# Predicted Angular Distribution of Fast Charged Particles with Ionization

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#### Abstract

Molière theory of angular distribution for fast charged particles is improved to take into account ionization loss, by using Kamata-Nishimura formulation of the theory. Decrease of the particle energy along the passage hence increase of the screening angle brings a slight different results from those derived by Molière-Bethe formulation for fixed energies. The present results are reduced to the same Molière distribution with modified values of the expansion parameter and the unit of Molière angle. Properties of the new distribution and differences from the traditional one are discussed. Angular distributions of particles penetrating through the mixed or compound substances are also investigated both under the relativistic and the nonrelativistic conditions, together with the Kamata-Nishimura constants characterizing their formulation.

## 1 Introduction

Highly accurate theories of multiple Coulomb scattering are important when we design and analyze experiments concerning charged particle and trace charged particles in computer simulation. Among various theoretical predictions of the multiple scattering process, Molière theory [1, 2, 3] is recognized most advanced reflecting the single and the plural scatterings in the theory, so that it has been widely used in computer simulation codes [4, 5, 6]. In spite of its excellent formulation of the theory, it had been a defect of Molière theory that almost no theoretical improvements and applications to other problems were achieved after his original constructions [1, 2, 7].

Kamata and Nishimura proposed another formulation of Molière theory in their description of cascade shower theory [8, 9], which is equivalent with the Molière-Bethe formulation within the expansion errors [10]. They described the theory in a differential form with traversed thickness, so that we can regard it as a thorough extension of Fermi-Yang formulation [11, 12, 13, 14], and it made applications of the Molière theory very easy to other problems, for example, Kamata and Nishimura could add the next higher term reflecting the single and the plural scatterings to their shower theory [8, 9] and the author could discuss the Molière effect on the actual path length problem [13].

Recently we have found another superior aspect of the Kamata-Nishimura formulation that we can easily take into account ionization loss in the Molière angular distribution by only modifying parameter values in the Molière theory [15, 16, 17, 18]. It improves the accuracy and the reliability of Molière distribution. It has another important effect from the practical point of view that it improves sampling efficiency in computer simulations. In case using the traditional Molière theory of fixed energies, the sampling path length had to be restricted short so as not the distribution deformed due to the decrease of particle energy [4, 19]. By using our distribution this restriction will be removed.

Unfortunately for us, Kamata-Nishimura formulation of Molière theory is written for electron in the relativistic condition and the characteristic constants are indicated for only restricted substances [8, 9]. So we have attempted to describe the formulation suitable for general energy range, and applicable to variety of particles irrespective of mass and charge. The characteristic constants appearing in the formulation are tabulated for various substances. Method to obtain the distribution for particles traversing through mixed or compound substances is also discussed.

# 2 The Angular Distribution With Ionization Under The Relativistic Condition

Kamata and Nishimura proposed a very simple formulation of Molière theory for electrons of relativistic condition. Let  $f(\theta, t)2\pi\theta d\theta$  be the angular distribution of electrons after traversing through a thickness of t measured in radiation unit [11], receiving multiple Coulomb scattering under the axially symmetric condition. The diffusion equation is described as

$$\frac{\partial \tilde{f}}{\partial t} = -\frac{K^2 \zeta^2}{4E^2} \tilde{f} \{ 1 - \frac{1}{\Omega} \ln \frac{K^2 \zeta^2}{4E^2} \},\tag{1}$$

in the Fourier space [8, 9]. The equation possesses only two constants specific to the substance. Under the fixed energy condition, the solution of equation becomes

$$\tilde{f} = \frac{1}{2\pi} \exp\{-\frac{\theta_{\rm G}^2 \zeta^2}{4} (1 - \frac{1}{\Omega} \ln \frac{\theta_{\rm G}^2 \zeta^2}{4t})\} \quad \text{with} \quad \theta_{\rm G}^2 = \frac{K^2 t}{E^2}.$$
(2)

Using the translation formula indicated in the Appendix, the Kamata-Nishimura formulation is reduced to the Molière-Bethe one and we get the Molière angular distribution characterized by the two parameters, the expansion parameter B and the unit of Molière angle  $\vartheta = \theta/\theta_M$ , determined by [13]

$$B - \ln B = \Omega - \ln \Omega + \ln t$$
 and  $\theta_{\rm M} = \theta_{\rm G} \sqrt{B/\Omega}$ . (3)

