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Kamata-Nishimura constants of Molière theory characterizing substances

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Abstract. Under the Kamata-Nishimura formulation of Molière theory, properties of substance were all reflected in two constants, Ω and K. It made the theory very simple and easy to apply to other problems. In the original formulation, the theory was described under the extreme relativistic condition. We have devised the theory also valuable under the moderate relativistic condition with ionization and defined the constants valid in both the extreme and the moderate relativistic conditions. Evaluations of the Kamata-Nishimura constants are made consistent with the values tabulated by the Particle Data Group, together with the Kamata-Nishimura constants for mixture applicable to mixed or compound substances. Dependences on representative screening models are also discussed.

1 Introduction

Molière theory of multiple Coulomb scattering (Molière, 1947, 1948; Bethe, 1953) is improved by use of Kamata-Nishimura formulation of the theory (Kamata and Nishimura, 1958; Nishimura, 1967); ionization loss through the passage is taken into account in the theory (Nakatsuka, 1999a) and the mechanism of depth-variation of Molière angular distribution is made clear (Nakatsuka, 1999b). Another superior aspect of the new formulation is that the properties of substance through which charged particles penetrate are all reflected in the Kamata-Nishimura constants, Ω and K (Kamata and Nishimura, 1958; Nishimura, 1967). By use of the constants, the diffusion equation has become very simple in the Fourier space and the derivation of angular distribution has become very easy obeying an algorithm of plain flow.

As the original formulation by Kamata and Nishimura was described only for the relativistic electrons and the Kamata-Nishimura constants were indicated only for a few substances, so we intended to describe the Kamata-Nishimura formulation even valid for charged particles of moderate relativistic energy and to evaluate the Kamata-Nishimura constants for more substances than the original paper.

The method to obtain Molière angular distribution for charged particles traversing through mixed or compound substances is also investigated under the Kamata-Nishimura formulation. It is proved that under some conditions or some screening models, the method has become as simple as that for pure substances by use of the Kamata-Nishimura constants for mixture, $\bar{\Omega}$ and $\bar{K}$.

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2 Derivation of Kamata-Nishimura Formulation and Definition of Kamata-Nishimura Constants

We take the single scattering formula as

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

under the small angle approximation (Scott, 1963). χ_{a} is called the characteristic screening angle (Bethe, 1953). Then the probability density to predict deflection angle θ after an infinitesimal passage of dx measured in g/cm^2 is

$$\begin{aligned}\frac{N}{A}\sigma(\theta)2\pi\theta d\theta dx &= \frac{4N}{A}\frac{z^2 Z(Z+1)e^4}{p^2v^2}\theta^{-4}2\pi\theta d\theta dx \\ &= \frac{1}{4\pi L}\frac{E_{\mathrm{s}}^2}{p^2v^2}\theta^{-4}2\pi\theta d\theta\frac{z^2dx}{X_0}, \quad (2)\end{aligned}$$

where X_0 denotes the radiation length (Particle Data Group, 2000) and L the so-called radiation logarithm with its correction term (Dovzhenko and Pomanskii, 1964; Linsley, 1985).

Let $f(\boldsymbol{\theta}, x)d\boldsymbol{\theta}$ be the angular distribution of charged particles having traversed through substances of thickness x. The diffusion equation for the angular distribution becomes (Kamata and Nishimura, 1958; Nishimura, 1967)

$$df = \frac{N}{A}dx \iint \{f(\boldsymbol{\theta}-\boldsymbol{\theta}') - f(\boldsymbol{\theta})\}\sigma(\boldsymbol{\theta}')d\boldsymbol{\theta}', \quad (3)$$

where we assume continuous dissipations of energy along the traversed thickness without fluctuation. Under the azimuthally symmetrical condition, Fourier transforms of the

Table 1. Screening potentials adopted by representative authors. Bohr radius and the Born parameter, $a_0 = \hbar^2/me^2$ and $\alpha = zZ/137\beta$, are used in the table.

