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THE CROSS-SECTION DIVIDING METHOD AND A STOCHASTIC INTERPRETATION OF THE MOLIÈRE EXPANSION

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Abstract

Properties of Molière scattering process are investigated through the cross-section dividing method. We divide the single-scattering at an adequate angle into the moderate scattering and the large-angle scattering. We have found the expansion parameter or the shape parameter B of Molière, which corresponds to the splitting angle of the single scattering at $e^{B/2}$ times the screening angle, acts as the probability parameter to receive the large-angle scattering. A mathematical formulation to derive the angular distribution through the cross-section dividing method is proposed. Small distortions from the gaussian distribution were found in the central distribution produced by the moderate scattering of Molière, due to the higher Fourier components. Smaller splitting angles than Molière, e.g. the one-scattering angle χ_C, will be effective for rapid sampling sequences of Molière angular distribution, giving almost gaussian central distributions as the product of moderate scatterings and low-frequent single-scatterings as the product of large-angle scatterings.

1 Introduction

We are investigating the properties and the mechanism of Molière scattering process and Molière expansion [1]. We found Molière expansion [2, 3, 4] was well explained by dividing of the single-scattering cross-section into the high frequent moderate scattering and the low frequent large-angle scattering. The splitting angle corresponds to $e^{B/2}$ times the screening angle in case of Molière expansion, when the large-angle scattering does not interfere the shape of the central distribution and the angular distribution is expressed by a simple single series. The probability of receiving the large-angle scattering in this case is evaluated as B^{-1} multiplied by a constant factor. So we find the Molière series implies the expansion by the probability of the large-angle scattering.

Based on these experiences, we have attempted to establish a mathematical formulation of the cross-section dividing method to reconstruct the Molière angular distributions.

2 The cross-section dividing method under the ionization process

The single-scattering formula is described as

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

where the screening angle $\sqrt{e}\chi_a$ is described as

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

The screening angle increases as E^{-1} with dissipation of energy. We took the splitting angle of the cross-section as a constant factor $e^{B'/2}$ greater than the screening angle the last time [1]. We take the splitting angle as a constant $\chi'_{\rm B}$, this time:

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

Then we have

$$\int_0^t \frac{2dt}{\Omega}\frac{K^2}{E^2}\int_{\sqrt{e}\chi_{\rm a}}^{\chi'_{\rm B}}[J_0(\zeta\theta)-1]\theta^{-3}d\theta \simeq -\frac{1}{\Omega}\frac{K^2\zeta^2 t}{4E_0E}\ln\frac{\chi'^2_{\rm B}}{(\sqrt{e}\hat{\chi}_{\rm a})^2}, \tag{4}$$

$$\int_0^t \frac{2dt}{\Omega}\frac{K^2}{E^2}\int_{\chi'_{\rm B}}^{\infty}[J_0(\zeta\theta)-1]\theta^{-3}d\theta \simeq \frac{1}{\Omega}\frac{K^2\zeta^2 t}{4E_0E}\ln\frac{\chi'^2_{\rm B}\zeta^2}{4e^{2-2C}}, \tag{5}$$

where the effective screening angle $\sqrt{e}\hat{\chi}_{\rm a}$ under the ionization process is defined as

$$\sqrt{e}\hat{\chi}_{\rm a} = \frac{K}{\sqrt{\nu E_0 E}}e^{-\Omega/2+1-C} \tag{6}$$

with

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

ν was a scaling factor appearing in the ionization process. Then introducing B' as

$$B' = 2\ln\frac{\chi'_{\rm B}}{\sqrt{e}\hat{\chi}_{\rm a}} \quad \text{or} \quad \chi'_{\rm B} = e^{B'/2}\sqrt{e}\hat{\chi}_{\rm a}, \tag{8}$$

we have the same generalized expansion formula

$$\begin{aligned} 2\pi f(\vartheta) = f^{(0)}(\vartheta) \quad &+ \quad \frac{1}{B'}\{f^{(1)}(\vartheta) + f_1^{(1)}(\vartheta)\ln\tau\} \\ &+ \quad \frac{1}{B'^2}\{f^{(2)}(\vartheta) + f_1^{(2)}(\vartheta)\ln\tau + f_2^{(2)}(\vartheta)(\ln\tau)^2\} + \cdots \end{aligned} \tag{9}$$

as last [1], where

$$\vartheta \equiv \theta/\theta'_{\rm M} \tag{10}$$

and

$$\theta'^2_{\rm M} \equiv \frac{B'}{\Omega}\theta^2_{\rm G} = \frac{B'}{\Omega}\frac{K^2 t}{E_0 E}, \tag{11}$$

