Accuracy of numerical functional transforms applied to derive Molière series terms and comparison with analytical results

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Abstract: Accuracies of numerical Fourier and Hankel transforms are examined with the Takahasi-Mori theory of error evaluation. The higher Molière terms both for spatial and projected distributions derived by these methods agree very well with those derived analytically. The methods will be valuable to solve other transport problems concerning fast charged particles.

Introduction

To solve diffusion equations in theoretical studies of particle transport, method of the functional transforms is effective. In the final stage of applying this method we usually use analytical methods to search for exact solutions in mathematical tables and/or to apply approximation methods e.g. the saddle point method [1, 2] or others. If numerical methods for functional transforms were applicable, our knowledge of particle transport problems would be increased.

Andreo, Medin, and Bielajew applied a numerical method of functional transforms on derivation of Molière's series function [3, 4, 5] by using a tool in mathematical libraries and their own integrations [6]. It will be necessary and interesting to confirm reliability of numerical functional transforms by error analyses. We apply Takahasi-Mori theory of error evaluation based on the complex function theory [7] to investigate accuracy and efficiency of the method. Accuracy of our analytical results on Molière's series function of higher orders [8] will also be confirmed in these investigations.

Numerical functional transforms for Molière's series function

We evaluate the spatial and the projected Molière series functions [5] by numerical integration using trapezoidal method:

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

$$\simeq \frac{h}{n!}{\sum_{k=0}^{\infty}}' k J_0(\vartheta hk) e^{-\frac{h^2k^2}{4}} \left(\frac{h^2k^2}{4}\ln\frac{h^2k^2}{4}\right)^n, \quad (1)$$

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

$$\simeq \frac{2h}{\pi n!}{\sum_{k=0}^{\infty}}' \cos(\varphi hk) e^{-\frac{h^2k^2}{4}} \left(\frac{h^2k^2}{4}\ln\frac{h^2k^2}{4}\right)^n, \quad (2)$$

where $\sum'$ denotes the values of the both ends of summation should be taken half. The results agree very well with those derived by analytical method [8], as indicated for $f^{(6)}(\vartheta)$ and $f_{\mathrm{P}}^{(6)}(\varphi)$ in Figs. 1 and 2.

Error analyses of numerical integrations with Takahasi-Mori theory

Takahasi and Mori developed a new method to evaluate errors of numerical integration based on

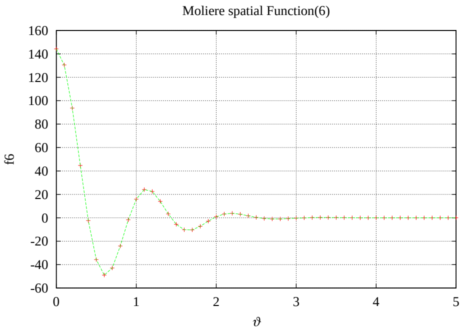

Figure 1: Comparison of $f^{(6)}(\vartheta)$, derived by the numerical method (dots) and the analytical method (lines).

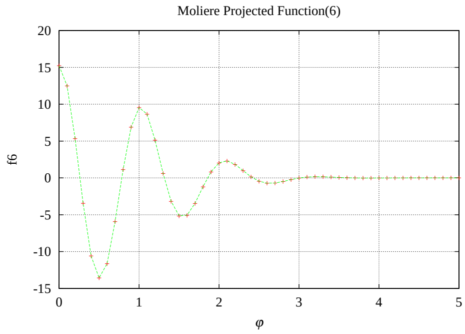

Figure 2: Comparison of $f_{\mathrm{P}}^{(6)}(\varphi)$, derived by the numerical method (dots) and the analytical method (lines).