Author	Screening Potential $V(r)$	Atomic Radius a	Born Screening Angle χ_0	The Characteristic Screening Angle $\chi_{\rm a}$
Goudsmit-Saunderson	$\frac{Ze^2}{r}\exp(-r/a)$	$a_0 Z^{-1/3}$	$\hbar/(ap)$	χ_0
Snyder-Scott	$\frac{Ze^2}{r}\exp(-r/a)$	$a_0 Z^{-1/3}$	$\hbar/(ap)$	χ_0
Molière	$\frac{zZe^2}{r}\omega(r/a)$	$0.885 a_0 Z^{-1/3}$	$\hbar/(ap)$	$\sqrt{1.13+3.76\alpha^2}\chi_0$

probability density is reduced to the Hankel transforms,

$$\begin{aligned} \tilde{f}(\boldsymbol{\zeta}, x) &\equiv \frac{1}{2\pi}\iint e^{i\boldsymbol{\zeta\theta}} f(\boldsymbol{\theta}, x) d\boldsymbol{\theta} \\ &= \int_0^\infty J_0(\zeta\theta) f(\theta, x)\theta d\theta, \end{aligned} \tag{4}$$

$$\begin{aligned} f(\boldsymbol{\theta}, x) &\equiv \frac{1}{2\pi}\iint e^{-i\boldsymbol{\theta\zeta}} \tilde{f}(\boldsymbol{\zeta}, x) d\boldsymbol{\zeta} \\ &= \int_0^\infty J_0(\theta\zeta)\tilde{f}(\zeta, x)\zeta d\zeta, \end{aligned} \tag{5}$$

so that the equation in the Fourier space is got as

$$\begin{aligned} d\tilde{f} &= -2\pi\frac{N}{A}\tilde{f}dx\int_0^\infty[1-J_0(\zeta\theta)]\sigma(\theta)\theta d\theta \\ &= -\frac{E_{\rm s}^2}{2L}\frac{z^2dt}{p^2v^2}\tilde{f}\int_{\sqrt{e}\chi_{\rm a}}^\infty[1-J_0(\zeta\theta)]\theta^{-3}d\theta, \end{aligned} \tag{6}$$

where t denotes the traversed thickness measured in radiation length:

$$t \equiv x/X_0. \tag{7}$$

Evaluating the integration using the Eq. (14) of Bethe (1953), we get the following differential equation

$$\begin{aligned} -\frac{d}{z^2dt}\ln\tilde{f} &= \frac{E_{\rm s}^2}{8L}\frac{\zeta^2}{p^2v^2}[1+\ln 2 - C - \ln(\sqrt{e}\chi_{\rm a}\zeta)] \\ &= \frac{E_{\rm s}^2}{4L}\frac{\zeta^2}{4p^2v^2}[1-2C+\ln\frac{\beta^2E_{\rm s}^2/(4Lp^2v^2\chi_0^2)}{[\chi_{\rm a}^2/\chi_0^2]_{\rm rel}} \\ &\quad -\ln\frac{\beta^2\chi_{\rm a}^2/\chi_0^2}{[\chi_{\rm a}^2/\chi_0^2]_{\rm rel}} - \ln(\frac{E_{\rm s}^2}{4L}\frac{\zeta^2}{4p^2v^2})], \end{aligned} \tag{8}$$

where we introduced the angular constant χ_0 (Bethe, 1953) called as the Born screening angle (Scott, 1963),

$$\chi_0 = \hbar/(ap), \tag{9}$$

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

Now we define the Kamata-Nishimura constants as

$$\Omega - \ln\Omega = 1 - 2C + \ln\frac{E_{\rm s}^2/(4Lp^2c^2\chi_0^2)}{[\chi_{\rm a}^2/\chi_0^2]_{\rm rel}}, \tag{10}$$

$$K^2 = \frac{E_{\rm s}^2}{4L}\Omega, \tag{11}$$

then Ω 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 (1967) defined in the extreme relativistic condition. We also introduce the factor

$$\beta'^2 = \frac{\chi_{\rm a}^2/\chi_0^2}{[\chi_{\rm a}^2/\chi_0^2]_{\rm rel}}\beta^2, \tag{12}$$

reflecting the velocity of penetrating particle and the difference of the characteristic screening angle from the Born screening angle. Then the diffusion equation becomes

$$-\frac{d}{z^2dt}\ln\tilde{f} = \frac{K^2}{\Omega}\frac{\zeta^2}{4p^2v^2}[\Omega - \ln\Omega - \ln(\frac{K^2}{\Omega}\frac{\beta'^2\zeta^2}{4p^2v^2})]. \tag{13}$$

