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ABSTRACT

We present a new fast algorithm for computing the Boys function using a nonlinear approximation of the integrand via exponentials. The resulting algorithms evaluate the Boys function with real and complex valued arguments and are competitive with previously developed algorithms for the same purpose.

I. INTRODUCTION

The Boys function[1]

$$F(n,z) = \int_0^1 e^{-zt^2} t^{2n} dt = \frac{1}{2}\int_0^1 e^{-zs} s^{n-1/2} ds \tag{1}$$

appears in problems of computing Gaussian integrals, and over the years, there were many algorithms proposed for its evaluation; see, e.g., Refs. 2–10. The Boys function is related to a number of special functions, for example, the error function and the incomplete Gamma function, and (for a pure imaginary argument) to the Fresnel integrals.

It is common (see, e.g., Refs. 5 and 7) to use recursion to compute the Boys function for different n. The recursion is obtained via integration by parts,

$$\begin{aligned} F(n,z) &= -\frac{1}{2z}\int_0^1 \frac{d}{ds}\left(e^{-zs}\right) s^{n-1/2} ds \\ &= \frac{n-1/2}{z} F(n-1,z) - \frac{1}{2z} e^{-z}, \end{aligned} \tag{2}$$

and can be run starting with $n = 1$ so that we need to have the value $F(0,z)$ or starting from a large $n = n_{\max}$ and going to $n = 1$,

$$F(n-1,z) = \frac{z}{n-1/2} F(n,z) + \frac{1}{2(n-1/2)} e^{-z}, \tag{3}$$

so that we need to have the value $F(n_{\max},z)$. In order to avoid a loss of accuracy, the choice of which recursion to use depends on the size z and $n_{\max}$. Iterating recursion (2), the dominant term expressing $F(n,z)$ via $F(0,z)$ is $\prod_{j=1}^{n}(j-1/2)/z^n$. We set

$$z^* = \left(\prod_{j=1}^{n}(j-1/2)\right)^{1/n}$$

and choose (2) when $|z| \geq z^*$ and (3) if $|z| < z^*$. For example, if $n_{\max} = 18$, then $z^* \approx 6.75$. We note that other choices of the parameter z^* are possible.

At each step, recursions (2) and (3) require only three multiplications and one addition (since the coefficients can be computed in advance and stored), so it is hard to obtain a more efficient alternative if one needs to compute these functions for a range of n, $1 \leq n \leq n_{\max}$. In order to initialize these recursions, we need fast algorithms for computing $F(0,z)$ and $F(n_{\max},z)$. Computing $F(0,z)$ for real z is straightforward since

$$F(0,z) = \int_0^1 e^{-zt^2} dt = \frac{\sqrt{\pi}\,\mathrm{Erf}\left(\sqrt{z}\right)}{2\sqrt{z}}. \tag{4}$$

For a real argument, an optimized implementation of the error function Erf is available within programming languages. For a complex argument, we present an algorithm for computing $F(0,z)$ using a nonlinear approximation of the integrand following the approach in Ref. 11. We obtain a rational approximation of $F(0,z)$ with an additional exponential factor.

We note that, as a function of complex argument, the Boys function $F(0,z)$ can be highly oscillatory. In particular, if z is purely imaginary, then the Boys function is related to the Fresnel integrals,

$$S(y) = \int_0^y \sin\left(\frac{\pi}{2}t^2\right)dt,\ C(y) = \int_0^y \cos\left(\frac{\pi}{2}t^2\right)dt$$

so that

$$C(y) - iS(y) = \int_0^y e^{-i\frac{\pi}{2}t^2}dt = y\int_0^1 e^{-i\frac{\pi}{2}y^2s^2}ds = yF\left(0, i\frac{\pi}{2}y^2\right). \quad (5)$$

For computing $F(n_{\max}, z)$, instead of tabulating this function as it is performed for a real argument in, e.g., Refs. 2, 5, 7, and 9, we use a nonlinear approximation of the integrand in (1) (see Ref. 11), leading to an approximation of the Boys function valid for the complex argument $\mathcal{Re}(z) \geq 0$ with tight error estimates. For $\mathcal{Re}(z) < 0$, we compute $e^z F(n,z)$ instead of $F(n,z)$. Based on these approximations, we develop two algorithms, for real and complex valued arguments. We refer to Refs. 3, 4, and 8 for previously developed algorithms for the Boys function with the complex argument. The complex argument appears in a number of problems, for example, in calculations with mixed Gaussian/plane wave bases in molecules and scattering problems,[12–16] in the context of complex scaling calculations of excited states,[17] and in using gauge invariant basis functions for calculating magnetic properties.[18]

