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# **Practical and efficient derivations of Molière angular distribution** with ionization

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Abstract. Molière theory of multiple Coulomb scattering has been far improved to take account ionization loss by use of Kamata-Nishimura formulation of the theory. The new formulation only introduce the scale factor  $\nu$  to the traversed thickness for effects of ionization process, and is simply reduced to the traditional Molière-Bethe formulation by use of our translation formula. Introducing Kamata-Nishimura constants  $\Omega$  and K specific to the traversed substance, we can simplify the configuration of Molière theory, so that the sequence to derive Molière angular distributions has become much easy. Based on the new formulation, we propose a practical and efficient method to obtain Molière angular distributions. The method is accurate enough to apply in Monte Carlo simulations as well as designings and analyses of experiments concerning charged particles.

#### 1 Introduction

Reconstruction of Molière's multiple scattering theory (Molière, 2 1947, 1948; Bethe, 1953) by Kamata-Nishimura formulation (Kamata and Nishimura, 1958; Nishimura, 1967) is continuing. The new formulation is equivalent to the traditional Molière-Bethe formulation, both cutting off the higher terms of Fourier component at the same order (Nakatsuka, 1999b). We have found various superior aspects of the new formulation: ionization loss is taken into account (Nakatsuka, 1999a); properties of substance are all reflected in the Kamata-Nishimura, 1967; Nakatsuka, 2001a); mixed or compound substances can easily be treated; the formulation is simple as a thorough extension of the Rossi-Greisen or the Fermi-Yang theory (Rossi and Greisen, 1941; Yang, 1951); the theory is easily applicable to other problems; and so on.

Although the Molière theory has been improved by the new formulation, a few problems still remain in actual applications. In case we take account ionization loss, the scale factor  $\nu$  is newly introduced (Nakatsuka, 1999a). It makes the expansion parameter *B* of the Molière angular distribution smaller. Namely, we should take the smaller value of *B* at the  $\nu$  times shallower thickness, compared with the fixed energy condition. Under the moderate relativistic condition, evaluation of the scale factor  $\nu$  requires heavy calculations of numerical integration. In case we get the Molière angular distribution for charged particles propagating through mixed or compound substances, we have to carry out multiple sequence of evaluations according to the number of mixed substances to get the stochastic mean among substances (Nakatsuka, 2001a). These facts will bring serious inefficiencies to our frequent derivations of the distribution.

In this paper, we derive simple methods to avoid these complicated sequences, and propose a practical and efficient procedure of getting Molière angular distribution with ionization applicable widely in simulations and analyses (Heck et al., 1998).

## 2 Sequence to Obtain Exact Molière Angular Distribution With Ionization

For derivations of Molière angular distribution under the moderate relativistic condition with ionization, we found it is enough to introduce a scale factor  $\nu$  for the traversed thickness (Nakatsuka, 2001b). If we assume ionization loss of charged particles of z with a constant rate as

$$E = E_0 - z^2 \varepsilon t,\tag{1}$$

where traversed thickness t is measured in radiation length (Particle Data Group, 2000), then the scale factor  $\nu$  is derived as

$$\ln \frac{\nu}{\beta'^2} = \ln \frac{\theta_{\rm G}^2}{4z^2 t} - \frac{4z^2}{\theta_{\rm G}^2} \int_0^t \frac{1}{w^2} \ln \frac{\beta'^2}{w^2} dt,$$
 (2)

with (Nakatsuka, 2001a)

$$w = 2pv/K,\tag{3}$$

$$\beta^{\prime 2} = \frac{1 + 3.34z^2 Z^2 / (137\beta)^2}{1 + 3.34Z^2 / 137^2} \beta^2, \tag{4}$$

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**Fig. 1.** Comparison of the exact scale factors  $\nu$  (thick lines) and their approximations (thin lines).

and the gaussian mean square angle (Nakatsuka, 1999a) with the scattering constant K,

$$\theta_{\rm G}^2 = \frac{K^2}{2\varepsilon mc^2} \left\{ \frac{mc^2}{pv} - \frac{mc^2}{p_0 v_0} + \frac{1}{2} \ln \frac{(E_0 - mc^2)/(E - mc^2)}{(E_0 + mc^2)/(E + mc^2)} \right\}.$$
(5)

Then we get the expansion parameter B and the unit of Molière angle  $\theta_{M}$ ;

$$B - \ln B = \Omega - \ln \Omega + \ln(\nu z^2 t/\beta'^2), \tag{6}$$

$$\theta_{\rm M} = \theta_{\rm G} \sqrt{B/\Omega}.\tag{7}$$

Using the both parameters we get the Molière angular distributions  $f(\vartheta)$  and  $f_{\rm P}(\varphi)$  for polar angle  $\theta$  and projected angle  $\phi$ , respectively:

$$f(\vartheta) = f^{(0)}(\vartheta) + B^{-1}f^{(1)}(\vartheta) + B^{-2}f^{(2)}(\vartheta) + \dots, \quad (8)$$

$$f_{\rm P}(\varphi) = f_{\rm P}^{(0)}(\varphi) + B^{-1} f_{\rm P}^{(1)}(\varphi) + B^{-2} f_{\rm P}^{(2)}(\varphi) + \dots, \quad (9)$$

with

$$\vartheta = \theta/\theta_{\rm M} \quad \text{and} \quad \varphi = \phi/\theta_{\rm M}.$$
(10)

