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

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Abstract: General higher terms of Molière series are solved analytically, in Molière-Heisenberg definite integral and/or Goldstein series. 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 $f(\vartheta)\vartheta d\vartheta$ is expressed with power series of B^{-1} by

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

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

$$f^{(n)}(\vartheta) = \frac{1}{n!}\int_0^\infty y dy J_0(\vartheta y) e^{-\frac{y^2}{4}} \left(\frac{y^2}{4}\ln\frac{y^2}{4}\right)^n \quad (2)$$

Likewise, probability density of the projected angular distribution $f_{\mathrm{P}}(\varphi)d\varphi$ is expressed as

$$f_{\mathrm{P}}(\varphi) = f_{\mathrm{P}}^{(0)}(\varphi)+B^{-1}f_{\mathrm{P}}^{(1)}(\varphi)+B^{-2}f_{\mathrm{P}}^{(2)}(\varphi)+\ldots, \quad (3)$$

where the coefficient $f_{\mathrm{P}}^{(n)}(\varphi)$ is determined as

$$f_{\mathrm{P}}^{(n)}(\varphi) = \frac{2}{\sqrt{\pi}n!}\int_0^\infty dy \cos(\varphi y) e^{-\frac{y^2}{4}} \left(\frac{y^2}{4}\ln\frac{y^2}{4}\right)^n \quad (4)$$

Molière described the coefficient $f^{(n)}(\vartheta)$ and $f_{\mathrm{P}}(\varphi)$ for general n in complex integral as

$$f^{(n)}(\vartheta) = \frac{1}{n!}\int_0^\infty d\xi e^{-\xi}\xi^n \times \frac{1}{\pi i}\int_C \frac{d\eta}{\eta^{n+1}(1+\eta)}\left[\ln\frac{\eta}{\xi} - i\pi\right]^n e^{-\frac{\vartheta^2}{1+\eta}}, \quad (5)$$

$$f_{\mathrm{P}}^{(n)}(\varphi) = \frac{2}{\sqrt{\pi}n!}\int_0^\infty d\xi e^{-\xi}\xi^n \times \frac{1}{2\pi i}\int_C \frac{d\eta}{\eta^{n+1}\sqrt{1+\eta}}\left[\ln\frac{\eta}{\xi} - i\pi\right]^n e^{-\frac{\varphi^2}{1+\eta}} \quad (6)$$

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 ${}_nM_j$.

$n\backslash j$	0	1	2	3	4	5
1	1					
2	2	-1.84557				
3	3	-7.53671	-4.28464			
4	4	-18.0734	-9.60186	41.9884		
5	5	-34.1224	-5.93123	219.544	-150.143	
6	6	-56.1835	22.2599	664.563	-1120.4	169.714

Table 2: Value of ${}_{n-\frac{1}{2}}C_{j-\frac{1}{2}}$.

$n\backslash j$	0	1	2	3	4	5	6
1	$\frac{1}{2}$	1					
2	$\frac{3}{8}$	$\frac{3}{2}$	1				
3	$\frac{5}{16}$	$\frac{15}{8}$	$\frac{5}{4}$	1			
4	$\frac{35}{128}$	$\frac{35}{16}$	$\frac{35}{8}$	$\frac{7}{2}$	1		
5	$\frac{63}{256}$	$\frac{315}{128}$	$\frac{105}{16}$	$\frac{63}{8}$	$\frac{9}{2}$	1	
6	$\frac{231}{1024}$	$\frac{693}{256}$	$\frac{1155}{128}$	$\frac{231}{16}$	$\frac{99}{8}$	$\frac{11}{2}$	1

