Методы и алгоритмы для расчета ионизационных потерь энергии релятивистскими тяжелыми ионами, моделирования электромагнитных каскадных ливней экстремально высоких энергий и некоторых сложных физико-химических систем

О.О. Воскресенская
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I. Ионизационные потери энергии релятивистскими тяжелыми ионами при их прохождении через вещество

1. **Corrections to the higher moments of the heavy ion energy-loss distribution beyond the Born approximation: β-dependence of the Mott corrections.**
   Olga Voskresenskaya. **Journal of Astrophysics & Aerospace Technology, 6, 65, 2018, DOI:10.4172/2329-6542-C6-033; arXiv:1810.00542 [hep-ph].**
2. **Corrections to the Bethe formula for average ionization energy loss of relativistic charged particles in solids: Mott's corrections**
   O. Voskresenskaya, **arXiv:1912.10547 v1 [nucl-th] 22 Dec 2019**
3. **Comparison of the Lindhard–Sorensen and Mott–Bloch Corrections to the Bethe Stopping Formula at Moderately Relativistic Energies.**
   P.B. Kats, K.V. Halenka, O.O. Voskresenskaya, **Particles and Nuclei, Letters, JINR, Dubna, 18, 3, 267-276, 2021**
4. **Normalized Mott Cross Section in Different Approaches**
   P. B. Kats, K.V. Halenka, O.O. Voskresenskaya, **Particles and Nuclei, Letters, JINR, Dubna, 18, 3, 277-283, 2021**
5. **Аналитические выражения для поправки Мотта, полученные на основе метода Лиджиана-Кинга-Чжэнминга,**
   О.О. Воскресенская, П.Б. Кац, Е.В. Голенко. **Менделеевские чтения 2021, БрГУ, Брест, Беларусь : сборник материалов республиканской научно-практич. конференции, Брест, 26 февраля 2021 г. / Брест. гос. ун-т им. А.С. Пушкина; редколлегия: Э.А. Тур, Н.Ю. Колбас, Н.С. Ступень; под общ. ред. Н.Ю. Колбас. Брест : БрГУ, 2021, 2021 С. 26-29**

6. **Сравнение различных методов расчета нормированного моттовского сечения рассеяния**
***О.О. Воскресенская, П.Б. Кац, Е.В. Голенко*. Менделеевские чтения 2021, БрГУ, Брест, Беларусь : сборник материалов республиканской научно-практической конференции, Брест, 26 февраля 2021 г. / Брест. гос. ун-т им. А.С. Пушкина; редколлегия: Э.А. Тур, Н.Ю. Колбас, Н.С. Ступень; под общ. редакцией Н.Ю. Колбас. – Брест: БрГУ, 2021. С. 21-25**
7. **Some Approaches to the Calculation of the Normalized Mott Cross Section, Displacement Cross Section, and the Mott Correction to the Bethe formula**
***P.B. Kats, K.V. Halenka, I.D. Halenka, O.O. Voskresenskaya.* Radiation Physics and Chemistry (Q2), ISSN:0969-806X, eISSN:1879-0895, Изд:Elsevier Science Limited, 192, 3, 109919(1-13), 2022**
8. **Comparative Study of the Energy-Loss Straggling Calculation Methods**
***P.B. Kats, A.V. Kudravets, A.S. Rymasheuskaya, O.O. Voskresenskaya.* Radiation Physics and Chemistry (Q2), 193, submitted, 2023**
9. **Some Approaches to the Energy-Loss Straggling Calculation**
***P.B. Kats, A.V. Kudravets, A.S. Rymasheuskaya, O.O. Voskresenskaya.* https: // doi.org/10.48550/arXiv.2309.12558, 2023**

От ЛИТ: Воскресенская О. Сотрудничество: доц. П.Б. Кац и др. (Каф. общей и теоретической физики Брестского государственного университета им. А.С. Пушкина, Беларусь).

II. Развитие теоретической и математической базы для исследования электромагнитных каскадных ливней экстремально высоких энергий (ЛПМ-ливней)

1. **Coulomb correction to the spectral bremsstrahlung rate in the quantum Migdal theory of the Landau-Pomeranchuk effect**
   ***O. Voskresenskaya*, hep-preprint, 2018, arXiv:1809.10760 [hep-ph]**

2. **978-5-7904-2288-126h Extended European Cosmic Ray Symposium and 35th Russian Cosmic Ray Conference, Altai State University (Barnaul), Max Planck Institute for Physics (Munich), Skobeltsyn Institute of Nuclear Physics (Moscow), Novosibirsk State University, Barnaul, Russia. Application of a Revised Moliere Theory to the Description of the Landau-Pomeranchuk-Migdal Effect**
   ***Olga Voskresenskaya and Hrach Torosyan*, 209-210, Publishing house of Altai State University, BOOK OF ABSTRACTS, 978-5-7904-2288-1, 2018**

3. **Application of an Improved Moliere Theory to the Description of the Landau-Pomeranchuk-Migdal Effect**
   ***O.O. Voskresenskaya and H.T. Torosyan*, Journal of Physics: Conference Series, IOPSCIENCE, 1181, 012087(1-6), 2019**

4. **Essential Characteristics of Electromagnetic Cascades in PeV Neutrino Energy Region**
   K. Kato (Kyowa. Ltd), T. Tanemori (Saitama University), A. Misaki (Saitama University), N. Takahashi (Hirosaki University), Y. Mizumoto (Tokyo Astronomical Observatory), O.O. Voskresenskaya (LIT JINR), H.T. Torosyan (DLNP JINR),
   work in progress

5. Systematic Studies on Energy Estimation of Partially Contained Events in High Energy Neutrino Astrophysics. Part I: Detailed Examination of the Inevitable Uncertainties Due to Purely Stochastic Processes Amoung Partially Contained Events

N. Tkahashi [a], Y. Okumura[a] , M. Tamada[b], M. Kato[c], Misaki[d], T. Tanemori[d], K. Mitsui[e], Y. Mizumoto[f], T. Ohyama[g], Kudoh[h], O. Voskresenskaya[i], H. Torosyan[i], V. Galkin[j]

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Revised on 14th, March 2023. Work in progress

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III. Математическая и вычислительная поддержка проекта DIRAC

Dimesoatom Breakup in the Coulomb Field
***L.G. Afanasyev, S.R. Gevorkyan, O.O. Voskresenskaya,* The European Physical Journal A (Q2), ISSN:1434-6001, eISSN:1434-601X, Изд:Springer Berlin Heidelberg, 56, 10(1-8), 2020**

От ЛИТ: Воскресенская О.О. Сотрудничество: Афанасьев Л.Г. (ЛЯП ОИЯИ, DIRAC Collaboration), Геворкян С.Р. (ЛФВЭ ОИЯИ)

IV. Моделирование некоторых сложных физико-химических процессов, “неравновесная термодинамика” и корреляционный анализ

1. **ISBN 978-963-454-694-82nd Intarnational Conference on Reaction Kinetics, Mechanism and Catalysis, Akademiai Kiado, Budapest, Budapest, Hungary Kinetic and mechanistic investigation for the ceric sulfate–oxalic acid redox reaction as an integral part of the cerium-catalyzed BZ reaction, *Olga Voskresenskaya*, 122-123, Akademiai Kiado, Budapest, Book of Abstracts 2nd Intarnational Conference on Reaction Kinetics, Mechanism and Catalysis, 20-22 May 2021, Budapest, Hungary, 978-963-454-694-8, 2021**
2. **6th Edition of International Conference and Exhibition on Organic Chemistry, EuroSciCon, Dublin, Ireland. Characteristics of Intermediate Complexes in the Oxidation Reactions of Some Dicarboxylic Acids by Cerium(IV),**
   ***O. Voskresenskaya*, 6th Edition of International Conference and Exhibition on Organic Chemistry, Dublin, 16 - 17 August, 2018, Book of Abstracts, Ireland, Dublin, 2018**
3. **Pure and Applied Chemistry 18th International Conference, IPAC, Toronto, Canada. Thermodynamic and Kinetic Parameters of Cerium(IV) Complexes with Some Dicarboxylic Acids. doi:10.4172/2161-0444-C2-043, *O. Voskreesnskaya*, P. 48, OMICIES, Med. Chem. (Los Angeles) ISSN:2161-0444, 8, 3, 2161-0444, 2018**

4. **Thermodynamic and Kinetic Parameters of Cerium(IV) Complexes with Some Dicarboxylic Acids**
   ***O.O. Voskresenskaya, N.A. Skorik, and Yu.V. Yuzhakova*, Russ. J. General Chem., ISSN:1070-3632, eISSN:1608-3350, Pleiades Publishing, Springer, 88, 4, 640-649, 2018**
5. **Stability constants of cerium(IV) complexes with 8-hydroxyquinoline and 8-hydroxy-7-iodoquinoline-5-sulfonic acid**
   ***Olga O. Voskresenskaya and Nina A. Skorik*, J. Analyt. Pharm. Research, eISSN:eISSN:2473-0831, MedCrave Publishing Group, 7, 5, 517-520, 2018**
6. **Kinetic and Thermodynamic Stability of Intermediate Complexes in the Reactions of Oxidation of Some Heterocyclic Compounds with Cerium(IV).**
   ***O.O. Voskresenskaya, N.A. Skorik, and E.N. Naprienko*, Russ. J. Inorg. Chem., ISSN:0036-0236, eISSN:1531-8613, Pleiades Publishing, Ltd., 64, 4, 511-519, 2019**

