Analytical solutions of the Molière series terms of higher orders for multiple Coulomb scattering

T. NAKATSUKA1, K. OKE1, N. TAKAHASHI3

1Okayama Shoka University, Okayama 700-8601, Japan
2Dept. of Information Sciences, Kawasaki Medical School, Kurashiki 701-0192, Japan
3Grad. School of Natural Science and Technology, Okayama University, Okayama 700-8530, Japan
nakatuka@osu.ac.jp

Abstract: General higher terms of Molière series are solved analytically, in Molière-Heisenberg definite integral and/or Goldstein series [3]. The terms of higher orders up to n=6 are practically obtained. Applicable region of Molière series is extended to shorter depths of penetration down to B = 5 by the results. Integrated Molière angular distribution is also obtained using general Goldstein series, which will be useful for rapid sampling of the Molière angular distribution.

Introduction

Molière formulated the accurate theory of multiple Coulomb scattering in power series [1, 2, 3] and indicated the analytical solutions for the first three series terms up to the second higher order of accuracy, by applying superior complex function theories with advices of Heisenberg [2]. We propose analytical solutions for the general higher expansion term of Molière series both for the spatial and the projected Molière distributions, in Molière definite integral and Goldstein series [3].

Molière’s solution for the angular distribution by series expansion

According to Molière’s theory [1, 2, 3], probability density of the spatial angular distribution \( f(\theta)d\theta \) is expressed with power series of \( B^{-1} \) by

\[
f(\theta) = f^{(0)}(\theta) + B^{-1} f^{(1)}(\theta) + B^{-2} f^{(2)}(\theta) + \ldots,
\]

(1)

where \( B^{-1} \) is determined from the probability of the scarce large-angle scattering [4] and \( \theta \) is the deflection angle measured in Molière’s scale angle \( \theta_M \) [5]. The coefficient \( f^{(n)}(\theta) \) is determined as

\[
f^{(n)}(\theta) = \frac{1}{n!} \int_{0}^{\infty} y dy J_0(\theta y) e^{-\frac{y^2}{4}} \left( \frac{y^2}{4} \ln \frac{y^2}{4} \right)^n.
\]

(2)

Likewise, probability density of the projected angular distribution \( f_P(\varphi)d\varphi \) is expressed as

\[
f_P(\varphi) = f_P^{(0)}(\varphi) + B^{-1} f_P^{(1)}(\varphi) + B^{-2} f_P^{(2)}(\varphi) + \ldots,
\]

(3)

where the coefficient \( f_P^{(n)}(\varphi) \) is determined as

\[
f_P^{(n)}(\varphi) = \frac{2}{\sqrt{\pi n!}} \int_{0}^{\infty} dy \cos(\varphi y) e^{-\frac{y^2}{4}} \left( \frac{y^2}{4} \ln \frac{y^2}{4} \right)^n.
\]

(4)

Molière described the coefficient \( f^{(n)}(\theta) \) and \( f_P^{(n)}(\varphi) \) for general \( n \) in complex integral as

\[
f^{(n)}(\theta) = \left[ \frac{1}{\pi i} \int_{C} \frac{d\eta}{\eta^{n+1}(1+\eta)} \left[ \ln \frac{\eta}{\xi} - i\pi \right]^{n} e^{-\frac{\eta^2}{\xi}} \right] x e^{-\xi n} \times
\]

\[
\frac{1}{\pi i} \int_{C} \frac{d\eta}{\eta^{n+1}(1+\eta)} \left[ \ln \frac{\eta}{\xi} - i\pi \right]^{n} e^{-\frac{\eta^2}{\xi}} \times
\]

but indicated the explicit expressions only up to \( n = 2 \) using the normal distribution, the exponential integral, and a definite integral [2, 3].
Table 1: Value of $nM_j$.

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The solution for general terms of Molière series

We find the explicit expressions of Eqs. (5) and (6) to carry out the complex integrals by the real integration.

Modifying the integral variable by $-1 = 1/(1 + \eta)$ as Molière did [2], we have

\[
\begin{align*}
\int_{-1}^{1} f(n)(t) &= \frac{2}{n!} \int_{0}^{\infty} d\xi e^{-\xi} \frac{\alpha^{n-2}}{2\pi i} \int_{0}^{\infty} dt \frac{(1-t)^n}{t^{n+1}} \\
&\times e^{t \beta^2} \sum_{j=0}^{n} nC_j \left( \ln \frac{t}{t-1} \right)^j (-\ln \xi)^{n-j} (\xi) \\
\int_{-1}^{1} f(n)(\phi) &= \frac{2}{\sqrt{\pi n!}} \int_{0}^{\infty} d\xi e^{-\xi} \frac{\alpha^{n-2}}{2\pi i} \int_{0}^{\infty} dt \frac{(1-t)^n}{t^{n+1}} \\
&\times e^{t \beta^2} \sum_{j=0}^{n} nC_j \left( \ln \frac{t}{t-1} \right)^j (-\ln \xi)^{n-j} (\xi)
\end{align*}
\]

where the complex integral with $t$ are performed along a closed path surrounding $t = 0$ and $t = 1$.