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 $1-t=1/(1+\eta)$ as Molière did [2], we have

$$f^{(n)}(\vartheta) = \frac{2}{n!}\int_0^\infty d\xi e^{-\xi}\xi^n \frac{e^{-\vartheta^2}}{2\pi i}\oint dt \frac{(1-t)^n}{t^{n+1}} \times e^{t\vartheta^2}\sum_{j=0}^n {}_nC_j\left(\ln\frac{t}{t-1}\right)^j(-\ln\xi)^{n-j} \quad (7)$$

$$f_{\rm P}^{(n)}(\varphi) = \frac{2}{\sqrt{\pi}n!}\int_0^\infty d\xi e^{-\xi}\xi^n \frac{e^{-\varphi^2}}{2\pi i}\oint dt \frac{(1-t)^{n-\frac{1}{2}}}{t^{n+1}} \times e^{t\varphi^2}\sum_{j=0}^n {}_nC_j\left(\ln\frac{t}{t-1}\right)^j(-\ln\xi)^{n-j} \quad (8)$$

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

Integrals with ξ are evaluated as

$$\int_0^\infty d\xi e^{-\xi}\xi^n(\ln\xi)^{n-j} = \Gamma^{(n-j)}(n+1). \quad (9)$$

Next we evaluate a complex integral of

$$T_{\rm n} \equiv \frac{1}{2\pi i}\oint f(s)\left[\ln\frac{s-\alpha}{s-\beta}\right]^n ds, \quad (10)$$

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

$$\begin{aligned} T_{\rm n} &= \frac{1}{2\pi i}\oint ds f(s)\left[\int_\alpha^\beta \frac{du}{s-u}\right]^n \\ &= \int_\alpha^\beta du_1\int_\alpha^\beta du_2\cdots\int_\alpha^\beta du_n \\ &\quad \times\frac{1}{2\pi i}\oint ds f(s)\sum_{k=1}^n\frac{a_k}{s-u_k}, \end{aligned} \quad (11)$$

where

$$a_k = \prod_j^{j\neq k}\frac{1}{u_k-u_j}. \quad (12)$$

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

$$\frac{1}{2\pi i}\oint\frac{f(s)}{s-z}ds = f(z) - \sum_{\rm pole}{\rm PP} \equiv f^*(z), \quad (13)$$

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

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

where the sign $\pm$ is determined by the mutual relation between the location u_1 and the path of u_2 from α to β on the complex plane, as indicated in Figs. 1 and 2. So

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

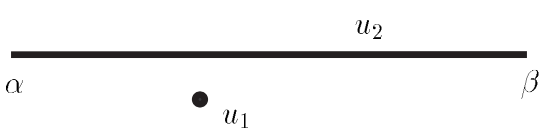

Figure 1: Situation of $\int_\alpha^\beta\frac{du_2}{u_1-u_2} = \ln\frac{u_1-\alpha}{\beta-u_1}+\pi i$.

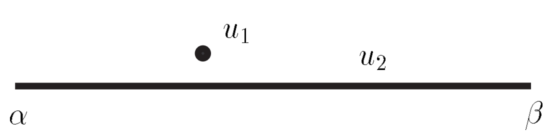

Figure 2: Situation of $\int_\alpha^\beta\frac{du_2}{u_1-u_2} = \ln\frac{u_1-\alpha}{\beta-u_1}-\pi i$.

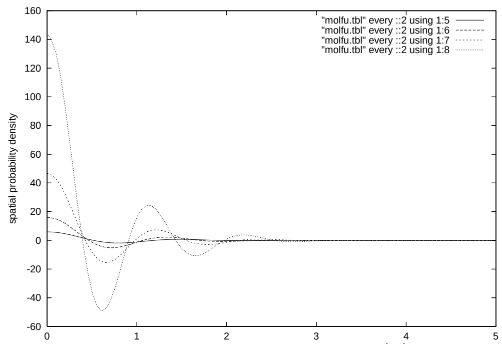

Figure 3: Molière series function $f^{(n)}(\vartheta)$ with n from 3 to 6, for spatial angular distribution.

$$= \sum_{k=1}^{[(n+1)/2]} {}_nC_{2k-1}(-\pi^2)^{k-1} \times \int_\alpha^\beta dt f^*(t)\left(\ln\frac{t-\alpha}{\beta-t}\right)^{n-2k+1}, \qquad (15)$$