7. **Relative Kinetic Stability of Cerium(IV) Complexes with Some Organic Compounds of the Aliphatic Series**
   ***O.O. Voskresenskaya, N.A. Skorik*, Russ. J. General Chem., ISSN:1070-3632, eISSN:1608-3350, Pleiades Publishing, Springer, 90, 3, 434–443, 2020**
8. **Relative kinetic stability towards redox decomposition of cerium(IV) complexes with some organic compounds**
   ***Olga O. Voskresenskaya, Nina A. Skorik*, Monatshefte für Chemie – Chemical Monthly, ISSN:0026-9247, eISSN:1434-4475, Springer Nature, 151, 4, 533-542, 2020**
9. **Stability Constants and Rate Constants of Intramolecular Redox Decomposition of Cerium(IV) Complexes with Certain Hydroxycarboxylic Acids in Nitrate Medium**
   ***O.O. Voskresenskaya, N.A. Skorik, N.I. Sokovikova*, Russ. J. Inorg. Chem., ISSN:0036-0236, eISSN:1531-8613, Pleiades Publishing, Ltd., 64, 10, 1288-1296, 2019.**
10. **Hydrolysis and Complexation of Cerium(IV) with 2,3-Dihydroxysuccinic Acid in Sulfate Media**
    ***O.O. Voskresenskaya,* Russ. J. Inorg. Chem., ISSN:0036-0236, eISSN:1531-8613, Pleiades Publishing, Ltd., 67, 7, 1069-1079, 2022**

11. Thermodynamics of the Formation of Intermediate Complexes in the Oxidation of Citric Acid by Cerium(IV) and Kinetics of Their Intramolecular Redox Decomposition
***Voskresenskaya O.O.*, *Skorik N.A.*, Russ. J. of Physical Chem., ISSN:0036-0244, Pleiades Publishing Ltd., 97, 4, 663-671, 2023**

12. Kinetics, Mechanism, and Reactivity of Intermediates of the Cerium(IV)-Oxalate Reaction in a Sulfate Medium
***O.O. Voskresenskayaa*, *N.A. Skorik*, Kinetics and Catalysis, Pleiades Publishing, 64, 6, accepted, 2023**

От ЛИТ: Воскресенская О.О. Сотрудничество: проф. Скорик Н.А. и др. (Национальный исследовательский Томский государственный университет)

I-1 Numerical and analytical calculations of the normalized Mott cross section in different approaches

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Particles and Nuclei, Letters, JINR, Dubna, 18, 3, 277-283, 2021; arXiv:2007.03622[nucl-th];
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Scattering cross section of relativistic electrons through the Coulomb potential MDCS

,

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

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

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

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

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

,

$$\boxed{F_M(\theta) = F_0(\theta) + F_1(\theta)}$$

$$\boxed{G_M(\theta) = G_0(\theta) + G_1(\theta)}$$

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

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

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

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

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

$$F_0(\theta) = \frac{i}{2}\frac{\Gamma(1-i\eta)}{\Gamma(1+i\eta)}\sin^{2i\eta}\left(\frac{\theta}{2}\right)$$

$$G_0(\theta) = -i\eta\frac{F_0(\theta)}{\tan^2(\theta/2)}$$

normalized Mott cross section (NMCS)

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

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

$$G_M(\theta) = -\frac{1}{\tan^2(\theta/2)}\frac{dF_M}{d\theta} \equiv -\frac{1}{\tan^2(\theta/2)}F_M{}'$$

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

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

$$\omega_Z(\theta) = \left[\xi^2 + \eta^2\cos^2\left(\frac{\theta}{2}\right)\right]/\sin^2\left(\frac{\theta}{2}\right) \equiv \omega_B(\theta)$$

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. 64, 604−607.

- Разработан новый эффективный алгоритм расчета нормализованного мотовского дифференциального сечения (НМДС) рассеяния релятивистских электронов кулоновским потенциалом на основе предложенного авторами точного представления данного сечения в терминах моттовских парциальных амплитуд (см. следующий слайд; результаты расчета представлены таблицами 1, 2).

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

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

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

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

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

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

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

Table 1: Comparison of the *R*(*θ*) values obtained by different methods for the scattering of electrons on nuclei of charge number Z=80 (R_M: summation up to N=200; R_{KHV}: summation up to N=80; $R_M^{(2)}$: summation up to N=150 of the series «reduced» with m=2 by Sherman's method*)

θ/β	0.2	0.4	0.5	0.6	0.7	0.8	0.9
30°	R_M=1.02 R_{KHV} =1.01 $R_M^{(2)}$=1.01	R_M=0.991 R_{KHV} =1.00 $R_M^{(2)}$=1.00	R_M=1.04 R_{KHV} =1.03 $R_M^{(2)}$=1.03	R_M=1.09 R_{KHV} =1.08 $R_M^{(2)}$=1.08	R_M=1.14 R_{KHV} =1.15 $R_M^{(2)}$=1.15	**R_M=1.19** R_{KHV} =1.22 $R_M^{(2)}$=1.22	**R_M=1.26** R_{KHV} =1.29 $R_M^{(2)}$=1.29
60°	**R_M=0.986** R_{KHV} =0.979 $R_M^{(2)}$=0.979	R_M=1.12 R_{KHV} =1.12 $R_M^{(2)}$=1.12	R_M=1.28 R_{KHV} =1.27 $R_M^{(2)}$=1.27	**R_M=1.39** R_{KHV} =1.42 $R_M^{(2)}$=1.41	**R_M=1.52** R_{KHV} =1.55 $R_M^{(2)}$=1.55	R_M=1.68 R_{KHV} =1.67 $R_M^{(2)}$=1.67	**R_M=1.82** R_{KHV} =1.78 $R_M^{(2)}$=1.78
90°	**R_M=0.956** R_{KHV} =0.963 $R_M^{(2)}$=0.963	**R_M=1.38** R_{KHV} =1.41 $R_M^{(2)}$=1.41	**R_M=1.62** R_{KHV} =1.58 $R_M^{(2)}$=1.58	**R_M=1.69** R_{KHV} =1.71 $R_M^{(2)}$=1.71	**R_M=1.74** R_{KHV} =1.80 $R_M^{(2)}$=1.80	**R_M=1.83** R_{KHV} =1.86 $R_M^{(2)}$=1.86	**R_M=1.93** R_{KHV} =1.89 $R_M^{(2)}$=1.89
120°	**R_M=1.35** R_{KHV} =1.33 $R_M^{(2)}$=1.33	**R_M=1.79** R_{KHV} =1.75 $R_M^{(2)}$=1.75	**R_M=1.75** R_{KHV} =1.81 $R_M^{(2)}$=1.80	R_M=1.79 R_{KHV} =1.79 $R_M^{(2)}$=1.79	**R_M=1.82** R_{KHV} =1.72 $R_M^{(2)}$=1.72	**R_M=1.67** R_{KHV} =1.60 $R_M^{(2)}$=1.60	**R_M=1.42** R_{KHV} =1.44 $R_M^{(2)}$=1.44
150°	**R_M=1.95** R_{KHV} = 1.92 $R_M^{(2)}$=1.93	**R_M=2.13** R_{KHV} = 2.06 $R_M^{(2)}$=2.06	**R_M=1.89** R_{KHV} =1.95 $R_M^{(2)}$=1.95	R_M=1.75 R_{KHV} =1.76 $R_M^{(2)}$=1.76	**R_M=1.66** R_{KHV} =1.50 $R_M^{(2)}$=1.50	**R_M=1.33** R_{KHV} =1.18 $R_M^{(2)}$=1.18	**R_M=0.817** R_{KHV} =0.810 $R_M^{(2)}$=0.810

*Sherman, N., 1956. Coulomb Scattering of Relativistic Electrons by Point Nuclei. Phys. Rev. 103, 1601–1607.

Wolfram Mathematica

Table 2: Comparison of the $R(\theta)$ values obtained by different methods for the scattering of electrons with an energy of 10 MeV on nuclei of charge number Z=47

R	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
R_{LQZ}	1.118	1.214	1.255	1.225	1.123	0.959	0.753	0.532	0.323	0.153	0.043	0.0041
R_{JWM}	1.143	1.228	1.240	1.171	1.042	0.867	0.667	0.463	0.278	0.131	0.036	0.0032
R_{MF}	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_{FB}	0.983	0.933	0.854	0.751	0.630	0.501	0.372	0.252	0.149	0.069	0.019	0.0026

- The results obtained are compared with the results of the calculations by other exact and approximate methods in wide ranges of the ion nucleus charge number Z, electron energies, and their scattering angle (Figure 1).

