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PRACTICAL DERIVATION OF MOLIÈRE ANGULAR DISTRIBUTION WITH IONIZATION

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Abstract

Approximation methods for practical and efficient derivations of Molière angular distribution are attempted. The scale factor ν characterizing the ionization process, solved in numerical integrals, is well approximated by a series expansion of the solution with rest-mass up to the second order. Molière screening model is found well approximated by a simpler Born-type model for wide variety of substances, so that the characteristic constants B and θ_{M} of angular distribution for mixed or compound substances are derived far simply and enough accurately from the Kamata-Nishimura constants for mixture without taking as many integrations as the number of mixed substances for stochastic means. These confirmations will be valuable for rapid derivations of Molière angular distribution, especially in tracing tracks of charged particle in Monte Carlo simulations.

1 Introduction

Molière theory of multiple Coulomb scattering [1, 2, 3] is one of the most accurate theories [4, 5, 6] to describe stochastic aspects of charged particle traversing through substance, taking account single scattering other than multiple scattering in the theory. Kamata and Nishimura proposed another formulation of Molière theory in their construction of cascade shower theory. Their formulation will be characterized by that they remain the equation differential with traversed thickness even after integrating with scattering angle in Hankel transforms and that they introduce the Kamata-Nishimura constants to reflect all the properties of substance. So the Molière theory has become far simple and convenient to get the result and to apply it on other problems.

One superior aspect of Kamata-Nishimura formulation to the Molière-Bethe formulation is that we can easily get Molière angular distribution with ionization. The multiple scattering theory with ionization is especially valuable for our application of the theory to Monte Carlo simulations, because we can trace tracks of charged particle more effectively by taking comparatively longer passages.

Kamata and Nishimura described their formulation for relativistic electrons of fixed energy. We have attempted an improvement to make the formulation applicable to other charged particles of moderate relativistic conditions with ionization. It required tedious numerical integrations in the solution of the scale factor ν characterizing the ionization process. And in the derivation of angular distribution for mixed or compound substances, it required as many times of integration as the number of the mixed substances in the evaluation of stochastic mean. In this report we propose practical and efficient approximations [7, 8] to conquest the above defects, found after the previous international workshop of EGS [9].

2 Derivation of Molière Angular Distribution with Ionization

The diffusion equation of the Molière angular distribution for charged particles of moderate relativistic energy with charge z, rest-mass mc^2, and velocity β is described as

$$\frac{\partial \tilde{f}}{z^2 \partial t} = -\frac{\zeta^2}{w^2} \tilde{f} \{1 - \frac{1}{\Omega} \ln \frac{\beta'^2 \zeta^2}{w^2}\} + \varepsilon \frac{\partial \tilde{f}}{\partial E}, \tag{1}$$

in the Fourier space [9]. The last term of the right hand side means charged particle lose energy of $z^2\varepsilon$ in unit radiation length, so that we have

$$E = E_0 - z^2 \varepsilon t. \tag{2}$$

We use almost the same variable

$$w = 2pv/K = \frac{2E}{K}\{1 - (\frac{mc^2}{E})^2\} \tag{3}$$

as in Rossi and Greisen [10], and introduce the correction factor of velocity due to the non-proportional relation of the Molière angle to the Born angle;

$$\beta'^2 = \frac{1.13 + 3.76\alpha^2}{1.13 + 3.76\alpha_0^2} \beta^2 \tag{4}$$

where

$$\alpha = \frac{zZ}{137\beta} \quad \text{and} \quad \alpha_0 = \frac{Z}{137}. \tag{5}$$

