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## A SINGLE-SCATTERING DIVIDING MODEL TO INTERPRET THE MOLIÈRE SCATTERING PROCESS

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#### Abstract

Molière process of multiple Coulomb scattering is attempted to be interpreted by dividing the single scattering cross-section at a separation angle into moderate scattering and large-angle scattering. The high-frequent moderate scattering produces the central gaussian distribution although the low-frequent large-angle scattering interferes the central gaussian distribution to change the width, which causes the angular distribution to be described in double series. Only when we adopt the separation angle adequately, the large-angle scattering does not interfere the shape of the central gaussian distribution and the angular distribution is described in the single series of Molière. Magnitude of the expansion parameter B is determined by the ratio of the width of central gaussian distribution to the screening angle, as a first approximation. Under the fixed-energy condition, the central gaussian distribution broadens monotonously but the screening angle stays constant, so that B increases monotonously. On the other hand under the ionization process, the central gaussian distribution broadens rapidly at first stage and broadens later as  $E^{-1/2}$  as dissipation of energy although the screening angle increases as  $E^{-1}$ , so that B increases at first but begins to decrease at the latter stage of propagation.

#### 1 Introduction

We have found the analytical solution of Molière angular distribution with ionization [1] by using Kamata-Nishimura formulation of the theory [2, 3]. The angular distribution indicated in Fig. 1 is expressed by series expansion of the same universal functions as Molière [4, 5] and Bethe [6], only with the increased scale angle  $\theta_{\rm M}$  and the decreased expansion parameter B. Although there exist many excellent investigations about Molière theory [7, 8], there remain yet difficult properties to understand in Molière process: Why does Molière-Bethe formulation give the effective single series although Kamata-Nishimura gives the double series ? Why does the *shape* parameter B begin to decrease at the latter stage of propagation under the ionization process, in spite it increased monotonusly under the fixed-energy process ?

We have attempted to interpret by dividing the single scattering cross-section into the moderate scattering and the large-angle scattering, and investigated the interference of the large-angle scattering to the central gaussian distribution produced by the moderate scattering. We have found the large-angle scattering does not change the shape of the central gaussian distribution when the separation angle is adequately selected depending on the traversed thickness, and just under this condition the angular distribution is described by the single series and the parameter B changes as above with the traverse.

We will do our investigations under the extreme relativistic conditions.

## 2 Separation of the Single Scattering into Moderate and Large-Angle Scatterings

We start with the single scattering formula of

$$\frac{N}{A}\sigma(\theta)2\pi\theta d\theta dx = \frac{1}{\pi\Omega}\frac{K^2}{E^2}\theta^{-4}2\pi\theta d\theta dt \quad \text{with} \quad \theta > \sqrt{e}\chi_a,\tag{1}$$



Figure 1: Angular distributions multiplied by  $\theta^2$ . Solid lines correspond to those at  $t/(E_0/\varepsilon)$  of 0.1, 0.3, 0.5, 0.7, and 0.9 from left to right. Dot lines indicate accumulated distributions of the single scattering.  $\Omega e^{-\Omega}$  of order of  $10^{-6}$  agrees with  $e^{2C-2}$  times mean-free-path of the single scattering.

where we used the scattering constants  $\Omega$  and K defined by Kamata and Nishimura [2, 3], assuming the extreme relativistic condition:

$$E \gg mc^2. \tag{2}$$

We temporarily separate the single-scattering cross-section  $\sigma$  into the moderate scattering  $\sigma_{\rm M}$ and the large-angle scattering  $\sigma_{\rm L}$  at an angle of  $\chi'_{\rm B}$ , locating at  $e^{B'/2}$  times large angle of the screening angle  $\sqrt{e}\chi_{\rm a}$ , as indicated in Fig. 2:

$$\sigma(\theta) = \sigma_{\rm M}(\theta) + \sigma_{\rm L}(\theta), \tag{3}$$

where B' is taken as a temporary constant irrespective of dissipation of the energy. Thus we have

$$\sqrt{e}\chi_{\mathbf{a}} = (K/E)e^{-\Omega/2 + 1 - C},\tag{4}$$

$$\chi'_{\rm B} \equiv e^{B'/2} \sqrt{e} \chi_{\rm a}.$$
 (5)

## 3 The Diffusion Equation

Then the diffusion equation to determine the angular distribution  $f(\vec{\theta}, t)d\vec{\theta}$  is described as

$$\frac{d}{dx}f(\vec{\theta},t) = \frac{N}{A} \iint \{f(\vec{\theta}-\vec{\theta'},t) - f(\vec{\theta},t)\}\sigma(\vec{\theta'})d\vec{\theta'}.$$
(6)