If we assume ionization loss of constant rate

$$E = E_0 - \varepsilon t. \tag{4}$$

the diffusion equation becomes

$$\frac{\partial \tilde{f}}{\partial t} = -\frac{K^2 \zeta^2}{4E^2} \tilde{f} \{ 1 - \frac{1}{\Omega} \ln \frac{K^2 \zeta^2}{4E^2} \} + \varepsilon \frac{\partial \tilde{f}}{\partial E}.$$
(5)

Then we have the solution

$$\tilde{f} = \frac{1}{2\pi} \exp\{-\frac{\theta_{\rm G}^2 \zeta^2}{4} (1 - \frac{1}{\Omega} \ln \frac{\theta_{\rm G}^2 \zeta^2}{4\nu t})\} \quad \text{with} \quad \theta_{\rm G}^2 = \frac{K^2 t}{E_0 E},\tag{6}$$

where

$$\nu = e^2 (E/E_0)^{(E_0 + E)/(E_0 - E)}.$$
(7)

The characteristic parameters B and  $\theta_{\rm M}$  are determined by

$$B - \ln B = \Omega - \ln \Omega + \ln \nu t$$
 and  $\theta_{\rm M} = \theta_{\rm G} \sqrt{B/\Omega}$ . (8)

The angular distributions with ionization are compared with those without ionization in Fig. 1. The width of distribution increases rapidly with dissipation of energy.

# 3 The Angular Distribution With Ionization Under The General Energy Condition

The diffusion equation for the angular distribution in Kamata-Nishimura formulation equivalent with that in Molière-Bethe one is described as

$$\frac{\partial \tilde{f}}{z^2 \partial t} = -\frac{\zeta^2}{w^2} \tilde{f} \{ 1 - \frac{1}{\Omega} \ln \frac{\beta'^2 \zeta^2}{w^2} \}$$
(9)

in the Fourier space. We define

$$w = 2pv/K = \frac{2E}{K} \{1 - (\frac{mc^2}{E})^2\}$$
(10)

and

$$\beta^{\prime 2} = \frac{1.13 + 3.76\alpha^2}{1.13 + 3.76\alpha_0^2}\beta^2, \quad \text{with} \quad \alpha = \frac{zZ}{137\beta} \quad \text{and} \quad \alpha_0 = \frac{Z}{137}.$$
 (11)

K and  $\Omega$  denote Kamata-Nishimura constants [8, 9].

Under the ionization process of

$$E = E_0 - \varepsilon z^2 t, \tag{12}$$

we get the solution as

$$\tilde{f} = \frac{1}{2\pi} \exp\{-\frac{\theta_{\rm G}^2 \zeta^2}{4} (1 - \frac{1}{\Omega} \ln \frac{\theta_{\rm G}^2 \zeta^2}{4\nu z^2 t/\beta'^2})\},\tag{13}$$

where  $\theta_{\rm G}$  denotes the gaussian root-mean-square angle with  $E_{\rm s}$  replaced by K,

$$\theta_{\rm G}^2 = \int_0^t \frac{4z^2}{w^2} dt = \frac{K^2}{2\varepsilon mc^2} \{ \frac{mc^2}{pv} - \frac{mc^2}{p_0v_0} + \frac{1}{2} \ln \frac{(E_0 - mc^2)/(E - mc^2)}{(E_0 + mc^2)/(E + mc^2)} \},\tag{14}$$

and  $\nu$  denotes the scale factor derived by

$$\ln \frac{\nu}{\beta'^2} = \ln \frac{\theta_{\rm G}^2}{4z^2 t} - \frac{4z^2}{\theta_{\rm G}^2} \int_0^t \frac{1}{w^2} \ln \frac{\beta'^2}{w^2} dt.$$
(15)

So that the angular distribution is determined by the expansion parameter B and the unit of Molière angle  $\theta_{\rm M}$ , derived from

$$B - \ln B = \Omega - \ln \Omega + \ln(\nu z^2 t/\beta'^2)$$
 and  $\theta_{\rm M} = \theta_{\rm G} \sqrt{B/\Omega}$ . (16)

In case of  $\beta' \approx \beta$ , which is realized for e.g. light substances of  $\alpha \ll 1$  or for singly-charged relativistic particle of  $\alpha \approx \alpha_0$ ,  $\nu$  determined from Eq. (15) becomes the function of  $E_0/mc^2$  and  $E/mc^2$ .  $\nu$  in this case is plotted against fractional thickness,  $t/(E_0/\varepsilon)$ , in Fig. 2 for various  $E_0/mc^2$ . B and  $\theta_{\rm M}$  in this case are plotted against the traversed thickness in Fig. 3 and Fig. 4. Differences of B and  $\theta_{\rm M}$  due to different  $E_0/mc^2$  are small.