#### 3 Approximated Expression of The Scale Factor

In case of small Born parameter,  $zZ/137\beta \ll 1$ , it satisfies  $\beta' \simeq \beta$ . Then, applying the partial integration on Eq. (2), we get

$$\ln \nu = \ln \frac{\theta_{\rm G}^2 p^2 v^2}{K^2 z^2 t} - \frac{2z^2 \varepsilon}{\theta_{\rm G}^2} \int_0^t \frac{\theta_{\rm G}^2}{p v} dt.$$
(11)

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

$$pv = E(1 - \frac{m^2 c^4}{E^2}),$$
(12)

$$\theta_{\rm G}^2 \simeq \frac{K^2 z^2 t}{E_0 E} \{ 1 + \frac{2}{3} \frac{m^2 c^4}{E^2} (1 + \frac{E}{E_0} + \frac{E^2}{E_0^2}) \},$$
(13)

we have

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

The first two terms agree with the scale factor under the extreme relativistic approximation, indicated in the formula (11) of Nakatsuka (1999a). The third term shows the contribution of the next higher term with rest-mass. The exact and the approximated results of the scale factor  $\nu$  are compared against the fraction of energy loss in Fig. 1. Both agree well within the error of 1 percent up to the traversed thickness of energy loss of about 70 percents.

# 4 Molière Angular Distribution in Mixed or Compound Substance and Its Approximation Using The Constants For Mixture

The two parameters B and  $\theta_M$  for charged particles traversing through mixed or compound substances are derived from

$$B - \ln B = \frac{\int_{0}^{x} \Pr[\frac{1}{X_{0}w^{2}}(1 - \frac{1}{\Omega}\ln\frac{\beta^{\prime 2}}{w^{2}})]z^{2}dx}{\bar{\theta}_{G}^{2}/4\bar{\Omega}} + \ln\frac{\bar{\theta}_{G}^{2}}{4\bar{\Omega}},$$
(15)

$$\theta_{\rm M} = \bar{\theta}_{\rm G} \sqrt{B/\bar{\Omega}},$$
(16)

where we used the Kamata-Nishimura constants for mixture (Kamata and Nishimura, 1958; Nishimura, 1967; Nakatsuka, 2001a).  $\bar{\theta}_{\rm G}^2$  in the formula denotes the mean square angle  $\theta_{\rm G}^2$  derived using the constants for mixture,  $\bar{K}$  and  $\bar{\varepsilon}$ ,

$$\bar{\theta}_{\rm G}^2 = \frac{\bar{K}^2}{2\bar{\varepsilon}mc^2} \left\{ \frac{mc^2}{pv} - \frac{mc^2}{p_0v_0} + \frac{1}{2} \ln \frac{(E_0 - mc^2)/(E - mc^2)}{(E_0 + mc^2)/(E + mc^2)} \right\},\tag{17}$$

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:

$$\Pr[Q] = \sum_{i} p_i Q_i. \tag{18}$$

Although this method gives the accurate results, it requires multiple sequence of calculations in evaluation of the stochastic mean, as many integrations as the number of mixed substances. In case it satisfies  $\beta' \simeq \beta$  on the propagation, the stochastic mean becomes simple and B and  $\theta_{\rm M}$  in Eqs. (15), (16) are reduced to  $\bar{B}$  and  $\bar{\theta}_{\rm M}$  defined as

$$\bar{B} - \ln \bar{B} = \bar{\Omega} - \ln \bar{\Omega} + \ln(\nu z^2 t/\beta^2), \tag{19}$$

$$\bar{\theta}_{\rm M} = \bar{\theta}_{\rm G} \sqrt{\bar{B}/\bar{\Omega}}.$$
(20)



Fig. 2. Comparison of the exact and the approximated expansion parameters, B and  $\overline{B}$ , for H<sub>2</sub>O. Unit of abscissa,  $\overline{\Omega}e^{-\overline{\Omega}}$ , 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  $E_0/\overline{\varepsilon}$  of 10,  $10^2$ ,  $10^3$ , and  $10^4$  in unit of  $\overline{\Omega}e^{-\overline{\Omega}}$ , from left to right.