II. APPROXIMATION OF $F(0,z)$ FOR COMPLEX VALUED ARGUMENT

We have

$$F(0,z) = \int_0^1 e^{-zt^2}dt = \frac{1}{2}\int_0^1 e^{-zs}s^{-1/2}ds \quad (6)$$

and use the integral

$$s^{-1/2} = \frac{2}{\sqrt{\pi}}\int_0^\infty e^{-st^2}dt \quad (7)$$

to obtain

$$F(0,z) = \frac{1}{\sqrt{\pi}}\int_0^\infty \frac{1-e^{-(t^2+z)}}{t^2+z}dt = \frac{1}{\sqrt{\pi}}\int_0^\infty q\left(t^2+z\right)dt, \quad (8)$$

where

$$q(\xi) = \left(1 - e^{-\xi}\right)/\xi, \xi \in \mathbb{C},$$

is an analytic function. An algorithm for computing $F(0,z)$ is essentially a quadrature for the integral in (8). Note that if, instead, we were to use a quadrature to compute $F(0,z)$ via integrals in (6), then, for each z, we would need to evaluate as many exponentials as the number of quadrature terms. Importantly, when using (8), we need to evaluate e^{-z} only once and then use the result as a factor.

A. The case $\mathcal{Re}(z) \geq 0$.

We split integral (8) into three terms

$$F(0,z) = \frac{1}{\sqrt{\pi}}\int_0^\infty \frac{1}{t^2+z}dt - \frac{e^{-z}}{\sqrt{\pi}}\int_0^{t_{\max}} \frac{e^{-t^2}}{t^2+z}dt - \frac{e^{-z}}{\sqrt{\pi}}\int_{t_{\max}}^\infty \frac{e^{-t^2}}{t^2+z}dt \quad (9)$$

and observe that the last term in (9) (without the factor e^{-z}) is estimated as

$$\left|\frac{1}{\sqrt{\pi}}\int_{t_{\max}}^\infty \frac{e^{-t^2}}{t^2+z}dt\right| \leq \frac{1}{\sqrt{\pi}}\int_{t_{\max}}^\infty \frac{e^{-t^2}}{|t^2+z|}dt \leq \frac{1}{\sqrt{\pi}}\int_{t_{\max}}^\infty \frac{e^{-t^2}}{t^2}dt = \frac{1}{\sqrt{\pi}}\left(\frac{e^{-t_{\max}^2}}{t_{\max}} - \sqrt{\pi}\mathrm{Erfc}(t_{\max})\right) = \epsilon_{t_{\max}}. \quad (10)$$

Select $t_{\max} = e^{7/4}$ to obtain $\varepsilon_{t_{\max}} \approx 5.9 \cdot 10^{-18}$. For the first term in (9), we have

$$\frac{1}{\sqrt{\pi}}\int_0^\infty \frac{1}{t^2+z}dt = \frac{1}{2}\sqrt{\frac{\pi}{z}}.$$

For $|z| \geq r_0 = 0.35$, we use quadrature (see the Appendix for details) to approximate the second term in (9) as

$$\left|\frac{1}{\sqrt{\pi}}\int_0^{t_{\max}} \frac{e^{-t^2}}{t^2+z}dt - \sum_{m=1}^{M}\frac{w_m e^{-\eta_m}}{\eta_m+z}\right| \leq \varepsilon, \quad (11)$$

where $M = 22$ and nodes and weights are given in Table I. We note that it is possible to use the standard Gauss–Legendre quadrature on the interval $[0, t_{\max}]$, but the number of terms, M, will be larger. As a result, we obtain approximation

$$\left|F(0,z) - \left(\frac{1}{2}\sqrt{\frac{\pi}{z}} - \frac{1}{2\sqrt{\pi}}e^{-z}\sum_{m=1}^{22}\frac{w_m e^{-\eta_m}}{\eta_m+z}\right)\right| \leq 2\varepsilon + \varepsilon_{t_{\max}}, |z| \geq r_0. \quad (12)$$

B. The case $\mathcal{Re}(z) < 0$

In this case, we compute $e^z F(0,z)$ rather than $F(0,z)$. Since the denominator in (8) can be zero, we cannot separate terms in $q\left(t^2+z\right)$ as in (9). Instead, we split integral (8) into two terms and obtain

$$e^z F(0,z) = \frac{e^z}{\sqrt{\pi}}\int_0^{t_{\max}} \frac{1-e^{-(t^2+z)}}{t^2+z}dt + \frac{1}{\sqrt{\pi}}\int_{t_{\max}}^\infty \frac{e^z - e^{-t^2}}{t^2+z}dt. \quad (13)$$

The first term in (13) is approximated by using the Gauss–Legendre quadrature on the interval $[0, t_{\max}]$. The function q is analytic, and therefore, there is no singularity at $t^2 = -z$. Since we can compute derivatives of q, the error introduced by this quadrature can be estimated using results in Sec. 5.2 of Ref. 19. For example,

TABLE I. The poles and weights in (12).