Проведено сопоставление результатов расчетов указанного сечения точными и приближенными методами в широких диапазонах значений зарядового числа ядра иона *Z*, энергий электронов и угла их рассеяния (Рисунок 1).

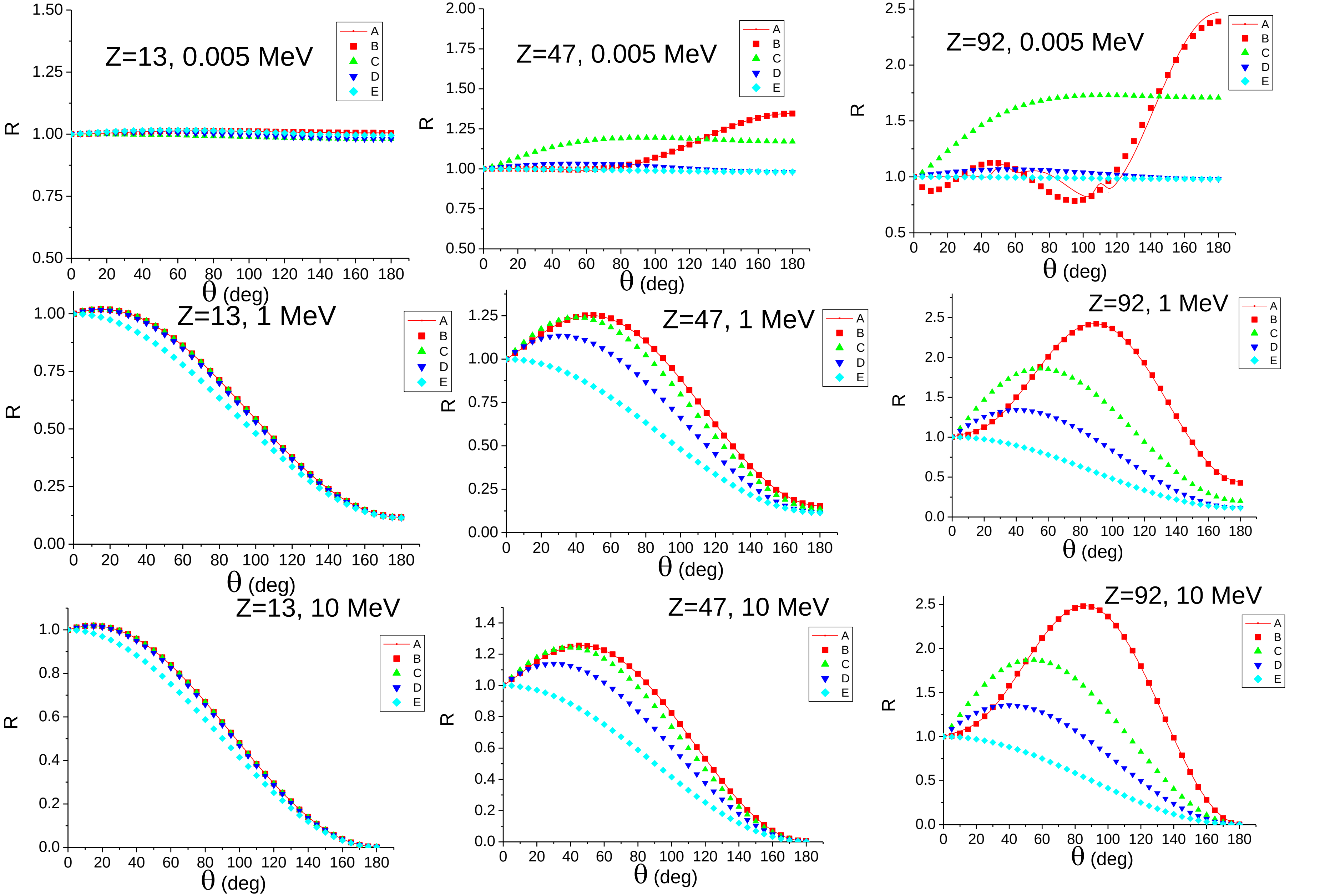

Figure 1: NMDS computation by approximate (blue-green lines) and exact methods (red discrete line) as a function of the scattering angle of electrons with energies of 0.005 MeV, 1 MeV and 10 MeV on nuclei with the charge numbers Z 13, 47, and 90.

- Показано, что тогда как для легких элементов все методы дают удовлетворительное согласие (левый столбец рисунков), а для тяжелых элементов приближенные методы неприменимы (правый столбец), расчеты, полученные на основе нового точного представления, а также представления Мотта, крайне неудобного в вычислительном отношении (верхняя красная дискретная линия), дают прекрасное согласие во всей рассматриваемой зарядовой и энергетической области.
- It is shown It is shown that while all approximations give fairly accurate results for light elements (left column) and the approximate methods are not applicable for heavy elements (right column), the computations based on the new exact representation and also Mott representations, which is extremely computationally inconvenient (upper red discrete line) give excellent agreement in the entire charge and energy region considered.

Conclusions

- A 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), ii) the approximate Lijian−Qing−Zhengming expression, iii) the Johnson−Weber−Mullin formula , iv) the McKinley−Feshbach expression , and v) the Mott−Born result.
- 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 degrees.
- 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 results of the rigorous methods considered are remarkably consistent. Thus, we can conclude that the both methods, 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 $R(\theta)$.

I-2 Computation of the Mott, Mott–Bloch, and Lindhard–Sørensen corrections to the Bethe stopping formula at moderately relativistic energies

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Particles and Nuclei, Letters, JINR, Dubna, 18, 3, 267-276, 2021; arXiv:2008.04819 [nucl-th]

- **New efficient algorithms are developed to compute the exact Mott and total Mott and Bloch corrections to the Bethe formula for average ionization energy losses by heavy relativistic ions in solids based on previously obtained analytical results**

Expression for the Mott corrections to the Bethe−Bloch formula in terms of the Mott partial amplitudes*

$$\Delta L_{MVSTT} = \frac{mc^2\beta^2}{4\pi(Ze^2)^2} \lim_{\varepsilon\to 0} \int_{\varepsilon}^{E_m} E\left[\left(\frac{d\sigma}{dE}\right)_M - \left(\frac{d\sigma}{dE}\right)_{FB}\right] dE,$$

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

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

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

***Voskresenskaya O.O., Sissakyan, A.N., Tarasov, A.V., Torosyan, G.T. JETP Lett. 1996, 64, 604−607.**

Bloch's correction as a series

$$\Delta L_B = \sum_{k=0}^{\infty} \left(\frac{k+1}{(k+1)^2 + \eta^2} - \frac{1}{k+1} \right)$$

Total Mott-Bloch's correction as a series

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

- **It is shown (i) great computational advantages of the developed method over the standard method for computing the exact Mott corrections, (ii) an excellent agreement of the obtained values of total Mott−Bloch's and Lindhard−Sørensen's corrections over the Z and β ranges $6 \leq Z \leq 114$ and $0.85 \leq \beta \leq 0.99$ (Tables 3.1 and 3.2), as well as (iii) an excellent agreement of the obtained Mott corrections with the corrections computed by an alternative Lindhard− Sørensen method in the entire range $1 \lesssim \gamma \lesssim 15$ of the gamma factor considered (Figs. 1A, 1B), and (iv) a sharp contrast of the exact results with the results of known approximate methods (Figs. 2C, 2D, 2E) having very limited range of applicability for medium-*Z* (Fig. 2, left) and high-*Z* (Fig. 2, right) ions (see below).**

