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On the computation of generalized Fermi–Dirac and Bose–Einstein integrals *

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Gauss-type quadrature formulae based on rational functions are proposed to evaluate generalized Fermi–Dirac and Bose–Einstein integrals to high accuracy. The method is compared with recent quadrature methods of B. Pichon and R.P. Sagar.

1. Introduction

The computation of the generalized Fermi–Dirac integrals

$$F_k(\eta, \theta) = \int_0^\infty \frac{x^k\sqrt{1+\frac{1}{2}\theta x}}{\mathrm{e}^{-\eta+x}+1}\,\mathrm{d}x, \qquad \theta \geqslant 0, \quad \eta \in \mathbb{R}, \tag{1.1}$$

where $k = \frac{1}{2}, \frac{3}{2}, \frac{5}{2}$, has been the subject of two recent communications [1,2]. The former proposes Gauss–Laguerre quadrature (with weight function $x^k\,\mathrm{e}^{-ax}$) after dividing and multiplying the integrand by e^{-ax} with $a > 0$ suitably chosen, the latter a "Gauss–Fermi" quadrature (with weight function $x^k(\mathrm{e}^x+1)^{-1}$), after dividing and multiplying by $(\mathrm{e}^x+1)^{-1}$. Both methods disregard the major obstacle to rapid convergence (when θ is relatively small), namely the poles at

$$x = \eta \pm (2\nu - 1)\mathrm{i}\pi, \quad \nu = 1, 2, 3, \ldots. \tag{1.2}$$

In this note we write

$$F_k(\eta, \theta) = \int_0^\infty f(x)\, x^k\, \mathrm{e}^{-x}\,\mathrm{d}x, \tag{1.3}$$

with

$$f(x) = \frac{\sqrt{1+\frac{1}{2}\theta x}}{\mathrm{e}^{-\eta}+\mathrm{e}^{-x}}, \tag{1.4}$$

and propose a quadrature rule of the form

$$\int_0^\infty g(x)\, x^k\, \mathrm{e}^{-x}\,\mathrm{d}x \approx \sum_{r=1}^n w_r g(x_r), \tag{1.5}$$

which is exact for the n pairs of rational functions

$$g(x) = (1+\zeta_\nu x)^{-1}, \qquad g(x) = (1+\xi_\nu^* x)^{-1}, \qquad \nu = 1, 2, \ldots, n, \tag{1.6}$$

where

$$\zeta_\nu = -\frac{1}{\eta + (2\nu-1)\mathrm{i}\pi} \tag{1.7}$$

and the asterisk means complex conjugation. In this way, we take into account the first n paris of

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(conjugate complex) poles in eq. (1.2). Thus,

$$F_k(\eta, \theta) \approx \sum_{r=1}^{n} w_r f(x_r), \tag{1.8}$$

where the quadrature nodes and weights depend on n, k and η,

$$x_r = x_r^{(n)}(k, \eta), \qquad w_r = w_r^{(n)}(k, \eta). \tag{1.9}$$

An integral similar to (1.1), but arising from Bose–Einstein distributions, is

$$G_k(\eta, \theta) = \int_0^\infty \frac{x^k\sqrt{1+\frac{1}{2}\theta x}}{e^{-\eta+x}-1}\,dx, \quad \theta \geq 0, \quad \eta \leq 0, \tag{1.10}$$

for which analytic methods of evaluation, again for $k = \frac{1}{2}, \frac{3}{2}, \frac{5}{2}$, were discussed in the appendix of ref. [1]. Here we develop a quadrature method analogous to the one proposed above for $F_k(\eta, \theta)$ and compare it with other quadrature methods in the spirit of refs. [1,2].

It will be seen that the choice of quadratures proposed here significantly improves the accuracy of the results at the expense of requiring a sequence of quadrature rules to be generated for each k and η. Methods for generating such "rational Gauss" formulae will be briefly described in section 2. In section 3 we present numerical results and compare our method with those in refs. [1,2].