$$\tau \equiv (\theta'^2_{\rm M}/\chi'^2_{\rm B})e^{2-2C}. \tag{12}$$

$\chi'_{\rm B}$ or B' was as an arbitrary constant, so we can take $\chi'_{\rm B}$ as $\ln\tau$ vanishes,

$$\chi_{\rm B} \equiv \theta_{\rm M}e^{1-C} = e^{B/2}\sqrt{e}\hat{\chi}_{\rm a}, \tag{13}$$

or

$$B - \ln B = \Omega - \ln\Omega + \ln(\nu t). \tag{14}$$

Then we have the simple single series of Molière:

$$2\pi f(\vartheta) = f^{(0)}(\vartheta) + \frac{1}{B}f^{(1)}(\vartheta) + \frac{1}{B^2}f^{(2)}(\vartheta) + \cdots. \tag{15}$$

The probability to receive the large-angle scattering within the penetrating depth in this condition is evaluated as

$$p \quad \equiv \quad \int_0^t dt\int_0^\infty \sigma_{\rm L}(\chi)2\pi\chi d\chi = \frac{t}{\Omega}e^{-B+\Omega-2+2C} = \frac{1}{B}e^{2C-2}, \tag{16}$$

so that we find the expansion parameter B also acts as the probability parameter, besides the shape parameter. This fact tells us that Molière expansion is consisted of the leading gaussian distribution produced by the moderate scatterings followed by the correction terms due to the single large-angle scattering, the double, the triple, and so on, weighted by the respective probabilities.

3 Mathematical formulation of the cross-section dividing method

The diffusion equation for the angular distribution

$$\frac{d}{dt}f(\vec{\theta},t) = \iint [f(\vec{\theta}-\vec{\theta'},t) - f(\vec{\theta},t)]\sigma(\vec{\theta'})d\vec{\theta'} \tag{17}$$

is described as

$$\frac{d\tilde{f}}{dt} = 2\pi\tilde{f}\int_0^\infty [J_0(\zeta\theta)-1]\sigma(\theta)\theta d\theta \tag{18}$$

in the frequency space under the azimuthally symmetric condition, so that we have

$$\begin{aligned}\tilde{f} &= \frac{1}{2\pi}\exp\{\int_0^t 2\pi dt\int_0^\infty [J_0(\zeta\theta)-1][\sigma_{\mathrm{M}}(\theta)+\sigma_{\mathrm{L}}(\theta)]\theta d\theta\} \\ &= \tilde{f}_{\mathrm{M}}\sum_{k=0}^\infty \frac{1}{k!}\{\int_0^x 2\pi dt\int_0^\infty [J_0(\zeta\theta)-1]\sigma_{\mathrm{L}}(\theta)\theta d\theta\}^k,\end{aligned} \tag{19}$$

where

$$\tilde{f}_{\mathrm{M}} = \frac{1}{2\pi}\exp\{\int_0^t 2\pi dt\int_0^\infty [J_0(\zeta\theta)-1]\sigma_{\mathrm{M}}(\theta)\theta d\theta\} \tag{20}$$

denotes the Hankel transforms of the central distribution $f_{\mathrm{M}}(\vartheta)d\vec{\vartheta}$ produced by the moderate scatterings. Then we have the Molière angular distribution by the probability series expansion:

$$f(\vartheta)d\vec{\vartheta} = d\vec{\vartheta}\sum_{k=0}^\infty \frac{1}{k!}p^k f_{\mathrm{M}} * \{\sigma_{\mathrm{L}}-1\}^{(k)} \tag{21}$$

with p defined in Eq. (16), where the operation $f * g^{(k)}$ denotes the k-times sequential folding integrals of g on f. It is easily confirmed that this expansion is also expressed by the poisson series expansion:

$$f(\vartheta)d\vec{\vartheta} = e^{-p}d\vec{\vartheta}\sum_{k=0}^\infty \frac{1}{k!}p^k f_{\mathrm{M}} * \sigma_{\mathrm{L}}^{(k)}. \tag{22}$$

4 The single and the double scattering folded with the gaussian distribution

The poisson series expansion (22) requires the large-angle double scattering distribution. We derive the distribution generally for the normalized single scattering σ_1 of

$$\sigma_1(\rho)d\vec{\rho} = \pi^{-1}\rho^{-4}d\vec{\rho} \quad \text{with} \quad \rho > 1. \tag{23}$$