Under the azimuthally symmetric condition, the equation is converted to

$$\frac{d\tilde{f}}{dt} = -2\pi \frac{N}{A} X_0 \tilde{f} \int_0^\infty [1 - J_0(\zeta \theta)] \{\sigma_{\rm M}(\theta) + \sigma_{\rm L}(\theta)\} \theta d\theta \tag{7}$$



Figure 2: Separation of the single scattering  $\sigma$  at  $\chi_{\rm B}$  to the moderate scattering  $\sigma_{\rm M}$  and the large-angle scattering  $\sigma_{\rm L}$ .

by the Hankel transforms, where the traversed thickness x in  $g/cm^2$  is converted to t in radiation length [9]. Using the Bethe's evaluation [6]

$$I_1(x) \equiv 4 \int_x^\infty t^{-3} [1 - J_0(t)] dt \simeq 1 + \ln 2 - C - \ln x + O(x^2), \tag{8}$$

there hold

$$\frac{N}{A}X_0 \int_0^\infty [1 - J_0(\zeta\theta)] \sigma_{\rm M}(\theta) 2\pi\theta d\theta \simeq \frac{B'}{\Omega} \frac{K^2 \zeta^2}{4E^2},\tag{9}$$

$$\frac{N}{A}X_0 \int_0^\infty [1 - J_0(\zeta\theta)]\sigma_{\rm L}(\theta) 2\pi\theta d\theta \simeq -\frac{1}{B'}\frac{B'}{\Omega}\frac{K^2\zeta^2}{4E^2}\ln\left(\frac{K^2\zeta^2}{4E^2}e^{B'-\Omega}\right),\tag{10}$$

so the differential equation (7) becomes

$$\frac{d\tilde{f}}{dt} = -\frac{B'}{\Omega} \frac{K^2 \zeta^2}{4E^2} \tilde{f} \{ 1 - \frac{1}{B'} \ln\left(\frac{K^2 \zeta^2}{4E^2} e^{B' - \Omega}\right) \}.$$
(11)

Kamata-Nishimura equation [2, 3]

$$\frac{d\tilde{f}}{dt} = -\frac{K^2 \zeta^2}{4E^2} \tilde{f} \{ 1 - \frac{1}{\Omega} \ln \frac{K^2 \zeta^2}{4E^2} \}$$
(12)

is a special case of replacing B' with  $\Omega$ . It should be reminded that an application of factor (9) or (10) changes any angular distribution by one more single scattering of  $\sigma_{\rm M}$  or  $\sigma_{\rm L}$ , in the frequency space.

## 4 Integration of the Diffusion Equation and the Meaning of Terms

Eq. (11) can be integrated as

$$\tilde{f} = \frac{1}{2\pi} \exp\{-\langle \frac{B'}{\Omega} \frac{K^2 \zeta^2}{4E^2} \rangle_{av} t + \langle \frac{1}{B'} \frac{B'}{\Omega} \frac{K^2 \zeta^2}{4E^2} \ln(\frac{K^2 \zeta^2}{4E^2} e^{B'-\Omega}) \rangle_{av} t\}, 
= \frac{1}{2\pi} \exp\{-\langle \frac{B'}{\Omega} \frac{K^2 \zeta^2}{4E^2} \rangle_{av} t\} \sum_{0}^{\infty} \frac{1}{k!} \{\langle \frac{1}{B'} \frac{B'}{\Omega} \frac{K^2 \zeta^2}{4E^2} \ln(\frac{K^2 \zeta^2}{4E^2} e^{B'-\Omega}) \rangle_{av} t\}^k,$$
(13)

where the average  $\langle Q \rangle_{\rm av}$  of the variable Q is taken along the traversed thickness:

$$\langle Q \rangle_{\rm av} \equiv t^{-1} \int_0^t Q(t') dt'.$$
<sup>(14)</sup>

The solution can be expressed in a series expansion with  $B'^{-1}$  as

$$\tilde{f} = \tilde{f}_0 + B'^{-1}\tilde{f}_1 + B'^{-2}\tilde{f}_2 + \cdots,$$
(15)

where we distinguished  $f_k$  from  $f^{(k)}$  of Molière-Bethe [5, 6], then  $B'^{-k}\tilde{f}_k$  can be got from Eq. (13):

$$B'^{-k}\tilde{f}_{k} = \frac{1}{2\pi} \frac{1}{k!} \{ \langle \frac{1}{B'} \frac{B'}{\Omega} \frac{K^{2} \zeta^{2}}{4E^{2}} \ln(\frac{K^{2} \zeta^{2}}{4E^{2}} e^{B'-\Omega}) \rangle_{\mathbf{av}} t \}^{k} \exp\{-\frac{B'}{\Omega} \langle \frac{K^{2} \zeta^{2}}{4E^{2}} \rangle_{\mathbf{av}} t \}.$$
(16)