So, introducing the variable

$$w = 2pv/K, \tag{14}$$

we get the fundamental differential equation of the Molière angular distribution under the Kamata-Nishimura formulation:

$$\frac{d}{z^2dt}\tilde{f} = -\frac{\zeta^2}{w^2}[1-\frac{1}{\Omega}\ln\frac{\beta'^2\zeta^2}{w^2}]\tilde{f}. \tag{15}$$

3 Kamata-Nishimura Constants for Molière Screening Model

Many authors evaluated $\chi_{\rm a}$ and χ_0 respectively in their multiple scattering theories (Goudsmit and Saunderson, 1940; Snyder and Scott, 1949) as listed in Table 1, depending on their models of screening potential. If we adopt the Molière screening model (Molière, 1947), we get the equations for Ω and K as

$$\Omega - \ln\Omega = 1 - 2C + \ln\frac{137^3\pi(0.885Z^{-1/3})^2}{(1.13+3.76Z^2/137^2)L}, \tag{16}$$

$$K^2 = \frac{E_{\rm s}^2\Omega}{4L}. \tag{17}$$

Using the value of radiation length X_0 (Tsai, 1974)

$$\frac{1}{X_0} = \frac{4N}{137A}Z(Z+1)r_{\rm e}^2L \tag{18}$$

instead of L, we can determine Ω and K consistent with widely-used table of material constants indicated by Particle Data Group (2000):

$$\Omega - \ln\Omega = \ln\frac{6680(Z+1)Z^{1/3}X_0}{(1+3.34Z^2/137^2)A}, \tag{19}$$

$$K^2 = 3.49\times 10^{-4}\frac{Z(Z+1)}{A}X_0\Omega E_{\rm s}^2. \tag{20}$$

Table 2. Kamata-Nishimura constants Ω and K for pure substances derived under the Molière screening model.

Substance	Z	A	X_0 g/cm^2	Ω	K MeV
H	1	1.008	61.28	16.40	17.69
He	2	4.003	94.32	16.07	18.88
Li	3	6.941	82.76	15.80	18.83
C	6	12.011	42.70	15.34	18.96
N	7	14.007	37.99	15.25	19.06
O	8	15.999	34.24	15.17	19.15
Al	13	26.982	24.01	14.85	19.43
Si	14	28.086	21.82	14.80	19.47
S	16	32.066	19.50	14.71	19.54
Ar	18	39.948	19.55	14.63	19.60
Fe	26	55.845	13.84	14.34	19.79
Cu	29	63.546	12.86	14.25	19.84
Br	35	79.904	11.42	14.08	19.94
Ag	47	107.868	8.97	13.77	20.13
I	53	126.904	8.48	13.62	20.22
W	74	183.840	6.76	13.15	20.52
Pb	82	207.200	6.37	12.99	20.65

In this case Kamata-Nishimura equation becomes Eq. (15), with

$$\beta'^2 = \frac{1+3.34z^2Z^2/(137\beta)^2}{1+3.34Z^2/137^2}\beta^2. \tag{21}$$

Kamata-Nishimura constants under the Molière screening model, so obtained, are listed in Table 2.

4 Angular Distribution of Charged Particles Traversing Through Mixed or Compound Substance

We will derive the method to obtain the Molière angular distribution for charged particles, traversing through mixed or compound substances with ionization. The increase of Fourier component of the angular distribution is expressed as

$$d\tilde{f} = -\frac{\zeta^2}{w^2}\tilde{f}(1-\frac{1}{\Omega}\ln\frac{\beta'^2\zeta^2}{w^2})z^2dt. \tag{22}$$

Separating the terms by independent Fourier component, we have

$$\begin{aligned} -d\ln\tilde{f} \;&=\; \frac{1}{X_0w^2}(1-\frac{1}{\Omega}\ln\frac{\beta'^2}{w^2})\zeta^2z^2dx \\ &\quad - \frac{1}{X_0w^2\Omega}(\zeta^2\ln\zeta^2)z^2dx. \end{aligned} \tag{23}$$