Then the probability density of the double scattering $\sigma_1^{(2)}$ of the normalized single scattering $\sigma_1^{(1)}$ can be derived as

$$\begin{aligned}\sigma_1^{(2)}(\rho)d\vec{\rho} &= \pi^{-2}d\vec{\rho}\iint_{\rho'>1,|\vec{\rho}-\vec{\rho}'|>1}|\vec{\rho}-\vec{\rho}'|^{-4}\rho'^{-4}d\vec{\rho} \\ &= 4\pi^{-2}d\vec{\rho}\int_1^\infty \rho'^{-3}d\rho'\int_{\phi_0}^\pi (\rho^2+\rho'^2-2\rho\rho'\cos\phi)^{-2}d\phi,\end{aligned} \tag{24}$$

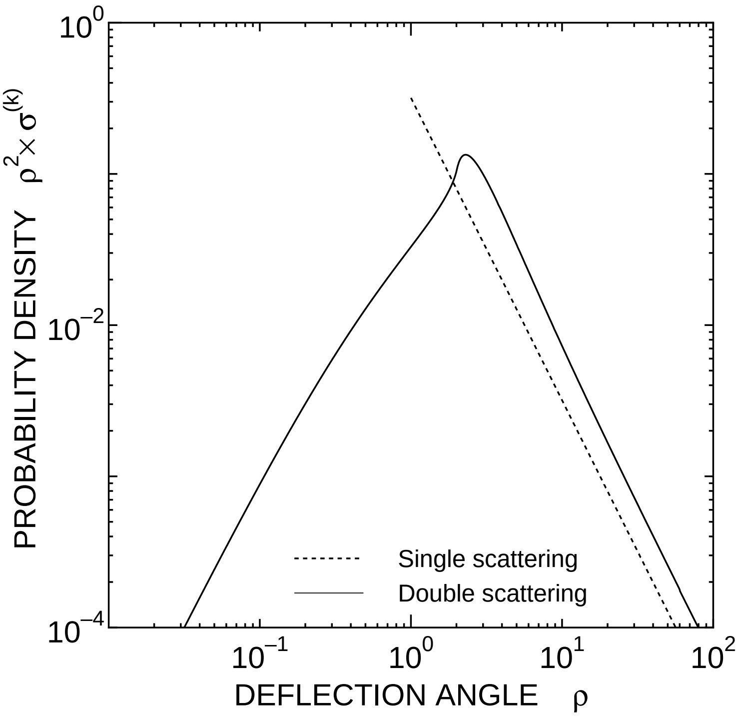

Figure 1: Probability density of the single and the double scattering.

where

$$\cos\phi_0 = \mathrm{Min}[1, \rho/2\rho']. \tag{25}$$

Asymptotic values are effective as

$$\begin{aligned}\sigma_1^{(2)}(\rho)d\vec{\rho} &\simeq (3\pi)^{-1}(1 - 6\rho/\pi + 3\rho^2)d\vec{\rho} \qquad (\rho < 0.06) &(26)\\ &\simeq 2\pi^{-1}\rho^{-4}\{1 + 4\rho^{-2}(2C - 3 + 2\ln\rho)\}d\vec{\rho} \qquad (\rho > 60). &(27)\end{aligned}$$

The results are indicated in Fig. 1.

Then we derive the folding integrals between the normal distribution with the mean square angle of a^2

$$N_{\mathrm{a}}d\vec{\rho} = (\pi a^2)^{-1}e^{-\rho^2/a^2}d\vec{\rho} \tag{28}$$

and the single scattering (23) and the double scattering (24):

$$\begin{aligned}N_{\mathrm{a}} * \sigma_1^{(k)}d\vec{\rho} &= (\pi a^2)^{-1}d\vec{\rho}\iint \sigma^{(k)}(\rho')e^{-(\vec{\rho}-\vec{\rho}')^2/a^2}d\vec{\rho}'\\ &= a^{-2}e^{-\rho^2/a^2}d\vec{\rho}\int_0^\infty I_0(2\rho\rho'/a^2)\sigma^{(k)}(\rho')e^{-\rho'^2/a^2}2\rho' d\rho'. &(29)\end{aligned}$$

At $\rho \gg 1$, we have the following asymptotic formulae:

$$N_{\mathrm{a}} * \sigma_1^{(1)}d\vec{\rho} \simeq \pi^{-1}\rho^{-4}d\vec{\rho}(1 + 4a^2\rho^{-2} + 18a^4\rho^{-4} + \cdots), \tag{30}$$

$$N_{\mathrm{a}} * \sigma_1^{(2)}d\vec{\rho} \simeq 2\pi^{-1}\rho^{-4}d\vec{\rho}[1 + 4\rho^{-2}(2\ln\rho + a^2 - 1) + 18a^2\rho^{-4}(4\ln\rho + a^2 - 10/3) + \cdots]. \tag{31}$$

The results are indicated in Figs. 2 and 3.

