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ORIGINAL PAPER

Efficient spherical surface integration of Gauss functions in three-dimensional spherical coordinates and the solution for the modified Bessel function of the first kind

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Abstract

An efficient solution of calculating the spherical surface integral of a Gauss function defined as $h(s,\mathbf{Q}) = \int_0^{2\pi}\int_0^{\pi}(\mathbf{s}+\mathbf{Q})_x^i(\mathbf{s}+\mathbf{Q})_y^j(\mathbf{s}+\mathbf{Q})_z^k e^{-\gamma(\mathbf{s}+\mathbf{Q})^2}\sin\theta d\theta d\varphi$ is provided, where $\gamma \geq 0$, and i, j, k are nonnegative integers. A computationally concise algorithm is proposed for obtaining the expansion coefficients of polynomial terms when the coordinate system is transformed from cartesian to spherical. The resulting expression for $h(s,\mathbf{Q})$ includes a number of cases of elementary integrals, the most difficult of which is $II(n,\mu) = \int_0^{\pi}\cos^n\theta e^{-\mu\cos\theta}d\theta$, with a nonnegative integer n and positive μ. This integral can be formed by linearly combining modified Bessel functions of the first kind $B(n,\mu) = \frac{1}{\pi}\int\limits_0^{\pi} e^{\mu\cos\theta}\cos(n\theta)d\theta$, with a nonnegative integer n and negative μ. Direct applications of the standard approach using Mathematica and GSL are found to be inefficient and limited in the range of the parameters for the Bessel function. We propose an asymptotic function for this expression for $n = 0,1,2$. The relative error of asymptotic function is in the order of 10^{-16} with the first five terms of the asymptotic expansion. At last, we give a new asymptotic function of $B(n,\mu)$ based on the expression for $e^{-\mu}II(n,\mu)$ when n is an integer and μ is real and large in absolute value.

Keywords Bessel function · Gauss function · Recursive relation · Computational algorithm

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1 Introduction

In this paper, we provide a solution for the following surface integral in the spherical coordinates (s, θ, φ), where the integrand is a Gauss function situated at point $\mathbf{Q}$:

$$h(s, \mathbf{Q}) = \int_0^{2\pi} \int_0^{\pi} g(\mathbf{s}, \mathbf{Q}) \sin\theta d\theta d\varphi, \quad (1)$$

where

$$g(\mathbf{s}, \mathbf{Q}) = (\mathbf{s}+\mathbf{Q})_x^i (\mathbf{s}+\mathbf{Q})_y^j (\mathbf{s}+\mathbf{Q})_z^k e^{-\gamma(\mathbf{s}+\mathbf{Q})^2}, \\ \gamma \geq 0. \quad (2)$$

Gauss functions in the form of Eq. (2) is routinely applied in numerical solutions in science and engineering. The surface integral Eq. (1) is often encountered when the field strength pertains to the distance s only, e.g. quantum exchange effect [1, 2].

Critically, the solution includes a solution for the following novel integral:

$$II(n, \mu) = \int_0^{\pi} \cos^n \theta e^{-\mu \cos\theta} d\theta, \quad (3)$$

where

$$\mu \geq 0,\ n \in \mathbb{Z}^*.\ (\mathbb{Z}^* \text{ is the set of non - negative integer}).$$

This integral can be formed by linearly combining of the modified Bessel functions of the first kind [3, 4]:

$$B(n, \mu) = \frac{1}{\pi} \int_0^{\pi} e^{\mu \cos\theta} \cos(n\theta) d\theta. \quad (4)$$

In this paper, we provide a solution for the spherical surface integration Eq. (1). We also provide a new efficient solution for $B(n, \mu)$ when n is an integer and μ is real and large in absolute value. The solutions involve a recursive relation for n and an asymptotic expansion for large $|\mu|$. We note that an apparently different approach for solving Eq. (1) is mentioned in ref. [5].

