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# RATIONAL FUNCTION APPROXIMATIONS FOR FERMI-DIRAC INTEGRALS

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## ABSTRACT

Rational function minimax approximations are given for the complete Fermi-Dirac integrals of orders $-\frac{1}{2}, \frac{1}{2}, \frac{3}{2}$, and $\frac{5}{2}$. In each case, three sets of approximations are provided with maximum relative error $\approx 10^{-4}$, $10^{-8}$, and $10^{-12}$, respectively. These approximations can be used to compute the Fermi-Dirac integrals efficiently over the entire range. Approximations to the corresponding inverse functions with an accuracy of $\approx 10^{-4}$ and $10^{-8}$ are also obtained.

*Subject headings:* atomic processes — methods: analytical

## 1. INTRODUCTION

The complete Fermi-Dirac integrals are usually defined by

$$F_n(x) = \int_0^\infty \frac{t^n dt}{e^{t-x}+1}, \quad n > -1 . \tag{1}$$

These integrals appear in various applications of Fermi-Dirac statistics in the nonrelativistic limit, the most frequently used values of $n$ being $-\frac{1}{2}, \frac{1}{2}, \frac{3}{2}$, and $\frac{5}{2}$. In physical problems, one often needs the inverse function which we denote by $X_n(f)$ where for a given value of $F_n(x)$ we have to find the corresponding value of $x$. For example, the number density of electrons in a degenerate electron gas is given by

$$n_e = \frac{4\pi}{h^3}(2m_e k_B T)^{3/2} F_{1/2}(\eta) , \tag{2}$$

where $n_e$ is the number density of electron, $h$ is Planck's constant, $m_e$ is the rest mass of an electron, $k_B$ is the Boltzmann's constant, $T$ is the temperature, and $\eta$ is the degeneracy parameter. In many physical problems, the number density may be known, and one has to calculate the corresponding value of the degeneracy parameter $\eta$.

A direct evaluation of the integral involves significant effort and may not be very useful, particularly when a large number of integrals at different values of $x$ are needed. As a result, a number of tables for these integrals are available (for example, McDougall & Stoner 1939; Cox & Giuli 1968). Recently, Cloutman (1989) has given extensive tables for $F_n(x)$ which are accurate to 12 significant figures for the range $-5 \le x \le 25$. Beyond this range the known asymptotic approximation for the integrals can be used to calculate $F_n(x)$, while interpolation within the tables can give the function value at nontabulated points. In fact, Cloutman (1989) has also given an interpolation routine which is claimed to give a relative accuracy of $10^{-10}$. But, this interpolation procedure requires a table of 1200 entries to be stored in the computer memory. Further, this interpolation routine can not be used to calculate $F_{-1/2}(x)$.

Most transcendental functions like trigonometric or exponential function can be evaluated much more efficiently using rational function approximations. It would therefore be interesting to try rational function approximation for evaluating Fermi-Dirac integrals. A number of rational function approximations for $F_{-1/2}(x)$, $F_{1/2}(x)$, and $F_{3/2}(x)$ have been given by Cody & Thacher (1967). The maximum relative error in these approximations varies between $10^{-2}$ and $10^{-8}$. In this work, we propose to use a slightly different form for approximation and aim to extend the relative accuracy to the $10^{-12}$ level in order to match the tables of Cloutman (1989). For each value of $n$, three sets of approximations are obtained with maximum relative error approximately $10^{-4}$, $10^{-8}$, and $10^{-12}$. Depending on the required accuracy either of these sets can be used to compute $F_n(x)$ efficiently for any given value of $x$. The evaluation of the rational function is more efficient by a factor of 2 as compared to the interpolation routine and requires much less computer memory, since only about 40 coefficients need to be stored.

For this purpose, it is best to obtain the minimax approximations where the coefficients in the rational function are chosen to minimize the maximum error over the required interval. Such approximations can be generated using the second algorithm of Remes (see Antia 1991). Once an approximation to $F_n(x)$ is obtained, the corresponding inverse function can be easily calculated by solving the nonlinear equation for $x$. This process may require several evaluations of $F_n(x)$, which would entail considerable effort if the integrals are calculated directly. In fact, it is possible to obtain approximations to the inverse function also.