the complex function theory [7]. We can approximate a definite integral

$$I \equiv \int_a^b f(x)dx \tag{3}$$

by a numerical integration

$$I_a \equiv \sum A_k f(a_k). \tag{4}$$

According to Takahasi and Mori, applying Cauchy integral theorem

$$f(x) = \frac{1}{2\pi i}\oint \frac{f(z)}{z-x}dz, \tag{5}$$

error of the numerical integration ΔI can be evaluated as

$$\begin{aligned} & \Delta I \equiv I - I_a \\ = & \frac{1}{2\pi i}\oint \left(\int_a^b dx \frac{f(z)}{z-x} - \sum \frac{A_k}{z-a_k} f(z) \right) dz \\ = & \frac{1}{2\pi i}\oint \left(\ln\frac{z-a}{z-b} - \sum \frac{A_k}{z-a_k} \right) f(z)dz \\ \equiv & \frac{1}{2\pi i}\oint \Phi(z) f(z) dz, \end{aligned} \tag{6}$$

where $\Phi(z)$ is called the characteristic function of error evaluation determined by the method of numerical integration irrespective of the integrand function.

In case of a numerical integration for infinite interval $(-\infty, \infty)$ by the trapezoidal method,

$$I = \int_{-\infty}^{\infty} g(x)dx \simeq h \sum_{k=-\infty}^{\infty} g(hk). \tag{7}$$

Then the characteristic function $\Phi(z)$ is determined as

$$\begin{aligned} \Phi(z) &= \lim_{k\to\infty} \ln\frac{z+kh}{z-kh} - \sum_{k=-\infty}^{\infty} \frac{h}{z-kh} \\ &= \lim_{k\to\infty} \ln\left(-1-\frac{h}{kh}\right) + \frac{h}{z} - 2hz\sum_{k=0}^{\infty}\frac{1}{z^2-k^2h^2} \\ &= -\pi\left\{ i\ \mathrm{Sign}(\mathrm{Im}\ z) + \cot\frac{\pi z}{h} \right\} \\ &\simeq \pm 2\pi i e^{\pm 2\pi i z/h}, \end{aligned} \tag{8}$$

where the sign $\pm$ should agree with the sign of the imaginary component of z.

In case of a numerical integration for semi-infinite interval $(0, \infty)$ by the trapezoidal method,

$$I = \int_0^{\infty} g(x)dx \simeq h \sum_{k=0}^{\infty} g(hk). \tag{9}$$

Then the characteristic function $\Phi(z)$ is determined as

$$\begin{aligned} \Phi(z) &= \ln(-\frac{z}{h}) + \frac{h}{2z} - \psi(-\frac{z}{h}) \\ &= \ln(-\frac{z}{h}) - \frac{h}{2z} - \psi(\frac{z}{h}) - \pi\cot\frac{\pi z}{h}. \end{aligned} \tag{10}$$

As it approximately satisfies

$$\psi(z) \simeq \ln z - \frac{1}{2z}, \tag{11}$$

$\Phi(z)$ can be well approximated as

$$\Phi(z) \simeq -\pi\left\{ i\ \mathrm{Sign}(\mathrm{Im}\ z) + \cot\frac{\pi z}{h} \right\}, \tag{12}$$

by that for infinite interval [7].

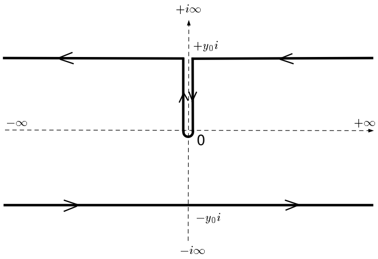

Figure 3: Path of complex integral for $\Delta I_{\rm P}^{(n)}$ with $n \geq 1$.

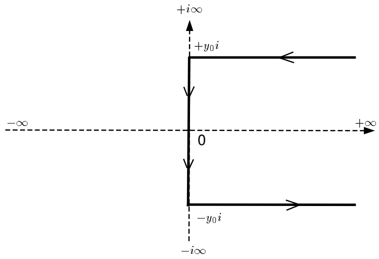

Figure 4: Path of complex integral for $\Delta I^{(n)}$ with $n \geq 0$.