m	η_m	$w_m \cdot e^{-\eta_m}$	m	η_m	$w_m \cdot e^{-\eta_m}$
1	$0.147\,787\,826\,379\,695\,65 \times 10^{-02}$	$0.866\,431\,027\,201\,416\,54 \times 10^{-01}$	12	$0.125\,395\,022\,879\,192\,93 \times 10^{+01}$	$0.574\,448\,042\,214\,302\,23 \times 10^{-01}$
2	$0.133\,172\,764\,137\,258\,17 \times 10^{-01}$	$0.857\,720\,608\,434\,394\,68 \times 10^{-01}$	13	$0.172\,446\,342\,335\,733\,95 \times 10^{+01}$	$0.420\,819\,943\,469\,454\,42 \times 10^{-01}$
3	$0.370\,635\,914\,520\,525\,41 \times 10^{-01}$	$0.839\,350\,436\,829\,178\,76 \times 10^{-01}$	14	$0.237\,152\,482\,627\,818\,63 \times 10^{+01}$	$0.258\,385\,394\,482\,232\,72 \times 10^{-01}$
4	$0.727\,525\,124\,228\,827\,62 \times 10^{-01}$	$0.809\,661\,970\,413\,229\,21 \times 10^{-01}$	15	$0.326\,137\,969\,960\,783\,55 \times 10^{+01}$	$0.124\,450\,241\,572\,555\,60 \times 10^{-01}$
5	$0.120\,236\,941\,228\,785\,68 \times 10^{+00}$	$0.769\,089\,548\,492\,978\,56 \times 10^{-01}$	16	$0.448\,513\,016\,905\,959\,11 \times 10^{+01}$	$0.429\,254\,159\,259\,983\,68 \times 10^{-02}$
6	$0.179\,574\,293\,958\,937\,73 \times 10^{+00}$	$0.731\,552\,078\,711\,821\,68 \times 10^{-01}$	17	$0.616\,806\,213\,512\,248\,38 \times 10^{+01}$	$0.935\,434\,298\,773\,596\,86 \times 10^{-03}$
7	$0.253\,534\,046\,984\,087\,27 \times 10^{+00}$	$0.726\,950\,035\,163\,157\,20 \times 10^{-01}$	18	$0.848\,247\,187\,231\,786\,981 \times 10^{+01}$	$0.108\,408\,854\,665\,025\,05 \times 10^{-03}$
8	$0.350\,388\,652\,780\,721\,95 \times 10^{+00}$	$0.752\,842\,556\,089\,304\,00 \times 10^{-01}$	19	$0.116\,653\,054\,862\,967\,931 \times 10^{+02}$	$0.527\,186\,796\,676\,167\,36 \times 10^{-05}$
9	$0.482\,109\,575\,931\,276\,68 \times 10^{+00}$	$0.770\,943\,953\,645\,196\,33 \times 10^{-01}$	20	$0.160\,424\,171\,322\,883\,281 \times 10^{+02}$	$0.776\,597\,403\,975\,041\,90 \times 10^{-07}$
10	$0.663\,028\,993\,158\,374\,16 \times 10^{+00}$	$0.754\,250\,625\,677\,530\,40 \times 10^{-01}$	21	$0.220\,619\,295\,181\,470\,89 \times 10^{+02}$	$0.221\,381\,724\,226\,800\,93 \times 10^{-09}$
11	$0.911\,814\,736\,856\,590\,87 \times 10^{+00}$	$0.689\,686\,192\,650\,315\,33 \times 10^{-01}$	22	$0.303\,401\,120\,947\,083\,07 \times 10^{+02}$	$0.659\,416\,176\,003\,770\,69 \times 10^{-13}$

we obtain

$$\left| \frac{1}{\sqrt{\pi}} \int_0^{t_{\max}} \frac{e^z - e^{-t^2}}{t^2 + z} dt - \frac{1}{\sqrt{\pi}} \sum_{m=1}^{M^g} w_m^g \frac{e^z \left(1 - e^{-\left(t_m^2 + z\right)}\right)}{t_m^2 + z} \right| \le \varepsilon^g$$

with $M^g = 16$ and $\varepsilon^g \approx 10^{-14}$, where t_m, w_m^g are the standard Gauss–Legendre nodes and weights on the interval $[0, t_{\max}]$. In the second term in (13), we drop e^{-t^2} (since its contribution is less than $e^{-t_{\max}^2} \approx 4.2 \cdot 10^{-15}$) and obtain

$$\frac{1}{\sqrt{\pi}} \int_{t_{\max}}^{\infty} \frac{e^z}{t^2 + z} dt = \frac{e^z}{\sqrt{\pi z}} \operatorname{Arctan}\left(\frac{\sqrt{z}}{t_{\max}}\right). \tag{14}$$

While we obtain an explicit expression, computing arctangent of a complex argument is relatively expensive. For a complex argument, we evaluate arctangent using

$$\operatorname{Arctan}(z) = \frac{1}{2} i \log \frac{1 - iz}{1 + iz}.$$

As a result of dropping e^{-t^2} in the second term of (13), our approximation in (14) has a singularity at $z = -t_{\max}^2$. In order to avoid using (14) in the vicinity of singularity, we use two different parameters $t_{\max}$ and $t_{\max,1}$ and switch to the version with $t_{\max,1}$ if $\left|z + t_{\max}^2\right| \le 1/2$, where $t_{\max,1} = \sqrt{t_{\max}^2 + 1}$.