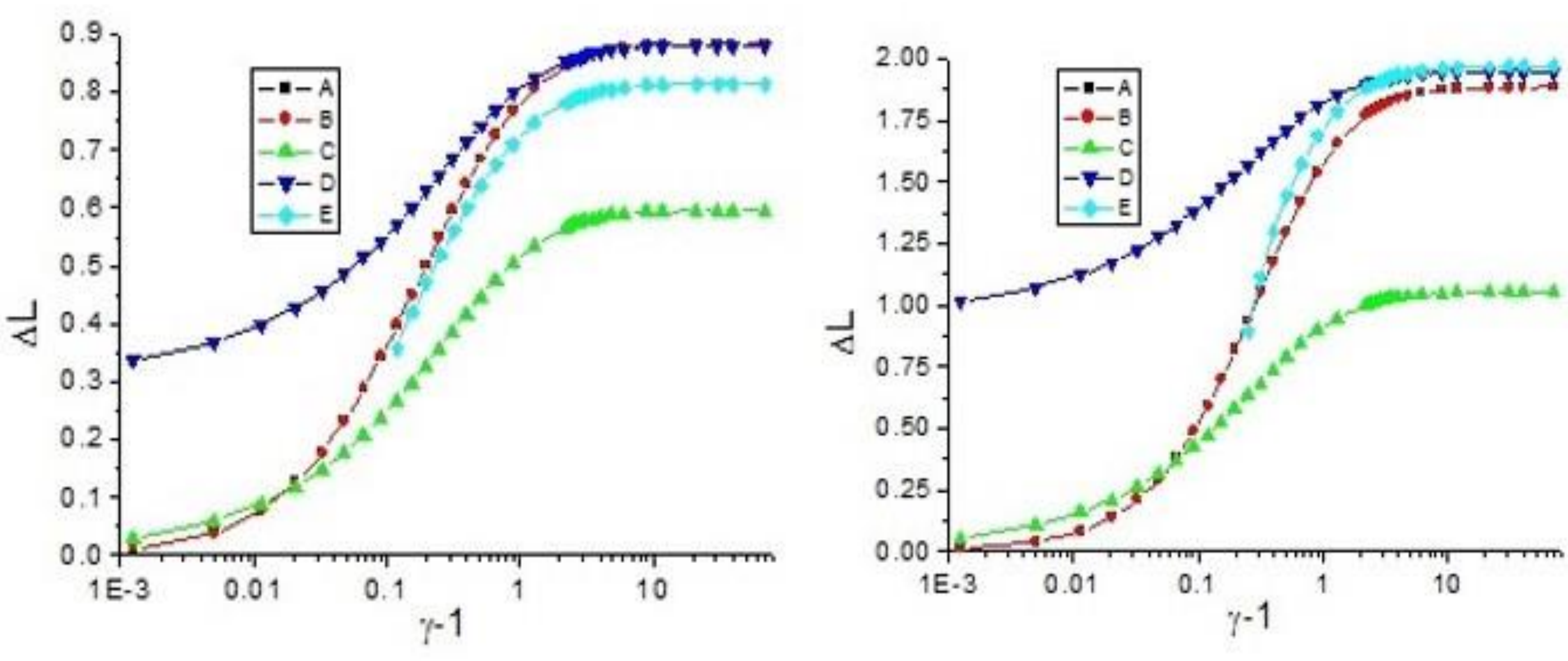

Figure 2: Mott's corrections obtained by the rigorous Lindhard–Sørensen (A) and the proposed (B) methods, as well as the approximate methods of Jackson and McCarthy (C), Morgan and Eby (D), and Ahlen (E) over the range $0.0500 \le \beta \le 0.9999$ for Z = 52 (left) and 92 (right).

Table 3.1: Lindhard-Sørensen's correction in the point nucleus approximation and the Mott-Bloch correction obtained by the VSTT, MT, and ME methods over the Z and β ranges $6 \leq Z \leq 114$ and $0.85 \leq \beta \leq 0.99$.

β/Z	6	12	26	36	52
0.85	ΔL_{LS} =0.059 ΔL_{MBVSTT} =0.059 ΔL_{MBMT} =0.061 ΔL_{MBME} =0.065	ΔL_{LS} =0.120 ΔL_{MBVSTT} =0.120 ΔL_{MBMT} =0.110 ΔL_{MBME} =0.125	ΔL_{LS} =0.267 ΔL_{MBVSTT} =0.267 ΔL_{MBMT} =0.258 ΔL_{MBME} =0.269	ΔL_{LS} =0.377 ΔL_{MBVSTT} =0.377 ΔL_{MBMT} =0.380 ΔL_{MBME} =0.379	ΔL_{LS} =0.562 ΔL_{MBVSTT} =0.562 ΔL_{MBMT} =0.583 ΔL_{MBME} =0.564
0.90	ΔL_{LS} =0.063 ΔL_{MBVSTT} =0.063 ΔL_{MBMT} =0.065 ΔL_{MBME} =0.069	ΔL_{LS} =0.128 ΔL_{MBVSTT} =0.128 ΔL_{MBMT} =0.111 ΔL_{MBME} =0.125	ΔL_{LS} =0.288 ΔL_{MBVSTT} =0.288 ΔL_{MBMT} =0.273 ΔL_{MBME} =0.293	ΔL_{LS} =0.411 ΔL_{MBVSTT} =0.411 ΔL_{MBMT} =0.409 ΔL_{MBME} =0.413	ΔL_{LS} =0.621 ΔL_{MBVSTT} =0.621 ΔL_{MBMT} =0.644 ΔL_{MBME} =0.622
0.95	ΔL_{LS} =0.067 ΔL_{MBVSTT} =0.067 ΔL_{MBMT} =0.067 ΔL_{MBME} =0.073	ΔL_{LS} =0.136 ΔL_{MBVSTT} =0.136 ΔL_{MBMT} =0.118 ΔL_{MBME} =0.143	ΔL_{LS} =0.309 ΔL_{MBVSTT} =0.309 ΔL_{MBMT} =0.284 ΔL_{MBME} =0.313	ΔL_{LS} =0.443 ΔL_{MBVSTT} =0.443 ΔL_{MBMT} =0.434 ΔL_{MBME} =0.443	ΔL_{LS} =0.676 ΔL_{MBVSTT} =0.676 ΔL_{MBMT} =0.701 ΔL_{MBME} =0.675
0.97	ΔL_{LS} =0.068 ΔL_{MBVSTT} =0.068 ΔL_{MBMT} =0.068 ΔL_{MBME} =0.076	ΔL_{LS} =0.139 ΔL_{MBVSTT} =0.139 ΔL_{MBMT} =0.119 ΔL_{MBME} =0.146	ΔL_{LS} =0.317 ΔL_{MBVSTT} =0.317 ΔL_{MBMT} =0.288 ΔL_{MBME} =0.321	ΔL_{LS} =0.455 ΔL_{MBVSTT} =0.455 ΔL_{MBMT} =0.443 ΔL_{MBME} =0.457	ΔL_{LS} =0.698 ΔL_{MBVSTT} =0.698 ΔL_{MBMT} =0.723 ΔL_{MBME} =0.705
0.99	ΔL_{LS} =0.070 ΔL_{MBVSTT} =0.070 ΔL_{MBMT} =0.069 ΔL_{MBME} =0.112	ΔL_{LS} =0.142 ΔL_{MBVSTT} =0.142 ΔL_{MBMT} =0.120 ΔL_{MBME} =0.185	ΔL_{LS} =0.325 ΔL_{MBVSTT} =0.325 ΔL_{MBMT} =0.291 ΔL_{MBME} =0.367	ΔL_{LS} =0.467 ΔL_{MBVSTT} =0.467 ΔL_{MBMT} =0.451 ΔL_{MBME} =0.502	ΔL_{LS} =0.718 ΔL_{MBVSTT} =0.718 ΔL_{MBMT} =0.744 ΔL_{MBME} =0.752

Table 3.2: Lindhard-Sørensen's correction in the point nucleus approximation and the Mott-Bloch correction obtained by the VSTT, MT, and ME methods over the Z and β ranges $6 \leq Z \leq 114$ and $0.85 \leq \beta \leq 0.99$.

β/Z	60	80	92	104	114
0.85	ΔL_{LS} =0.659 ΔL_{MBVSTT} =0.659 ΔL_{MBMT} =0.681 ΔL_{MBME} =0.662	ΔL_{LS} =0.903 ΔL_{MBVSTT} =0.903 ΔL_{MBMT} =0.912 ΔL_{MBME} =0.914	ΔL_{LS} =1.040 ΔL_{MBVSTT} =1.040 ΔL_{MBMT} =1.039 ΔL_{MBME} =1.051	ΔL_{LS} =1.145 ΔL_{MBVSTT} =1.145 ΔL_{MBMT} =1.157 ΔL_{MBME} =1.150	ΔL_{LS} =1.170 ΔL_{MBVSTT} =1.170 ΔL_{MBMT} =1.251 ΔL_{MBME} =1.17
0.90	ΔL_{LS} =0.733 ΔL_{MBVSTT} =0.733 ΔL_{MBMT} =0.762 ΔL_{MBME} =0.736	ΔL_{LS} =1.024 ΔL_{MBVSTT} =1.024 ΔL_{MBMT} =1.042 ΔL_{MBME} =1.033	ΔL_{LS} =1.196 ΔL_{MBVSTT} =1.196 ΔL_{MBMT} =1.199 ΔL_{MBME} =1.202	ΔL_{LS} =1.338 ΔL_{MBVSTT} =1.338 ΔL_{MBMT} =1.346 ΔL_{MBME} =1.343	ΔL_{LS} =1.392 ΔL_{MBVSTT} =1.392 ΔL_{MBMT} =1.462 ΔL_{MBME} =1.392
0.95	ΔL_{LS} =0.802 ΔL_{MBVSTT} =0.802 ΔL_{MBMT} =0.838 ΔL_{MBME} =0.804	ΔL_{LS} =1.140 ΔL_{MBVSTT} =1.140 ΔL_{MBMT} =1.169 ΔL_{MBME} =1.148	ΔL_{LS} =1.345 ΔL_{MBVSTT} =1.345 ΔL_{MBMT} =1.354 ΔL_{MBME} =1.354	ΔL_{LS} =1.527 ΔL_{MBVSTT} =1.527 ΔL_{MBMT} =1.529 ΔL_{MBME} =1.534	ΔL_{LS} =1.614 ΔL_{MBVSTT} =1.614 ΔL_{MBMT} =1.667 ΔL_{MBME} =1.613
0.97	ΔL_{LS} =0.829 ΔL_{MBVSTT} =0.829 ΔL_{MBMT} =0.867 ΔL_{MBME} =0.831	ΔL_{LS} =1.184 ΔL_{MBVSTT} =1.184 ΔL_{MBMT} =1.218 ΔL_{MBME} =1.196	ΔL_{LS} =1.404 ΔL_{MBVSTT} =1.404 ΔL_{MBMT} =1.415 ΔL_{MBME} =1.419	ΔL_{LS} =1.601 ΔL_{MBVSTT} =1.601 ΔL_{MBMT} =1.600 ΔL_{MBME} =1.723	ΔL_{LS} =1.702 ΔL_{MBVSTT} =1.702 ΔL_{MBMT} =1.746 ΔL_{MBME} =1.723
0.99	ΔL_{LS} =0.855 ΔL_{MBVSTT} =0.855 ΔL_{MBMT} =0.896 ΔL_{MBME} =0.889	ΔL_{LS} =1.228 ΔL_{MBVSTT} =1.228 ΔL_{MBMT} =1.266 ΔL_{MBME} =1.262	ΔL_{LS} =1.461 ΔL_{MBVSTT} =1.461 ΔL_{MBMT} =1.474 ΔL_{MBME} =1.506	ΔL_{LS} =1.675 ΔL_{MBVSTT} =1.675 ΔL_{MBMT} =1.671 ΔL_{MBME} =1.719	ΔL_{LS} =1.789 ΔL_{MBVSTT} =1.789 ΔL_{MBMT} =1.825 ΔL_{MBME} =1.825