K and Ω denote Kamata-Nishimura constants specific to the substance [11, 12, 9]. The solution of Eq. (1) can be expressed as

$$\tilde{f} = \frac{1}{2\pi} \exp\{-\frac{\theta_{\mathrm{G}}^2 \zeta^2}{4}(1 - \frac{1}{\Omega} \ln \frac{\beta'^2 \theta_{\mathrm{G}}^2 \zeta^2}{4\nu z^2 t})\}, \tag{6}$$

where θ_{G}^2 denotes the gaussian mean-square angle taking account rest-mass [9], derived from

$$\theta_{\mathrm{G}}^2 = \int_0^t \frac{4z^2}{w^2} dt = \frac{K^2}{2\varepsilon mc^2}\{\frac{mc^2}{pv} - \frac{mc^2}{p_0 v_0} + \frac{1}{2} \ln \frac{(E_0 - mc^2)/(E - mc^2)}{(E_0 + mc^2)/(E + mc^2)}\}, \tag{7}$$

and the scale factor ν is determined from

$$\ln \frac{\nu}{\beta'^2} = \ln \frac{\theta_{\mathrm{G}}^2}{4z^2 t} - \frac{4z^2}{\theta_{\mathrm{G}}^2} \int_0^t \frac{1}{w^2} \ln \frac{\beta'^2}{w^2} dt. \tag{8}$$

Applying the translation formula [13], the solution (6) is reduced to the Molière form,

$$\tilde{f} = \frac{1}{2\pi} \exp\{-\frac{\theta_{\mathrm{M}}^2 \zeta^2}{4}(1 - \frac{1}{B} \ln \frac{\theta_{\mathrm{M}}^2 \zeta^2}{4})\}, \tag{9}$$

where the expansion parameter B and the unit of Molière angle θ_{M} are derived from

$$B - \ln B = \Omega - \ln \Omega + \ln(\nu z^2 t/\beta'^2), \tag{10}$$

$$\theta_{\mathrm{M}} = \theta_{\mathrm{G}} \sqrt{B/\Omega}. \tag{11}$$

Thus we get the Molière angular distributions $f(\vartheta)2\pi\vartheta d\vartheta$ and $f_{\mathrm{P}}(\varphi)d\varphi$ for polar angle θ and projected angle ϕ, respectively:

$$f(\vartheta) = f^{(0)}(\vartheta) + B^{-1} f^{(1)}(\vartheta) + B^{-2} f^{(2)}(\vartheta) + \ldots, \tag{12}$$

$$f_{\mathrm{P}}(\varphi) = f_{\mathrm{P}}^{(0)}(\varphi) + B^{-1} f_{\mathrm{P}}^{(1)}(\varphi) + B^{-2} f_{\mathrm{P}}^{(2)}(\varphi) + \ldots, \tag{13}$$

with

$$\vartheta = \theta/\theta_{\mathrm{M}} \quad \text{and} \quad \varphi = \phi/\theta_{\mathrm{M}}. \tag{14}$$

The functions $f^{(k)}$ and $f_{\mathrm{P}}^{(k)}$ are the universal functions defined in [1, 2], except the factor of 2π for the polar distribution.

Molière angular distributions are characterized by two parameters, the expansion parameter B and the unit of Molière angle θ_{M}. So we want to discuss the dispersions of Molière angular distribution due to various conditions, by these parameters.

3 Composite Variables To Describe Molière Angular Distribution Irrespective of Substances

Under the extreme relativistic condition,

$$E \gg mc^2, \tag{15}$$

we have

$$w \simeq 2E/K, \tag{16}$$

$$\beta \simeq 1 \tag{17}$$

from Eq. (3), so that the two parameters B and θ_{M} are determined by

$$B - \ln B = \Omega - \ln \Omega + \ln \nu z^2 t, \tag{18}$$

$$\theta_{\mathrm{M}} = \theta_{\mathrm{G}} \sqrt{B/\Omega}, \tag{19}$$

where

$$\nu = e^2 (E/E_0)^{(E_0+E)/(E_0-E)} \tag{20}$$

and

$$\theta_{\mathrm{G}}^2 = \frac{K^2 z^2 t}{E_0 E}. \tag{21}$$

As it holds

$$B - \ln B = \ln(\nu \frac{z^2 t}{\Omega e^{-\Omega}}), \tag{22}$$

$$\theta_{\mathrm{M}}^2 / \frac{K^2 e^{-\Omega}}{E_0^2} = \frac{B}{E/E_0} \frac{z^2 t}{\Omega e^{-\Omega}}, \tag{23}$$