We note that it is possible to increase the number of terms in the quadrature in order to avoid evaluating arctangent. This might be of interest on a parallel [Graphics Processing Unit (GPU) or multi-core] computer since computation of quadrature terms is trivially parallel. As a result, we obtain approximation

$$\left| e^z F(0, z) - \frac{e^z}{\sqrt{\pi z}} \operatorname{Arctan}\left(\frac{\sqrt{z}}{t_{\max}}\right) - \frac{1}{\sqrt{\pi}} \sum_{m=1}^{M^g} w_m^g \frac{e^z \left(1 - e^{-\left(t_m^2 + z\right)}\right)}{t_m^2 + z} \right| \le \tilde{\varepsilon}, \left|z + t_{\max}^2\right| > 1/2, \tag{15}$$

where $\tilde{\varepsilon} \approx 10^{-14}$. For $|z| > t_{\max}^2$, we have a converging series for the second integral in (9) as follows:

$$\begin{aligned} \int_0^{t_{\max}} \frac{e^{-t^2}}{t^2 + z} dt &= \frac{1}{z} \int_0^{t_{\max}} \frac{e^{-t^2}}{t^2/z + 1} dt \\ &= \frac{1}{z} \sum_{j=0}^{\infty} (-1)^j z^{-j} \int_0^{t_{\max}} e^{-t^2} t^{2j} dt \\ &= \frac{1}{2z} \sum_{j=0}^{\infty} (-1)^j z^{-j} \left(\Gamma(j + 1/2) - \Gamma\left(j + 1/2, t_{\max}^2\right)\right) \\ &= \frac{1}{z} \sum_{j=0}^{\infty} (-1)^j z^{-j} t_{\max}^{2j+1} F\left(j, t_{\max}^2\right) \end{aligned} \tag{16}$$

so that we can use

$$\left| F(0, z) - \left[\frac{\sqrt{\pi}}{2\sqrt{z}} - \frac{e^{-z}}{2\sqrt{\pi z}} \sum_{j=0}^{J} (-1)^j z^{-j} (\Gamma(j + 1/2) - \Gamma\left(j + 1/2, t_{\max}^2\right)) \right] \right| \le \epsilon_{t_{\max}}, |z| > t_{\max}^2, \tag{17}$$

instead of (12) and

$$\left| e^z F(0, z) - \left[\frac{e^z \sqrt{\pi}}{2\sqrt{z}} - \frac{1}{2\sqrt{\pi z}} \sum_{j=0}^{J} (-1)^j z^{-j} (\Gamma(j + 1/2) - \Gamma\left(j + 1/2, t_{\max}^2\right)) \right] \right| \le \epsilon_{t_{\max}}, |z| > t_{\max}^2, \tag{18}$$

instead of (15). Since the parameter $t_{\max}$ is fixed, the coefficients of the series are computed offline.

Note that the series in (16) and (17) is related to the asymptotic expansion of $F(0, z)$ (see, e.g., Ref. 4),

$$\begin{aligned} F(0, z) &\sim \frac{1}{2} \frac{\sqrt{\pi}}{\sqrt{z}} - \frac{\sqrt{\pi}}{2} \frac{e^{-z}}{z} \sum_{j=0}^{J} \frac{z^{-j}}{\Gamma\left(\frac{1}{2} - j\right)} \\ &= \frac{1}{2} \frac{\sqrt{\pi}}{\sqrt{z}} - \frac{e^{-z}}{2\sqrt{\pi z}} \sum_{j=0}^{J} (-1)^j z^{-j} \Gamma(j + 1/2). \end{aligned} \tag{19}$$

We use (17) and (18) for $|z| \geq 100$ so that it is sufficient to keep only seven terms, yielding an error of less than 10^{-13}.

For $|z| \leq r_0$, we use the Taylor expansion of (6),

$$F(0,z) = \sum_{j=0}^{\infty} \frac{(-1)^j z^j}{j!(2j+1)}, \tag{20}$$

and we need 10 terms to maintain an accuracy of about 13 digits. While selecting parameters as above leads to algorithms with a reasonable speed, we did not optimize these choices as they may depend on several factors, e.g., computer architecture.