Error analyses for projected angular distribution

The integral in (2) for semi-infinite interval can be evaluated by the integral for infinite interval with the integrand extended on the negative real axis, as the integrand is even. So we can evaluate the error of numerical integration (2) by the formula for infinite interval, thus the error can be evaluated as

$$\Delta I_{\rm P}^{(n)} = \frac{1}{2\pi i}\oint \Phi(z)g(z)dz, \quad \text{where} \quad (13)$$

$$g(z) = \frac{1}{\pi n!}\cos(\varphi z)e^{-\frac{z^2}{4}}\left(\frac{z^2}{4}\ln\frac{z^2}{4}\right)^n, \quad (14)$$

with $\Phi(z)$ of Eq. (8). The path of complex integration is a pair of parallel straight lines, from $iy_0 + i\infty$ to $iy_0 - i\infty$ with y_0 positive and from $iy_0 - i\infty$ to $iy_0 + i\infty$ with y_0 negative.

For $n = 0$,

$$\Delta I_{\rm P}^{(n)} = \frac{1}{\pi}\frac{1}{2\pi i}\oint \Phi(z)\cos(\phi z)e^{-\frac{z^2}{4}}dz. \quad (15)$$

This integral can be well evaluated by the saddle point method [1, 2]:

$$\Delta I_{\rm P}^{(n)} \simeq -\frac{2}{\sqrt{\pi}}e^{-\frac{y_0^2}{4}}, \quad (16)$$

where the saddle points exist at

$$\bar{z} = \pm y_0 i, \quad \text{where} \quad \frac{y_0}{2} \equiv \frac{2\pi}{h} - \varphi. \quad (17)$$

For $n \geq 1$, the integrand $g(z)$ has a branch point at the origin. So we take a schnitt between the origin and the saddle point $z = y_0 i$ defined above and take the path as shown in Fig. 3. The contribution to $\Delta I_{\rm P}^{(n)}$ from the saddle points is about $(2/\sqrt{\pi})e^{-y_0^2/4}$ and is negligible. The value of $\Delta I_{\rm P}^{(n)}$ is determined from the line integral at both sides of the schnitt:

$$\Delta I_{\rm P}^{(n)} = \frac{-1}{2\pi i}\int_0^{y_0}\frac{idy}{\pi n!}\frac{\pi i e^{-\pi y/h}}{\sinh(\pi y/h)}\cosh(\varphi y)e^{\frac{y^2}{4}} \times \left(-\frac{y^2}{4}\right)^n\left\{\left(\ln\frac{y^2}{4}+4\pi i\right)^n - \left(\ln\frac{y^2}{4}\right)^n\right\}. \quad (18)$$

For enough small step size of numerical integration the factor $e^{y^2/4}\cosh(\varphi y)$ can be neglected as they satisfy $\pi/h \gg \varphi$ and $\pi/h \gg 1$, so we have

$$\begin{aligned}\Delta I_{\rm P}^{(n)} &\simeq \frac{2(-1)^n}{(n-1)!}\int_0^{y_0}\frac{e^{-\pi y/h}dy}{\sinh(\pi y/h)}\left(\frac{y^2}{4}\right)^n\left(\ln\frac{y^2}{4}\right)^{n-1} \\ &\simeq \frac{2(-1)^n}{(n-1)!}\left[\frac{d^{n-1}}{dp^{n-1}}\int_0^{\infty}\left(\frac{y^2}{4}\right)^p\frac{e^{-\pi y/h}dy}{\sinh(\pi y/h)}\right]_{p=n} \\ &\simeq -2n(2n-1)!!\zeta(2n+1) \\ &\quad \times\left(\ln\frac{2\pi}{h}\right)^{n-1}\left(\frac{2\pi}{h}\right)^{-2n-1}, \quad (19)\end{aligned}$$

where $\zeta(k)$ denotes ζ-function [9]. The results of $\Delta I_{\rm P}^{(n)}$ are indicated in Fig. 5 for n of 1 and 6.