2 Spherical surface integration

In Eq. (2), we notice that the original coordinate is not convenient for the exponential term $e^{-\gamma(\mathbf{s}+\mathbf{Q})^2}$. Thus, we rotate the coordinate to make the direction of $\mathbf{Q}$ be the new z-axis. Suppose

$$\mathbf{Q} = \left(Q\sin\tilde{\theta}\cos\tilde{\varphi} \;\; Q\sin\tilde{\theta}\sin\tilde{\varphi} \;\; Q\cos\tilde{\theta} \right)^T, \quad (5)$$

$$\begin{pmatrix} x \\ y \\ z \end{pmatrix} = \begin{pmatrix} (\mathbf{s}+\mathbf{Q})_x \\ (\mathbf{s}+\mathbf{Q})_y \\ (\mathbf{s}+\mathbf{Q})_z \end{pmatrix}. \tag{6}$$

The relationship between (x, y, z) and new coordinate $(\tilde{x}, \tilde{y}, \tilde{z})$ after the rotation is:

$$\begin{pmatrix} x \\ y \\ z \end{pmatrix} = A^{-1} \begin{pmatrix} \tilde{x} \\ \tilde{y} \\ \tilde{z} \end{pmatrix}, \tag{7}$$

where

$$A = A_2 A_1 \tag{8}$$

$$A_1 = \begin{pmatrix} \cos\tilde{\varphi} & \sin\tilde{\varphi} & 0 \\ -\sin\tilde{\varphi} & \cos\tilde{\varphi} & 0 \\ 0 & 0 & 1 \end{pmatrix}, \; A_2 = \begin{pmatrix} \cos\tilde{\theta} & 0 & -\sin\tilde{\theta} \\ 0 & 1 & 0 \\ \sin\tilde{\theta} & 0 & \cos\tilde{\theta} \end{pmatrix}. \tag{9}$$

Now we need to collect the new coefficients in terms of new coordinates. We notice that once we have the rotation matrix A, the function $g(\mathbf{s}, \mathbf{Q})$ can be expressed as:

$$\begin{aligned} g(\mathbf{s}, \mathbf{Q}) &= x^i y^j z^k e^{-\gamma(\mathbf{s}+\mathbf{Q})^2} \\ &= f\left(a_1\tilde{x} + b_1\tilde{y} + c_1\tilde{z}\right)^i \left(a_2\tilde{x} + b_2\tilde{y} + c_2\tilde{z}\right)^j \left(a_3\tilde{x} + b_3\tilde{y} + c_3\tilde{z}\right)^k e^{-2\gamma\mathbf{sQ}-2\gamma sQ}, \end{aligned} \tag{10}$$

where

$$f = e^{-\gamma\left(s^2+Q^2\right)+2\gamma sQ}.$$

The $e^{-\gamma\mathbf{sQ}}$ inside Eq. (10) can be simplified as $e^{-\gamma sQ\cos\theta}$ within the rotation, where θ is the angle between $\mathbf{s}$ and $\mathbf{Q}$. In Eq. (10), $g(\mathbf{s}, \mathbf{Q})$ will be linear combination of new coordinate $(\tilde{x}, \tilde{y}, \tilde{z})$. That is, we want to get the form of:

$$g(\mathbf{s}, \mathbf{Q}) = \sum_t \sum_s \sum_r f_{tsr} \tilde{x}^t \tilde{y}^s \tilde{z}^r e^{-\mu(\cos\theta+1)}, \tag{11}$$

where

$$\mu = 2\gamma sQ.$$

The original integral $h(s, \mathbf{Q})$ now becomes a linear combination of the following term in general:

$$F_{ijkl} = \int_0^{2\pi} \int_0^{\pi} \sin^i\theta \cos^j\theta \sin^k\varphi \cos^l\varphi e^{-\mu(\cos\theta+1)} d\theta d\varphi. \tag{12}$$

It is tedious and cumbersome to expand directly the products of the polynomials in Eq. (10) and collect the coefficients for different F_{ijkl}. Here we provide an algorithm that speeds up this step. We define

$$p(\tilde{x}) = \left(a_1\tilde{x} + Y_1\right)^i \left(a_2\tilde{x} + Y_2\right)^j \left(a_3\tilde{x} + Y_3\right)^k, \quad (13)$$

where

$$Y_s = b_s\tilde{y} + C_s$$
$$Z_s = c_s\tilde{z}.$$

Then, we have:

$$p(\tilde{x}) = \sum_{t=0}^{i+j+k} f'(t,i,j,k)\tilde{x}^t, \quad (14)$$

where

$$f'(t,i,j,k) = \sum_{l=\max\{0,t-(j+k)\}}^{\min\{i,t\}} \sum_{m=\max\{0,t-l-k\}}^{\min\{t-l,j\}} a_1^l a_2^m a_3^{t-l-m} \binom{i}{l}\binom{j}{m}\binom{k}{t-l-m} Y_1^{i-l} Y_2^{j-m} Y_3^{k+l+m-t}.$$

$Y_1^{i-l} Y_2^{j-m} Y_3^{k+l+m-t}$ can be done using Eqs. (13) and (14) again to obtain the coefficients for various powers of $\tilde{y}$ and $\tilde{z}$. Those coefficients are multiplied together to yield f_{tsr} in Eq. (11). The advantage of this formalism over the direct expansion is that the coefficient for $\tilde{x}^t$ is only calculated once when $\tilde{y}$ and $\tilde{z}$ terms are expanded.