Since the Boys function $F(0,z)$ is related to the error function (and can be used to compute it), we compared the speed of our algorithm with that of the well-known algorithm by Gautschi[20] for computing the error function with a complex argument using a rational approximation of the closely related Faddeeva function. The speed of that algorithm was measured in comparison with the speed of computing $\exp(z)$. In Ref. 20, it is stated that with an accuracy of ~10 digits, the code is 7–15 times slower than the speed of computing $\exp(z)$. Using the same comparison for our algorithm, this ratio is ~12 for an accuracy of about 13 digits. Our algorithm is implemented using Fortran 90 compiled by Intel's ifort with compiler flags -O3 -ipo -static and running on a laptop with ≈2.3 GHz chipset. We timed our code by performing 10^6 evaluations, yielding $\approx 0.92 \cdot 10^{-7}$ s/evaluation in comparison with $\approx 0.79 \cdot 10^{-8}$ s/evaluation for $\exp(z)$ with a complex argument.

While algorithms for computing the Fresnel integrals appear to be somewhat faster than using the Boys function in (5) (see, e.g., Ref. 21), we note that the generalized Fresnel integrals, e.g., $\int_0^x e^{it^n}\,dt$, $n \geq 2$, can be evaluated using our approach and plan to consider algorithms for these oscillatory special functions elsewhere.

III. APPROXIMATION OF $F(n_{\max}, z)$ FOR REAL AND COMPLEX ARGUMENTS

The function

$$g_n(s) = (1-s)^{n-1/2} \tag{21}$$

decays monotonically on $[0,1]$, and we use Algorithm 1 in Ref. 22 to construct its near optimal approximation via exponentials. We refer to Ref. 22 and references therein for the details of the algorithm that we use to obtain the necessary parameters (for an example, see Table II).

We obtain approximation

$$\left| g_n(s) - \sum_{m=1}^{M} w_m e^{\eta_m s} \right| \leq \varepsilon \quad \text{for } s \in [0,1], \tag{22}$$

where $w_m, \eta_m \in \mathbb{C}$. We note that n should be sufficiently large (e.g., $n \geq 7$) to avoid the impact on the approximation of the singularity of the nth derivative of g_n. Its numerical effect makes the accuracy of the current double precision implementation of Algorithm 1 in Ref. 22 insufficient to reliably produce approximation (22) for $1 \leq n \leq 6$.

Substituting the approximation of $g_n(1-s)$ into the integral (1), we arrive at

$$F(n,z) - \frac{1}{2}\sum_{m=1}^{M} w_m \int_0^1 e^{-zs} e^{\eta_m(1-s)}\,ds = \frac{1}{2}\int_0^1 e^{-zs}\left(s^{n-1/2} - \sum_{m=1}^{M} w_m e^{\eta_m(1-s)}\right)ds$$

and estimate

$$\left| F(n,z) - \frac{1}{2}\sum_{m=1}^{M} w_m \int_0^1 e^{-zs} e^{\eta_m(1-s)}\,ds \right| \leq \frac{\varepsilon}{2}\int_0^1 e^{-\mathscr{R}e(z)s}\,ds = \frac{\varepsilon}{2}\,\frac{1-e^{-\mathscr{R}e(z)}}{\mathscr{R}e(z)}.$$

Since

$$\frac{1}{2}\sum_{m=1}^{M} w_m \int_0^1 e^{-zs} e^{\eta_m(1-s)}\,ds = \frac{1}{2}\sum_{m=1}^{M} w_m e^{\eta_m}\,\frac{1-e^{-(z+\eta_m)}}{z+\eta_m},$$

TABLE II. Weights and exponents of the approximation of $g_{12}(s)$ on $[0,1]$ in (22). With these parameters, the absolute error in (23) is $\varepsilon \approx 2.5 \cdot 10^{-13}$.