- **The developed algorithms provide simple and efficient computation of the specified corrections to the ionization energy losses by relativistic heavy ions passing through matter, which is relevant in many areas of nuclear physics, astrophysics, and physics of elementary particles.**

Bethe's stopping power formula

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

$$-\frac{d\bar{E}}{dx} = \zeta L$$

in the first Born approximation $Z\alpha / \beta << 1$

$$L = L_0 = \ln\left(\frac{E_m}{I}\right) - \beta^2 - \frac{\delta}{2}$$

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

$$-\frac{d\bar{E}}{\rho dx} = \tilde{\zeta} L, \qquad \tilde{\zeta} = 4\pi r^2 mc^2 \cdot \tilde{N}_e \cdot \left(\frac{Z}{\beta}\right)^2 = 0.307075 \frac{Z'}{A}\left(\frac{Z}{\beta}\right)^2 \text{ MeV g}^{-1}\text{cm}^2$$

Fermi, E. 1940. The Ionization Loss of Energy in Gases and in Condensed Materials. Phys. Rev. 571, 485–493.

Bloch correction

Bloch, F., 1933. Zur Bremsung rasch bewegter Teilchen beim Durchgang durch Materie. Ann. Physik. 16, 285–320

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

Mott correction

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

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

Eby, P. B., Morgan, S. H., Jr., 1972. Charge Dependence of Ionization Energy Loss for Relativistic Heavy Nuclei. Phys. Rev. A 6, 2536 –2541.
Morgan, S. H., Jr., Eby, P. B., 1973. Corrections to the Bethe−Bloch Formula for Average Ionization Energy Loss of Relativistic Heavy Nucley. Nucl. Instr. Meth. 106, 429 –435.

$$\Delta L_{MJM} = \frac{\tilde{N}_e}{\tilde{\zeta}} \int_{\varepsilon}^{E_m} E \left[\left(\frac{d\sigma}{dE} \right)_{MMF} - \left(\frac{d\sigma}{dE} \right)_{B} \right] dE = \frac{1}{2} \pi \alpha \beta Z$$

Jackson, J. D., McCarthy, R.L., 1972. z^3 Corrections to Energy Loss and Range. Phys. Rev. B 6, 4131–4141.

$$\Delta L_{MME3} = \frac{\tilde{N}_e}{\tilde{\zeta}} \int_{\varepsilon}^{E_m} E \left[\left(\frac{d\sigma}{dE} \right)_{MJWM} - \left(\frac{d\sigma}{dE} \right)_{FB} \right] dE =$$

$$= \frac{1}{2} \left\{ \pi \alpha \beta Z + \left(\alpha Z \right)^2 \left[\pi^2 / 3 + 1 + \beta^2 \left(3/4 - \ln 2 \right) + 0.5 \left(\zeta(3) - 3 \right) \right] \right\}$$

Morgan, S. H., Jr., Eby, P. B., 1973. Corrections to the Bethe−Bloch Formula for Average Ionization Energy Loss of Relativistic Heavy Nucley. Nucl. Instr. Meth.106, 429–435.

$$\Delta L_{MA} = \frac{1}{2}\eta\beta^2 \left\{[1.725 + 0.52\pi\cos\chi] + \eta[3.246 - 0.451\beta^2] + \right.$$
$$+\eta^2[0.987 + 1.552\beta^2] + \eta^3[-2.696 + \beta^2(4.569 - 0.494\beta^2)] +$$
$$\left. +\eta^4[-1.170 + \beta^2(0.222 + 1.254\beta^2)]\right\}$$

$$\cos\chi = \mathrm{Re}\frac{\Gamma(1/2 - i\eta)\Gamma(1 + i\eta)}{\Gamma(1/2 + i\eta)\Gamma(1 - i\eta)}$$

Ahlen, S.P., 1978. Z_1^7 stopping-power formula for fast heavy ions. Phys. Rev. A 17, 1236–1239.

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

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

Matveev, V.I., 2002. Effective stopping of relativistic composite heavy ions colliding with atoms. Tech. Phys. 47, 523–528.

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. 64, 604−607

$$\Delta L_{MVSTT} = \frac{mc^2\beta^2}{4\pi(Ze^2)^2}\lim_{\varepsilon\to 0}\int_{\varepsilon}^{E_m} E\left[\left(\frac{d\sigma}{dE}\right)_M - \left(\frac{d\sigma}{dE}\right)_{FB}\right]dE$$

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

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

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

The Lindhard-Sørensen correction for pointlike nuclei

$$\Delta L_{LS} = \frac{\beta^2}{2} + \frac{1}{\eta^2}\sum_{k=1}^{\infty} k\left[\frac{k-1}{2k-1}\sin^2(\delta_k - \delta_{k-1}) + \frac{k+1}{2k+1}\sin^2(\delta_{-k} - \delta_{-k-1}) + \frac{\eta^2}{(4k^2-1)(\gamma^2 k^2 + \eta^2)} - \frac{\eta^2}{k^2}\right]$$

$$\delta_k = \varphi_k - \arg\Gamma(\rho_k + 1 + i\eta) + \frac{\pi}{2}(l - \rho_k), \quad e^{2i\varphi_k} = \frac{k - i\xi}{\rho_k - i\eta}, \quad l = \begin{cases} k, & k > 0, \\ -k-1, & k < 0. \end{cases}$$

Lindhard, J., Sørensen, A.H. 1996. Relativistic theory of stopping for heavy ions. Phys. Rev. A 53, 2443–2456.

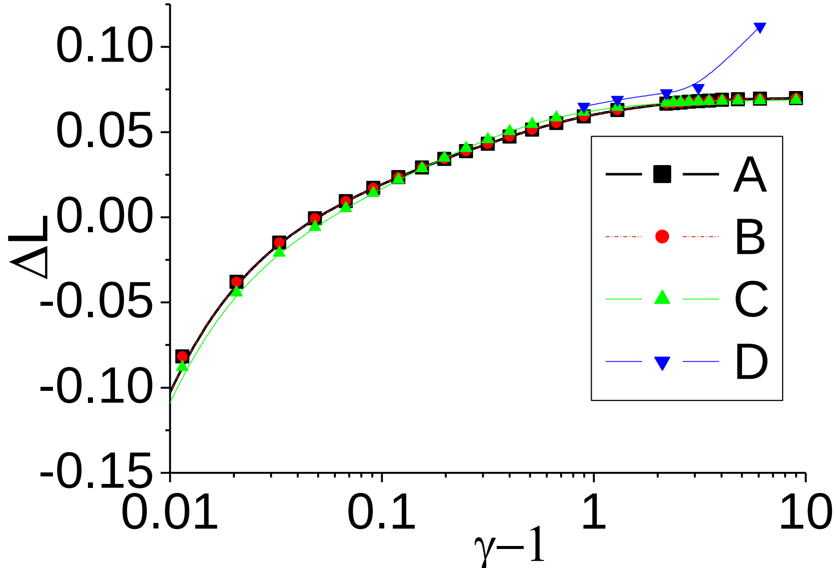

Figure 3.1: Z = 6. A: ΔL_{LS}; B: $\Delta L_{\mathrm{MBVSTT}}$; C: ΔL_{MBMT}; D: ΔL_{MBME}.