Integrals with $\xi$ are evaluated as

\[
\int_{0}^{\infty} d\xi e^{-\xi} \xi^n (\ln \xi)^{n-j} = \Gamma(n-j)(n+1).
\]

Next we evaluate a complex integral of

\[
T_n = \frac{1}{2\pi i} \int f(s) \left[ \ln \frac{s-\alpha}{s-\beta} \right]^n ds,
\]

\[
\int_{0}^{\infty} d\xi e^{-\xi} \xi^n (\ln \xi)^{n-j} = \Gamma(n-j)(n+1).
\]

Figure 1: Situation of $\int_{0}^{\infty} d\xi e^{-\xi} \xi^n (\ln \xi)^{n-j} = \Gamma(n-j)(n+1)$.

Table 2: Value of $nM_j$.

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against general functions of $f(s)$ for $n \geq 1$. We have

\[
T_n = \frac{1}{2\pi i} \int f(s) \left[ \int_{-1}^{1} \frac{du}{s-u} \right]^n
\]

\[
= \int_{-1}^{1} du_1 \int_{-1}^{1} du_2 \cdots \int_{-1}^{1} du_n
\]

\[
\times \frac{1}{2\pi i} \int ds f(s) \sum_{k=1}^{n} \frac{a_k}{s-u_k},
\]

where

\[
a_k = \prod_{j \neq k} \frac{1}{u_k - u_j}.
\]

Then, for a function $f(s)$ to have poles within a certain area, the Cauchy integral enclosing the area is evaluated as [6]

\[
\frac{1}{2\pi i} \int f(s) ds = f(z) - \sum_{\text{pole}} \text{PP} \equiv f^*(z),\quad (13)
\]

where PP denotes the principal part or the terms with negative power for poles in the area. Also we have

\[
\int_{-1}^{1} du_2 = [\ln(u_1 - u_2)]_{u_2=\beta} = \ln \frac{u_1 - \alpha}{u_2 - \beta + \pi i},\quad (14)
\]

where the sign $\pm$ is determined by the mutual relation between the location $u_1$ and the path of $u_2$.

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Figure 2: Situation of $\int_{-1}^{1} du_2 = [\ln(u_1 - u_2)]_{u_2=\beta} = \ln \frac{u_1 - \alpha}{u_2 - \beta + \pi i}$. 
from $\alpha$ to $\beta$ on the complex plane, as indicated in Figs. 1 and 2. So

$$T_n = \frac{1}{2\pi i} \int_{\alpha}^\beta \left\{ \left( \frac{t - \alpha}{\beta - t} + \pi i \right)^n - \left( \frac{t - \alpha}{\beta - t} - \pi i \right)^n \right\} f^*(t) \, dt$$

$$= \sum_{k=1}^{[(n+1)/2]} n C_{2k-1} (-\pi^2)^{k-1}$$

$$\times \int_{\alpha}^\beta dt f^*(t) \left( \frac{t - \alpha}{\beta - t} \right)^{n-2k+1}$$

(15)

where $[x]$ denotes the largest integer not exceeding $x$.

So we have the solution for general terms of Molière series, expressed explicitly by definite integrals in the real space:

$$f^{(n)}(\theta) = 2 e^{-\theta^2} \frac{\Gamma(n+1)}{\Gamma(n+1)} \sum_{j=0}^{n} n C_j (-\theta^2)^j j!$$

$$+ 2 e^{-\theta^2} \int_0^1 \left\{ \frac{(1-t)^n}{\Gamma(n+1)} e^{\theta^2 t} \right\}^*$$

$$\times \sum_{j=0}^{n} n M_j \left( \ln \frac{t}{1-t} \right)^{n-1-j} \, dt,$$

(16)

$$f_p^{(n)}(\varphi) = \frac{2 e^{-\varphi^2}}{\sqrt{\pi}} \frac{\Gamma(n+1)}{\Gamma(n+1)} \sum_{j=0}^{n-1} n^{-\frac{1}{2}} C_j \frac{(-\varphi^2)^j}{j!}$$

$$+ \frac{2 e^{-\varphi^2}}{\sqrt{\pi}} \int_0^1 \left\{ \frac{(1-t)^{n-\frac{1}{2}}}{\Gamma(n+1)} e^{\varphi^2 t} \right\}^*$$

$$\times \sum_{j=0}^{n-1} n M_j \left( \ln \frac{t}{1-t} \right)^{n-1-j} \, dt,$$