# 4 Derivation of Kamata-Nishimura Formulation and Definition of Kamata-Nishimura Constants

We take the single scattering formula as

$$\sigma(\theta)2\pi\theta d\theta = \frac{4z^2 Z(Z+1)e^4}{p^2 v^2} \theta^{-4} 2\pi\theta d\theta \quad \text{with} \quad \theta > \sqrt{e}\chi_{a},\tag{17}$$

where  $\chi_a$  is called the characteristic screening angle [3]. Then the probability density to receive deflection angle  $\theta$  after an infinitesimal passage of dx measured in g/cm<sup>2</sup> is

$$\frac{N}{A}\sigma(\theta)2\pi\theta d\theta dx = \frac{4N}{A} \frac{z^2 Z(Z+1)e^4}{p^2 v^2} \theta^{-4} 2\pi\theta d\theta dx$$

$$= \frac{1}{4\pi L} \frac{E_s^2}{p^2 v^2} \theta^{-4} 2\pi\theta d\theta \frac{z^2 dx}{X_0},$$
(18)

where  $X_0$  denotes the radiation length [20] and L the so-called radiation logarithm with its correction term [21].

The diffusion equation for Molière angular distribution becomes [8, 9]

$$df = \frac{N}{A} dx \iint \{ f(\vec{\theta} - \vec{\theta'}) - f(\vec{\theta}) \} \sigma(\vec{\theta'}) d\vec{\theta'}.$$
(19)

Under the azimuthally symmetrical condition, Hankel transforms of Eq. (19) becomes

$$d\tilde{f} = -2\pi \frac{N}{A} \tilde{f} dx \int_{0}^{\infty} [1 - J_{0}(\zeta \theta)] \sigma(\theta) \theta d\theta$$
  
$$= -\frac{E_{s}^{2}}{2L} \frac{z^{2} dt}{p^{2} v^{2}} \tilde{f} \int_{\sqrt{e}\chi_{a}}^{\infty} [1 - J_{0}(\zeta \theta)] \theta^{-3} d\theta, \qquad (20)$$

where t denotes the traversed thickness measured in radiation unit:

$$t \equiv x/X_0. \tag{21}$$

Evaluating the integration using the formula (14) of Bethe [3], we get the following differential equation

$$\frac{d}{z^{2}dt}\ln\tilde{f} = \frac{E_{s}^{2}}{8L}\frac{\zeta^{2}}{p^{2}v^{2}}[1+\ln 2 - C - \ln(\sqrt{e}\chi_{a}\zeta)] \\
= \frac{E_{s}^{2}}{4L}\frac{\zeta^{2}}{4p^{2}v^{2}}[1-2C+\ln\frac{\beta^{2}E_{s}^{2}/(4Lp^{2}v^{2}\chi_{0}^{2})}{[\chi_{a}^{2}/\chi_{0}^{2}]_{\text{rel}}} - \ln\frac{\beta^{2}\chi_{a}^{2}/\chi_{0}^{2}}{[\chi_{a}^{2}/\chi_{0}^{2}]_{\text{rel}}} - \ln(\frac{E_{s}^{2}}{4L}\frac{\zeta^{2}}{4p^{2}v^{2}})], \quad (22)$$

where we introduced the angular constant  $\chi_0$  [3] called the Born screening angle [22],

$$\chi_0 = \hbar/(ap), \tag{23}$$

and  $[\chi_a^2/\chi_0^2]_{\rm rel}$  denotes the value of  $\chi_a^2/\chi_0^2$  for electrons of high energy limit.