## 2. RATIONAL FUNCTION APPROXIMATIONS

It would not be very effective to obtain rational function (or any other) approximation to $F_n(x)$ over the infinite range. Cody & Thacher (1969) divided the range into three parts and obtained the approximating rational function over each of these three intervals separately. In this paper, we break the range into two parts and seek approximations of the form

$$F_n(x) \approx \begin{cases} e^x R^1_{m_1k_1}(e^x) & \text{for} \quad x < 2 \\ x^{n+1} R^2_{m_2k_2}(x^{-2}) & \text{for} \quad x \ge 2 , \end{cases} \tag{3}$$

where

$$R^1_{m_1k_1}(x) = \frac{a_0 + a_1x + \cdots + a_{m_1}x^{m_1}}{b_0 + b_1x + \cdots + b_{k_1}x^{k_1}}$$

$$R^2_{m_2k_2}(x) = \frac{c_0 + c_1x + \cdots + c_{m_2}x^{m_2}}{d_0 + d_1x + \cdots + d_{k_2}x^{k_2}}. \quad (4)$$

For fixed values of $m_1$, $k_1$, the coefficients $a_i$, $b_i$ are chosen to minimize the maximum relative error in the approximation

$$1 - \frac{e^x R^1_{m_1k_1}(e^x)}{F_n(x)}, \quad (5)$$

over the interval $0 \le e^x \le e^2$. Similarly, the coefficients in $R^2_{m_2k_2}(x^{-2})$ are determined by minimizing the maximum relative error over the interval $0 \le x^{-2} \le \frac{1}{4}$. The degrees $m_1$, $k_1$, $m_2$, $k_2$ are chosen to achieve the required precision.

The coefficients of rational function approximation can be obtained using the second algorithm of Remes. For this purpose, the subroutine REMES described in Antia (1991) was used with some minor modifications. It was found that in many cases the iteration in the Remes algorithm has to be terminated because the number of extrema in the error curve are less than the required number (i.e., $m + k + 2$). To improve the chances of convergence an additional extremum was introduced between the first two when the number of extrema was less than required. This modification was found to be fairly effective in improving the chances of convergence.

The Remes algorithm requires the function value to be evaluated at any required point within the specified range. Further, to obtain approximations with relative error of less than $10^{-12}$ the function value should be accurate to more than 20 significant figures. Since a large number of function evaluations are required, the function value was calculated using polynomial interpolation in a table of approximately 1000 entries. In order to achieve the specified relative accuracy of $10^{-25}$, a polynomial of degree 20–30 was required. For low-accuracy approximations, a polynomial of degree eight was found to be enough to yield an accuracy of $10^{-13}$. By varying the spacing within the table it should be possible to reduce the degree of required interpolating polynomial, but that was not attempted. The table of values itself was generated using either the asymptotic formulas (see Cloutman 1989) or by explicit evaluation of the integral using an adaptive quadrature routine.

The results are summarized in Table 1, which gives the values of $m_1$, $k_1$, $m_2$, $k_2$, as well as the maximum relative error in these approximations. Comparing these results with those of Cody & Thacher (1969) it can be seen that we require a slightly higher degree of rational function to achieve the same level of accuracy. This difference is mainly because the range for $R^2_{m_2k_2}(x^{-2})$ is curtailed to $0 \le x^{-2} \le \frac{1}{16}$ in their work since the infinite interval is divided into three subintervals, instead of two, in the present work. It may be noted that at lower accuracy of $10^{-4}$ there is no significant difference in the required degree in the two cases. On the other hand, if we attempt to generate one rational function approximation, even over a limited range of $-5 \le x \le 25$ considered by Cloutman (1989), then it requires $m = k = 6$ to get an accuracy of approximately $10^{-4}$. Higher accuracy with single approximation over such a range is rather difficult to achieve.