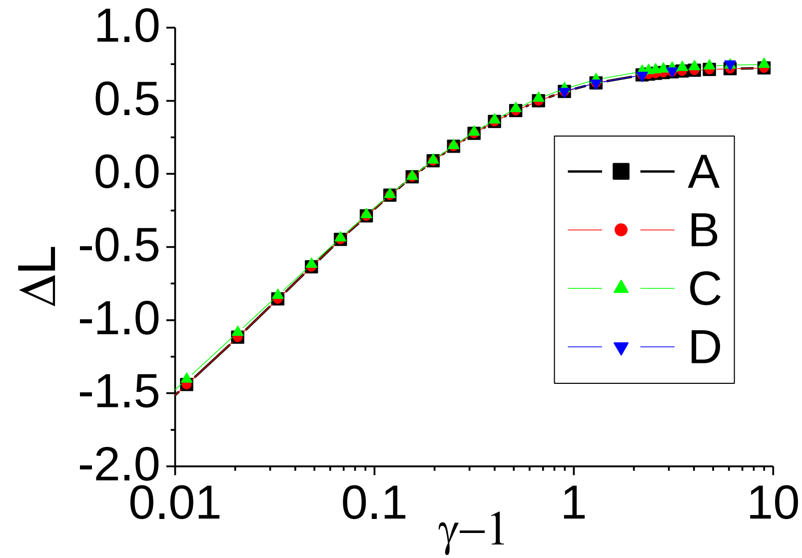

Figure 3.2: Z = 52. A: ΔL_{LS}; B: $\Delta L_{\mathrm{MBVSTT}}$; C: ΔL_{MBMT}; D: ΔL_{MBME}

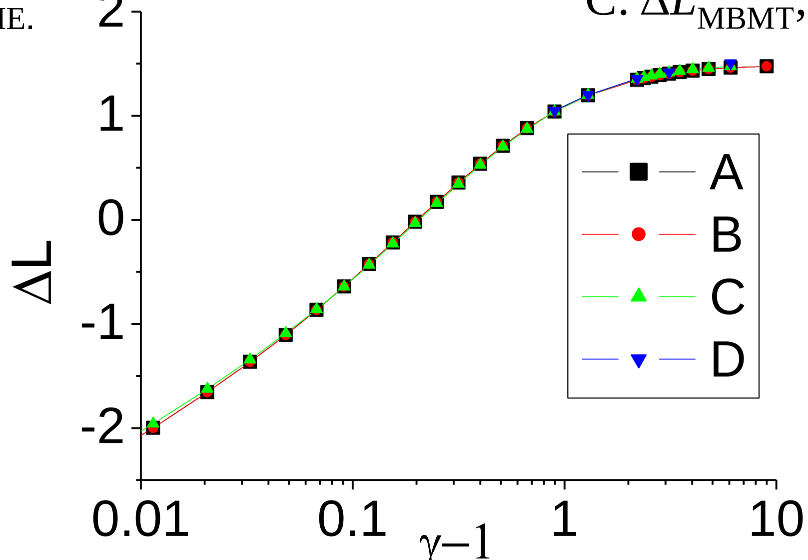

Figure 3.3: Z = 92. A: ΔL_{LS}; B: $\Delta L_{\mathrm{MBVSTT}}$; C: ΔL_{MBMT}; D: ΔL_{MBME}.

Figure 3: Lindhard−Sørensen's correction (A) in the point nucleus approximation and the Mott− Bloch correction obtained by the VSTT (B) MT (C), and ME (D) methods over the range $0.15 \leq \beta \leq 0.995$ for $Z = 6$ (3.1), 52 (3.2), and 92 (3.3).

Relative difference between the Lindhard−Sørensen and Mott−Bloch corrections

$$\delta\Delta L = \frac{\Delta L_{MBVSTT} - \Delta L_{LS}}{\Delta L_{LS}} 100\%$$

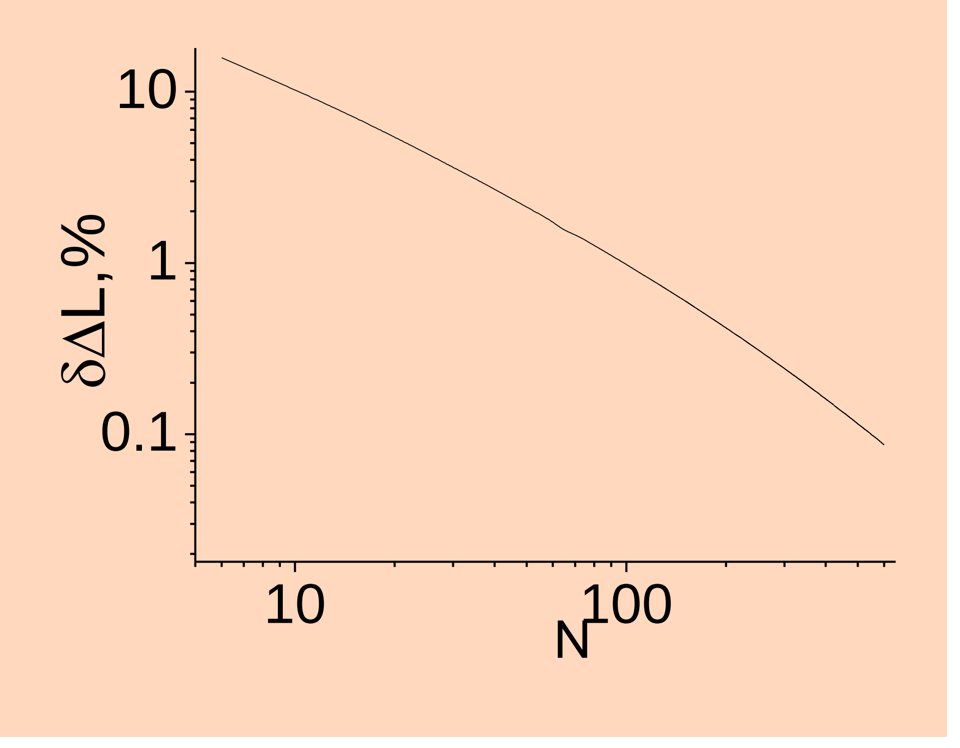

Figure 4: Dependence of the relative difference between the Lindhard−Sørensen and Mott−Bloch corrections on the upper summation limit N (for $Z = 118$, $\beta = 0.6$).

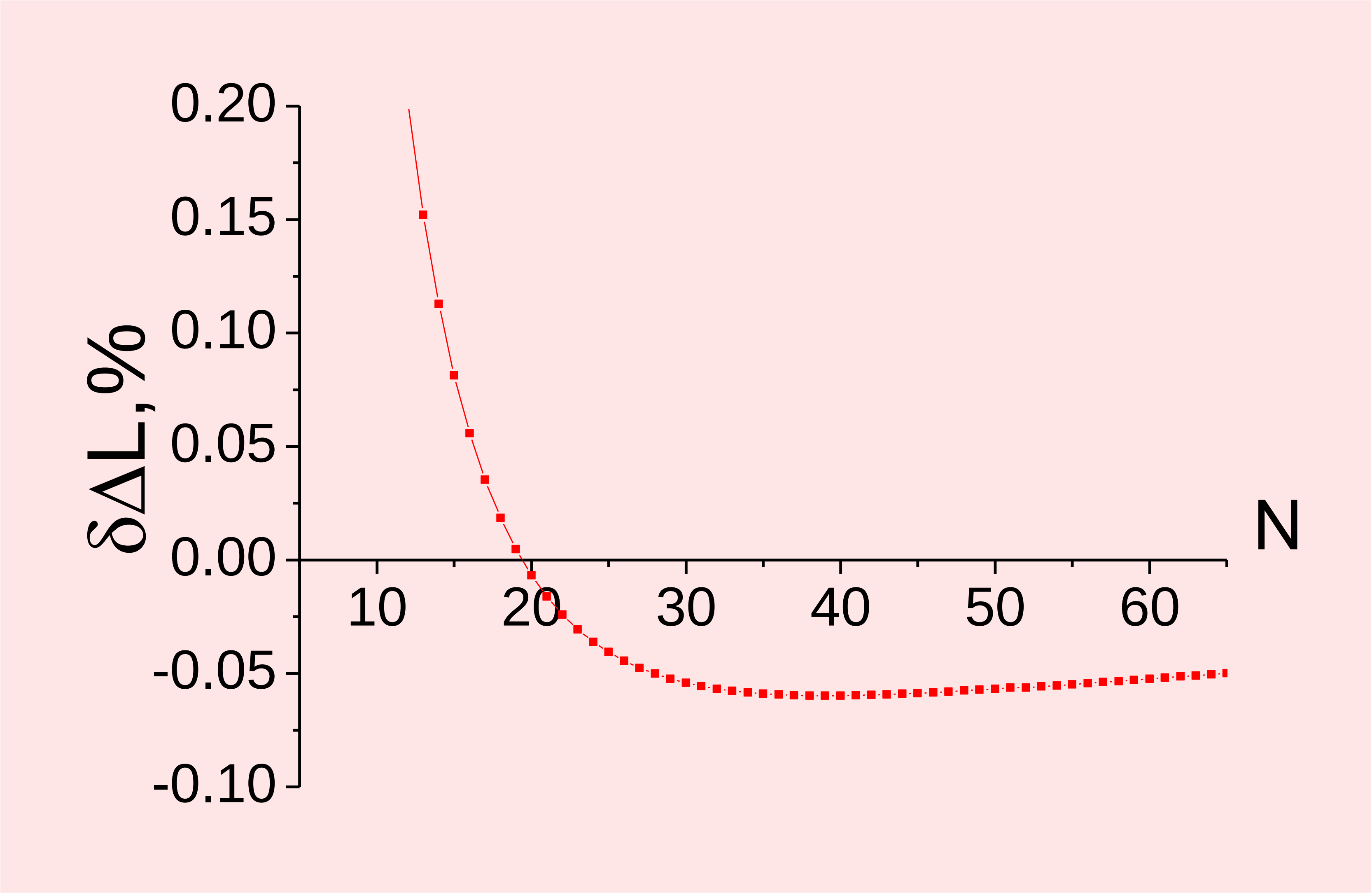

Figure 4.1: Dependence of the relative difference between the Lindhard−Sørensen and Mott−Bloch corrections on the upper summation limit N (for Z = 118, β = 0.6).