(17)

Goldstein series and the integrated Molière angular distribution

Goldstein proposed another expression of the solution for the term of $n = 2$ [3]. We apply his method to general higher Molière terms. Putting $x = \theta^2$ and $y = \varphi^2$, we have

$$n M_j \equiv n C_{j+1} (-y)^j$$

$$\times \sum_{k=0}^{[j/2]} \frac{\Gamma(j-2k) (n+1)}{\Gamma(n+1)} (-\pi^2)^k,$$

(18)

Molière series up to $n = 6$ so obtained are confirmed to extend the reliable region of the series to shorter passages down to $B = 5$.
so definite integrals $I_n$ and $J_n$ in Eqs. (16) and (17), respectively, can be expressed in power series as

$$I_n = \sum_{k=0}^{\infty} \sum_{l=0}^{n-1} \frac{x^{n+l+1-k}}{(n+l+1-k)!} \times \sum_{j=0}^{n-1} Q_{lj} n M_{n-1-j}$$

$$= \sum_{l=0}^{\infty} G_{ln} \sum_{k=0}^{n} \frac{x^{n+l+1-k}}{(n+l+1-k)!}$$

$$J_n = \sum_{k=0}^{n-1} \frac{x^{n+1-k}}{(n+1-k)!} \sum_{l=0}^{n-1} Q_{lj} n M_{n-1-j}$$

$$= \sum_{l=0}^{\infty} G_{ln} \sum_{k=0}^{n} \frac{x^{n+l+1-k}}{(n+l+1-k)!}$$

where

$$Q_{lj} \equiv \int_0^{\frac{1}{l}} l^j \left( \ln \frac{1}{l} \right)^j dt,$$  \text{and (23)}

$$G_{ln} \equiv \sum_{j=0}^{n-1} Q_{lj} n M_{n-1-j}. \quad (24)$$

We can easily integrate the spatial Molière angular distribution (1), utilizing the result. Defining

$$F(\bar{\theta}) \equiv \int_{\theta}^{\bar{\theta}} f(\theta) d\theta = \frac{1}{2} \int_{x}^{\infty} f(\bar{\theta}) dx$$

$$= F^{(0)}(\bar{\theta}) + B^{-1} F^{(1)}(\bar{\theta}) + B^{-2} F^{(2)}(\bar{\theta}) + \ldots, \quad (25)$$

we have $F^{(n)}(\bar{\theta})$ for $n \geq 1$ as

$$F^{(n)}(\bar{\theta}) = \frac{\Gamma^{(n)}(n+1)}{\Gamma(n+1)} e^{-x} \sum_{k=1}^{n} \frac{x^k}{k!} \sum_{j=k}^{n} n C_j (-)^j$$

$$+ e^{-x} \sum_{l=0}^{n} \sum_{k=l+1}^{n} \frac{x^k}{k!} \sum_{j=0}^{n-l+1-k} n C_j (-)^j. \quad (26)$$

The results for $n = 0, 1, 2$ are practically expressed as

$$F^{(0)}(\bar{\theta}) = e^{-x}, \quad (27)$$

Figure 5: Integrated Molière terms, $F^{(0)}(\bar{\theta})$ (solid line), $F^{(1)}(\bar{\theta})$ (broken line), and $F^{(2)}(\bar{\theta})$ (dot line).

$$F^{(1)}(\bar{\theta}) = \left\{ \gamma - 1 + \int_0^{x} e^{x} - 1 - \frac{x}{x^2} dx \right\} x e^{-x}$$

$$= e^{-x} - 1 + \left\{ E_i(x) - \ln x \right\} x e^{-x}, \quad (28)$$

$$F^{(2)}(\bar{\theta}) = \left\{ \psi(3) + \psi(3)^2 \right\} \left\{ \frac{x}{2} - 1 \right\} x e^{-x}$$

$$+ 2e^{-x} \sum_{l=0}^{\infty} \psi(l+1) + \gamma - \psi(3)$$

$$\times \left\{ \frac{x^{l+3}}{(l+3)!} - \frac{x^{l+2}}{(l+2)!} \right\}, \quad (29)$$

as indicated in Fig. 5.

Conclusions and discussions

Higher expansion terms of Molière series are solved generally in analytical form both with the definite integral and the series expansion. The formula for Cauchy integral with functions possessing poles in the closed path of integration [6] was valuable to get the solution. Integrated functions of Molière distribution were proposed in power series, which could realize rapid samplings of Molière’s angular and lateral distributions through the Newton method.

References