The integral of F_{ijkl} in Eq. (12) involves two parts: I_{ij} and J_{kl}:

$$F_{ijkl} = I_{ij} J_{kl}, \quad (15)$$

where

$$I_{ij} = \int_0^{\pi} \sin^i\theta \cos^j\theta e^{-\mu(\cos\theta+1)} d\theta, \quad (16)$$

$$J_{kl} = \int_0^{2\pi} \sin^k\varphi \cos^l\varphi d\varphi. \quad (17)$$

We show the details of integral J_{kl} first. It has two cases:

Case 1: Either k or l is odd or both are odd in Eq. (17). Let k be odd and define P:

$$P(\varphi) = \sin^k\varphi \cos^l\varphi \quad (18)$$

We notice that the function $P(\varphi)$ is an odd function centered at π. That is $P(\pi - \varphi) = -P(\pi + \varphi)$.

$$\begin{aligned} P(\pi - \varphi) &= \sin^k(\pi - \varphi)\cos^l(\pi - \varphi) \\ &= (-1)^k \sin^k(\varphi - \pi)\cos^l(\varphi - \pi) \\ &= -P(\pi + \varphi). \end{aligned} \tag{19}$$

Proof

. □

Thus, the integral J_{kl} will be zero. If l is an odd number and k is an even number, we can find that $P(\varphi)$ is still an odd function centered by $\pi/2$ with period π. That is $P(\pi/2 - \varphi) = -P(\pi/2 + \varphi)$.

$$\begin{aligned} P(\pi/2 - \varphi) &= \sin^k(\pi/2 - \varphi)\cos^l(\pi/2 - \varphi) \\ &= (-1)^k \sin^k(-\pi/2 + \varphi)\cos^l(-\pi/2 + \varphi) \\ &= (-1)^{2k+l} \sin^k(\pi/2 + \varphi)\cos^l(\pi/2 + \varphi) \\ &= -P(\pi/2 + \varphi) \end{aligned} \tag{20}$$

Proof

□

All the above shows $J_{kl} = 0$ in this case.

Case 2: Both of k and l are even. $\left(k = 2k',\ l = 2l'\right)$

$$\begin{aligned} J_{kl} &= \int_0^{2\pi} \sin^{2k'}\varphi\cos^{2l'}\varphi d\varphi \\ &= \int_0^{2\pi} \left(\frac{1-\cos 2\varphi}{2}\right)^{k'}\left(\frac{1+\cos 2\varphi}{2}\right)^{l'} d\varphi \\ &= 2^{-\left(k'+l'+1\right)} \sum_{t=0}^{k'+l'} f\left(t, k', l'\right) \int_0^{2\pi} \cos^t 2\varphi d2\varphi, \end{aligned} \tag{21}$$

where

$$f\left(t, k', l'\right) = \sum_{s=\max\{0, t-l'\}}^{\min\{k', t\}} \binom{k'}{s}\binom{l'}{t-s}(-1)^s \tag{22}$$

The trigonometric integral $\int_0^{\pi} \cos^t \varphi' d\varphi' \left(\varphi' = 2\varphi\right)$ has the following recursive relation:

$$\int \cos^n x dx = \frac{\cos^{n-1} x \sin x}{n} + \frac{n-1}{n} \int \cos^{n-2} x dx \tag{23}$$

The integral I_{ij} has two cases too, depending on the parity of i.

