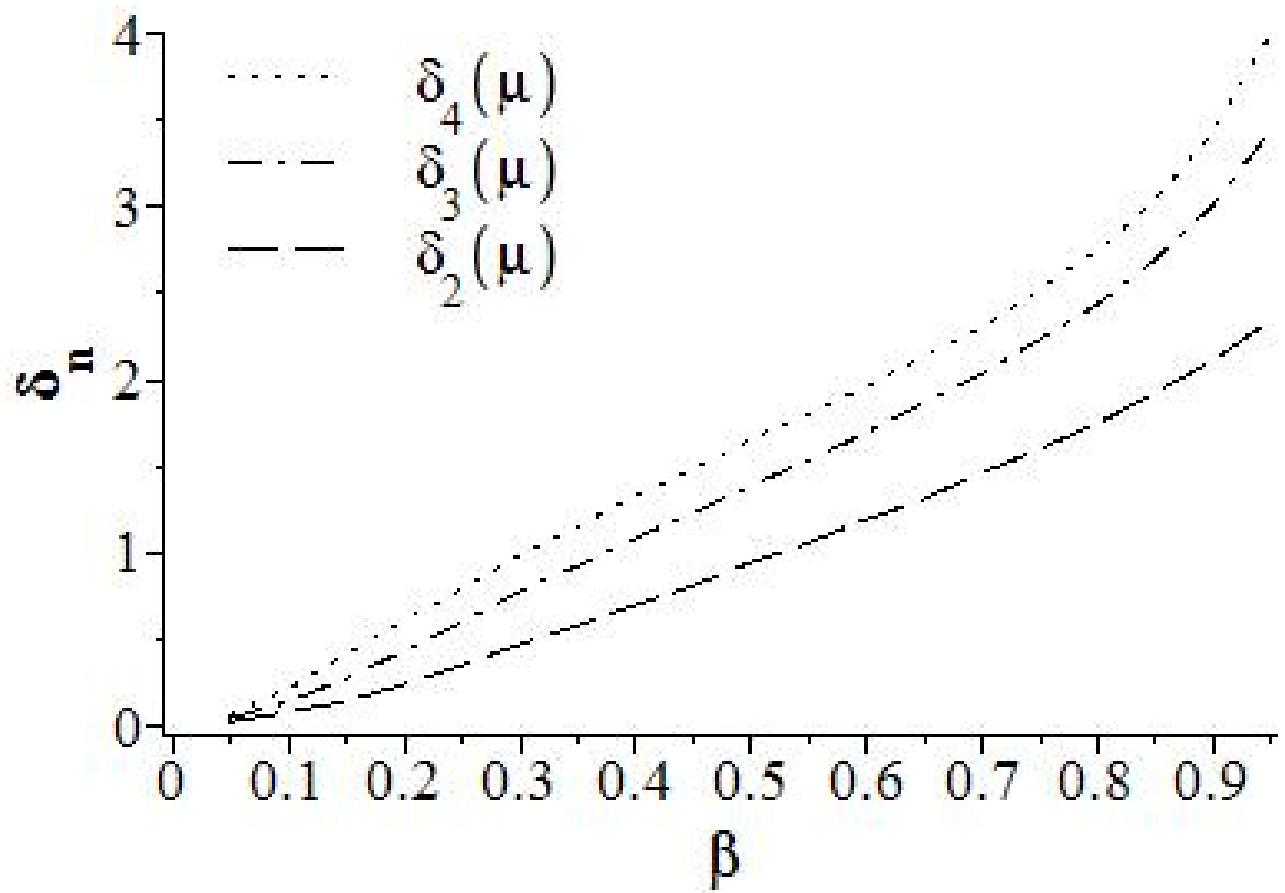


Figure 1: Relative Mott's corrections δ_n to the first-order Born central moments $\mu_{n,B}$ $(n = 2, 3, 4)$ of the heavy ion energy-loss distribution depending on the relative ion velocity β for $Z = 92$.

Table 1. β dependence of the relative corrections $\delta_n(\mu)$ to the first-order Born central moments $\mu_{n,B}$ $(n = \overline{2-4})$ for $Z = 92$.

β	$\delta_2(\mu)$	$\delta_3(\mu)$	$\delta_4(\mu)$
0.0500	0.0155	0.0362	0.0570
0.1500	0.1383	0.2675	0.3879
0.2500	0.3336	0.5877	0.7841
0.3500	0.5617	0.9129	1.1478
0.4500	0.8016	1.2242	1.4766
0.5500	1.0481	1.5290	1.7893
0.6500	1.3055	1.8467	2.1137
0.7500	1.5865	2.2105	2.4950
0.8500	1.9140	2.6838	3.0261
0.9500	2.3303	3.4152	3.9685

It can be seen from Fig. 1 and Table 1 that the relative Mott corrections $\delta_n(\mu)$ can reach a very large value.