In case of 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 stochastic mean of it, then we have

$$\begin{aligned} -\ln 2\pi\tilde{f} \;&=\; \zeta^2\int_0^x \mathrm{Pr}[\frac{1}{X_0w^2}(1-\frac{1}{\Omega}\ln\frac{\beta'^2}{w^2})]z^2dx \\ &\quad -\zeta^2\ln\zeta^2\int_0^x \mathrm{Pr}[\frac{1}{X_0\Omega w^2}]z^2dx, \end{aligned} \tag{24}$$

where the stochastic mean is evaluated as the weighted mean value by the fractions p_i of mass:

$$\mathrm{Pr}[Q] \equiv \sum_i p_iQ_i. \tag{25}$$

Thus we get the solution,

$$\begin{aligned} \tilde{f} \;&=\; \frac{1}{2\pi}\exp\{-\zeta^2\int_0^x \mathrm{Pr}[\frac{1}{X_0w^2}(1-\frac{1}{\Omega}\ln\frac{\beta'^2}{w^2})]z^2dx \\ &\quad +\zeta^2\ln\zeta^2\int_0^x \mathrm{Pr}[\frac{1}{X_0\Omega w^2}]z^2dx\}. \end{aligned} \tag{26}$$

The Molière angular distribution is got by applying Hankel transforms on the solution. Using the translation formula indicated in Nakatsuka (1999b), we get the characteristic parameters of the Molière angular distribution, as are the expansion parameter B and the unit of Molière angle θ_M:

$$\begin{aligned} B-\ln B &= \frac{\int_0^x \mathrm{Pr}[\frac{1}{X_0w^2}(1-\frac{1}{\Omega}\ln\frac{\beta'^2}{w^2})]z^2dx}{\int_0^x \mathrm{Pr}[\frac{1}{X_0\Omega w^2}]z^2dx} \\ &\quad +\ln\int_0^x \mathrm{Pr}[\frac{1}{X_0\Omega w^2}]z^2dx, \end{aligned} \tag{27}$$

$$\theta_\mathrm{M} = 2\sqrt{B\int_0^x \mathrm{Pr}[\frac{1}{X_0\Omega w^2}]z^2dx}. \tag{28}$$

In homogeneous mixture of substances, integration of the stochastic mean along the thickness becomes

$$\int_0^x \mathrm{Pr}[f(x)]dx = \bar{X}_\mathrm{R}\mathrm{Pr}[\int_0^{x/\bar{X}_\mathrm{R}} f(X_\mathrm{R}u)du], \tag{29}$$

where X_R denote the respective ranges of particle in mixed substances, and $\bar{X}_\mathrm{R}$ denotes their stochastic mean, measured in g/cm^2:

$$X_\mathrm{R} \equiv E_0/\frac{dE}{dx}, \tag{30}$$

$$\bar{X}_\mathrm{R} \equiv E_0/\mathrm{Pr}[\frac{dE}{dx}]. \tag{31}$$

In case we adopt the screening model where the characteristic screening angle χ_a is proportional to the Born angle χ_0 (Born-type screening angle), it satisfies $\beta' = \beta$. Or in case we adopt the Molière screening model with the small Born parameter, $zZ \ll 137\beta$, it satisfies the similar relation, $\beta' \approx \beta$. Then we have

$$\begin{aligned} -d\ln\tilde{f} \;&=\; \{\frac{K^2}{X_0}(1-\frac{1}{\Omega}\ln K^2)\frac{\zeta^2}{4p^2v^2} \\ &\quad -\frac{K^2}{X_0\Omega}\frac{\zeta^2}{4p^2v^2}\ln\frac{\beta^2\zeta^2}{4p^2v^2}\}dx, \end{aligned} \tag{32}$$

thus

$$\begin{aligned} -\ln 2\pi\tilde{f} \;&=\; \int_0^x \mathrm{Pr}[\frac{K^2}{X_0}(1-\frac{1}{\Omega}\ln K^2)]\frac{\zeta^2}{4p^2v^2}dx \\ &\quad -\int_0^x \mathrm{Pr}[\frac{K^2}{X_0\Omega}]\frac{\zeta^2}{4p^2v^2}\ln\frac{\beta^2\zeta^2}{4p^2v^2}dx. \end{aligned} \tag{33}$$

Table 3. The Kamata-Nishimura constants for mixture, $\bar{\Omega}$ and $\bar{K}$, for mixed or compound substances derived from the Molière screening model.