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:

$$\begin{aligned} f^{(n)}(\vartheta) &= 2e^{-\vartheta^2}\frac{\Gamma^{(n)}(n+1)}{\Gamma(n+1)}\sum_{j=0}^{n} {}_nC_j\frac{(-\vartheta^2)^j}{j!} \\ &\quad + 2e^{-\vartheta^2}\int_0^1\left\{\frac{(1-t)^n}{t^{n+1}}e^{\vartheta^2 t}\right\}^* \\ &\quad \times\sum_{j=0}^{n-1} {}_nM_j\left(\ln\frac{t}{1-t}\right)^{n-1-j}dt \qquad (16) \\ f_{\mathrm{P}}^{(n)}(\varphi) &= \frac{2e^{-\varphi^2}}{\sqrt{\pi}}\frac{\Gamma^{(n)}(n+1)}{\Gamma(n+1)}\sum_{j=0}^{n} {}_{n-\frac12}C_{j-\frac12}\frac{(-\varphi^2)^j}{j!} \\ &\quad + \frac{2e^{-\varphi^2}}{\sqrt{\pi}}\int_0^1\left\{\frac{(1-t)^{n-\frac12}}{t^{n+1}}e^{\varphi^2 t}\right\}^* \\ &\quad \times\sum_{j=0}^{n-1} {}_nM_j\left(\ln\frac{t}{1-t}\right)^{n-1-j}dt \qquad (17) \end{aligned}$$

where

$$\begin{aligned} {}_nM_j &\equiv {}_nC_{j+1}(-)^j \\ &\times\sum_{k=0}^{[j/2]} {}_{j+1}C_{2k+1}\frac{\Gamma^{(j-2k)}(n+1)}{\Gamma(n+1)}(-\pi^2)^k \qquad (18) \end{aligned}$$

Molière series up to $n = 6$ so obtained are confirmed to extend the reliable region of the series to shorter passages down to $B = 5$.

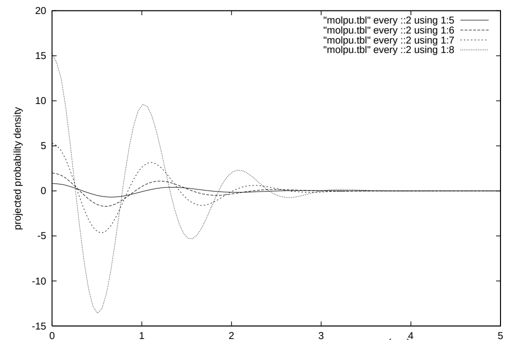

Figure 4: Molière series function $f_{\mathrm{P}}^{(n)}(\varphi)$ with n from 3 to 6, for projected angular distribution.

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 $x \equiv \vartheta^2$ and $y \equiv \varphi^2$, we have

$$\begin{aligned} &\left\{\frac{(1-t)^n}{t^{n+1}}e^{xt}\right\}^* \\ &= \frac{1}{t^{n+1}}\sum_{k=0}^{n} {}_nC_k(-t)^k\sum_{l=n+1-k}^{\infty}\frac{1}{l!}x^l t^l \\ &= \sum_{l=0}^{\infty}t^l\sum_{k=0}^{n} {}_nC_k\frac{(-)^k x^{n+l+1-k}}{(n+l+1-k)!}, \qquad (19) \\ &\left\{\frac{(1-t)^{n-\frac12}}{t^{n+1}}e^{yt}\right\}^* \\ &= \frac{1}{t^{n+1}}\sum_{k=0}^{n} {}_{n-\frac12}C_k(-t)^k\sum_{l=n+1-k}^{\infty}\frac{1}{l!}y^l t^l \\ &= \sum_{l=0}^{\infty}t^l\sum_{k=0}^{\infty} {}_{n-\frac12}C_k\frac{(-)^k y^{n+l+1-k}}{(n+l+1-k)!}, \qquad (20) \end{aligned}$$

so definite integrals I_n and J_n in Eqs. (16) and (17), respectively, can be expressed in power series as