Calculation results for the MCs to the central moments

- So the energy-loss straggling (ELS) in the Mott approximation $\mu_{2,M}$ is larger than that in the Born approximation $\mu_{2,B}$ by a factor of 3 for $Z = 92$ ($R = \mu_{2,M}/\mu_{2,B} = \delta_2(\mu) + 1 \sim 3$), which is consistent with the results of the ELS measurements for $Z = 92$[5].
- The magnitudes of $\mu_{n,M}$ ($n = 3, 4$) in the Mott approximation are larger than those in the Born approximation $\mu_{n,B}$ ($n = 3, 4$) by a factors of 4 and 5, correspondingly, for $Z = 92$.

Thus, we can conclude that the Born approximation can not be used to adequate estimation of the higher moments of the heavy ion energy-loss distribution. Their estimation requires going beyond this approximation using, in particular, the Mott corrections.

[5] C. Scheidenberger, H. Geissel, H. H. Mikkelsen et al. 1996 Phys. Rev. Lett. **77**, No. 19, 3987

Mott's corrections to the normalized k-th central moments

The relative Mott corrections to the normalized 3rd and 4th central moments $\rho_{k,B}$ $(k = 3, 4)$ of the relativistic ion energy-loss distribution may be defined as follows:

$$\delta_k \equiv \delta_k(\rho) = \frac{\rho_{k,M} - \rho_{k,B}}{\rho_{k,B}}, \quad k = 3, 4, \tag{14}$$

where

$$\rho_{3,M} = \frac{\mu_{3,M}}{\left(\mu_{2,M}\right)^{3/2}}, \qquad \rho_{4,M} = \frac{\mu_{4,M}}{\left(\mu_{2,M}\right)^{4/2}}. \tag{15}$$

The normalized third central moment is called the "skewness". A distribution that is skewed to the left will have a negative skewness. A distribution that is skewed to the right will have a positive skewness. The normalized fourth central moment characterizes the degree to which the distribution is peaked.
Let us evaluate these corrections for some highly charged particles (e.q., for $_{92}$U ions). Figure 2 demonstrates the numerical results of the $\delta_k(\rho)$ calculations and shows the dependence of these corrections on the relative particle velocity β for $Z = 92$. Table 2 listed their values over the range $0.35 \leq \beta \leq 0.95$.