Now we define the Kamata-Nishimura constants as

$$\Omega - \ln \Omega = 1 - 2C + \ln \frac{E_{\rm s}^2 / (4Lp^2 c^2 \chi_0^2)}{[\chi_{\rm a}^2 / \chi_0^2]_{\rm rel}},\tag{24}$$

$$K^2 = \frac{E_s^2}{4L}\Omega,\tag{25}$$

then  $\Omega$  and K are constants specific to the substance. It can be easily confirmed that these definitions agree with (A.3.26) and (A.3.28) of Nishimura defined in the relativistic condition [9]. We also introduce the factor

$$\beta^{\prime 2} = \frac{\chi_{a}^{2}/\chi_{0}^{2}}{[\chi_{a}^{2}/\chi_{0}^{2}]_{\rm rel}}\beta^{2},$$
(26)

reflecting the velocity of penetrating particle and the difference between the characteristic screening angle and the Born screening angle.

Then the diffusion equation becomes

$$-\frac{d}{z^2 dt} \ln \tilde{f} = \frac{K^2}{\Omega} \frac{\zeta^2}{4p^2 v^2} [\Omega - \ln \Omega - \ln(\frac{K^2}{\Omega} \frac{\beta'^2 \zeta^2}{4p^2 v^2})], \qquad (27)$$

so that we get

$$\frac{d}{z^2 dt} \ln \tilde{f} = -\frac{\zeta^2}{w^2} \left[1 - \frac{1}{\Omega} \ln \frac{\beta'^2 \zeta^2}{w^2}\right] \quad \text{where} \quad w = 2pv/K.$$

$$(28)$$

Many authors evaluated  $\chi_a$  and  $\chi_0$  respectively in their multiple scattering theories, depending on their models of screening potential. We listed in Table 1 some screening models adopted by representative authors of multiple scattering theory.

Table 1: Screening potentials adopted by representative authors. V(r), a,  $\chi_0$ ,  $\chi_a$  denote screening potential, atomic radius, Born screening angle, and the characteristic screening angle, respectively. Bohr radius and the Born parameter,  $a_0 = \hbar^2/me^2$  and  $\alpha = zZ/137\beta$ , are used in the table.

| Author              | V(r)                        | a                    | $\chi_0$     | $\chi_{ m a}$                  |
|---------------------|-----------------------------|----------------------|--------------|--------------------------------|
| Goudsmit-Saunderson | $rac{Ze^2}{r}\exp(-r/a)$   | $a_0 Z^{-1/3}$       | $\hbar/(ap)$ | $\chi_0$                       |
| Molière             | $rac{zZe^2}{r}\omega(r/a)$ | $0.885 a_0 Z^{-1/3}$ | $\hbar/(ap)$ | $\sqrt{1.13+3.76lpha^2}\chi_0$ |
| ${ m Snyder-Scott}$ | $rac{Ze^2}{r}\exp(-r/a)$   | $a_0 Z^{-1/3}$       | $\hbar/(ap)$ | $\chi_0$                       |

## 5 Evaluation of Kamata-Nishimura Constants for Pure Substances

#### 5.1 Molière screening model

If we adopt the Molière screening model [1], we get the equations for  $\Omega$  and K as

$$\Omega - \ln \Omega = 1 - 2C + \ln \frac{137^3 \pi (0.885 Z^{-1/3})^2}{(1.13 + 3.76 Z^2 / 137^2)L},$$
(29)

$$K^2 = \frac{E_{\rm s}^2 \Omega}{4L}.\tag{30}$$

Using the value of radiation length  $X_0$  [23] of

$$\frac{1}{X_0} = \frac{4N}{137A} Z(Z+1) r_{\rm e}^2 L \tag{31}$$

instead of L, we can determine  $\Omega$  and K consistent with widely-used table of material constants indicated by Particle Data Group [24]:

$$\Omega - \ln \Omega = \ln \frac{6680(Z+1)Z^{1/3}X_0}{(1+3.34Z^2/137^2)A},$$
(32)

$$K^{2} = 3.49 \times 10^{-4} \frac{Z(Z+1)}{A} X_{0} \Omega E_{s}^{2}.$$
(33)

In this case Kamata-Nishimura equation becomes

$$\frac{d}{z^2 dt} \ln \tilde{f} = -\frac{\zeta^2}{w^2} \left[1 - \frac{1}{\Omega} \ln \frac{\beta'^2 \zeta^2}{w^2}\right] \quad \text{where} \quad \beta'^2 = \frac{1 + 3.34 z^2 Z^2 / (137\beta)^2}{1 + 3.34 Z^2 / 137^2} \beta^2. \tag{34}$$

Kamata-Nishimura constants so obtained are listed in Table 2.