Case 1: When i is odd $\left(i = 2i' + 1\right)$, with i' being an integer,

$$
\begin{aligned}
I_{ij} &= \int_0^{\pi} \sin^{2i'+1}\theta \cos^j \theta e^{-\mu(\cos\theta+1)} d\theta \\
&= -\int_0^{\pi} \left(1-\cos^2\theta\right)^{i'} \cos^j \theta e^{-\mu(\cos\theta+1)} d\cos\theta \\
&= \sum_{s=0}^{i'} (-1)^{s+1} \binom{i'}{s} e^{-\mu} \int_0^{\pi} \cos^{j+2s}\theta e^{-\mu\cos\theta} d\cos\theta.
\end{aligned}
\tag{24}
$$

The trigonometric integral inside Eq. (24) can be calculated as the following:

$$
\int_1^{-1} x'^{j'} e^{-\mu x'} dx' = e^{-\mu x'} \sum_{s=0}^{j'} (-1)^{j'-s} \frac{j'!}{s!(-u)^{j'-s+1}} x'^s \Bigg|_1^{-1}, \tag{25}
$$

where

$$
x' = \cos\theta,\ j' = j + 2s
$$

Case 2: When i is even, i.e. $i = 2i'$ with i' being an integer,

$$
\begin{aligned}
I_{ij} &= \int_0^{\pi} \sin^{2i'}\theta \cos^j \theta e^{-\mu(\cos\theta+1)} d\theta \\
&= \int_0^{\pi} \left(1-\cos^2\theta\right)^{i'} \cos^j \theta e^{-\mu(\cos\theta+1)} d\theta \\
&= \sum_{s=0}^{i'} (-1)^{s} \binom{i'}{s} \int_0^{\pi} \cos^{j+2s}\theta e^{-\mu(\cos\theta+1)} d\theta.
\end{aligned}
\tag{26}
$$

We define $I(n, \mu)$:

$$
I(n,\mu) = \int_0^{\pi} \cos^n \theta e^{-\mu(\cos\theta+1)} d\theta \tag{27}
$$

We tried to use Mathematica [6] and GSL [7] to evaluate Eq. (27). The solution from Mathematica involves modified Bessel functions of the first kind. It is slow and the computational time grows exponentially with respect n, as show in Fig. 1. This is undesirable when Eq. (27) is computed repeatedly in a practical application with numerous μ and n combinations.

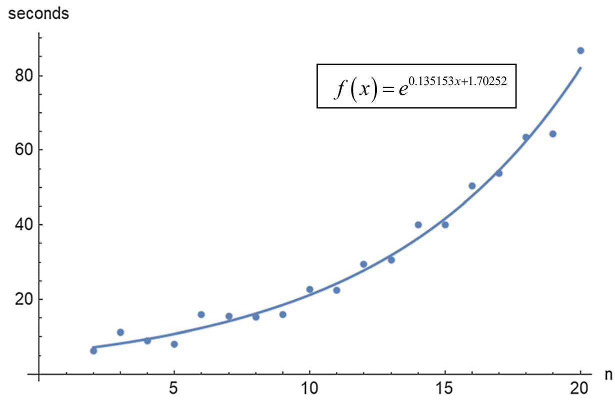

Fig. 1 Time of $I(n,\mu)=\int_0^\pi \cos^n\theta e^{-\mu(\cos\theta+1)}d\theta$ ($\mu=20$) with respect to n using Mathematica on an Intel(R) Core™ i5-4300U

Second, the computation of the Bessel function $B(n, \mu)$ (Eq. (4)) in Mathematica and GSL has the drawback that the result is out of range quickly for large μ. To our knowledge, the current way of computing $B(n, \mu)$ uses the following formula [8]:

$$B(n,\mu)=C_n\left(\frac{d}{d\mu}\right)B(0,\mu), \tag{28}$$

where $C_n(\mu)$ is the Chebyshev polynomial of the first kind [9]. $B(0, \mu)$ is computed with the following expansion [8]:

$$B(0,\mu)=\sum_{k=0}^{\infty}\frac{\left(\mu^2/4\right)^k}{(k!)^2}. \tag{29}$$

This expansion can be long for a large μ, causing an overflow on a computer. In practice, we find that GSL library fails when $\mu \geq 500$.