Difference between the Lindhard–Sørensen and Bloch corrections

Bloch correction as a series

$$\Delta L_B = \sum_{k=1}^{\infty}\left(\frac{k}{k^2+\eta^2}-\frac{1}{k}\right)$$

$$\Delta L_{LS-B} = \frac{\beta^2}{2} + \frac{1}{\eta^2}\sum_{k=1}^{\infty} k\left[\frac{k-1}{2k-1}\sin^2(\delta_k - \delta_{k-1}) + \frac{k+1}{2k+1}\sin^2(\delta_{-k} - \delta_{-k-1}) + \frac{\eta^2}{(4k^2-1)(\gamma^2 k^2+\eta^2)} - \frac{\eta^2}{k^2+\eta^2}\right]$$

Table 4: Difference between the Lindhard–Sørensen correction in the point nucleus approximation and the Bloch correction, as well as the Mott correction (10) obtained by the VSTT method for $Z = 92$ over the β range $0.1 \le \beta \le 0.9$.

β	0.1	0.2	0.3	0.4	0.5	0.6	0.7	0.8	0.9
$\Delta L_{LS\text{-}B}$	0.0372735	0.139856	0.293763	0.485402	0.703029	0.936563	0.177409	1.418710	1.655487
ΔL_{MVSTT}	0.0372735	0.139856	0.293763	0.485402	0.703029	0.936563	0.177409	1.418710	1.655487

Numerical results for stopping power

$$S_E \equiv -dE/(\rho dx)$$

Table 5 : Electronic stopping power $S(E)$ in MeVcm^{2}g^{-1}, calculated without ΔL, with the total Mott−Bloch corrections ΔL_{MBJM} , ΔL_{MBA}, ΔL_{MBMT}, and ΔL_{MBVSTT}, as well as with the Lindhard− Sørensen correction ΔL_{LS} In comparison with experimental data from [8].

Low-Z particles.

Projectile	Target	S_0	S_{MBJM}	S_{MBA}	S_{MBMT}	S_{MBVSST}	S_{LS}	Experiment
$^{18}_{8}O$ 690 MeV/u (β=0.819)	Be	0.125035	0.125933	0.126061	0.126004	0.126022	0.126022	0.125±0.002
	C	0.137066	0.138077	0.138220	0.138156	0.138178	0.138178	0.138±0.004
	Al	0.122963	0.123937	0.124076	0.124014	0.124035	0.124035	0.123±0.004
	Pb	0.082791	0.083591	0.083705	0.083655	0.083671	0.083671	0.084±0.002
$^{40}_{18}Ar$ 985 MeV/u (β=0.874)	Be	0.573850	0.582735	0.585039	0.583828	0.584732	0.584732	0.578±0.016
	C	0.628435 (0.629)	0.638435	0.641029	0.639665	0.640683	0.640683	0.640±0.019
	Al	0.568963	0.578608	0.581110	0.579794	0.580776	0.580776	0.584±0.019
	Cu	0.494021	0.503157	0.505526	0.504280	0.505210	0.505210	0.494±0.016
	Pb	0.386315	0.394237	0.396292	0.395211	0.396018	0.396018	0.389±0.012

Table 6 : Electronic stopping power $S(E)$ in MeVcm^{2}g^{-1}, calculated without ΔL, with the total Mott−Bloch corrections ΔL_{MBJM} , ΔL_{MBA}, ΔL_{MBMT}, and ΔL_{MBVSTT}, as well as with the Lindhard− Sørensen correction ΔL_{LS} In comparison with experimental data from [8].

Medium-Z particles.

Projectile	Target	S_0	S_{MBJM}	S_{MBA}	S_{MBMT}	S_{MBVSST}	S_{LS}	Experiment
$^{86}_{36}Kr$ 900 MeV/u (β=0.861)	Be	2.34572	2.40567	2.43801	2.43794	2.43738 (2.438)	2.43738	2.432±0.037
$^{136}_{54}Xe$ 780 MeV/u (β=0.839)	Be	5.48721 (5.488)	5.65418	5.70788	5.82166	5.81012 (5.812)	5.81012	5.861±0.076
	C	6.01291 (6.014)	6.20084	6.26128	6.38934	6.37635 (6.378)	6.37635	6.524±0.084
	Al	5.40984 (5.404)	5.59110	5.64940	5.77291	5.76038 (5.755)	5.76038	5.806±0.121
	Cu	4.70236 (4.703)	4.87404	4.92926	5.04624	5.03438 (5.036)	5.03438	5.077±0.066

Scheidenberger, C. et al ., 1994. Direct Observation of Systematic Deviations from the Bethe Stopping Theory for Relativistic Heavy Ions. Phys. Rev. Lett. 73, 50–53.

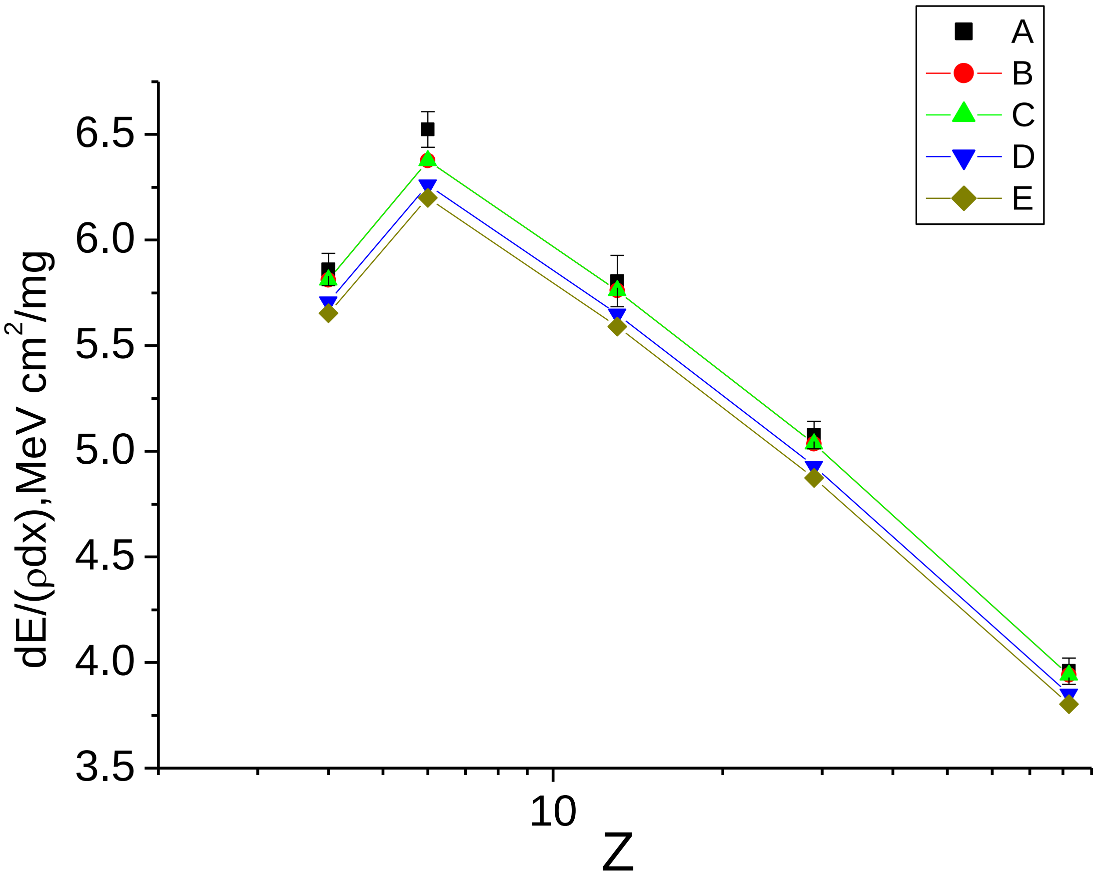

Figure 6: Ionization losses of relativistic (β = 0.839) Xe particles in the Be, C, Al, Cu, and Pb targets (left to right): experimental (A) and calculated values with the corrections ΔL_{LS} (B), ΔL_{MBVSTT} (C), ΔL_{MBA} (D), and ΔL_{MBJM} (E).