TABLE 1

MAXIMUM ERROR IN MINIMAX APPROXIMATIONS FOR $F_n(x)$

| $n$ | $m_1$ | $k_1$ | $\mathrm{err_{max}}$ | $m_2$ | $k_2$ | $\mathrm{err_{max}}$ |
|---|---|---|---|---|---|---|
| −0.5 ...... | 2 | 3 | $1.35 \times 10^{-5}$ | 2 | 2 | $4.75 \times 10^{-5}$ |
| 0.5 ...... | 2 | 3 | $1.54 \times 10^{-5}$ | 2 | 2 | $5.54 \times 10^{-5}$ |
| 1.5 ...... | 2 | 2 | $6.54 \times 10^{-5}$ | 2 | 2 | $4.59 \times 10^{-5}$ |
| 2.5 ...... | 2 | 2 | $2.63 \times 10^{-5}$ | 2 | 2 | $7.02 \times 10^{-5}$ |
| −0.5 ...... | 4 | 5 | $3.31 \times 10^{-9}$ | 6 | 7 | $1.93 \times 10^{-9}$ |
| 0.5 ...... | 4 | 5 | $3.82 \times 10^{-9}$ | 6 | 6 | $5.33 \times 10^{-9}$ |
| 1.5 ...... | 4 | 5 | $1.94 \times 10^{-9}$ | 6 | 6 | $4.51 \times 10^{-10}$ |
| 2.5 ...... | 4 | 4 | $5.84 \times 10^{-9}$ | 6 | 5 | $1.10 \times 10^{-9}$ |
| −0.5 ...... | 7 | 7 | $1.30 \times 10^{-13}$ | 11 | 11 | $1.23 \times 10^{-12}$ |
| 0.5 ...... | 7 | 7 | $1.51 \times 10^{-13}$ | 10 | 11 | $5.47 \times 10^{-13}$ |
| 1.5 ...... | 6 | 7 | $5.07 \times 10^{-13}$ | 9 | 10 | $3.50 \times 10^{-13}$ |
| 2.5 ...... | 6 | 7 | $1.80 \times 10^{-13}$ | 10 | 9 | $2.47 \times 10^{-13}$ |

Tables 2–5 give the coefficients $a_i$, $b_i$, $c_i$, and $d_i$ in the rational function approximations for $F_{-1/2}(x)$, $F_{1/2}(x)$, $F_{3/2}(x)$, and $F_{5/2}(x)$, respectively. These coefficients are not independent, since all of them can be multiplied by any nonzero constant without changing the value of the rational function. The coefficients listed in the tables are normalized to make the coefficient of the highest degree term in the numerator unity. Using this normalization one multiplication can be saved while evaluating the rational function at any value of its argument. Once the coefficients are calculated, the evaluation of the rational function $R_{mk}(x)$ requires $2(m + k) + 1$ floating point operations. In addition, $e^x$ or $x^{n+1}$ has to be evaluated once. The number of floating point operations can be reduced by almost a factor of 2 if the rational function is converted to equivalent continued fraction (see Antia 1991). This number may be compared with about 60 floating point operations required by the interpolation routine of Cloutman (1989). A FORTRAN function routine FERMI to calculate $F_{1/2}(x)$ to an accuracy of $10^{-4}$ is given in the Appendix. This routine can be easily modified to use more accurate approximations or to calculate $F_n(x)$ for different values of $n$.

The Remes algorithm also yields the maximum error in these approximations. However, the coefficients appearing in the tables are rounded versions of the coefficients calculated by the subroutine, and hence it is necessary to estimate the maximum error in these approximations independently. This estimate can be obtained by finding all extrema of the relative error. In all cases, the maximum error in approximations with rounded coefficients was found to be only marginally higher than that obtained by the Remes algorithm. Further, each of the approximations was separately checked at about 2000 random arguments against the original function routine. The function routine itself was checked against the tables of Cloutman (1989).

## 3. APPROXIMATIONS TO THE INVERSE FUNCTIONS

After having obtained approximations to $F_n(x)$, we can easily calculate the value of $x$ corresponding to a given $F$ by iteratively solving the corresponding nonlinear equation. However, if a large number of such values are required, it will be more efficient to use direct approximation to the inverse function $X_n(f)$ itself. Such approximations can once again be generated using the Remes algorithm. Since $X_n(f)$ vanishes for some

