Corrections to the Bethe formula for average ionization energy loss of relativistic charged particles in solids. I. Mott’s corrections

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Abstract

Based on the proposed representation of the Mott corrections $\Delta_M$ to the Bethe stopping formula in the form of rapidly convergent series of quantities bilinear in the Mott partial amplitudes, the numerical calculations were performed for these corrections over the range of nuclear charge number $4 \leq Z \leq 92$ of the incident particles at various values of their relative velocity $\beta$. 
1 Introduction

Stopping power (the average energy loss of a particle per unit path length) is a necessary ingredient for many parts of nuclear and particle physics, as well as for a wide variety of application areas within materials and surface science and engineering, micro and nano science and technology, radiation medicine and biology [1, 2, 3]. Stopping power of a relativistic particle is described by the relativistic version of the Bethe formula [4, 5]

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

with

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

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 \(\beta c\), \(m\) is the electron mass, \(Z'\) 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. F. Bloch showed that the mean excitation potential of the atoms is approximately given by \(I = (10\text{ eV})Z'\) [6]. In this approximation the formula (1) is often called the ‘Bethe–Bloch formula’ [7].

The importance of the Mott higher-order-correction term \(\Phi_{Mott}/2\) [8] to the formula (1)

\[- \frac{d\bar{E}}{dx} = 2\zeta \left[ \ln \left( \frac{E_m}{I} \right) - \beta^2 + \frac{\Phi_{Mott}}{2} \right], \quad \Phi_{Mott} = \frac{1}{\zeta} \Delta_{Mott} \left( \frac{d\bar{E}}{dx} \right), \quad \Delta_{Mott} \left( \frac{d\bar{E}}{dx} \right) = N \int \left( \frac{d\sigma_{Mott}}{d\varepsilon} - \frac{d\sigma_{Born}}{d\varepsilon} \right) \varepsilon d\varepsilon, \tag{2}\]

was noted in various works (see, e.g., [9]). In the above formula \(\Delta_{Mott}\) denotes the Mott correction (MC), \(N = N_A Z'/A\) is the number of target electrons per unit volume, and \(\sigma_{Born}\) represents the first-order Born approximation to the Mott exact cross section \(\sigma_{Mott}\).

The expression for the MCs in (2) is extremely inconvenient for practical application. In this regard, obtaining convenient and accurate representations for the MCs become significant. Ref. [10] gives an exact expression for the Mott correction in the form of
a rather fast converging series of the quantities bilinear in the Mott partial amplitudes, which can be quite simply calculated.

The aim of the presented work is to obtain numerical results for the Mott corrections to the Bethe formula over a wide range of nuclear charge number of the incident particles at various values of their relative velocity $\beta$ based on results of [10] and also to estimate the Bloch and total corrections to (1) over the $Z$ and $\beta$ ranges under consideration. The presented communication is organized as follows. Section 2 considers an analytical result for the $\Delta_{\text{Mott}}$ correction in the form of a quite rapidly converging series. Section 3 gives the numerical results of their computation over the ranges $4 \leq Z \leq 92$ and $0.75 \leq \beta \leq 0.95$. In Section 4 we briefly sum up our results and outline some prospects.

### 2 Analytical result for Mott’s correction to the Bethe stopping formula

Switching in expression for $\Delta_{\text{Mott}}$ (3) from integration over the energy $\varepsilon$ energy transferred to a target electron to integration over the a center-of-mass scattering angle $\vartheta$, we rewrite this expression in the form

$$
\Delta_{\text{Mott}} \left( \frac{dE}{dx} \right) = \frac{N \pi}{m_j \hbar} \int_{\vartheta_0}^{\pi} \left[ \omega_{\text{Mott}}(\vartheta) - \omega_{\text{Born}}(\vartheta) \right] \sin^2(\vartheta/2) \sin \vartheta \, d\vartheta ,
$$

where

$$
\omega_{\text{Mott}}(\vartheta) = \frac{\hbar^2}{4p^2 \sin^2(\vartheta/2)} \left[ \xi^2 |F_{\text{Mott}}(\vartheta)|^2 + |G_{\text{Mott}}(\vartheta)|^2 \right] ,
$$

$$
F_{\text{Mott}}(\vartheta) = \sum_l F_l P_l(x), \quad x = \cos \vartheta, \quad G_{\text{Mott}}(\vartheta) = \sum_l G_l P_l(x),
$$

$$
F_l = lC_l - (l + 1)C_{l+1}, \quad G_l = l^2 C_l + (l + 1)^2 C_{l+1}, \quad C_l = \frac{\Gamma(\rho_l - i\nu)}{\Gamma(\rho_l + 1 + i\nu)} e^{i\pi(l-\rho_l)},
$$

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

$$
\omega_{\text{Born}}(\vartheta) = \frac{\nu^2}{\sin^4(\vartheta/2)} \left[ 1 - \beta^2 \sin^2(\vartheta/2) \right] .
$$
Here, $P_l$ is the Legendre polynomial of order $l$ and $\Gamma(\mu)$ designates the Euler gamma function.