# 5.2 Other simple models which do not distinguish the characteristic screening angle from the Born screening angle

According to Goudsmit and Saunderson [25], Snyder and Scot [26], and Rossi [20], they do not distinguish the characteristic screening angle from the Born screening angle;

$$\chi_{\rm a} = \chi_0. \tag{35}$$

In those cases, it satisfies

$$\beta' = \beta, \tag{36}$$

| Material            | Z  | A       | $X_0$       | Ω            | K            |
|---------------------|----|---------|-------------|--------------|--------------|
|                     |    |         | $ m g/cm^2$ |              | ${ m MeV}$   |
| Н                   | 1  | 1.008   | 61.28       | 16.40(16.54) | 17.69(17.76) |
| ${\rm He}$          | 2  | 4.003   | 94.32       | 16.07(16.20) | 18.88(18.96) |
| ${ m Li}$           | 3  | 6.941   | 82.76       | 15.80(15.93) | 18.83(18.91) |
| С                   | 6  | 12.011  | 42.70       | 15.34(15.48) | 18.96(19.04) |
| Ν                   | 7  | 14.007  | 37.99       | 15.25(15.39) | 19.06(19.15) |
| 0                   | 8  | 15.999  | 34.24       | 15.17(15.31) | 19.15(19.24) |
| Al                  | 13 | 26.982  | 24.01       | 14.85(15.02) | 19.43(19.53) |
| Si                  | 14 | 28.086  | 21.82       | 14.80(14.97) | 19.47(19.58) |
| S                   | 16 | 32.066  | 19.50       | 14.71(14.89) | 19.54(19.66) |
| $\operatorname{Ar}$ | 18 | 39.948  | 19.55       | 14.63(14.82) | 19.60(19.73) |
| Fe                  | 26 | 55.845  | 13.84       | 14.34(14.60) | 19.79(19.96) |
| Cu                  | 29 | 63.546  | 12.86       | 14.25(14.53) | 19.84(20.03) |
| $\operatorname{Br}$ | 35 | 79.904  | 11.42       | 14.08(14.42) | 19.94(20.19) |
| Ag                  | 47 | 107.868 | 8.97        | 13.77(14.25) | 20.13(20.48) |
| Ι                   | 53 | 126.904 | 8.48        | 13.62(14.19) | 20.22(20.63) |
| W                   | 74 | 183.840 | 6.76        | 13.15(14.02) | 20.52(21.19) |
| Pb                  | 82 | 207.200 | 6.37        | 12.99(13.97) | 20.65(21.42) |

Table 2: Kamata-Nishimura constants  $\Omega$  and K for pure substances derived from the Molière screening model, together with those (embraced) from the simple model of  $\chi_a = \chi_0$ .

so that we get the Kamata-Nishimura constants from

$$\Omega - \ln \Omega = 1 - 2C + \ln \frac{137^3 \pi (0.885 Z^{-1/3})^2}{L},$$
(37)

$$K^2 = \frac{E_s^2 \Omega}{4L},\tag{38}$$

or by using  $X_0$  we get

$$\Omega - \ln \Omega = \ln \frac{1.13 \times 6680(Z+1)Z^{1/3}X_0}{A},$$
(39)

$$K^{2} = 3.49 \times 10^{-4} \frac{Z(Z+1)}{A} X_{0} \Omega E_{\rm s}^{2}.$$
(40)

This time, Kamata-Nishimura equation becomes

$$\frac{d}{z^2 dt} \ln \tilde{f} = -\frac{\zeta^2}{w^2} [1 - \frac{1}{\Omega} \ln \frac{\beta^2 \zeta^2}{w^2}].$$
(41)

Kamata-Nishimura constants obtained in this case are tabulated in Table 2, embraced by brackets.