Conclusions

- Numerical implementation of the VSTT method based on the calculation of the Mott exact cross section is given and the preference for using this method instead of the standard method of integrating the Mott cross section is demonstrated for the case when the lower integration limit tends to zero.
- Using the latter result, the Mott correction (ΔL_M) and the total the Mott−Bloch corrections were computed for the ranges of a gamma factor of approximately $1 \lesssim \gamma \lesssim 10$ and the ion nuclear charge number $6 \leq Z \leq 114$.
- The Lindhard−Sorensen corrections in the point nucleus approximation and also the difference between the Lindhard−Sorensen and Bloch corrections ($\Delta L_{LS\text{-}B}$) were also calculated in the γ and Z ranges under consideration.
- It is shown that the difference between the Lindhard−Sorensen and Bloch corrections and the Mott correction obtained by the exact in $Z\alpha$ VSTT method coincide up to the seventh decimal digit over the range of approximately $1 \lesssim \gamma \lesssim 15$.
- In contrast by the two above-mentioned rigorous methods, the approximate methods have a very limited range of applicability and either (i) give a large difference in the ΔL_M values (as, for example, the Jackson−McCarthy method in the γ range about from 1.01 to 15), or (ii) have an incorrect threshold behavior (e.g. the Morgan−Eby method in the γ range from 1 to 2), or (iii) are characterized by an uncertain accuracy (for example, Ahlen's method in the γ range about from 1.01 to 15, which also gives non-physical negative values at γ less than 1.01) for medium and high Z materials

For low Z materials, these methods give the ΔL_M values rather close to those obtained by rigorous methods.

- Calculation of the total Mott−Bloch correction (ΔL_{MB}) by the VSTT methods and the Lindhard−Sorensen correction (ΔL_{LS}) over the γ and Z ranges $0.01 \le \gamma - 1 \le 10$ and $6 \le Z \le 114$ gives excellent agreement. The relative difference between these two corrections is less than 0.1% at the upper summation limit $N > 600$.
- We also showed that the results of stopping power calculations obtained by the LS and VSTT methods coincide with each other also up to the seventh significant digit and provide the best agreement with experimental data, while the approximate methods of Ahlen and Jackson−McCarthy give understated values in comparison with the experiment for intermediate-Z particles ($Z = 36, 54$).

Thus, we can conclude that at intermediate energies, when a heavy ion can be considered as a point-like particle, both methods, the method based on calculating the Mott-exact cross section and the Lindhard−Sørensen method, can be successfully used in electronic stopping calculations for relativistic heavy ions.

I-3 Corrections to the higher moments of the relativistic ion energy-loss distributions beyond the Born approximation

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- Based on the representation of the Mott corrections to the Bethe-Bloch formula in the form of rapidly convergent series of quantities bilinear in the Mott partial amplitudes, **an algorithm is proposed for computing the most important parameters of the average energy-loss distributions of relativistic ions in the Mott approximation**.
- Using its implementation, the parameters of the energy-loss distributions were calculated for incident charged particles of charge number Z from 5 to 95 and relative velocity β from 0.05 to 0.95.
- The relative Mott corrections δ_n to the Born values of the central moments and normalized central moments of the particle average energy-loss rates in the irradiated material were also computed.

It is shown that the relative Mott corrections δ_n to the Born central moments $\mu_{n,B}$ ($n = \overline{2,4}$) of the distributions can reach several hundred percent for heavy relativistic ions.

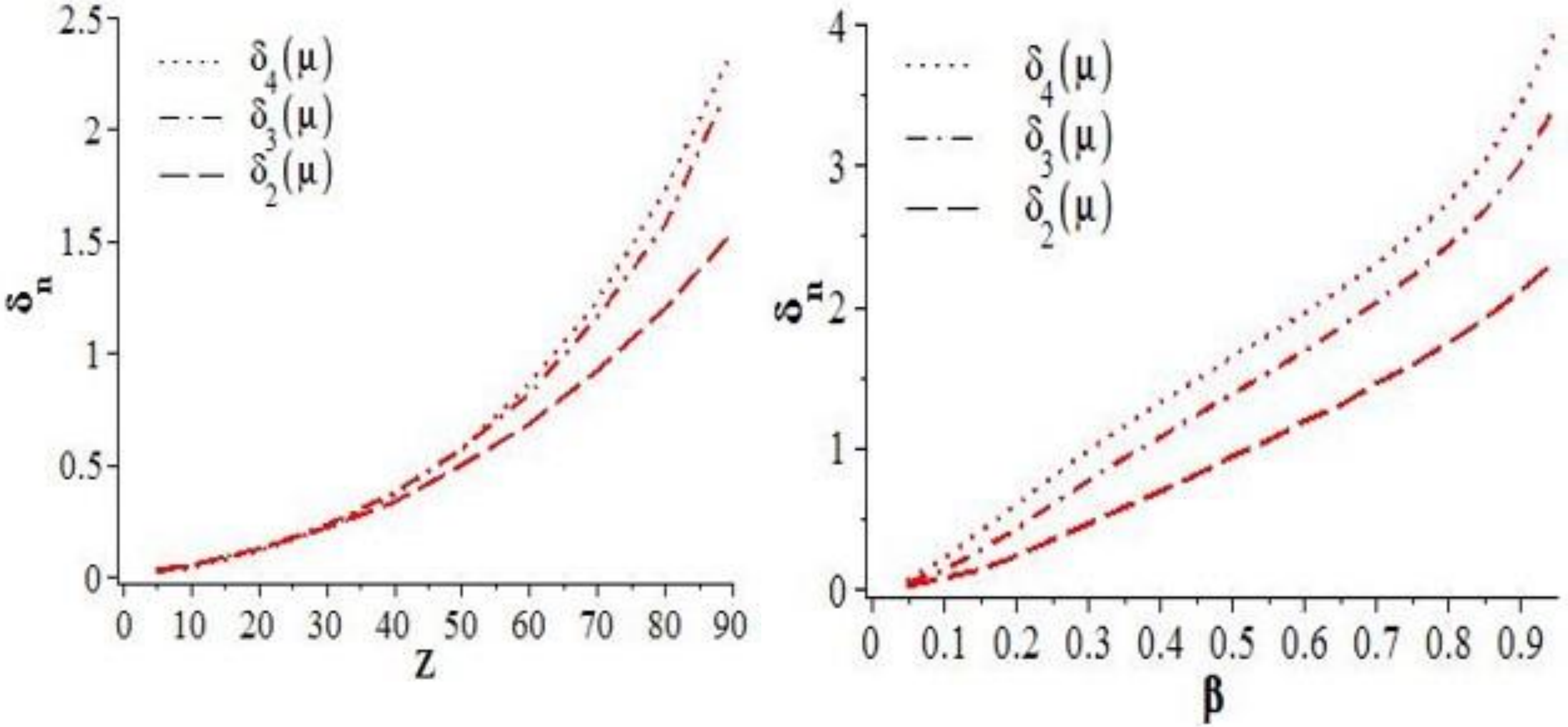

Figure 7: Relative Mott's corrections δ_n to the Born central moments $\mu_{n,B}$ ($n = \overline{2,4}$) of the energy-loss distribution of incident charged particles: Z dependence of $\delta_n(\mu)$ for $\beta = 0.75$ (at the left) and β dependence of $\delta_n(\mu)$ for $Z = 92$ (on the right).

I-4 Some Approaches to the Energy-Loss Straggling Calculation

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- Some exact and approximate methods commonly used to calculate corrections to the Bethe stopping formula are modified and adapted by the authors to the calculation of the energy loss straggling (ELS).
- An intercomparison is carried out for results of approaches developed in the present work.
- An excellent agreement obtained between the results for ELS, calculated with an exact method previously proposed by one of the authors and the results of the Lindhard–Sørensen method for moderate relativistic energies.

Table 7 Relative correction to the first Born approximation δ on the data of works [Lindhard and Sørensen, 1996] [1] and [Voskresenskaya, 2018] [2] for $\beta = 0.75$ (1)

Z	10	20	30	40	50
[1]	0.0486257	0.117467	0.210810	0.333171	0.489170
[2]	0.0486257	0.117467	0.210810	0.333171	0.489170
Z	60	70	80	90	100
[1]	0.683263	0.919165	1.19858	1.51831	1.86377
[2]	0.683263	0.919165	1.19858	1.51831	1.86377

- Thus, when using the limits N = 3000, the results of calculations according to [Lindhard and Sørensen, 1996] and [Vosrresenskaya, 2018] coincide up to the seventh decimal digit over the range of approximately $1 \leq \gamma \leq 15$.

The calculation time for ten values of the relative correction according to [Lindhard and Sørensen, 1996] was 37 seconds, and according to [Voskresenskaya, 2018] it was 15 seconds. Therefore, and also because of the simpler expression, in our opinion, it is preferable to use the method developed in [Voskresenskaya, 2018].

Lindhard, J., Sørensen, A.H. 1996. Relativistic theory of stopping for heavy ions. Phys. Rev. A 53, 2443–2456
Voskresenskaya, O. 2018. Journal of Astrophysics & Aerospace Technology, 6, 65. DOI:10.4172/2329-6542-C6-033; arXiv:1810.00542 [hep-ph]