We derive the following recursive relation to improve the efficiency for large n:

$$I(n,\mu)=\frac{n-1}{\mu}I(n-1,\mu)+I(n-2,\mu)+\frac{n-1}{\mu}I(n-3,\mu). \tag{30}$$

The derivation of this recursive relation is based on integration by parts:

$$
\begin{aligned}
I(n,\mu) &= e^{-\mu}\int_0^{\pi} \cos^{n-1}\theta e^{-\mu\cos\theta} d\sin\theta \\
&= e^{-\mu}\left(\sin\theta \cos^{n-1}\theta e^{-\mu\cos\theta}\Big|_0^{\pi} - \int_0^{\pi} \sin\theta d\left(\cos^{n-1}\theta e^{-\mu\cos\theta}\right) \right) \\
&= e^{-\mu}\left(-\int_0^{\pi} (n-1)\left(-\sin^2\theta\right)\cos^{n-2}\theta e^{-\mu\cos\theta} + \mu\sin^2\theta\cos^{n-1}\theta e^{-\mu\cos\theta} d\theta \right) \\
&= (n-1)\int_0^{\pi} \cos^{n-2}\theta e^{-\mu(\cos\theta+1)}d\theta - (n-1)\int_0^{\pi} \cos^{n}\theta e^{-\mu(\cos\theta+1)}d\theta \\
&\quad - \mu\int_0^{\pi} \cos^{n-1}\theta e^{-\mu(\cos\theta+1)}d\theta + \mu\int_0^{\pi} \cos^{n+1}\theta e^{-\mu(\cos\theta+1)}d\theta
\end{aligned}
\tag{31}
$$

The first three terms need to be evaluated explicitly for this recursive relation. Using Mathematica yields the following results based on $B(n,\mu)$(Eq. (4)):

$$
I(0,\mu) = \pi e^{-\mu} B(0,\mu), \tag{32}
$$

$$
I(1,\mu) = \pi e^{-\mu} B(1,\mu), \tag{33}
$$

$$
I(2,\mu) = \frac{\pi e^{-\mu}}{\mu}(B(1,\mu) + \mu B(2,\mu)), \tag{34}
$$

We developed the following asymptotic expansions for $I(n,\mu)$ (n=0, 1, 2) for large μ since the standard method fails as explained above. $I(0,\mu)$ can be transformed into:

$$
I(0,\mu) = 2\int_0^{\pi/2} e^{-2\mu\cos^2\theta'} d\theta', \tag{35}
$$

where $\theta' = \theta/2$. Let $T = \cos\theta'$, the Eq. (35) becomes:

$$
I(0,\mu) = 2\int_0^{1} e^{-2\mu T^2} \frac{1}{\sqrt{1-T^2}} dT. \tag{36}
$$

$1/\sqrt{1-T^2}$ expanded by Taylor expansion:

$$
\frac{1}{\sqrt{1-T^2}} = \sum_{n=0}^{\infty} \binom{-1/2}{n} \left(-T^2\right)^n. \tag{37}
$$

Finally, we get the asymptotic function for $I(0,\mu)$:

$$I(0,\mu) = 2\sum_{n=0}^{\infty}\binom{-1/2}{n}(-1)^n\int_0^1 e^{-2\mu T^2}T^{2n}dT. \tag{38}$$

The formulas for $\int_0^1 e^{-2\mu T^2}T^{2n}dT$ can be obtained using Mathematica. The resulted expression involves the error function, which can be computed efficiently on modern computers. The formulas are listed in the appendix for the reader's convenience.

The formulas for $I(1, \mu)$ and $I(2, \mu)$ can be derived the same way:

$$\begin{aligned} I(1,\mu) &= 2\int_0^{\pi/2}\left(2\cos^2\theta' - 1\right)e^{-2\mu\cos^2\theta'}d\theta' \\ &= 4\int_0^1 e^{-2\mu T^2}\frac{T^2}{\sqrt{1-T^2}}dT - 2\int_0^1 e^{-2\mu T^2}\frac{1}{\sqrt{1-T^2}}dT \\ &= 4\sum_{n=0}^{\infty}\binom{-1/2}{n}(-1)^n\int_0^1 e^{-2\mu T^2}T^{2n+2}dT - 2\sum_{n=0}^{\infty}\binom{-1/2}{n}(-1)^n\int_0^1 e^{-2\mu T^2}T^{2n}dT, \end{aligned} \tag{39}$$

$$\begin{aligned} I(2,\mu) &= 2\int_0^{\pi/2}\left(2\cos^2\theta' - 1\right)^2 e^{-2\mu\cos^2\theta'}d\theta' \\ &= 4\sum_{n=0}^{\infty}\binom{-1/2}{n}(-1)^n\int_0^1 e^{-2\mu T^2}T^{2n+4}dT - 4\sum_{n=0}^{\infty}\binom{-1/2}{n}(-1)^n\int_0^1 e^{-2\mu T^2}T^{2n+2}dT \\ &\quad + 2\sum_{n=0}^{\infty}\binom{-1/2}{n}(-1)^n\int_0^1 e^{-2\mu T^2}T^{2n}dT. \end{aligned} \tag{40}$$