# 6 Angular Distribution of Charged Particles Traversing Through Mixed or Compound Substance

The diffusion equation for the angular distribution of charged particles is described as

$$d\tilde{f} = -\frac{\zeta^2}{w^2} \tilde{f}(1 - \frac{1}{\Omega} \ln \frac{\beta^{\prime 2} \zeta^2}{w^2}) z^2 dt,$$
(42)

in the Fourier space. So the increase of Fourier component in the differential passage becomes

$$-d\ln\tilde{f} = \frac{1}{X_0 w^2} (1 - \frac{1}{\Omega} \ln \frac{\beta'^2}{w^2}) \zeta^2 z^2 dx - \frac{1}{X_0 w^2 \Omega} (\zeta^2 \ln \zeta^2) z^2 dx.$$
(43)

In case of charged particles traversing through mixed or compound substance, the coefficients appearing in the right-hand side changes discontinuously corresponding to the atoms they encounter. So we take the value of coefficient as the expectation value of it. Thus we get

$$-\ln 2\pi \tilde{f} = \zeta^2 \int_0^x \Pr[\frac{1}{X_0 w^2} (1 - \frac{1}{\Omega} \ln \frac{\beta'^2}{w^2})] z^2 dx - \zeta^2 \ln \zeta^2 \int_0^x \Pr[\frac{1}{X_0 \Omega w^2}] z^2 dx, \tag{44}$$

where the expectation value is taken as the weighted mean value by the fractions of mass:

$$\Pr[Q] \equiv \sum_{i} p_i Q_i. \tag{45}$$

thus

$$\tilde{f} = \frac{1}{2\pi} \exp\{-\zeta^2 \int_0^x \Pr[\frac{1}{X_0 w^2} (1 - \frac{1}{\Omega} \ln \frac{\beta'^2}{w^2})] z^2 dx + \zeta^2 \ln \zeta^2 \int_0^x \Pr[\frac{1}{X_0 \Omega w^2}] z^2 dx\}.$$
(46)

So using the translation formula indicated in the Appendix, we get the angular distribution characterized by the expansion parameter B of

$$B - \ln B = \int_0^x \Pr\left[\frac{1}{X_0 w^2} \left(1 - \frac{1}{\Omega} \ln \frac{\beta'^2}{w^2}\right)\right] z^2 dx / \int_0^x \Pr\left[\frac{1}{X_0 \Omega w^2}\right] z^2 dx + \ln \int_0^x \Pr\left[\frac{1}{X_0 \Omega w^2}\right] z^2 dx$$
(47)

and the unit of Molière angle

$$\theta_{\rm M} = 2\sqrt{B\int_0^x \Pr[\frac{1}{X_0\Omega w^2}]z^2 dx}.$$
(48)

If we assume homogeneous mixture of substances, integration of the expectation value along the thickness should become

$$\int_0^x \Pr[f(x)]dx = \Pr[\frac{\bar{X}_{\mathrm{R}}}{X_{\mathrm{R}}} \int_0^{x/(\bar{X}_{\mathrm{R}}/X_{\mathrm{R}})} f(x)dx],\tag{49}$$

where  $X_{\rm R}$  denotes the range of particle measured in g/cm<sup>2</sup>,

$$X_{\rm R} \equiv E_0 / \frac{dE}{dx}$$
 and  $\bar{X}_{\rm R} \equiv E_0 / \Pr[\frac{dE}{dx}],$  (50)

In case of  $\beta' \approx \beta$ , which is realized for singly charged particles of relativistic condition or charged particles penetrating through light substances in such a condition as  $zZ \ll 137\beta$ , we have

$$-d\ln\tilde{f} = \{\frac{K^2}{X_0}(1 - \frac{1}{\Omega}\ln K^2)\frac{\zeta^2}{4p^2v^2} - \frac{K^2}{X_0\Omega}\frac{\zeta^2}{4p^2v^2}\ln\frac{\beta^2\zeta^2}{4p^2v^2}\}dx.$$
(51)

Thus

$$-\ln 2\pi \tilde{f} = \int_0^x \Pr[\frac{K^2}{X_0} (1 - \frac{1}{\Omega} \ln K^2)] \frac{\zeta^2}{4p^2 v^2} dx - \int_0^x \Pr[\frac{K^2}{X_0 \Omega}] \frac{\zeta^2}{4p^2 v^2} \ln \frac{\beta^2 \zeta^2}{4p^2 v^2} dx.$$
(52)