we find the characteristic parameters are described universally irrespective of substances, by using the composite variables $z^2 t/(\Omega e^{-\Omega})$ and $\theta_{\mathrm{M}}/(K e^{-\Omega/2}/E_0)$. The unit $\Omega e^{-\Omega}/z^2$ for the traversed thickness is almost the same as the mean free path of the single scattering larger than the screening angle, measured in the radiation length. It should be noted that the characteristic parameters represented in the composite variable, B and $\theta_{\mathrm{M}}/(K e^{-\Omega/2}/E_0)$, are functions of fractional energy E/E_0, in case of the extreme relativistic condition.

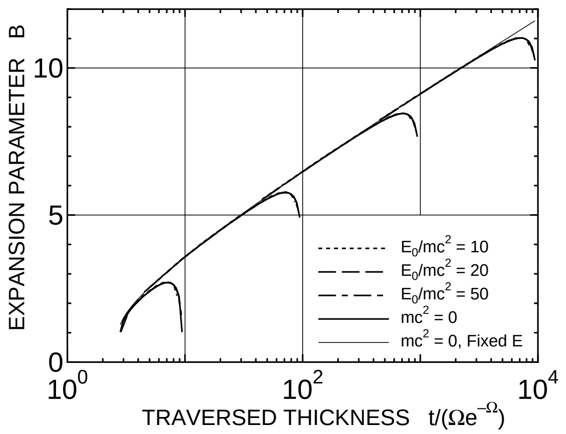

Figure 1: Discrepancies of B due to the different rest-masses. Incident energies E_0/ε correspond to 10, 10^2, 10^3, and 10^4 in unit of $\Omega e^{-\Omega}$, from left to right.

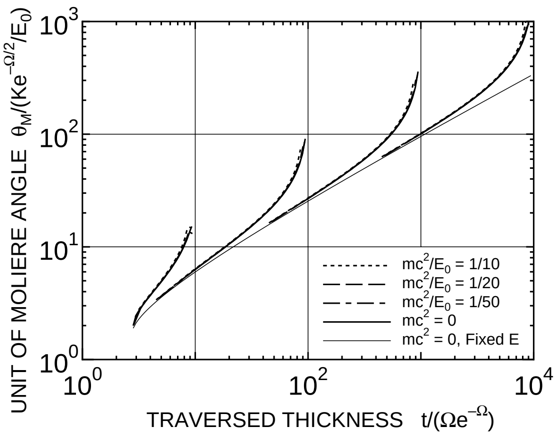

Figure 2: Discrepancies of θ_{M} due to the different rest-masses. Incident energies E_0/ε correspond to 10, 10^2, 10^3, and 10^4 in unit of $\Omega e^{-\Omega}$, from left to right.

4 Discrepancy of Molière Angular Distribution Arising From The Difference of Rest-Mass

We investigate dispersions of the characteristic parameters, B and θ_{M}, due to the difference of rest-mass mc^2, for singly charged particles with moderate relativistic energies. We assume the Born parameter be small enough, $zZ/137\beta \ll 1$, which is realized at e.g. the penetration through light substances. Then it satisfies $\beta' \simeq \beta$, and we can determine the characteristic parameters as

$$B - \ln B = \Omega - \ln \Omega + \ln(\nu t/\beta^2), \tag{24}$$

$$\theta_{\mathrm{M}} = \theta_{\mathrm{G}}\sqrt{B/\Omega}, \tag{25}$$

with θ_{G} from Eq. (7), and ν is derived from

$$\ln\frac{\nu}{\beta^2} = \ln\frac{\theta_{\mathrm{G}}^2}{4z^2 t} - \frac{4z^2}{\theta_{\mathrm{G}}^2}\int_0^t \frac{1}{w^2}\ln\frac{\beta^2}{w^2}dt. \tag{26}$$

The scale factor ν, so that B and θ_{M}, are functions of E_0/mc^2 and E/mc^2 in this case.