2. Gauss formulae for rational functions

2.1. Fermi–Dirac integrals

Let $\zeta_\nu = \xi_\nu + i\eta_\nu$, that is (cf. (1.7)),

$$\xi_\nu = -\frac{\eta}{\eta^2 + (2\nu-1)^2\pi^2}, \qquad \eta_\nu = \frac{(2\nu-1)\pi}{\eta^2 + (2\nu-1)^2\pi^2}, \qquad \nu = 1, \ldots, n, \tag{2.1}$$

and define

$$\omega_{2n}(x) = \prod_{\nu=1}^{n} \left[(1+\xi_\nu x)^2 + \eta_\nu^2 x^2\right]. \tag{2.2}$$

Then (1.5) is exact for the rational functions in (1.6) precisely if

$$x_r = x_r^{G}, \qquad w_r = w_r^{G}\omega_{2n}(x_r^{G}), \tag{2.3}$$

where x_r^G, w_r^G are the Gauss nodes and weights for the weight function $x^k\, e^{-x}/\omega_{2n}(x)$:

$$\int_0^\infty p(x)\, \frac{x^k\, e^{-x}}{\omega_{2n}(x)}\, dx = \sum_{r=1}^{n} w_r^G p(x_r^G), \quad \text{all } p \in \mathbb{P}_{2n-1} \tag{2.4}$$

(cf., e.g., ref. [3, Theorem 1.1 with $m = 2n$]). The orthogonal polynomials required for (2.4) can be generated, similarly as in ref. [2], by a discretized Stieltjes procedure. It is generally more efficient, however, to use a partial fraction decomposition of $[\omega_{2n}(x)]^{-1}$ and construct special Gauss formulae for each partial fraction prior to using the Stieltjes algorithm. This results in a finite algorithm, whereas the discretized Stieltjes procedure requires iteration. On the other hand, it may happen that the partial fractions involve large coefficients with varying signs, which will cause serious cancellation errors in the generation of the desired (rational) Gauss formulae. For details we refer to ref. [3].

2.2. Bose–Einstein integrals

For the integral (1.10), it is convenient to write

$$G_k(\eta, \theta) = \int_0^\infty f(x)\, x^{k-1}\, e^{-x}\, dx, \tag{2.5}$$

with

$$f(x) = \frac{x}{e^{-\eta} - e^{-x}}\sqrt{1+\tfrac{1}{2}\theta x}\,. \tag{2.6}$$

By splitting off a factor x, we insure that $f(x)$ remains regular as $x \to 0$ even when $\eta = 0$. The poles of f are now at

$$x = \eta \pm 2\nu i\pi, \quad \nu = 0, 1, 2, \ldots, \tag{2.7}$$

which suggests letting

$$\zeta_\nu = -\frac{1}{\eta + 2\nu \mathrm{i}\pi} \tag{2.8}$$

and proceeding similarly as in (1.5)–(1.7), except that k is to be replaced by $k-1$ in (1.5). The appropriate rational Gauss formulae (cf. ref. [3, Theorem 1.1 with $m = 2n-1$]) are then constructed similarly as in section 2.1, with

$$\xi_\nu = -\frac{\eta}{\eta^2 + 4\nu^2\pi^2}, \qquad \eta_\nu = \frac{2\nu\pi}{\eta^2 + 4\nu^2\pi^2}, \qquad \nu = 0, 1, 2, \ldots, n-1, \tag{2.9}$$

and (2.4) replaced by

$$\int_0^\infty p(x)\, \frac{x^{k-1}\,\mathrm{e}^{-x}}{\omega_{2n-1}(x)}\, \mathrm{d}x = \sum_{r=1}^{n} w_r^{\mathrm{G}} p(x_r^{\mathrm{G}}), \qquad \text{all } p \in \mathbb{P}_{2n-1}, \tag{2.10}$$

where ω_{2n-1} is defined by

$$\omega_{2n-1}(x) = (1 + \xi_0 x) \prod_{\nu=1}^{n-1} \left[(1 + \xi_\nu x)^2 + \eta_\nu^2 x^2 \right]. \tag{2.11}$$

3. Numerical results

All computations reported in this section were carried out in both single and double precision on the Cyber 205, which allows for precisions of approximately 14 and 28 decimal digits, respectively. Unless stated otherwise, our goal was to produce results with relative errors $\le \frac{1}{2} \times 10^{-10}$ in single precision, and $\le \frac{1}{2} \times 10^{-25}$ in double precision.