If we introduce the reduced Kamata-Nishimura constants for mixed or compound substance,  $\overline{\Omega}$  and  $\overline{K}$ , from the equations

$$\frac{\bar{K}^2}{\bar{X}_0}(1 - \frac{1}{\bar{\Omega}}\ln\bar{K}^2) = \Pr[\frac{K^2}{X_0}(1 - \frac{1}{\Omega}\ln K^2)],$$
(53)

$$\frac{\bar{K}^2}{\bar{X}_0\bar{\Omega}} = \Pr[\frac{K^2}{X_0\Omega}],\tag{54}$$

Table 3: The reduced Kamata-Nishimura constants,  $\overline{\Omega}$  and  $\overline{K}$ , for mixed or compound substances derived from the Molière screening model, together with those (embraced) from the simple model of  $\chi_{a} = \chi_{0}$ .

| Material         | $ar{X}_0$   | $\bar{\Omega}$ | $\bar{K}$    |
|------------------|-------------|----------------|--------------|
|                  | $ m g/cm^2$ |                | ${ m MeV}$   |
| Air              | 36.61       | 15.21(15.35)   | 19.10(19.19) |
| $\mathrm{SiO}_2$ | 27.04       | 14.95(15.11)   | 19.34(19.44) |
| $H_2O$           | 36.02       | 15.23(15.37)   | 19.06(19.15) |
| ${ m LiH}$       | 79.24       | 15.88(16.02)   | 18.65(18.73) |
| Emulsion         | 11.32       | 13.94(14.36)   | 20.01(20.31) |

then, taking  $\bar{X}_0$  as the radiation length for the compound substance [20], we get

$$\bar{\Omega} - \ln \bar{\Omega} = \Pr[\frac{K^2}{X_0} (1 - \frac{1}{\Omega} \ln K^2)] / \Pr[\frac{K^2}{X_0 \Omega}] + \ln \Pr[\frac{K^2}{X_0 \Omega}] + \ln \bar{X}_0,$$
(55)

$$\bar{K} = \sqrt{\bar{X}_0 \bar{\Omega} \Pr[\frac{K^2}{X_0 \Omega}]}.$$
(56)

In this case we can get the Molière angular distribution for mixed or compound substances by regarding they are pure materials with the reduced Kamata-Nishimura constants,  $\bar{\Omega}$  and  $\bar{K}$ . So that the distribution is determined by the expansion parameter B and the unit of Molière angle  $\theta_{\rm M}$  derived from

$$B - \ln B = \bar{\Omega} - \ln \bar{\Omega} + \ln(\nu z^2 t/\beta^2) \quad \text{and} \quad \theta_{\rm M} = \bar{\theta}_{\rm G} \sqrt{B/\bar{\Omega}}, \tag{57}$$

where  $\bar{\theta}_{\rm G}$  is derived from Eq. (14) with  $\Omega$  and K replaced by  $\bar{\Omega}$  and  $\bar{K}$ . The reduced Kamata-Nishimura constants,  $\bar{\Omega}$  and  $\bar{K}$ , for mixed or compound substance are tabulated in Table 3. The distribution for mixed or compound substances can also be got by the reduced constants in case we can neglect energy loss or in case assuming simple screening model of  $\chi_{\rm a} = \chi_0$ .

By using the reduced constants, we can slightly simplify Eqs. (47) and (48) for general energy conditions, as

$$B - \ln B = \int_0^x \Pr[\frac{1}{X_0 w^2} (1 - \frac{1}{\Omega} \ln \frac{\beta'^2}{w^2})] z^2 dx / \frac{\bar{\theta}_{\rm G}^2}{4\bar{\Omega}} + \ln \frac{\bar{\theta}_{\rm G}^2}{4\bar{\Omega}}$$
(58)

and the unit of Molière angle

$$\theta_{\rm M} = \bar{\theta}_{\rm G} \sqrt{B/\bar{\Omega}}.\tag{59}$$

In general energy conditions we should get exact B and  $\theta_{\rm M}$  from the above equations. But in practical use, the approximation to regard the mixed or compound substance as a pure one with the reduced Kamata-Nishimura constants will be available. The results of exact B and  $\theta_{\rm M}$  are compared with those from the approximate method for nuclear emulsion in Figs. 5 and 6. We used  $\Pr[Z]$  for the charge number in the approximate method. We cannot observe almost any differences.