We compare the results of B and θ_{M} for various E_0/mc^2 of 10, 20, 50, and ∞, in Figs. 1 and 2. A slight differences appear with increase of the fractional thickness $t/(E_0/\varepsilon)$ especially for curves of lower values of E_0/mc^2.

5 Discrepancy of Angular Distribution Arising From The Non-Proportional Relation of Molière Screening Angle to The Born Angle

Under the Molière screening model with moderate relativistic energies, the characteristic parameters B and θ_{M} derived from Eqs. (10), (11) still require the explicit Z in the term β' even if we use the above composite variables $t/(\Omega e^{-\Omega})$ and $\theta_{\mathrm{M}}/(Ke^{-\Omega/2}/E_0)$. Difference of β' from β arises from non-proportional relation of the Molière screening angle to the Born angle. In this case, we cannot describe the characteristic parameters irrespective of substances by the composite variables, in the definite sense. But in case it satisfies $\beta' \simeq \beta$, which is realized in case of Born parameter

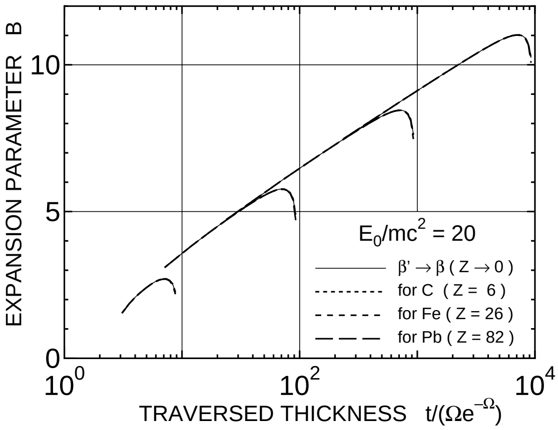

Figure 3: Discrepancies of B due to the different Molière screening angles from Born ones by substance. Incident energies E_0/ε correspond to 10, 10^2, 10^3, and 10^4 in unit of $\Omega e^{-\Omega}$, from left to right.

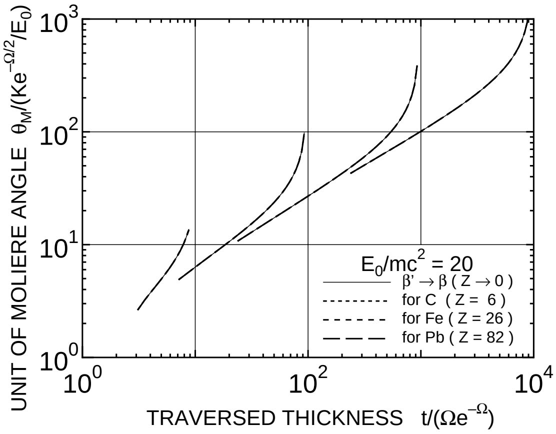

Figure 4: Discrepancies of $\theta_{\rm M}$ due to the different Molière screening angles from Born ones by substance. Incident energies E_0/ε correspond to 10, 10^2, 10^3, and 10^4 in unit of $\Omega e^{-\Omega}$, from left to right.

to be small enough, B and $\theta_{\rm M}$ could be described universally irrespective of substances from Eqs. (24), (25) by the composite variables.

We examine whether the relation $\beta' \simeq \beta$ still satisfies or not, so that the universal relations satisfy or not, on the practical substances around us. The B and $\theta_{\rm M}$ derived from β' by Eqs. (10), (11) and those from β by Eqs. (24), (25) are compared on substances C, Fe, and Pb in Figs. 3 and 4. We cannot find any visible differences more than 1 percent between them within passage of energy loss less than 80 percent.