m	η_m	w_m
1	$0.707\,194\,313\,205\,700\,10 \cdot 10^1 + 0.164\,872\,912\,507\,521\,15 \cdot 10^2 i$	$0.364\,436\,324\,028\,985\,01 \cdot 10^{-10} + 0.264\,117\,510\,721\,075\,04 \cdot 10^{-10} i$
2	$0.707\,194\,313\,205\,700\,10 \cdot 10^1 - 0.164\,872\,912\,507\,521\,15 \cdot 10^2 i$	$0.364\,436\,324\,028\,985\,01 \cdot 10^{-10} - 0.264\,117\,510\,721\,075\,04 \cdot 10^{-10} i$
3	$-0.571\,432\,717\,151\,916\,35 + 0.132\,785\,794\,532\,336\,33 \cdot 10^2 i$	$0.181\,852\,503\,467\,536\,33 \cdot 10^{-6} - 0.218\,604\,589\,713\,993\,52 \cdot 10^{-5} i$
4	$-0.571\,432\,717\,151\,916\,35 - 0.132\,785\,794\,532\,336\,33 \cdot 10^2 i$	$0.181\,852\,503\,467\,536\,33 \cdot 10^{-6} + 0.218\,604\,589\,713\,993\,52 \cdot 10^{-5} i$
5	$-0.471\,930\,213\,303\,925\,06 \cdot 10^1 + 0.998\,352\,571\,123\,710\,32 \cdot 10^1 i$	$-0.994\,891\,692\,720\,557\,48 \cdot 10^{-3} - 0.230\,490\,791\,052\,030\,73 \cdot 10^{-3} i$
6	$-0.471\,930\,213\,303\,925\,06 \cdot 10^1 - 0.998\,352\,571\,123\,710\,32 \cdot 10^1 i$	$-0.994\,891\,692\,720\,557\,48 \cdot 10^{-3} + 0.230\,490\,791\,052\,030\,73 \cdot 10^{-3} i$
7	$-0.717\,046\,627\,728\,950\,89 \cdot 10^1 + 0.667\,123\,608\,398\,207\,68 \cdot 10^1 i$	$-0.256\,252\,169\,858\,790\,06 \cdot 10^{-1} + 0.358\,183\,352\,748\,769\,82 \cdot 10^{-1} i$
8	$-0.717\,046\,627\,728\,950\,89 \cdot 10^1 - 0.667\,123\,608\,398\,207\,68 \cdot 10^1 i$	$-0.256\,252\,169\,858\,790\,06 \cdot 10^{-1} - 0.358\,183\,352\,748\,769\,82 \cdot 10^{-1} i$
9	$-0.848\,997\,470\,547\,246\,99 \cdot 10^1 + 0.334\,348\,041\,684\,674\,91 \cdot 10^1 i$	$0.165\,068\,015\,448\,807\,23 + 0.322\,739\,644\,717\,760\,45 i$
10	$-0.848\,997\,470\,547\,246\,99 \cdot 10^1 - 0.334\,348\,041\,684\,674\,91 \cdot 10^1 i$	$0.165\,068\,015\,448\,807\,23 - 0.32\,273\,964\,471\,776\,045 i$
11	$0.365\,644\,143\,631\,509\,73 \cdot 10^2$	$-0.201\,046\,416\,615\,651\,64 \cdot 10^{-25}$
12	$-0.324\,242\,392\,559\,219\,54 \cdot 10^1$	$-0.395\,635\,369\,550\,420\,78 \cdot 10^{-3}$
13	$-0.890\,660\,477\,331\,007\,53 \cdot 10^1$	$0.723\,499\,458\,050\,852\,92$

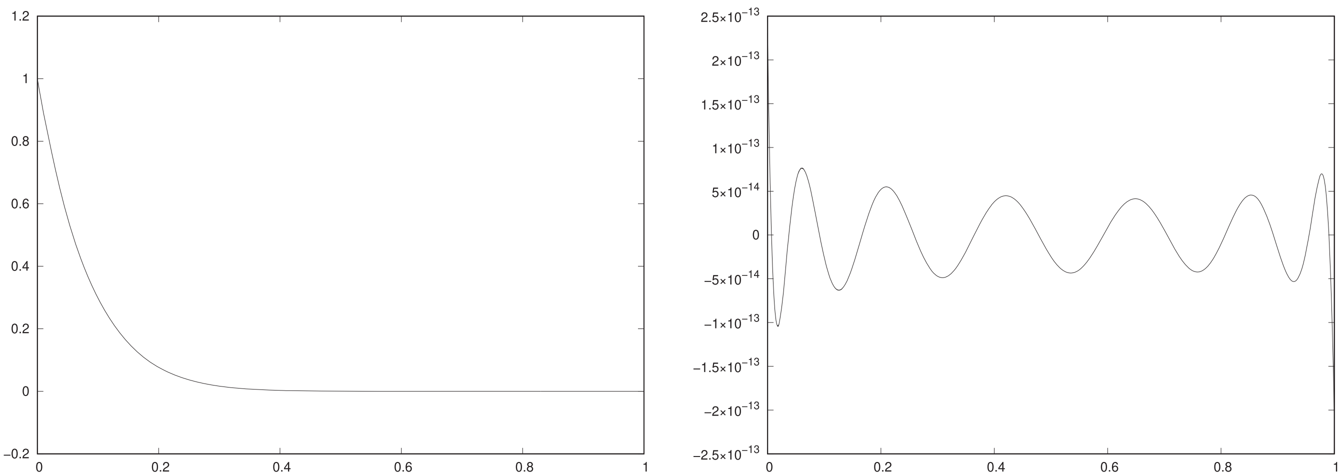

FIG. 1. The function $g_{12}(s)$ in (21) and the error of its near optimal approximation via exponentials in (22) with parameters described in Table II.