3.1. Fermi–Dirac integrals

For purposes of identification, we denote our method (1.8), (1.4), (2.3) by GR(n) (n-point Gauss Rational). The method in ref. [2], i.e.,

$$F_k(\eta, \theta) = \int_0^\infty f_1(x)\, \frac{x^k}{\mathrm{e}^x + 1}\, \mathrm{d}x \approx \sum_{r=1}^{n} w_r^{\mathrm{F}} f_1(x_r^{\mathrm{F}}),$$
$$f_1(x) = \frac{\sqrt{1 + \frac{1}{2}\theta x}}{\mathrm{e}^{-\eta + x} + 1}(\mathrm{e}^x + 1), \tag{3.1}$$

we denote by GF(n) (n-point Gauss–Fermi), while GL(n) (n-point Gauss–Laguerre) will refer to

$$F_k(\eta, \theta) = \int_0^\infty f(x)\, x^k\, \mathrm{e}^{-x}\, \mathrm{d}x \approx \sum_{r=1}^{n} w_r^{\mathrm{L}} f(x_r^{\mathrm{L}}) \tag{3.2}$$

(with f as in (1.4)), which is the case $a = 1$ of ref. [1]. The first 40 recursion coefficients for the orthogonal polynomials required in (3.1) are tabulated to 19 significant digits in ref. [2, table 1] for $k = \frac{1}{2}, \frac{3}{2}, \frac{5}{2}$. We have recomputed them to 25 digits and observed complete agreement to 19 digits (with the exception of occasional discrepancies of one unit in the last digit). Contrary to ref. [2], we computed the Gauss formulae from the respective Jacobi matrix via eigenvalue techniques (cf. refs. [4; 5, §6]).

All numerical examples in ref. [2] use $\theta = 1 \times 10^{-4}$, a comfortably small value that puts the square root singularity of the integrand in (1.1) at -2×10^4, sufficiently far away from the interval of integration to have any appreciable effect on the convergence properties of quadrature schemes. For ease of comparison, we use the

Table 1

Relative errors of three quadrature schemes for Fermi–Dirac integrals with $\eta = -1$ and $\theta = 1 \times 10^{-4}$.

k	n	GR(n)	GF(n)	GL(n)
$\frac{1}{2}$	5	8.1 (−9)	8.4(−5)	5.6(−5)
	10	5.9(−18)	2.7(−7)	1.6(−7)
	15	1.5(−25)	6.5(−9)	4.1(−9)
$\frac{3}{2}$	5	2.5 (−8)	1.3(−4)	9.5(−5)
	10	3.1(−17)	8.2(−7)	5.6(−7)
	15	1.6(−27)	1.5(−8)	1.1(−8)
$\frac{5}{2}$	5	5.6 (−8)	9.8(−5)	7.3(−5)
	10	1.1(−16)	7.7(−7)	5.7(−7)
	15	3.2(−25)	9.9(−9)	7.8(−9)

Table 2
Relative errors of three quadrature schemes for Fermi–Dirac integrals with $\eta = 1$ and $\theta = 1 \times 10^{-4}$.

k	n	GR(n)	GF(n)	GL(n)
$\frac{1}{2}$	5	2.1 (−8)	3.7(−4)	6.3(−4)
	10	1.7(−17)	7.4(−6)	1.5(−5)
	15	1.2(−25)	4.4(−7)	7.7(−7)
$\frac{3}{2}$	5	5.6 (−8)	4.7(−4)	9.5(−4)
	10	7.7(−17)	4.4(−6)	4.8(−6)
	15	2.4(−25)	2.7(−7)	6.7(−7)
$\frac{5}{2}$	5	1.1 (−7)	1.9(−5)	1.6(−4)
	10	2.5(−16)	1.3(−5)	2.4(−5)
	15	5.0(−26)	5.2(−7)	8.3(−7)

same value of θ in most of our examples, but experiment also with significantly larger values. Tables 1 and 2 are the analogues of tables 3 and 4 of ref. [2], showing relative errors of the three above quadrature methods for $\eta = -1$ and $\eta = 1$, respectively. As can be seen, GF and GL are very comparable in accuracy, in contrast to GR, which converges incomparably faster. The accuracy obtained with 15 quadrature points in the two former schemes is almost (if $\eta = -1$) or actually (if $\eta = 1$) achieved with 5 points in the latter, and considerably surpassed (not shown in the tables) when $n = 6$.

Table 3
Exact values of Fermi–Dirac integrals.

k	η	$F_k(\eta, 10^{-4})$
$\frac{1}{2}$	−1	0.2905124170194926626167642
$\frac{3}{2}$	−1	0.4608784541779919553534758
$\frac{5}{2}$	−1	1.186073501075755783982726
$\frac{1}{2}$	1	1.396441820349115339606362
$\frac{3}{2}$	1	2.661873279107150138112456
$\frac{5}{2}$	1	7.627256095653447632904998

The exact values to 25 digits (taken to be the limit values observed with our method) are given in table 3.