6 Approximated Expression of The Scale Factor ν

We have confirmed it satisfies $\beta' \simeq \beta$ in practical cases. Then, applying the partial integration on Eq. (26), we get

$$\ln\nu = \ln\frac{\theta_{\rm G}^2 p^2 v^2}{K^2 z^2 t} - \frac{2z^2\varepsilon}{\theta_{\rm G}^2}\int_0^t \frac{\theta_{\rm G}^2}{pv}dt. \tag{27}$$

This time we obtain the value of ν up to the second order of rest-mass mc^2. As

$$pv = E(1 - \frac{m^2c^4}{E^2}), \tag{28}$$

$$\theta_{\rm G}^2 \simeq \frac{K^2z^2t}{E_0E}\{1 + \frac{2}{3}\frac{m^2c^4}{E^2}(1 + \frac{E}{E_0} + \frac{E^2}{E_0^2})\}, \tag{29}$$

we have

$$\ln\nu \simeq 2 + \frac{E_0+E}{E_0-E}\ln\frac{E}{E_0} - \frac{m^2c^4}{9E_0^2}(14\frac{E_0^2}{E^2} + 5\frac{E_0}{E} + 5 + 12\frac{E_0}{E}\frac{E_0+E}{E_0-E}\ln\frac{E}{E_0}). \tag{30}$$

The first two terms describe the scale factor ν of Eq. (20) for the extreme relativistic condition. The third term shows the contribution of the next higher term with rest-mass. The exact and the approximated results of the scale factor ν are compared against the fraction of energy loss in Fig. 5. Both agree well within the error of 1 percent up to the traversed thickness of energy loss of about 70 percents.

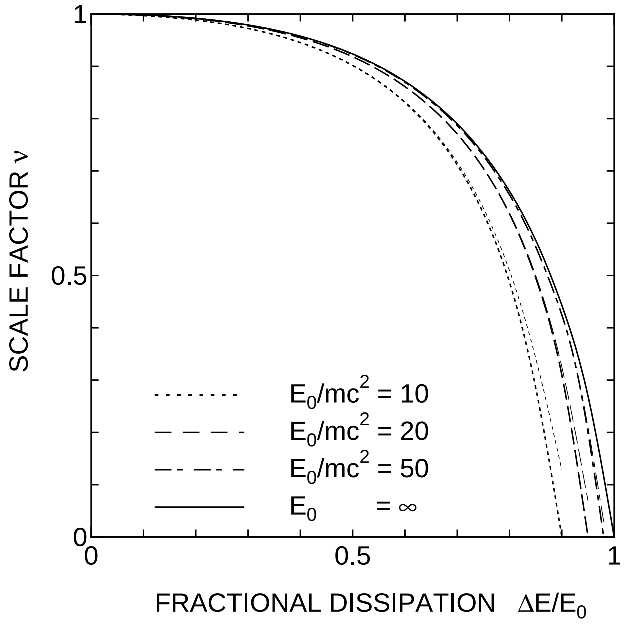

Figure 5: Comparison of the exact scale factors ν (thick lines) and their approximations (thin lines).

7 Approximated Derivation of Molière Angular Distribution for Mixed or Compound Substances

Exact results of the characteristic parameters B and θ_{M} for charged particles traversing through mixed or compound substances will be derived [9] from

$$B - \ln B = (\frac{\bar{\theta}_{\mathrm{G}}^2}{4\bar{\Omega}})^{-1} \int_0^x \Pr[\frac{1}{X_0 w^2}(1 - \frac{1}{\Omega}\ln\frac{\beta'^2}{w^2})] z^2 dx + \ln\frac{\bar{\theta}_{\mathrm{G}}^2}{4\bar{\Omega}}, \tag{31}$$

$$\theta_{\mathrm{M}} = \bar{\theta}_{\mathrm{G}}\sqrt{B/\bar{\Omega}}, \tag{32}$$

where we used the Kamata-Nishimura constants for mixture [11, 12, 9]. $\bar{\theta}_{\mathrm{G}}^2$ in the formula denotes the mean square angle θ_{G}^2 derived using the constants for mixture, $\bar{K}$ and $\bar{\varepsilon}$,