TABLE 2

COEFFICIENTS OF RATIONAL FUNCTION APPROXIMATIONS FOR $F_{-1/2}(x)$

| $i$ | $a_i$ | $b_i$ | $c_i$ | $d_i$ |
|---|---|---|---|---|
| | $m_1 = 2$ | $k_1 = 3$ | $m_2 = 2$ | $k_2 = 2$ |
| 0 ...... | 2.31456E+01 | 1.30586E+01 | 1.53602E−02 | 7.68015E−03 |
| 1 ...... | 1.37820E+01 | 1.70048E+01 | 1.46815E−01 | 7.63700E−02 |
| 2 ...... | 1.00000E+00 | 5.07527E+00 | 1.00000E+00 | 5.70485E−01 |
| 3 ...... | ... | 2.36620E−01 | ... | ... |
| | $m_1 = 4$ | $k_1 = 5$ | $m_2 = 6$ | $k_2 = 7$ |
| 0 ...... | 8.830316038E+02 | 4.981972343E+02 | −4.9141019880E−08 | −2.4570509894E−08 |
| 1 ...... | 1.183989392E+03 | 1.020272984E+03 | −7.2486358805E−06 | −3.6344227710E−06 |
| 2 ...... | 4.473770672E+02 | 6.862151992E+02 | −7.4382915429E−04 | −3.7345152736E−04 |
| 3 ...... | 4.892542028E+01 | 1.728621255E+02 | −3.2856045308E−02 | −1.6589736860E−02 |
| 4 ...... | 1.000000000E+00 | 1.398575990E+01 | −5.6853219702E−01 | −2.9154391835E−01 |
| 5 ...... | ... | 2.138408204E−01 | −1.9284139162E+00 | −1.1843742874E+00 |
| 6 ...... | ... | ... | 1.0000000000E+00 | 7.0985168479E−01 |
| 7 ...... | ... | ... | ... | −6.0197789199E−02 |
| | $m_1 = 7$ | $k_1 = 7$ | $m_2 = 11$ | $k_2 = 11$ |
| 0 ...... | 1.71446374704454E+7 | 9.67282587452899E+6 | −4.46620341924942E−15 | −2.23310170962369E−15 |
| 1 ...... | 3.88148302324068E+7 | 2.87386436731785E+7 | −1.58654991146236E−12 | −7.94193282071464E−13 |
| 2 ...... | 3.16743385304962E+7 | 3.26070130734158E+7 | −4.44467627042232E−10 | −2.22564376956228E−10 |
| 3 ...... | 1.14587609192151E+7 | 1.77657027846367E+7 | −6.84738791621745E−08 | −3.43299431079845E−08 |
| 4 ...... | 1.83696370756153E+6 | 4.81648022267831E+6 | −6.64932238528105E−06 | −3.33919612678907E−06 |
| 5 ...... | 1.14980998186874E+5 | 6.13709569333207E+5 | −3.69976170193942E−04 | −1.86432212187088E−04 |
| 6 ...... | 1.98276889924768E+3 | 3.13595854332114E+4 | −1.12295393687006E−02 | −5.69764436880529E−03 |
| 7 ...... | 1.00000000000000E+0 | 4.35061725080755E+2 | −1.60926102124442E−01 | −8.34904593067194E−02 |
| 8 ...... | ... | ... | −8.52408612877447E−01 | −4.78770844009440E−01 |
| 9 ...... | ... | ... | −7.45519953763928E−01 | −4.99759250374148E−01 |
| 10 ...... | ... | ... | 2.98435207466372E+00 | 1.86795964993052E+00 |
| 11 ...... | ... | ... | 1.00000000000000E+00 | 4.16485970495288E−01 |

TABLE 3

COEFFICIENTS OF RATIONAL FUNCTION APPROXIMATIONS FOR $F_{1/2}(x)$

| $i$ | $a_i$ | $b_i$ | $c_i$ | $d_i$ |
|---|---|---|---|---|
| | $m_1 = 2$ | $k_1 = 3$ | $m_2 = 2$ | $k_2 = 2$ |
| 0 ...... | 2.18168E+01 | 2.46180E+01 | 4.73011E−02 | 7.09478E−02 |
| 1 ...... | 1.31693E+01 | 2.35546E+01 | 5.48433E−01 | 7.37041E−01 |
| 2 ...... | 1.00000E+00 | 4.76290E+00 | 1.00000E+00 | 3.82065E−01 |
| 3 ...... | ... | 1.34481E−01 | ... | ... |
| | $m_1 = 4$ | $k_1 = 5$ | $m_2 = 6$ | $k_2 = 6$ |
| 0 ...... | 7.940307136E+02 | 8.959677183E+02 | 7.265461948E−08 | 1.089819298E−07 |
| 1 ...... | 1.072518408E+03 | 1.526979592E+03 | 1.678032858E−05 | 2.503603684E−05 |
| 2 ...... | 4.106017002E+02 | 8.307577602E+02 | 1.365376899E−03 | 2.017068914E−03 |
| 3 ...... | 4.607473842E+01 | 1.638158630E+02 | 4.647886226E−02 | 6.719888328E−02 |
| 4 ...... | 1.000000000E+00 | 9.960923624E+00 | 5.231390123E−01 | 7.001197631E−01 |
| 5 ...... | ... | 1.047712331E−01 | 1.567714263E+00 | 1.309399040E+00 |
| 6 ...... | ... | ... | 1.000000000E+00 | 1.727377764E−01 |
| | $m_1 = 7$ | $k_1 = 7$ | $m_2 = 10$ | $k_2 = 11$ |
| 0 ...... | 5.75834152995465E+6 | 6.49759261942269E+6 | 4.85378381173415E−14 | 7.28067571760518E−14 |
| 1 ...... | 1.30964880355883E+7 | 1.70750501625775E+7 | 1.64429113030738E−11 | 2.45745452167585E−11 |
| 2 ...... | 1.07608632249013E+7 | 1.69288134856160E+7 | 3.76794942277806E−09 | 5.62152894375277E−09 |
| 3 ...... | 3.93536421893014E+6 | 7.95192647756086E+6 | 4.69233883900644E−07 | 6.96888634549649E−07 |
| 4 ...... | 6.42493233715640E+5 | 1.83167424554505E+6 | 3.40679845803144E−05 | 5.02360015186394E−05 |
| 5 ...... | 4.16031909245777E+4 | 1.95155948326832E+5 | 1.32212995937796E−03 | 1.92040136756592E−03 |
| 6 ...... | 7.77238678539648E+2 | 8.17922106644547E+3 | 2.60768398973913E−02 | 3.66887808002874E−02 |
| 7 ...... | 1.00000000000000E+0 | 9.02129136642157E+1 | 2.48653216266227E−01 | 3.24095226486468E−01 |
| 8 ...... | ... | ... | 1.08037861921488E+00 | 1.16434871200131E+00 |
| 9 ...... | ... | ... | 1.91247528779676E+00 | 1.34981244060549E+00 |
| 10 ...... | ... | ... | 1.00000000000000E+00 | 2.01311836975930E−01 |
| 11 ...... | ... | ... | ... | −2.14562434782759E−02 |