$$\begin{aligned} I_n &= \sum_{k=0}^{\infty} {}_nC_k(-)^k\sum_{l=0}^{\infty}\frac{x^{n+l+1-k}}{(n+l+1-k)!} \\ &\quad \times\sum_{j=0}^{n-1}Q_{lj}\ {}_nM_{n-1-j} \\ &= \sum_{l=0}^{\infty}G_{ln}\sum_{k=0}^{n} {}_nC_k\frac{(-)^k x^{n+l+1-k}}{(n+l+1-k)!}, \qquad (21) \end{aligned}$$

$$
\begin{aligned}
J_n &= \sum_{k=0}^{\infty} {}_{n-\frac{1}{2}}C_k (-)^k \sum_{l=0}^{\infty} \frac{y^{n+l+1-k}}{(n+l+1-k)!} \\
&\quad \times \sum_{j=0}^{n-1} Q_{lj}\ {}_nM_{n-1-j} \\
&= \sum_{l=0}^{\infty} G_{ln} \sum_{k=0}^{n+1+l} {}_{n-\frac{1}{2}}C_k \frac{(-)^k y^{n+l+1-k}}{(n+l+1-k)!},
\end{aligned}
\tag{22}
$$

where

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

$$
G_{ln} \equiv \sum_{j=0}^{n-1} Q_{lj}\ {}_nM_{n-1-j}. \tag{24}
$$

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

$$
\begin{aligned}
F(\vartheta) &\equiv \int_{\vartheta}^{\infty} f(\vartheta)\vartheta d\vartheta = \frac{1}{2}\int_{x}^{\infty} f(\vartheta)dx \\
&= F^{(0)}(\vartheta)+B^{-1}F^{(1)}(\vartheta)+B^{-2}F^{(2)}(\vartheta)+\cdots,
\end{aligned}
\tag{25}
$$

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

$$
\begin{aligned}
F^{(n)}(\vartheta) &= \frac{\Gamma^{(n)}(n+1)}{\Gamma(n+1)} e^{-x} \sum_{k=1}^{n} \frac{x^k}{k!} \sum_{j=k}^{n} {}_nC_j (-)^j \\
&+ e^{-x} \sum_{l=0}^{\infty} G_{ln} \sum_{k=l+2}^{n+l+1} \frac{x^k}{k!} \sum_{j=0}^{n+l+1-k} {}_nC_j (-)^j
\end{aligned}
\tag{26}
$$

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

$$
F^{(0)}(\vartheta) = e^{-x}, \tag{27}
$$

$$
\begin{aligned}
F^{(1)}(\vartheta) &= \left\{\gamma-1+\int_0^x \frac{e^x-1-x}{x^2}dx\right\}xe^{-x} \\
&= e^{-x}-1+\{E_i(x)-\ln x\}xe^{-x}
\end{aligned}
\tag{28}
$$

$$
\begin{aligned}
F^{(2)}(\vartheta) &= \{\psi'(3)+\psi(3)^2\}\left\{\frac{x}{2}-1\right\}xe^{-x} \\
&+ 2e^{-x}\sum_{l=0}^{\infty} \frac{\psi(l+1)+\gamma-\psi(3)}{l+1} \\
&\quad \times \left\{\frac{x^{l+3}}{(l+3)!}-\frac{x^{l+2}}{(l+2)!}\right\},
\end{aligned}
\tag{29}
$$

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.

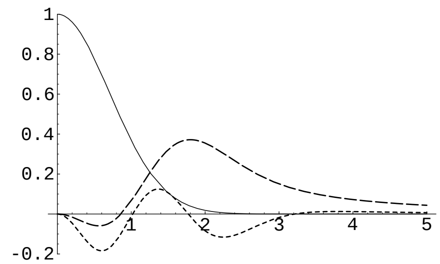

Figure 5: Integrated Molière terms, $F^{(0)}(\vartheta)$ (solid line), $F^{(1)}(\vartheta)$ (broken line), and $F^{(2)}(\vartheta)$ (dot line).

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