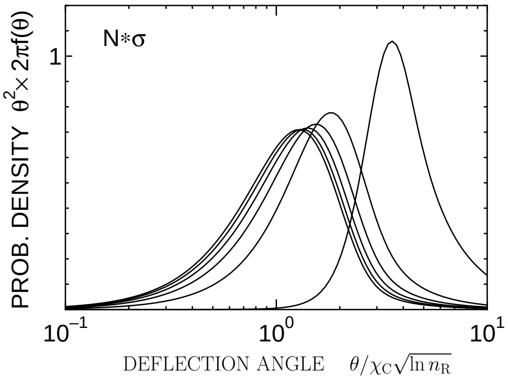

Figure 2: Normal distribution folded with single scattering. $t = e^k\Omega e^{-\Omega}$ with $k = 1, 2, 3, \cdots, 6$, from right to left.

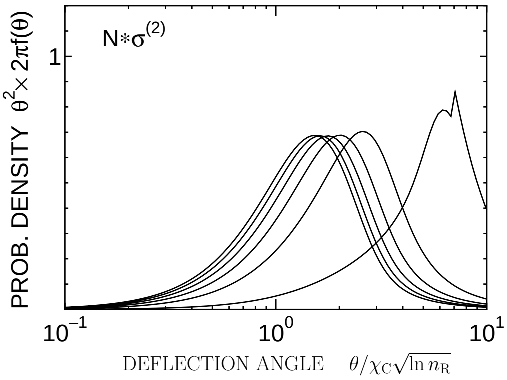

Figure 3: Normal distribution folded with double scattering. $t = e^k\Omega e^{-\Omega}$ with $k = 1, 2, 3, \cdots, 6$, from right to left.

5 The central distribution produced by the high-frequent moderate scatterings

The cross-section dividing method requires the accurate central distribution produced by the high-frequent moderate scatterings. The authors surmised the moderate scatterings defined by the Molière cut $\chi_{\rm B}$ of Eq. (13) would produce the good gaussian distribution. But we found small distortions from the gaussian in our close Monte Carlo examination [5] based on the Rutherford cross-section with the Molière screening. Distortions will arise as the penetrating depth is not enough for the moderate scattering to produce the gaussian distribution, or the angular range of the moderate scattering is too wide against the penetration depth. We will confirm in this section the reason by investigating the contribution of the next higher Fourier component. The adequate range of the moderate scattering to produce the central gaussian distribution for the given penetrating depth will be also predicted.

Central distribution produced by moderate scatterings $\sigma_{\rm M}(\theta)$ is predicted as Eq. (20). Taking account of the higher-order Fourier components indicated as e.g. (A12) of Scott [6], we have

$$2\pi \tilde{f}_{\rm M} = \exp[-\frac{\theta_{\rm M}^2\zeta^2}{4}]\{1 + \frac{1}{4B}(1 - e^{-B})e^{2-2C}(\frac{\theta_{\rm M}^2\zeta^2}{4})^2 + \cdots\} \tag{32}$$

for the Molière splitting angle of $\chi_{\rm B}$, so that

$$2\pi f_{\rm M}(\vartheta)d\vec{\vartheta} = d\vec{\vartheta}\{f^{(0)}(\vartheta) + \frac{1}{2B}(1 - e^{-B})e^{2-2C}f_2^{(2)}(\vartheta) + \cdots\} \tag{33}$$

with

$$\vartheta \equiv \theta/(\theta_{\rm G}\sqrt{B/\Omega}) \quad \text{and} \quad \theta_{\rm G} = (K/E)\sqrt{t}. \tag{34}$$

The resultant distributions are indicated in Fig. 4. Considerable distortion from the gaussian is seen in the central distribution, especially for shallow thickness.