we have

$$\left|F(n,z) - \frac{1}{2}\sum_{m=1}^{M} w_m e^{\eta_m} \frac{1-e^{-(z+\eta_m)}}{z+\eta_m}\right| \le \frac{\varepsilon}{2}\frac{1-e^{-\mathscr{R}e(z)}}{\mathscr{R}e(z)} \le \frac{\varepsilon}{2}. \tag{23}$$

Indeed, denoting the factor on the right-hand side of (23), $q(z) = \left(1-e^{-z}\right)/z$, we have

$$q(2z) = \frac{1}{2}\left(e^{-z}q(z) + q(z)\right),$$

and therefore, for $\mathscr{R}e(z) \ge 0$,

$$|q(2z)| \le |q(z)|.$$

This implies that $|q(z)|$ reaches it maximum at $z = 0$, where $q(0) = 1$.

If $\mathscr{R}e(z) < 0$, we compute $e^z F(0,z)$ instead of $F(0,z)$,

$$e^z F(n,z) = \frac{1}{2}\int_0^1 e^{z(1-s)} s^{n-1/2} ds = \frac{1}{2}\int_0^1 e^{zs}(1-s)^{n-1/2} ds.$$

Using (22), we obtain

$$e^z F(n,z) - \frac{1}{2}\sum_{m=1}^{M} w_m \int_0^1 e^{zs} e^{\eta_m s} ds = \frac{1}{2}\int_0^1 e^{zs}\left[g_n(s) - \sum_{m=1}^{M} w_m e^{\eta_m s}\right] ds$$

and the estimate

$$\left|e^z F(n,z) - \frac{1}{2}\sum_{m=1}^{M} w_m \frac{e^{z+\eta_m}-1}{z+\eta_m}\right| \le \frac{\varepsilon}{2}\frac{e^{\mathscr{R}e(z)}-1}{\mathscr{R}e(z)} \le \frac{\varepsilon}{2}.$$

For computing values of $e^z F(n,z)$ for $0 \le n \le n_{\max}$ for $\mathscr{R}e(z) < 0$, we use recursions

$$e^z F(n,z) = \frac{n-1/2}{z} e^z F(n-1,z) - \frac{1}{2z} \tag{24}$$

instead of (2) and

$$e^z F(n-1,z) = \frac{2x}{2n-1} e^z F(n,z) + \frac{1}{2n-1} \tag{25}$$

instead of (3).

IV. IMPLEMENTATION DETAILS

The speed of computation of values of $F(n_{\max}, z)$ for $n_{\max} \ge 7$ depends on the number of terms M in approximation (22). We demonstrate the results of approximating $F(12,z)$ and display function $g_{12}(s)$ in Fig. 1. Using only 13 terms (see Table II), we achieve accuracy for $F(12,z)$ $\varepsilon \approx 2 \cdot 10^{-14}$ [e.g., accuracy of evaluation of $F(12,0)$ is $2.08 \cdot 10^{-14}$].

In implementing this approximation, we need to isolate cases where z is close to $-\eta_m$ by using the Taylor expansion for $\frac{1-e^{-(z+\eta_m)}}{z+\eta_m}$. Since most of η_m have an imaginary part, it is a minimal effort if z is real since η_m is real in only three terms in our example in Table II. In addition, for the real argument z, we need to use only five terms with complex valued parameters as they come in complex conjugate pairs.

We implemented these algorithms using Fortran 90 on a laptop described in Sec. II. Computing the Boys functions $F(n,z)$ for $n = 0, \ldots, 12$ for the real argument takes $\approx 0.34 \cdot 10^{-7}$ s. The subroutine for the complex valued argument is slower and takes $\approx 0.21 \cdot 10^{-6}$ s.

V. CONCLUSION

Since their introduction in Ref. 1, the Boys functions with a real argument have widely been used for computing Gaussian integrals. When using mixed Gaussian/exponential bases, one needs to evaluate the Boys functions with complex argument. Such mixed bases are appropriate for scattering problems and for bound state problems where using only plane waves becomes too expensive near singularities. Consequently, mixed Gaussian/exponential bases provide a greater flexibility in formulation and solving problems of quantum chemistry, and we present our results, in part, to facilitate their use.

While for a real argument the Boys functions can be easily tabulated in regions where their asymptotic is not accurate, it is more difficult to apply such a straightforward implementation for a complex argument. A careful reading of Refs. 3, 4, and 8 reveals shortcomings of the existing approaches (relying mostly on expansions) to computing the Boys functions of a complex argument (see, e.g., conclusion in Ref. 8). For our approach, a better comparison is offered by Gautschi's algorithm[20] for the error function of complex argument since it is related to $F(0,z)$, as in (4); see Sec. II. Our approach of approximating a part of the integrand so that the resulting integral can be evaluated explicitly is simpler and yields tight accuracy estimates. Note that the part of the integrand we are approximating is real, while the Boys functions we are computing are complex valued. As a side remark, we note that the Boys function $F(0,z)$ remains bounded for a complex argument with $\mathscr{R}e(z) \geq 0$ [and $e^z F(0,z)$ for $\mathscr{R}e(z) < 0$] and, for this reason, provides a good alternative approach for computing the error function of a complex argument.