$$\bar{\theta}_{\mathrm{G}}^2 = \frac{\bar{K}^2}{2\bar{\varepsilon}mc^2}\{\frac{mc^2}{pv} - \frac{mc^2}{p_0v_0} + \frac{1}{2}\ln\frac{(E_0 - mc^2)/(E - mc^2)}{(E_0 + mc^2)/(E + mc^2)}\}, \tag{33}$$

and $\Pr[Q]$ denotes the stochastic mean of the quantity Q_i's defined as the weighted mean by the fraction p_i of mass:

$$\Pr[Q] = \sum_i p_i Q_i. \tag{34}$$

Although this method gives the accurate results, it requires tedious calculations of as many integrations as the number of mixed substances, in evaluation of the stochastic mean.

The evaluation becomes far simple in case it satisfies $\beta' \simeq \beta$ on the propagation, where B and θ_{M} in Eqs. (31), (32) are reduced [9] to $\bar{B}$ and $\bar{\theta}_{\mathrm{M}}$ defined as

$$\bar{B} - \ln\bar{B} = \bar{\Omega} - \ln\bar{\Omega} + \ln(\nu z^2 t/\beta^2), \tag{35}$$

$$\bar{\theta}_{\mathrm{M}} = \bar{\theta}_{\mathrm{G}}\sqrt{\bar{B}/\bar{\Omega}}. \tag{36}$$

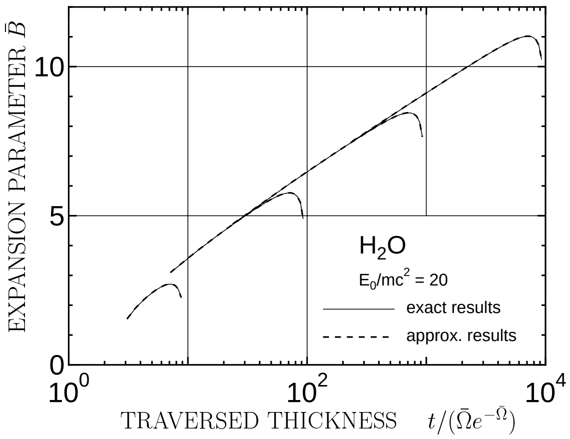

Figure 6: Comparison of the exact and the approximated expansion parameters, B and $\bar{B}$, for H_2O. Unit of abscissa, $\bar{\Omega}e^{-\bar{\Omega}}$, equals nearly to the mean thickness of single scattering larger than screening angle, and takes values of order 10^{-6}. Four branches of curve correspond to the incident energies by $E_0/\bar{\varepsilon}$ of 10, 10^2, 10^3, and 10^4 in unit of $\bar{\Omega}e^{-\bar{\Omega}}$, from left to right.

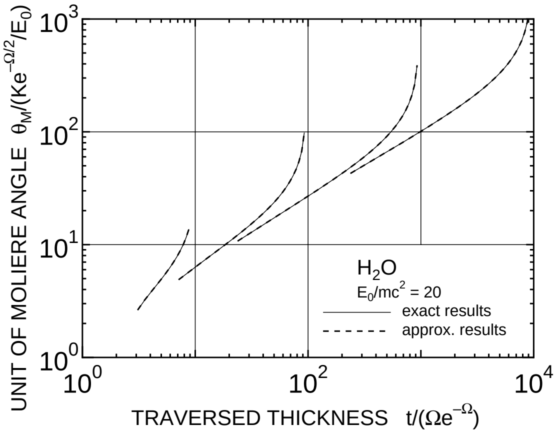

Figure 7: Comparison of the exact and the approximated units of Molière angle, θ_{M} and $\bar{\theta}_{\mathrm{M}}$, for H_2O. Unit of abscissa, $\bar{\Omega}e^{-\bar{\Omega}}$, equals nearly to the mean thickness of single scattering larger than screening angle, and takes values of order 10^{-6}. Four branches of curve correspond to the incident energies by $E_0/\bar{\varepsilon}$ of 10, 10^2, 10^3, and 10^4 in unit of $\bar{\Omega}e^{-\bar{\Omega}}$, from left to right.