This k-th term in the frequency space corrects the preceding series by one more large-angle scattering  $\sigma_{\rm L}$  than the preceding k - 1-th term, corresponding to its probability within the thickness.

## 5 Series Expansion Derived from the Arbitrarily-Selected Separation Angle

Under the ionization process of

$$E = E_0 - \varepsilon t, \tag{17}$$

there hold

$$\int_{0}^{t} \frac{K^{2}}{E^{2}} dt = \frac{K^{2}t}{E_{0}E},$$
(18)

$$\int_0^t \frac{K^2}{E^2} \ln \frac{K^2}{E^2} dt = \frac{K^2 t}{E_0 E} \ln \frac{K^2}{\nu E_0 E},\tag{19}$$

where  $\nu$  denotes a factor expressed as

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

appearing under the ionization process. Thus we have

$$\tilde{f} = \frac{1}{2\pi} \exp\{-\frac{B'}{\Omega} \frac{K^2 t \zeta^2}{4E_0 E} + \frac{1}{B'} \frac{B'}{\Omega} \frac{K^2 t \zeta^2}{4E_0 E} \ln(\frac{K^2 \zeta^2}{4\nu E_0 E} e^{B' - \Omega})\},\$$
  
$$= \frac{1}{2\pi} \exp\{-\frac{\theta_{\rm M}^{\prime 2} \zeta^2}{4} (1 - \frac{1}{B'} [\ln \frac{\theta_{\rm M}^{\prime 2} \zeta^2}{4} - \ln \tau])\},\$$
(21)

with

$$\theta_{\rm M}^{\prime 2} \equiv \frac{B'}{\Omega} \theta_{\rm G}^2 = \frac{B'}{\Omega} \frac{K^2 t}{E_0 E},\tag{22}$$

$$\tau \equiv \frac{\nu}{E/E_0} \frac{\theta_{\rm M}^{\prime 2}}{\chi_{\rm B}^{\prime 2}} e^{2-2C}, \qquad (23)$$

where  $\theta_{\rm G}^2$  denotes the gaussian mean-square angle [9], only with  $E_{\rm s}$  replaced by K:

$$\theta_{\rm G}^2 = K^2 t / (E_0 E). \tag{24}$$

If we introduce composite variables

$$\alpha \equiv \theta'_{\rm M} \zeta \quad \text{and} \quad \vartheta \equiv \theta/\theta'_{\rm M},$$
(25)

then the integration can be expanded as

$$\tilde{f} = \frac{1}{2\pi} \exp\{-\frac{\alpha^2}{4} (1 - \frac{1}{\Omega} [\ln \frac{\alpha^2}{4} - \ln \tau])\} = \frac{1}{2\pi} \exp\{-\frac{\alpha^2}{4}\} \sum_{k=0}^{\infty} \frac{1}{k!} \{\frac{1}{\Omega} \frac{\alpha^2}{4} (\ln \frac{alpha^2}{4} - \ln \tau)\}^k,$$
(26)

so that, applying Hankel transforms we have a double series with  $B'^{-1}$  and  $\ln \tau$ :

$$2\pi f(\vartheta) = f^{(0)}(\vartheta) + \frac{1}{B'} \{ f^{(1)}(\vartheta) + f_1^{(1)}(\vartheta) \ln \tau \} + \frac{1}{B'^2} \{ f^{(2)}(\vartheta) + f_1^{(2)}(\vartheta) \ln \tau + f_2^{(2)}(\vartheta) (\ln \tau)^2 \} + \cdots$$
(27)

Universal series functions  $f^{(0)}(\vartheta)$ ,  $f^{(1)}(\vartheta)$ , and  $f^{(2)}(\vartheta)$ , same as Molière-Bethe's, and others are expressed [10] as

$$f^{(0)}(\vartheta) = \int_{0}^{\infty} \alpha d\alpha J_{0}(\vartheta \alpha) e^{-\alpha^{2}/4}$$
  