Substance	$\bar{X}_0$ g/cm^2	$\bar{\varepsilon}$ MeV	$\bar{\Omega}$	$\bar{K}$ MeV
Air	36.61	66.5	15.21	19.10
SiO_2	27.04	47.0	14.95	19.34
H_2O	36.02	74.2	15.23	19.06
LiH	79.24	154.6	15.88	18.65
Emulsion	11.32	16.5	13.94	20.01

If we introduce the Kamata-Nishimura constants for mixture for mixed or compound substance, $\bar{\Omega}$ and $\bar{K}$, by the equations

$$\frac{\bar{K}^2}{\bar{X}_0}(1-\frac{1}{\bar{\Omega}}\ln\bar{K}^2) = \mathrm{Pr}[\frac{K^2}{X_0}(1-\frac{1}{\Omega}\ln K^2)], \qquad (34)$$

$$\frac{\bar{K}^2}{\bar{X}_0\bar{\Omega}} = \mathrm{Pr}[\frac{K^2}{X_0\Omega}], \qquad (35)$$

or, taking $\bar{X}_0$ as the radiation length for the compound substance (Particle Data Group, 2000),

$$\bar{\Omega}-\ln\bar{\Omega} = \frac{\mathrm{Pr}[\frac{K^2}{X_0}(1-\frac{1}{\Omega}\ln K^2)]}{\mathrm{Pr}[\frac{K^2}{X_0\Omega}]} + \ln\{\bar{X}_0\mathrm{Pr}[\frac{K^2}{X_0\Omega}]\}, \qquad (36)$$

$$\bar{K} = \sqrt{\bar{X}_0\bar{\Omega}\mathrm{Pr}[\frac{K^2}{X_0\Omega}]}, \qquad (37)$$

then we can get the Molière angular distribution for mixed or compound substances by regarding as if they are pure substances with the Kamata-Nishimura constants for mixture, $\bar{\Omega}$ and $\bar{K}$. So that the Molière angular distribution is determined by the characteristic parameters B and θ_{M} derived from

$$B-\ln B = \bar{\Omega}-\ln\bar{\Omega}+\ln(\nu z^2 t/\beta^2), \qquad (38)$$

$$\theta_{\mathrm{M}} = \bar{\theta}_{\mathrm{G}}\sqrt{B/\bar{\Omega}}, \qquad (39)$$

where

$$\bar{\theta}_{\mathrm{G}}^2 = \frac{\bar{K}^2}{2\bar{\varepsilon}mc^2}\{\frac{mc^2}{pv}-\frac{mc^2}{p_0v_0}+\frac{1}{2}\ln\frac{(E_0-mc^2)/(E-mc^2)}{(E_0+mc^2)/(E+mc^2)}\}, \qquad (40)$$

The Kamata-Nishimura constants for mixture, $\bar{\Omega}$ and $\bar{K}$, for mixed or compound substance are tabulated in Table 3.

It should be reminded that we can slightly simplify Eqs. (27) and (28) for the exact characteristic parameters, B and θ_{M}, by using the constants for mixture:

$$B-\ln B = \frac{\int_0^x \mathrm{Pr}[\frac{1}{X_0 w^2}(1-\frac{1}{\Omega}\ln\frac{\beta'^2}{w^2})]z^2dx}{\bar{\theta}_{\mathrm{G}}^2/4\bar{\Omega}} + \ln\frac{\bar{\theta}_{\mathrm{G}}^2}{4\bar{\Omega}}, \qquad (41)$$

$$\theta_{\mathrm{M}} = \bar{\theta}_{\mathrm{G}}\sqrt{B/\bar{\Omega}}. \qquad (42)$$

5 Conclusions and Discussions

Definition of the Kamata-Nishimura constants Ω and K for Molière scattering theory is devised to be valid for both the extreme and the moderate relativistic conditions of charged particle. The results for various substances are evaluated consistent with the widely used constant table of Particle Data Group (2000) and are tabulated in Table 2.

Method to get the Molière angular distribution for charged particles traversing through mixed or compound substances is described under the Kamata-Nishimura formulation. The description will be clearer than that under the Molière-Bethe formulation reviewed in Scott (1963). Representative screening models applied to the scattering theory are listed in Table 1. In case we adopt the Born-type screening angle or the Molière screening angle with the negligible Born parameter, the Molière angular distribution through the mixture can be obtained as simply as that through the pure substance (Nakatsuka and Nishimura, 2001) by using the Kamata-Nishimura constants for mixture $\bar{\Omega}$ and $\bar{K}$, indicated in Table 3.

Both for propagations through pure and mixed or compound substances, the method to derive Molière angular distribution has been far simplified by use of the Kamata-Nishimura constants.

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