In practice, we have confirmed in the section 5 the condition $\beta' \simeq \beta$ is satisfied for almost all the substances around us. We can expect the characteristic parameters B and θ_{M} for mixed or compound substances would be approximated by $\bar{B}$ and $\bar{\theta}_{\mathrm{M}}$. We have compared these approximated values with exact ones for substances of H_2O, Air, SiO_2, and Nuclear Emulsion in Figs. 6 to 13. Good agreements are confirmed between the approximated values from Eqs. (35), (36) and the exact ones from Eqs. (31), (32) within the differences of 1 percent.

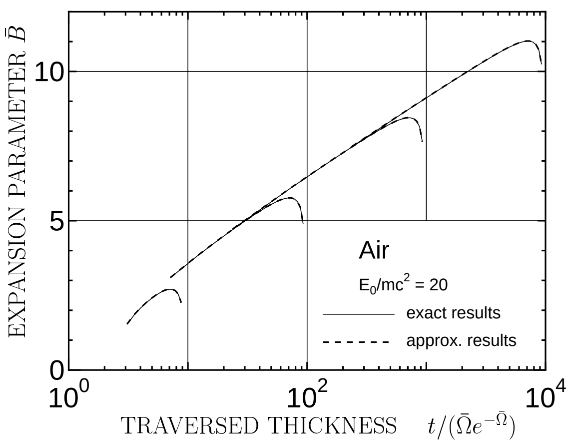

Figure 8: Comparison of B and $\bar{B}$ for Air.

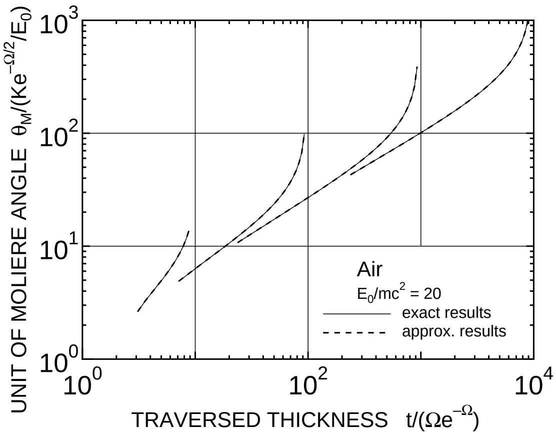

Figure 9: Comparison of θ_{M} and $\bar{\theta}_{\mathrm{M}}$ for Air.

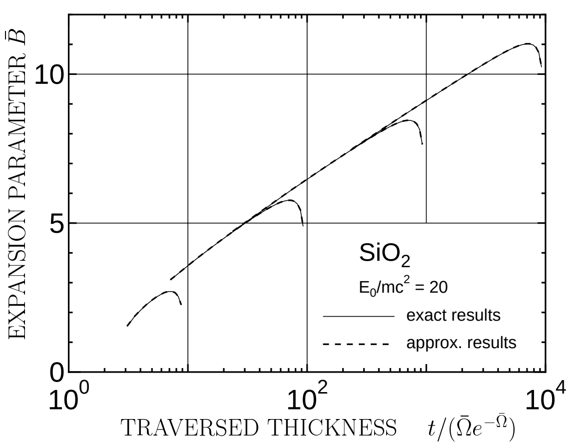

Figure 10: Comparison of B and $\bar{B}$ for SiO_2.

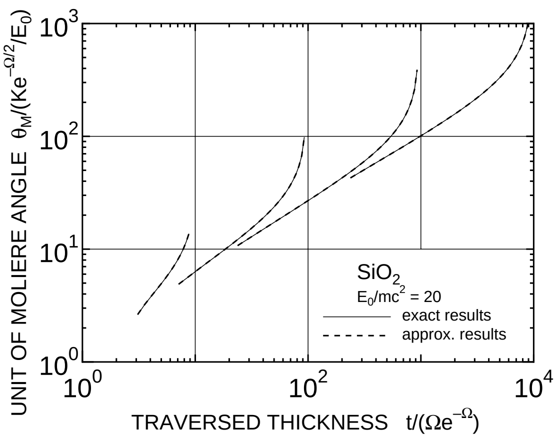

Figure 11: Comparison of θ_{M} and $\bar{\theta}_{\mathrm{M}}$ for SiO_2.