Error analyses for spatial angular distribution

Molière series function for spatial angular distribution (1) is derived from the integral over semi-infinite interval $(0, \infty)$. The error of numerical integration (1) can be evaluated by the complex integral (6) of Takahasi-Mori theory:

$$\Delta I^{(n)} = \frac{1}{2\pi i}\oint \Phi(z)g(z)dz, \text{ where} \quad (20)$$

$$g(z) = \frac{1}{n!}zJ_0(\vartheta z)e^{-\frac{z^2}{4}}\left(\frac{z^2}{4}\ln\frac{z^2}{4}\right)^n \quad (21)$$

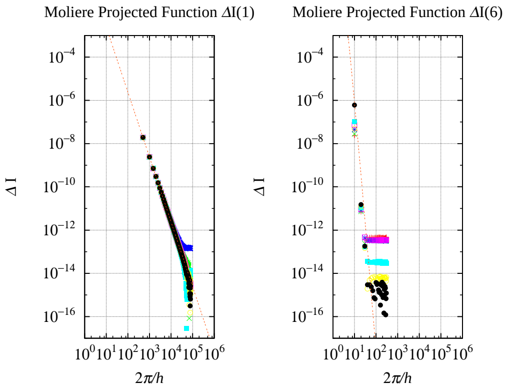

Figure 5: Error evaluation $\Delta I_{\rm P}^{(1)}$ (left) and $\Delta I_{\rm P}^{(6)}$ (right) vs the division rate in derivation of Molière series function for projected angular distribution. Our calculations (dots) agree well with Takahasi-Mori predictions (lines).

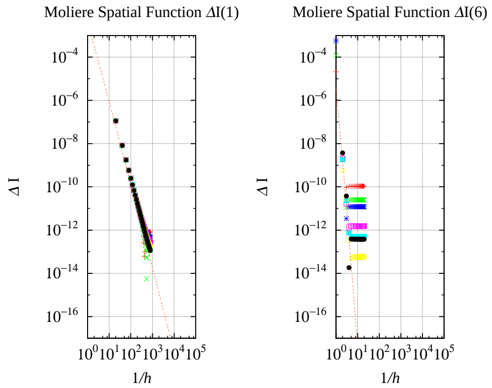

Figure 6: Error evaluation $\Delta I^{(1)}$ (left) and $\Delta I^{(6)}$ (right) vs the division rate in derivation of Molière series function for spatial angular distribution. Our calculations (dots) agree well with Takahasi-Mori predictions (lines).

with the characteristic function $\Phi(z)$ of Eq. (10), or its approximation (8). The path of complex integration is taken as a straight line parallel to the real axis with positive imaginary component y_0 and real component from ∞ to 0, a straight line on the imaginary axis from iy_0 to $-iy_0$, and a straight line parallel to the real axis with negative imaginary component $-y_0$ and real component from 0 to ∞, as shown in Fig. 4.

Taking account $g(z)$ is odd and $\Phi(z)$ falls extremely rapidly at positions far from the real axis, $\Delta I^{(n)}$ can be evaluated as

$$\begin{aligned}\Delta I^{(n)} &= \frac{1}{2\pi i}\int_{y_0 i}^{-y_0 i} dz \frac{\Phi(z)}{2n!} z J_0(\vartheta z) e^{-\frac{z^2}{4}} \left(\frac{z^2}{4}\ln\frac{z^2}{4}\right)^n \\ &\simeq \frac{(-1)^n}{2n!}\left[\frac{d^n}{dp^n}\int_0^\infty \left(\frac{y^2}{4}\right)^p \frac{e^{-\pi y/h}}{\sinh(\pi y/h)} y dy\right]_{p=n} \\ &\simeq \frac{1}{n!}|B_{2n+2}|\left(\ln\frac{2\pi}{h}\right)^n\left(\frac{2}{h}\right)^{-2n-2}, \qquad (22)\end{aligned}$$

where B_n denotes Bernoulli number [9]. The results of $\Delta I^{(n)}$ are indicated in Fig. 6 for n of 1 and 6.

Conclusions and discussions

We have evaluated Molière series functions by numerical functional transforms up to 6-th higher terms for both spatial and projected angular distributions. The results have agreed very well with those derived by analytical method [8] and Andreo et al.'s [6], and convergences of our numerical functional transforms are confirmed by Takahasi and Mori theory of error evaluation [7].

These results will prove reliability of numerical functional transforms applied in particle transport problems, as well as efficiencies of Takahasi-Mori theory in these problems.

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