We avoid the direct timing comparisons with existing algorithms since such comparisons are generally misleading. Given different hardware (single core, multi-core, GPU, etc.), different compilers and compiler flags, and different implementations, it is hard to compare algorithms by simply running them. Instead, one can look at algorithmic possibilities an approach offers. Our code is compact, and it is easy to simply count the total number of operations. We note that computation of each term in sums (12) and (23) is trivially parallel and only recursions in (2) and (3) require a sequential implementation (with just three multiplications and one addition per function). Thus, timing of our algorithms implemented on a multi-core or GPU computer will be much faster than the quoted timings of our implementation on a single central processing unit (CPU).

SUPPLEMENTARY MATERIAL

See the supplementary material for five Fortran 90 subroutines implementing, as an example, algorithms for computing the Boys function with indices $n = 0, \ldots, 12$. The subroutine dboysfun12.f90 evaluates the Boys functions $F(n,z)$ for real non-negative argument z. The subroutines zboysfun12.f90 and zboysfun00.f90 evaluate the Boys functions $F(n,z)$ for complex argument z with a non-negative real part. Finally, the subroutines zboysfun00nrp.f90 and zboysfun12nrp.f90 evaluate the functions $e^z F(n,z)$ for complex argument z with a negative real part.

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AUTHOR DECLARATIONS

Conflict of Interest

The authors have no conflicts to disclose.

DATA AVAILABILITY

The data that support the findings of this study are available within the article and its supplementary material.

APPENDIX: CONSTRUCTION OF QUADRATURE IN (11)

Changing variables in (7) $t = e^{\tau/2}$, we rewrite it as

$$s^{-1/2} = \frac{1}{\sqrt{\pi}} \int_{-\infty}^{\infty} e^{-se^{\tau}+\tau/2} d\tau, 0 \leq s \leq 1, \tag{A1}$$

and discretize it (following Ref. 23), yielding

$$\left| s^{-1/2} - \sum_{m=1}^{M} w_m e^{-\eta_m s} \right| \leq \epsilon s^{-1/2}, \quad \delta \leq s \leq 1, \tag{A2}$$

where $\eta_m, w_m > 0$ are arranged in an ascending order, and we estimate that

$$\begin{aligned} &\left| F(0,z) - \frac{1}{2}\int_0^1 e^{-zs} \left(\sum_{m=1}^{M} w_m e^{-\eta_m s} \right) ds \right| \\ &\leq \frac{1}{2}\int_0^1 e^{-\mathscr{R}e(z)s} \left| s^{-1/2} - \sum_{m=1}^{M} w_m e^{-\eta_m s} \right| ds \\ &\leq \frac{\epsilon}{2}\int_0^1 e^{-z\mathscr{R}e(z)} s^{-1/2} ds \\ &= \epsilon F(0, \mathscr{R}e(z)) \leq \epsilon. \end{aligned}$$

Using $\delta = \epsilon = 10^{-13}$ in (A2) results in approximation with $M = 210$. We also need this approximation to satisfy

$$\begin{aligned} &\left| \frac{1}{2\sqrt{\pi}} \int_{-\infty}^{\infty} \frac{1}{e^{\tau} + z} e^{\tau/2} d\tau - \sum_{m=1}^{M} \frac{w_m}{\eta_m + z} \right| \\ &= \left| \frac{1}{2}\sqrt{\frac{\pi}{z}} - \sum_{m=1}^{M} \frac{w_m}{\eta_m + z} \right| \leq \epsilon, \quad |z| \geq r_0, \end{aligned} \tag{A3}$$

in order to obtain

$$\left| F(0,z) - \left(\frac{1}{2}\sqrt{\frac{\pi}{z}} - \frac{e^{-z}}{2\sqrt{\pi}} \sum_{m=1}^{M} \frac{w_m e^{-\eta_m}}{\eta_m + z} \right) \right| \leq 2\epsilon. \tag{A4}$$

The exponents and the weights in (A2) grow as $\eta_m \approx e^{\tau_m}$ and $w_m \approx e^{\tau_m/2}$ (see Ref. 23) so that in (A4), it is sufficient to use a subset of terms with $\eta_m \leq e^{\tau_{\max}}$. Selecting $\tau_{\max} = 7/2$ so that $t_{\max} = e^{\tau_{\max}/2}$ in (10), the error $\epsilon_{t_{\max}} \approx 5.9 \cdot 10^{-18}$. Consequently, we only need the 22 terms displayed in Table I and obtain the approximation of (8) in (12).

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