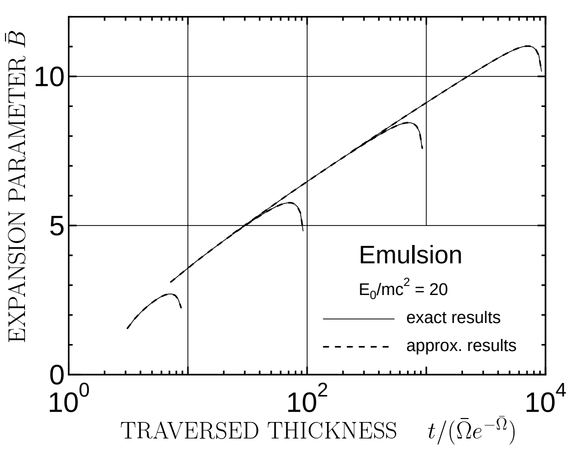

Figure 12: Comparison of B and $\bar{B}$ for Nuclear Emulsion.

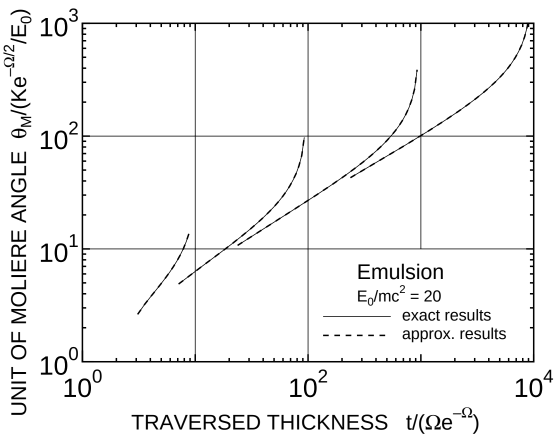

Figure 13: Comparison of θ_{M} and $\bar{\theta}_{\mathrm{M}}$ for Nuclear Emulsion.

8 Practical and Efficient Method to Obtain Molière Angular Distribution With Ionization

The Molière angular distribution for charged particles of moderate relativistic energy traversing through pure substances with ionization will be effectively derived as follows with enough accuracy. We derive B and θ_{M} from Eqs. (10), (11), replacing β' by β and substituting θ_{G} and ν from Eqs. (29), (30), then we get the spatial and projected angular distributions $f(\vartheta)$ and $f_{\mathrm{P}}(\varphi)$ by Eqs. (12) and (13).

The distribution for charged particles traversing through mixed or compound substances can be obtained practically in the same way by replacing the substance by a pure substance with the Kamata-Nishimura constants for mixture, $\bar{\Omega}$ and $\bar{K}$.

9 Conclusions and Discussions

A rapid and efficient method to derive Molière angular distribution is devised for charged particles traversing through pure or mixed substances with ionization. We have confirmed in Figs. 3 and 4 that Molière screening angle can be approximated regarding proportional to the Born screening angle in our applications to usual substances around us of wide energy range. Under this condition the scale factor ν characterizing the ionization process can be approximated enough accurately by series expansion with the rest-mass up to the second order as shown in Fig. 5. Also we have confirmed in Figs. 6 to 13 that the exact derivation of characteristic parameters B and θ_{M} for mixed or compound substances by as many integration as the number of mixed substances is approximated enough accurately by regarding the substance as a pure substance with the Kamata-Nishimura constants for mixture.

A proposed method in the section 8 for practical and efficient derivation of Molière angular distribution for charged particles with ionization will be valuable for rapid sampling of the distribution in Monte Carlo simulations [14, 15, 16] as well as for quick evaluation of the distributions in designing and analyses of experiments concerning charged particles.

Acknowledgments

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