Numerical results for the MCs to the normalized central moments

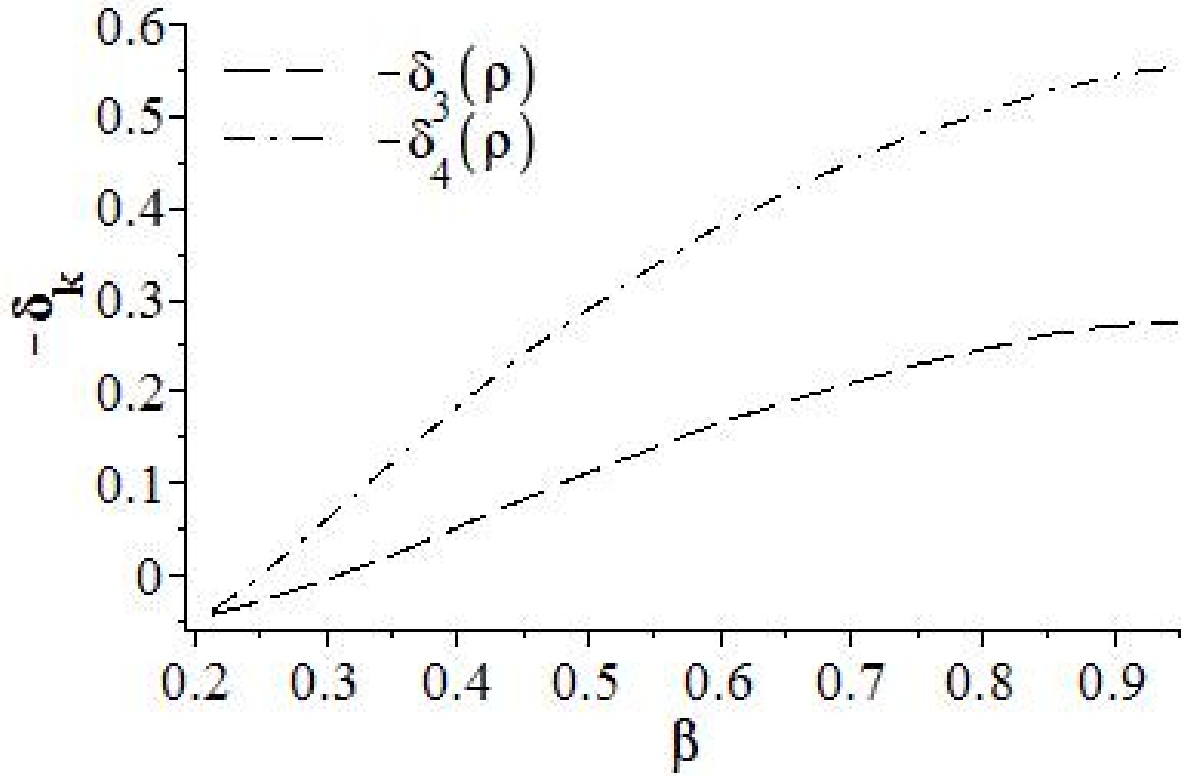


Figure 2: Relative Mott's corrections to the normalized Born central moments $\rho_{k,B}$ $(k = 3, 4)$ of the energy-loss distribution of heavy ions depending on the relative ion velocity β for $Z = 92$.

Table 2. β dependence of the relative corrections $\delta_k(\rho)$ to the normalized first-order Born central moments ρ_k $(k = 3, 4)$ for $Z = 92$.

β	$-\delta_3(\rho)$	$-\delta_4(\rho)$
0.3500	0.0198	0.1193
0.4500	0.0802	0.2370
0.5500	0.1371	0.3350
0.6500	0.1868	0.4142
0.7500	0.2282	0.4776
0.8500	0.2594	0.5259
0.9500	0.2735	0.5520

The modules of obtained relative Mott corrections to the normalized k-th central moments vary between 2–12% percent for $\beta = 0.35$ and 27–55% for $\beta = 0.95$ over the β range considered.

- The obtained results mean that the heavy ion energy-loss distributions, which were computed with the use of Mott's corrections, are less asymmetric and more close to Gaussian that those in the Born approximation.

Summary and outlook

- Based on the representation of the Mott correction Δ_M (2) in the form of rapidly convergent series of quantities bilinear in the Mott partial amplitudes, a method for computing the most important central moments $\mu_{n,M}$ ($n = 2, 3, 4$) of the energy-loss distributions of relativistic charged particles in the Mott approximation is proposed that reduces their calculation to the summation of rapidly convergent (as l^{-2n+1} at $l \to \infty$, $l \in \mathbb{N}_0$) infinite series (7), (8), (9).
- This algorithm is implemented using the numerical summation methods of convergent series for a given level of precision.
- Using the proposed method, the most common characteristics of the energy-loss distributions of highly charged particles were calculated in the Born and Mott approximations over a wide range of relative particle velocity.
- The relative Mott corrections δ_n and δ_k to the Born values of the central moments $\mu_{n,B}$ ($n = \overline{2,4}$) and the normalized central moments $\rho_{k,B}$ ($k = \overline{3,4}$) of the heavy ion energy-loss distribution are obtained in the irradiated material.

- It is shown that whereas the absolute values of the relative corrections $\delta_k(\rho)$ to the normalized first-order Born central moments $\rho_{n,B}$ of the distributions can reach several tens of percent for the heavy relativistic ions over the β range considered, the relative Mott corrections $\delta_n(\mu)$ to the central moments $\mu_{n,B}$ achieve several hundred percent over the range $0.05 \leq \beta \leq 0.95$ under consideration. This made it possible to explain the results of the experiment carried out in the works[6]
- A conclusion is drawn on the applicability of the Born approximation to the consideration of the higher moments of the relativistic heavy ions energy loss distributions (ELD) at best only for the purpose of qualitative evaluations.
- The obtained results mean the dominant contribution of close collisions to the higher moments of ELD.
- They also mean that ELDs which are calculated taking into account MCs are less asymmetric and more close to Gaussian than those in the Born approximation.

[6] C. Scheidenberger, H. Geissel, H. H. Mikkelsen et al. 1994 Phys. Rev. Lett. **73**, No. 1, 51; 1996 Phys. Rev. Lett. **77**, No. 19, 3987

- The choice of an efficient method for numerical calculations of the heavy ion ELDs and their parameters taking into account Mott's corrections within a transport model is planned later.
- It is of interest to find the Coulomb corrections to the higher moments of the ELDs and to estimate the total corrections to these quantities.
- Comparison of the computational results with the available experimental data will be the subject of a further research.

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Thank you for attention