We tested those asymptotic functions (Eqs. (38)–(40)) for $0 \le \mu \le 8000$ and found that the relative error is in the order of 10^{-16} by keeping the first 5 terms. The combination of this short expansion and the recursive relation ensures not only efficiency, but also precision. The integral $II(n, \mu)$ in Eq. (3) can be evaluated as:

$$II(n,\mu) = e^{\mu}I(n,\mu). \tag{41}$$

This concludes the solution for the surface integral in Eq. (1).

As one may see, the above derivations also provide a new way for solving Bessel function $B(n, \mu)$ (Eq. (4)). First, we recognize that $B(n, \mu)$ can be computed as $B(n, - \mu)$ when $\mu > 0$:

$$B(n,\mu) = (-1)^n B(n,-\mu). \tag{42}$$

This becomes obvious from the following ascending series [3]:

$$B(n, \mu) = (\mu/2)^n \sum_{k=0}^{\infty} \frac{\left(\mu^2/4\right)^k}{k!\Gamma(n+k+1)}. \tag{43}$$

Consider $B(n, \mu)$ when $\mu > 0$. It can be rewritten using $C_n(\cos\theta)$(Eq. (28)) [8, 9]:

$$B(n, \mu) = \frac{(-1)^n}{\pi} \int_0^{\pi} e^{-\mu\cos\theta} C_n(\cos\theta) d\theta, \tag{44}$$

The Chebyshev polynomial can also be defined as the following [9]:

$$C_n(\cos\theta) = \frac{n}{2} \sum_{r=0}^{\lfloor n/2 \rfloor} \frac{(-1)^r}{n-r} \binom{n-r}{r} 2^{n-2r} \cos^{n-2r}\theta \tag{45}$$

Combing Eqs. (27), (44) and (45) yields:

$$B(n, \mu) = \frac{(-1)^n n}{2\pi} e^{\mu} \sum_{r=0}^{\lfloor n/2 \rfloor} \frac{(-1)^r}{n-r} \binom{n-r}{r} 2^{n-2r} I(n-2r, \mu), \quad n \geq 1, \tag{46}$$

$$B(0, \mu) = \frac{e^{\mu}}{\pi} I(0, \mu). \tag{47}$$

$B(-n, \mu)$ has the same formula since $B(-n, \mu) = B(n, \mu)$.

3 Conclusion

An efficient solution of calculating the spherical surface integral of a Gauss function defined as $h(s, \mathbf{Q})$ in Eq. (1) is provided. A computationally concise algorithm is proposed for obtaining the expansion coefficients of polynomial terms when the coordinate system is transformed from cartesian to spherical. The resulting expression for $h(s, \mathbf{Q})$ includes a number of cases of elementary integrals, the most difficult of which is $e^{-\mu} II(n, \mu)$ as defined in Eq. (3). This integral can be formed by linearly combining of Bessel functions $B(n, \mu)$ (Eq. (4)) with a non-negative integer n and negative μ. Direct applications of the standard approach using Mathematica and GSL are found to be inefficient and limited in the range of the parameters for the Bessel function. We propose an asymptotic function for this expression for $n = 0,1,2$. The relative error of the asymptotic function is in the order of 10^{-16} with the first five terms of the asymptotic expansion. At last, we give a new asymptotic function of $B(n, \mu)$ based on the expression for $e^{-\mu} II(n, \mu)$ when n is an integer and μ is real and large in absolute value.

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Appendix

Formulas for $\int_0^1 e^{-2\mu T^2} T^{2n} dT$ used in Eqs. (38) to (40).

n	$\int_0^1 e^{-2\mu T^2} T^{2n} dT$
0	$\frac{1}{2}\sqrt{\frac{\pi}{2\mu}}Erf\left(\sqrt{2\mu}\right)$
1	$\frac{-4e^{-2u}\sqrt{u}+\sqrt{2\pi}Erf\left(\sqrt{2}\sqrt{u}\right)}{16u^{3/2}}$
2	$\frac{-4e^{-2u}\sqrt{u}(3+4u)+3\sqrt{2\pi}Erf\left(\sqrt{2}\sqrt{u}\right)}{64u^{5/2}}$

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