**Fig. 4.** Comparison of *B* and  $\overline{B}$  for Air.

In practice, we have confirmed the condition  $\beta' \simeq \beta$  is satisfied for almost all the substances around us (Nakatsuka, 2001b). We expect the characteristic parameters B and  $\theta_M$ for mixed or compound substances are approximated by  $\overline{B}$ and  $\overline{\theta}_M$ . We compare these approximated values with exact ones for substances of H<sub>2</sub>O, Air, SiO<sub>2</sub>, and Nuclear Emulsion in Figs. 2 to 9. Good agreements are confirmed between the approximated values from Eqs. (19), (20) and the exact ones from Eqs. (15), (16) within the differences of 1 percent.

### 5 Practical and Efficient Method to Obtain Molière Angular Distribution With Ionization

We propose a practical method to obtain the Molière angular distribution for charged particles of moderate relativistic energy traversing through pure substances with ionization. We



**Fig. 3.** Comparison of the exact and the approximated units of Molière angle,  $\theta_{\rm M}$  and  $\bar{\theta}_{\rm M}$ , for H<sub>2</sub>O. 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<sup>2</sup>, 10<sup>3</sup>, and 10<sup>4</sup> in unit of  $\bar{\Omega}e^{-\bar{\Omega}}$ , from left to right.



**Fig. 5.** Comparison of  $\theta_{\rm M}$  and  $\bar{\theta}_{\rm M}$  for Air.

derive B and  $\theta_{\rm M}$  from Eqs. (6), (7), replacing  $\beta'$  by  $\beta$  and substituting  $\theta_{\rm G}$  and  $\nu$  from Eqs. (5), (14), then we get the spatial and projected angular distributions  $f(\vartheta)$  and  $f_{\rm P}(\varphi)$  by Eqs. (8) and (9).

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,  $\overline{\Omega}$  and  $\overline{K}$ .

#### 6 Conclusions and Discussions

The scale factor  $\nu$  characterizing the ionization process, having been defined by a numerical integration for charged particles of moderate relativistic energies, is approximated by an expression expanding the exact formula up to the second order of rest-mass  $mc^2$ . We find good agreements between



**Fig. 6.** Comparison of B and  $\overline{B}$  for SiO<sub>2</sub>.



**Fig. 8.** Comparison of B and  $\overline{B}$  for Nuclear Emulsion.

the exact value and the approximated one within 1 percent up to traverse of about 70 percents of energy loss (Fig. 1).

Derivations of Molière angular distribution in mixed or compound substances, where multiple sequence of evaluations were needed according to the number of mixed substances, are also approximated. As the condition  $\beta' \simeq \beta$  is satisfied for almost all substances, the characteristic parameters B and  $\theta_M$  of Molière distribution are easily derived from simple stochastic means using the Kamata-Nishimura constants for mixture,  $\overline{\Omega}$  and  $\overline{K}$ . Visible discrepancies are not found between the approximated parameters  $\overline{B}$  and  $\overline{\theta}_M$  so obtained and the exact B and  $\theta_M$ , in mixtures of Air, H<sub>2</sub>O, SiO<sub>2</sub>, and Nuclear Emulsion (Figs. 2 to 9).

Based on these investigations we have proposed a practical and efficient method to derive the Molière angular distribution for charged particles with ionization, traversing through pure as well as mixed or compound substances. The method will be valuable for frequent derivations of the distribution in Monte Carlo simulations and for rapid evaluation of the distribution in designing and analyses of experiments concerning charged particles.



**Fig. 7.** Comparison of  $\theta_{\rm M}$  and  $\bar{\theta}_{\rm M}$  for SiO<sub>2</sub>.



**Fig. 9.** Comparison of  $\theta_{\rm M}$  and  $\overline{\theta}_{\rm M}$  for Nuclear Emulsion.

#### References

- H.A. Bethe, Phys. Rev. 89, 1256(1953).
- D. Heck, J. Knapp, J.N. Capdevielle, G. Shatz, and T. Thouw, Forschungszentrum Karlsruhe Report FZKA6019(1998).
- K. Kamata and J. Nishimura, Prog. Theor. Phys. Suppl. 6, 93(1958).
- G. Molière, Z. Naturforsch. 2a, 133(1947).
- G. Molière, Z. Naturforsch. 3a, 78(1948).
- T. Nakatsuka, "Proceedings of the 26th International Cosmic Ray Conference," HE2.5.25, Salt Lake City, 1999.
- T. Nakatsuka, "Proceedings of the 26th International Cosmic Ray Conference," HE2.5.16, Salt Lake City, 1999.
- T. Nakatsuka, 2001a in this conference.
- T. Nakatsuka, 2001b in this conference.
- J. Nishimura, in *Handbuch der Physik, Band 46*, edited by S. Flügge (Springer, Berlin, 1967), Teil **2**, p. 1.
- Particle Data Group, Eur. Phys. J. C15, 1(2000).
- B. Rossi and K. Greisen, Rev. Mod. Phys. 27, 240(1941).
- C. N. Yang, Phys. Rev. 84, 599(1951).