### 7 Conclusions and Discussions

Kamata-Nishimura formulation of the Molière theory, having been described for electrons of relativistic condition, is reconstructed to be valid in the general energy range and to wider variety of charged particles irrespective of mass and charge. Molière theory is simply described in the Kamata-Nishimura formulation by an ordinary differential equation of Fermi-Yang type in the Fourier space, possessing the two Kamata-Nishimura constants specific to the substance. We can obtain the Molière distribution much easily, moreover improve Molière angular distribution to take into account ionization loss, by the formulation. The Kamata-Nishimura constants are recalculated so that they should be consistent with the widely-used material constants of Particle Data Group [24] and are tabulated in Table 2.

The method to obtain the angular distribution for charged particles traversing through mixed or compound substance is investigated on the Kamata-Nishimura formulation. In general, Molière distribution in the substances can be obtained by taking the expectation values for coefficients in the equation as the weighted mean values by the fraction of mass. In case of e.g. fixed energy approximation, traversing through light substances, or assuming other simple screening model than Molière, we can regard the mixed or compound substance as a pure one with the reduced Kamata-Nishimura constants listed in Table 3. Approximated method to apply the reduced constants even in general cases have shown good accuracies in so far from our restricted investigations.

The present formulation will be valuable in cross check for other theoretical works or simulation results as a scarce multiple scattering theory with ionization. Examinations by and applications to experiments will also be followed using the Particle Telescope of Okayama University [28].

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## Appendix

We show a translation formula between the Kamata-Nishimura formulation and the Molière-Bethe one. Let the image function by Kamata-Nishimura be of a form [27]

$$\tilde{f} = \frac{1}{2\pi} \exp\{-a\zeta^2 + b\zeta^2 \ln(c\zeta^2)\}.$$
(60)

If we new define the expansion parameter B and the composite transform-variable u, as

$$B - \ln B = \frac{a}{b} - \ln \frac{c}{b}$$
 and  $u = 2\zeta \sqrt{bB}$ , (61)

then we get the well known Molière form

$$\tilde{f} = \frac{1}{2\pi} \exp\{-\frac{u^2}{4}\left(1 - \frac{1}{B}\ln\frac{u^2}{4}\right)\}.$$
(62)

So that the probability density can be represented in the Molière series of

$$f(\vartheta) = f^{(0)}(\vartheta) + B^{-1}f^{(1)}(\vartheta) + B^{-2}f^{(2)}(\vartheta) + \dots,$$
(63)

where the Molière angle is defined by the new unit,

$$\vartheta = \theta/\theta_{\rm M} \quad \text{with} \quad \theta_{\rm M} = (2\sqrt{bB}).$$
(64)

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Figure 1: Angular distributions multiplied by  $\theta^2$  at depth  $t/(E_0/\varepsilon)$  of 0.1, 0.3, 0.5, 0.7, and 0.9 from left to right. Dot lines indicate accumulations of single scatterings.



Figure 2: Variation of the scale factor  $\nu$  against t. Abscissa means  $t/(E_0/\varepsilon)$ . The curves correspond to incident energies  $E_0/(mc^2)$  of 10, 20, 50, and  $\infty$ .



Figure 3: Depth-variation of *B* for various incident energies,  $E_0/\varepsilon$  of 10, 10<sup>2</sup>, 10<sup>3</sup>, and 10<sup>4</sup> in unit of  $\Omega e^{-\Omega}$ , from left to right. Thin line indicates traditional *B* for fixed energy.



Figure 4: Depth-variation of  $\theta_{\rm M}$  for various incident energies,  $E_0/\varepsilon$  of 10, 10<sup>2</sup>, 10<sup>3</sup>, and 10<sup>4</sup> in unit of  $\Omega e^{-\Omega}$ , from left to right. Thin line indicates traditional  $\theta_{\rm M}$  for fixed energy.



Figure 5: Comparison of *B* for mixed or compound substance, between exact results and approximated ones. Four curves correspond to  $E_0/\varepsilon$  of 10, 10<sup>2</sup>, 10<sup>3</sup>, and 10<sup>4</sup> in unit of  $\Omega e^{-\Omega}$ , from left to right.



Figure 6: Comparison of  $\theta_{\rm M}$  for mixed or compound substance, between exact results and approximated ones. Four curves correspond to  $E_0/\varepsilon$  of 10, 10<sup>2</sup>, 10<sup>3</sup>, and 10<sup>4</sup> in unit of  $\Omega e^{-\Omega}$ , from left to right.