=  $2e^{-\vartheta^{2}},$  (28)

$$f^{(1)}(\vartheta) = \int_0^\infty \alpha d\alpha J_0(\vartheta \alpha) \frac{\alpha^2}{4} e^{-\alpha^2/4} \ln \frac{\alpha^2}{4}$$
$$= 2e^{-\vartheta^2}(\vartheta^2 - 1)[E_i(\vartheta^2) - \ln \vartheta^2] - 2(1 - 2e^{-\vartheta^2}),$$
(29)

$$f_1^{(1)}(\vartheta) = -\int_0^\infty \alpha d\alpha J_0(\vartheta \alpha) \frac{\alpha^2}{4} e^{-\alpha^2/4}$$
  
=  $2e^{-\vartheta^2}(\vartheta^2 - 1),$  (30)

$$f^{(2)}(\vartheta) = \frac{1}{2} \int_{0}^{\infty} \alpha d\alpha J_{0}(\vartheta \alpha) (\frac{\alpha^{2}}{4})^{2} e^{-\alpha^{2}/4} (\ln \frac{\alpha^{2}}{4})^{2}$$
  

$$= e^{-\vartheta^{2}} (\vartheta^{4} - 4\vartheta^{2} + 2) [\psi'(3) + \psi^{2}(3)]$$
  

$$+ 4e^{-\vartheta^{2}} \int_{0}^{1} t^{-3} [\ln \frac{t}{1-t} - \psi(3)] [(1-t)^{2} e^{\vartheta^{2}t} - 1 - (\vartheta^{2} - 2)t - \frac{1}{2} (\vartheta^{4} - 4\vartheta^{2} + 2)t^{2}] dt,$$
(31)

$$f_{1}^{(2)}(\vartheta) = -\int_{0}^{\infty} \alpha d\alpha J_{0}(\vartheta \alpha) (\frac{\alpha^{2}}{4})^{2} e^{-\alpha^{2}/4} \ln \frac{\alpha^{2}}{4} \\ = 2e^{-\vartheta^{2}} (\vartheta^{4} - 4\vartheta^{2} + 2) [E_{i}(\vartheta^{2}) - \ln \vartheta^{2}] + 4e^{-\vartheta^{2}} (2\vartheta^{2} - 3) - 2(\vartheta^{2} - 3),$$
(32)

$$f_2^{(2)}(\vartheta) = \frac{1}{2} \int_0^\infty \alpha d\alpha J_0(\vartheta \alpha) (\frac{\alpha^2}{4})^2 e^{-\alpha^2/4}$$
  
=  $e^{-\vartheta^2} (\vartheta^4 - 4\vartheta^2 + 2).$  (33)

We indicate these functions in Fig. 3.

## 6 Molière Single Series Derived From the Adequately-Selected Separation Angle

Only when the term  $\ln \tau$  vanishes,

$$\ln \tau = 0, \tag{34}$$

Eq. (21) gives the Molière single series:

$$2\pi f(\vartheta) = f^{(0)}(\vartheta) + \frac{1}{B'} f^{(1)}(\vartheta) + \frac{1}{B'^2} f^{(2)}(\vartheta) + \cdots$$
(35)



Figure 3: Universal series functions multiplied by  $\theta^2$  under the Kamata-Nishimura formulation of Molière theory.

In fact,  $\ln \tau = 0$  gives the equation for Molière expansion parameter B under the extreme relativistic condition proposed as Eq. (20) in our preceding paper [1]:

$$B - \ln B = \Omega - \ln \Omega + \ln(\nu t). \tag{36}$$

 $\nu$  appearing in the formula is a decreasing factor with t smaller than 1, so that we can call  $\nu$  as the contraction factor.

Existence of a term with  $\ln \tau$  in Eq. (21) would vary the mean-square angle  $\theta'^2_M$  of the central gaussian distribution by a factor of magnitude  $1 + B'^{-1} \ln \tau$ . In fact,  $f_1^{(1)}(\vartheta)$  appearing in the double series (27) was the term to broaden the central gaussian distribution. Under the gaussian approximation of fixed-energy condition, it satisfied

$$de^{-\theta_{\rm G}^2 \zeta^2/4} = -\frac{\alpha^2}{4} e^{-\alpha^2/4} d\ln t = \tilde{f}_1^{(1)}(\alpha) d\ln t, \qquad (37)$$

so that  $f_1^{(1)}(\vartheta)$  increased the width of gaussian distribution monotonously in the angular space.