For what follows, instead of the original expression (6) for $G_{Mott}(\vartheta)$, it is convenient to employ a somewhat different expression in terms of $F_{Mott}(\vartheta)$. Writing

$$G_{Mott}(\vartheta) = \sum_l \left[ l^2 C_l + (l + 1)^2 C_{l+1} \right] P_l(x) \equiv \sum_l (l + 1)^2 C_{l+1} \left[ P_l(x) + P_{l+1}(x) \right]$$

(9)

and taking account of the relation \[11\]

$$\Gamma(\rho l - i\nu) \Gamma(\rho l + 1 + i\nu),$$

we obtain by an elementary calculation

$$G_{Mott}(\vartheta) = \cos(\vartheta/2) \sum_l \left[ l C_l - (l + 1)^2 C_{l+1} \right] P_l^{(1)}(x) = -\cos(\vartheta/2) F'(\vartheta),$$

(11)

and, in consequence,

$$\omega_{Mott}(\vartheta) = \frac{\hbar^2}{4p^2 \sin^2(\vartheta/2)} \left[ \xi^2 |F_{Mott}(\vartheta)|^2 + |F'_{Mott}(\vartheta)|^2 \right].$$

(12)

It can now be shown that in terms of the quantities

$$\tilde{C}_l = \frac{\Gamma(\rho l - i\nu)}{\Gamma(\rho l + 1 + i\nu)},$$

(13)

which are obtained from the $C_l$ by the substitution $\rho l \to l$ and correspond the Sommerfeld–Moyer–Furry approximation \[12\] in the theory of $eZ$ scattering, and the corresponding quantities

$$\tilde{F}_l = l \tilde{C}_l - (l + 1) \tilde{C}_{l+1},$$

(14)

as well as using the orthogonality relation for the Legendre function

$$\int_{-1}^1 P_l^{(m)}(\cos \vartheta) P_l^{(m)}(\cos \vartheta) \sin \vartheta d\vartheta = \frac{2}{2l + 1} \frac{(l + |m|)!}{(l - |m|)!} \delta_{ll'},$$

(15)

the Mott correction can be expressed finally as

$$\Delta_{Mott} \left( \frac{d\bar{E}}{dx} \right) = \frac{2\pi Z N A}{mA} \sum_{l=0}^{L} \frac{l(l + 1) + \xi^2}{2l + 1} \left[ |F_l|^2 - |\tilde{F}_l|^2 \right].$$

(16)

It is easy to show that the terms of the series (16) behave asymptotically as as $l^{-2}$ and that the series converges absolutely.
3 Numerical results for Mott’s corrections to the Bethe formula

The obtained result (16) allows us to reduce the calculation of the Mott corrections \( \Delta_{Mott}(dE/dx) \) (3) to the summation of a series consisting of quantities bilinear in the Mott partial amplitudes. The computation results for the corrections \( \Phi_{Mott}/2 \) are given in Table; they give the dependence of the \( \Phi_{Mott}/2 \) corrections on the nuclear charge number of the incident particles and the values of their relative velocity.

**Table 1.** Z and \( \beta \) dependence of the Mott corrections \( \Phi_{Mott}/2 \) corrections to the Eq. (1).

| Particle | Z  | \( \frac{1}{2}\Phi_{Mott}|\beta=0.75 \) | \( \frac{1}{2}\Phi_{Mott}|\beta=0.85 \) | \( \frac{1}{2}\Phi_{Mott}|\beta=0.95 \) |
|----------|----|-------------------------------------|-------------------------------------|-------------------------------------|
| Be       | 04.000 | 00.031                              | 00.035                              | 00.039                              |
| C        | 06.000 | 00.041                              | 00.049                              | 00.075                              |
| Al       | 13.000 | 00.118                              | 00.151                              | 00.160                              |
| Ti       | 22.000 | 00.237                              | 00.248                              | 00.279                              |
| Fe       | 26.000 | 00.283                              | 00.302                              | 00.348                              |
| Ni       | 28.000 | 00.302                              | 00.339                              | 00.384                              |
| Mo       | 42.000 | 00.516                              | 00.552                              | 00.631                              |
| Sn       | 50.000 | 00.560                              | 00.670                              | 00.782                              |
| Ta       | 73.000 | 00.981                              | 01.142                              | 01.302                              |
| W        | 74.000 | 00.998                              | 01.158                              | 01.333                              |
| Pt       | 78.000 | 01.060                              | 01.241                              | 01.431                              |
| Au       | 79.000 | 01.076                              | 01.267                              | 01.450                              |
| Pb       | 82.000 | 01.118                              | 01.335                              | 01.499                              |
| U        | 92.000 | 01.251                              | 01.502                              | 01.759                              |

It can be seen from Table that the Mott corrections \( \delta_{n}(\mu) \) are becoming increasingly important with the growth of \( Z \) and \( \beta \), and they are significant for nuclei of high \( Z \).
4 Summary and outlook

- Based on the representation (16) of the Mott corrections $\Delta_{\text{Mott}}(d\bar{E}/dx)$ to the Bethe formula (1) in the form of quite rapidly converging series whose terms are bilinear in the Mott partial amplitudes, an algorithm is proposed to compute the $\Phi_{\text{Mott}/2}$ values in the wide ranges of $Z$ and $\beta$.

- This algorithm reduces the $\Phi_{\text{Mott}/2}$ computation to a summing the fast converging series (16) and can be simply implemented using the numerical summation methods of converging series for a given level of precision.

- Using the latter result, the $\Phi_{\text{Mott}/2}$ corrections to the Bethe stopping formula were calculated for charged particles over the ranges $4 \leq Z \leq 92$ and $0.75 \leq \beta \leq 0.95$.

- It is shown that these corrections are significant for nuclei of high $Z$.

- It is of interest to find the Coulomb and total corrections to the Bethe-Bloch stopping formula.

- Comparison of the computational results with the available experimental data will be the subject of a further research.

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