For convenience to the reader, and to illustrate the differences in the three quadrature rules, we list these in table 4 for $n = 5$, $k = \frac{1}{2}$ and $\eta = -1$. It can be seen that GR(5) has significantly smaller nodes than either of GL(5) and GF(5), presumably because of the "pull" exerted by the poles (1.2) in the complex plane located on the vertical line with real part $\eta = -1$. As this line is moved to the right, the nodes of GR(5) follow along and indeed become all larger than those of GL(5) and GF(5) by the time $\eta = 15$.

Convergence of the quadrature rule (1.8) speeds up as η is made larger negative, since the

Table 4
Nodes and weights of the three quadrature rules GF(n), GL(n), GR(n) for $n = 5$, $k = \frac{1}{2}$ and $\eta = -1$.

	nodes	weights
GF(5)	4.853282854052548902041607(−1)	2.528093182634590808714027(−1)
	1.873966916325342343159044 (0)	3.334462234469549285457945(−1)
	4.215862385021310462216175 (0)	8.691873578477134144754120(−2)
	7.846560736876599685022517 (0)	4.884285033837127451612712(−3)
	1.355305747901104375108016 (1)	3.533262407852899595773563(−5)
GL(5)	4.313988071478514844471342(−1)	3.704505700074585063243685(−1)
	1.759753698423696428573903 (0)	4.125843737694528821000270(−1)
	4.104465362828314989991953 (0)	9.777982005318070299139249(−2)
	7.746703779542557070882292 (0)	5.373415341171986513994744(−3)
	1.345767835205758002610472 (1)	3.874628149393571930106873(−5)
GR(5)	3.126398587450489212326774(−1)	2.556075807906894032848178(−1)
	1.255825743830479313965948 (0)	4.059161674922847483386820(−1)
	2.900866004335337302050356 (0)	1.924577586933245453743552(−1)
	5.481659473774843471464215 (0)	3.113158098682566730619157(−2)
	9.624406829641735767404573 (0)	1.113829627797498849117004(−3)

poles (1.2) then move further away from the interval of integration. For example, when $k = \frac{1}{2}$, double-precision accuracy $\approx 10^{-25}$ is attained with $n = 14$ for $\eta = -10$, with $n = 11$ for $\eta = -50$, and with $n = 9$ for $\eta = -100$. It is important, however, that the discretized Stieltjes procedure be used for constructing the quadrature rules in question, since the method of partial fraction decomposition gradually loses accuracy because of the cancellation problem mentioned at the end of section 2.1.

The case of large positive η is considerably more difficult: Not only is it harder to generate the rational Gauss formulae, but their convergence also slows down. When $\eta = 10$ (and $k = \frac{1}{2}$), double-precision accuracy 10^{-25} can still be attained with $n = 17$, but for $\eta = 50$, we obtain only 12 decimal places when $n = 17$, and the generation of n-point rational Gauss rules for larger values of n becomes increasingly subject to cancellation errors. Still, the results are far more accurate than those with Gauss–Fermi and Gauss–Laguerre quadrature, which for $n = 17$ yield about 3 respectively 2 correct decimal digits when $\eta = 10$ and $\eta = 50$, respectively.

We also experimented with larger values of θ, and $\eta = \pm 1$, $k = \frac{1}{2}$, to observe the damaging effect of the square root singularity at $x = -2/\theta$ as it moves toward the interval of integration $[0, \infty]$ (i.e., as θ increases). Interestingly, GF and GL seem to be less affected by this singularity than GR. For $\theta = 0.01$ and $\theta = 0.1$, the results are very similar to those in tables 1 and 2; for $\theta = 1$, they are shown in table 5.

Table 5
Relative errors of three quadrature schemes for Fermi–Dirac integrals with $\eta = \pm 1$, $k = \frac{1}{2}$ and $\theta = 1$.