As a result we can read the supplementary terms appearing in the double series (27) to the single series (35) of Molière are the correction terms arising from inadequately-selected widths of the central gaussian distribution.

# 7 Qualitative Interpretation for Variation of the Expansion Parameter B

We found in the preceding section that Molière expansion parameter B is determined from a free parameter B' when it satisfies  $\ln \tau = 0$ , or

$$\chi_{\rm B}^{\prime 2} = \frac{\nu}{E/E_0} \theta_{\rm M}^{\prime 2} e^{2-2C}.$$
(38)

We can also derive the Molière B by a successive method. Left-hand side of Eq. (38) depends on B' more strongly than the right-hand side. So substitution of a temporary B' in the right-hand



Figure 4: The expansion parameter B can be determined by a successive method.



Figure 5: *B* is evaluated by putting  $\theta_{\rm M} = \theta_{\rm G}$  as a first approximation under the fixed-energy process.

side gives a more accurate B' in the left-hand side, and successive application of this correction finally gives the Molière B as indicated in Fig. 4.

Qualitative feature of the Molière *B* is studied from a first approximation of *B* derived by substituting  $\theta_{\rm G}^2$  instead of  $\theta_{\rm M}'^2$  on the right-hand side of Eq. (38). Under the fixed-energy conditions, Eq. (38) becomes

$$\chi_{\rm B}^{\prime 2} = \theta_{\rm M}^{\prime 2} e^{2-2C} \tag{39}$$

and  $\theta_{\rm G}^2$  of Eq. (24) is expressed by

$$\theta_{\rm G}^2 = K^2 t / E^2. \tag{40}$$

So the first approximation of  $\chi_B$  increases monotonously as  $t^{1/2}$  with the traversed thickness, on the other hand  $\sqrt{e}\chi_a$  stays constant. B' is defined in (5) by a half of logarithm of the ratio  $\chi'_B/\sqrt{e}\chi_a$ . So we can understand B increases monotonously with the traversed thickness, as indicated in Fig. 5.

Under the ionization process,  $\nu$  and  $E/E_0$  in Eq. (38) both decrease monotonously with the traversed thickness. So a rough estimation of *B* could be made by neglecting the factor  $\nu/(E/E_0)$  and substituting  $\theta_G^2$  of (24) into  $\theta_M'^2$  on the right-hand side.  $\sqrt{e\chi_a}$  increases proportionally to  $E^{-1}$  with dissipation of energy in this condition, on the other hand  $\theta_G$  increases more rapidly at first stage but later it increases more slowly as proportional to  $E^{-1/2}$  than  $\sqrt{e\chi_a}$ , as indicated in Fig. 6.



Figure 6: *B* is evaluated by neglecting  $\nu/(E/E_0)$  and putting  $\theta_M = \theta_G$  as a first approximation under the ionization process.

So B increases at first stage of traverse, nevertheless it begins to decrease in the latter stage under the ionization process.

#### 8 Conclusions and Discussions

Molière series expansion is well reconstructed by dividing the single scattering cross-section at  $e^{B/2}$  times larger angle than the screening angle  $\sqrt{e}\chi_{a}$ , when the low-frequent large-angle scattering greater than the separation angle does not interfere the shape of central gaussian distribution. Andreo and Brahme [11] as well as Fernandez-Varea et al. [12] proposed hybrid methods where they divided the single scattering cross-section to improve the efficiency of their simulation algorithm. The Molière separation angle will be a candidate of adequate angle to be applied in those hybrid methods in the above sense, almost irrespective of the single scattering model [13, 14, 15].

Magnitude of the expansion parameter B is evaluated by the ratio of the width of central gaussian distribution  $\theta_{\rm G}$  to the screening angle  $\sqrt{e}\chi_{\rm a}$ , as a first approximation. Under the fixedenergy condition,  $\theta_{\rm G}$  increases monotonously instead  $\sqrt{e}\chi_{\rm a}$  stays constant, so that B increases monotonously with traverse. On the other hand under the ionization process,  $\theta_{\rm G}$  increases rapidly at the first stage and increases as  $E^{-1/2}$  with dissipation of energy instead  $\sqrt{e}\chi_{\rm a}$  increases as  $E^{-1}$ with dissipation, so that B increases at first stage but begins to decrease at the latter stage of traverse.

The single-scattering dividing model proposed this time to interpret Molière scattering process will help our understandings of Molière theory from the physical aspect of view and be valuable in our designing and analyses of experiments concerning to charged particles as well as in our tracing charged particles in Monte Carlo simulations.

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