We acquire central distributions produced by moderate scatterings with narrower range. In case of splitting at the one-scattering angle $\chi_{\rm C}$ [4],

$$\chi_{\rm C} = \theta_{\rm G}/\sqrt{\Omega}, \tag{35}$$

we have the central distribution of

$$2\pi f_{\rm M}(\vartheta)d\vec{\vartheta} = d\vec{\vartheta}\{f^{(0)}(\vartheta) + \frac{1}{2(\ln n_{\rm R})^2}(1 - \frac{1}{n_{\rm R}})f_2^{(2)}(\vartheta) + \cdots\} \tag{36}$$

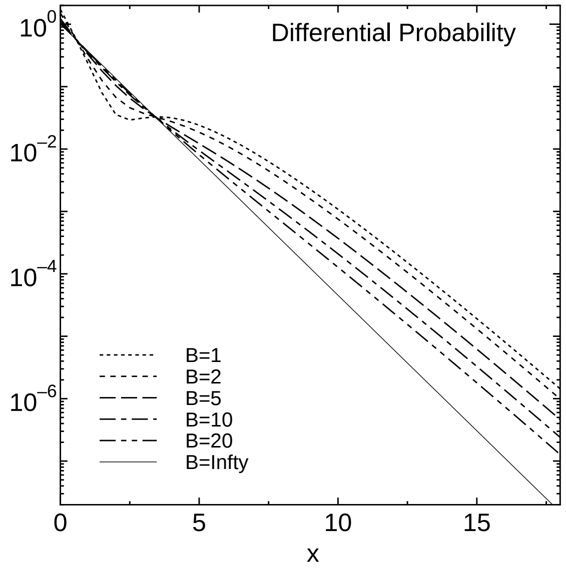

Figure 4: Central distribution produced by the moderate scattering, divided at $\chi_{\rm B}$. x denotes ϑ^2.

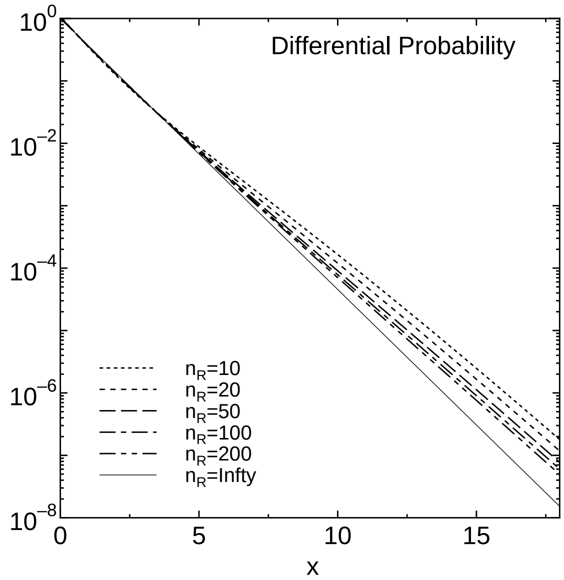

Figure 5: Central distribution produced by the moderate scattering, divided at $\chi_{\rm C}$. x denotes ϑ^2.

with

$$\vartheta \equiv \theta/(\chi_{\rm C}\sqrt{\ln n_{\rm R}}) \quad \text{with} \quad n_{\rm R} = t/(\Omega e^{-\Omega+2-2C}). \tag{37}$$

The resultant distributions agree with the gaussian well as indicated in Fig. 5.

6 Molière angular distribution reconstructed from the cross-section dividing method

In case of splitting at the one-scattering angle of $\chi_{\rm C}$, the central distribution $f_{\rm M}$ defined by Eq. (20) is well regarded as the gaussian distribution of width $\chi_{\rm C}\sqrt{\ln n_{\rm R}}$. So we can derive the Molière angular distribution by folding k-times the large-angle scattering on the central gaussian distribution as

$$f(\vartheta)d\vec{\vartheta} = \frac{1}{e}d\vec{\vartheta}\sum_{k=0}^{\infty}\frac{1}{k!}f_{\rm M} * \sigma_{\rm L}^{(k)}, \tag{38}$$

putting $\rho = \theta/\chi_{\rm C}$ and $a = \sqrt{\ln n_{\rm R}}$ in (23) and (28), respectively. The results evaluated by the first three terms (normalized) agree with those derived by Molière-Bethe theory, as indicated in Fig. 6.

7 Conclusions and discussions

The cross-section dividing method is effective to investigate the multiple scattering process. We have divided the single scattering at a splitting angle into high-frequent moderate scattering and low-frequent large-angle scattering. As the resultant angular distribution does not depend on the order of the scattering under the small angle approximations, we can derive the central distribution produced from moderate scatterings at first and correct the distribution by large-angle scatterings next. We have proposed a mathematical formulation of the cross-section dividing method, expressing the angular distribution with series expansion by the probability of large-angle scattering.