η	n	GR(n)	GF(n)	GL(n)
−1.0	5	8.6 (−8)	4.8(−5)	2.0 (−5)
	10	1.8(−10)	8.8(−8)	7.4 (−8)
	15	1.2(−12)	1.6(−9)	1.3(−10)
1.0	5	1.4 (−8)	2.7(−4)	4.0 (−4)
	10	1.6(−10)	9.5(−6)	1.8 (−5)
	15	1.1(−12)	3.8(−7)	6.1 (−7)

Table 6
Relative errors of three quadrature schemes for Bose–Einstein integrals with $\eta = -1$ and $\theta = 1 \times 10^{-4}$.

k	n	GR(n)	GE(n)	GL(n)
$\frac{1}{2}$	5	5.4(−8)	1.6(−3)	6.6(−3)
	10	4.1(−17)	4.3(−5)	2.0(−4)
	15	7.5(−26)	2.6(−6)	1.3(−5)
$\frac{3}{2}$	5	1.6(−7)	7.6(−4)	3.2(−3)
	10	2.3(−15)	2.3(−5)	1.1(−4)
	15	1.5(−25)	1.5(−6)	7.0(−6)
$\frac{5}{2}$	5	3.3(−7)	3.2(−4)	1.4(−3)
	10	8.1(−16)	9.5(−6)	4.6(−5)
	15	1.1(−24)	6.1(−7)	3.0(−6)

3.2. Bose–Einstein integrals

In analogy to Fermi–Dirac integrals, we consider three quadrature methods for evaluating the Bose–Einstein integral (2.5), (2.6), namely the n-point Gauss Rational formula GR(n) with weight function $x^{k-1}\,\mathrm{e}^{-x}$ (cf. section 2.2), the n-point "Gauss–Einstein" formula GE(n),

$$G_k(n, \theta) = \int_0^\infty f(x)\,\frac{1-\mathrm{e}^{-x}}{x}\,\frac{x^k}{\mathrm{e}^x - 1}\,\mathrm{d}x$$

$$\approx \Sigma_{r=1}^{n} w_r^{\mathrm{E}} f(x_r^{\mathrm{E}}) \frac{1-\mathrm{e}^{-x_r^{\mathrm{E}}}}{x_r^{\mathrm{E}}}, \tag{3.3}$$

and the n-point Gauss–Laguerre formula GL(n),

$$G_k(\eta, \theta) = \int_0^\infty f(x)\, x^{k-1}\,\mathrm{e}^{-x}\,\mathrm{d}x$$

$$\approx \sum_{r=1}^{n} w_r^{\mathrm{L}} f(x_r^{\mathrm{L}}), \tag{3.4}$$

Table 7
Exact values of Bose–Einstein integrals.

k	η	$G_k(\eta, 10^{-4})$
$\frac{1}{2}$	−1	0.37970886599807399070148O2
$\frac{3}{2}$	−1	0.5260888870796462905919174
$\frac{5}{2}$	−1	1.2665691265431175469322246

where f in (3.3) and (3.4) is given by (2.6). The results for $\eta = -1$ and $\theta = 1 \times 10^{-4}$ are shown in table 6. They are similar to those for Fermi–Dirac integrals in table 1, except that GR is now slightly less accurate and GE, GL both considerably less accurate. Exact values are shown in table 7.

As η decreases from -1 to larger negative values, convergence of all three quadrature schemes speeds up, particularly so for GE and GL. The opposite is true when η increases from -1 to 0: convergence slows down, particularly for GE and GL, but much less so for GR. On the other hand, GR becomes harder to generate, although there is no loss of accuracy as in the case of Fermi–Dirac integrals.

An increase of θ affects convergence similarly as in the case of Fermi–Dirac integrals. For $k = \frac{1}{2}$, $\eta = -1$, and $\theta = 1$, the results are shown in table 8.

Table 8
Relative errors of three quadrature schemes for Bose–Einstein integrals with $\eta = -1$, $k = \frac{1}{2}$ and $\theta = 1$.

n	GR(n)	GE(n)	GL(n)
5	5.5(−7)	3.7(−3)	8.8(−4)
10	3.2(−10)	1.1(−4)	2.4(−5)
15	1.9(−12)	6.9(−6)	1.4(−6)

4. Conclusions

We have shown that Gauss-type quadrature formulae based on rational functions are capable of producing very accurate approximations to generalized Fermi–Dirac and Bose–Einstein integrals, provided the poles of the rational functions are suitably matched with those exhibited by the integrals in question. The use of these formulae is costly in as much as they are parameter-dependent. This probably rules them out for purposes of large-scale production, but makes them eminently suitable for isolated high-precision calculation of generalized (as well as ordinary) Fermi–Dirac and Bose–Einstein integrals. Indeed, any integral whose integrand has sufficiently many poles (outside the interval of integration) is a natural candidate for evaluation by rational Gauss-type quadrature rules.

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