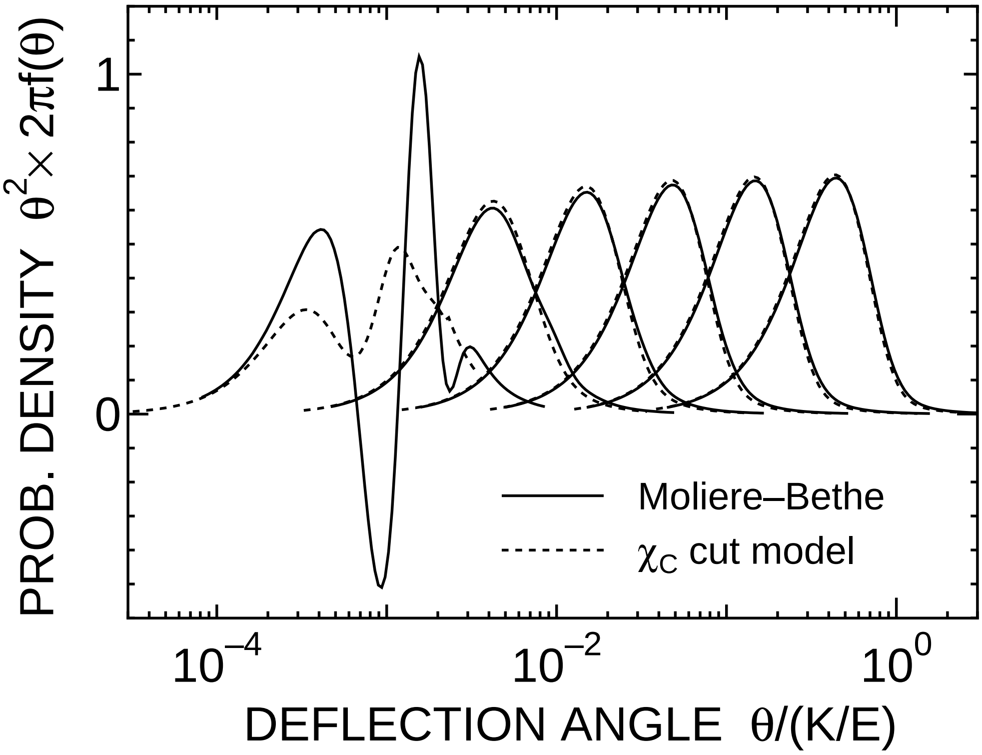

Figure 6: Molière angular distribution derived through the splitting cross-section method divided at χ_C. $t = e^{2k+1}\Omega e^{-\Omega}$ with $k = 0, 1, 2, \cdots, 5$, from left to right.

Molière expansion well corresponds to the cross-section dividing method with the splitting angle of $e^{B/2}$ times the screening angle. In fact the probability to receive the large-angle scattering is B^{-1} with a constant factor. The moderate scattering defined by Molière splitting gave a little-distorted distribution from the gaussian, due to having too wide angular range against the penetrating depth. The one-scattering angle χ_C was a good splitting angle for the moderate scattering to give the gaussian distribution. The angular distributions derived through the cross-section dividing method with the splitting angle of χ_C have shown good agreements with those through the Molière-Bethe method.

We have reached to the cross-section dividing method through the investigation of properties of Molière-Bethe theory. Almost the same concepts have been already applied by other groups [7, 8, 9]. Our investigations will give some helps in total understandings of these methods.

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References

[1] T. Nakatsuka, *"Proceedings of the Tenth EGS4 User's Meeting in Japan,"* KEK Proceedings 2002-18, 1(2002).

[2] G. Molière, Z. Naturforsch. **2a**, 133(1947).

[3] G. Molière, Z. Naturforsch. **3a**, 78(1948).

[4] H.A. Bethe, Phys. Rev. **89**, 1256(1953).

[5] K. Okei and T. Nakatsuka, in this proceedings.

[6] W.T. Scott, Rev. Mod. Phys. **35**, 231(1963).

[7] S.T. Butler, Proc. Phys. Soc. (London), **A69**, 599(1950).

[8] P. Andreo and A. Brahme, Radiat. Res. **100**, 16(1984).

[9] J.M. Fernandez-Varea, R. Mayol, J. Baro, and F. Salvat, Nucl. Instrum. Methods Phys. Res. **B73**, 447(1993).