TABLE 4

COEFFICIENTS OF RATIONAL FUNCTION APPROXIMATIONS FOR $F_{3/2}(x)$

| $i$ | $a_i$ | $b_i$ | $c_i$ | $d_i$ |
|---|---|---|---|---|
| | $m_1 = 2$ | $k_1 = 2$ | $m_2 = 2$ | $k_2 = 2$ |
| 0 ...... | 1.35863E+02 | 1.02210E+02 | 1.54699E−01 | 3.86765E−01 |
| 1 ...... | 4.92764E+01 | 5.50312E+01 | 1.20037E+00 | 6.08119E−01 |
| 2 ...... | 1.00000E+00 | 4.23365E+00 | 1.00000E+00 | −1.65665E−01 |
| | $m_1 = 4$ | $k_1 = 5$ | $m_2 = 6$ | $k_2 = 6$ |
| 0 ...... | 9.895512903E+02 | 7.443927085E+02 | 6.7384341042E−08 | 1.6846085253E−07 |
| 1 ...... | 1.237156375E+03 | 1.062245497E+03 | 7.4281282702E−06 | 1.7531170088E−05 |
| 2 ...... | 4.413986183E+02 | 4.720721124E+02 | 4.6220789293E−04 | 1.0476768850E−03 |
| 3 ...... | 4.693212727E+01 | 7.386867306E+01 | 1.1905625478E−02 | 2.3334235654E−02 |
| 4 ...... | 1.000000000E+00 | 3.424526047E+00 | 1.3661062300E−01 | 1.9947560547E−01 |
| 5 ...... | ... | 2.473929073E−02 | 6.5500705397E−01 | 4.7103657850E−01 |
| 6 ...... | ... | ... | 1.0000000000E+00 | −1.7443752246E−02 |
| | $m_1 = 6$ | $k_1 = 7$ | $m_2 = 9$ | $k_2 = 10$ |
| 0 ...... | 4.32326386604283E+4 | 3.25218725353467E+4 | 2.80452693148553E−13 | 7.01131732871184E−13 |
| 1 ...... | 8.55472308218786E+4 | 7.01022511904373E+4 | 8.60096863656367E−11 | 2.10699282897576E−10 |
| 2 ...... | 5.95275291210962E+4 | 5.50859144223638E+4 | 1.62974620742993E−08 | 3.94452010378723E−08 |
| 3 ...... | 1.77294861572005E+4 | 1.95942074576400E+4 | 1.63598843752050E−06 | 3.84703231868724E−06 |
| 4 ...... | 2.21876607796460E+3 | 3.20803912586318E+3 | 9.12915407846722E−05 | 2.04569943213216E−04 |
| 5 ...... | 9.90562948053193E+1 | 2.20853967067789E+2 | 2.62988766922117E−03 | 5.31999109566385E−03 |
| 6 ...... | 1.00000000000000E+0 | 5.05580641737527E+0 | 3.85682997219346E−02 | 6.39899717779153E−02 |
| 7 ...... | ... | 1.99507945223266E−2 | 2.78383256609605E−01 | 3.14236143831882E−01 |
| 8 ...... | ... | ... | 9.02250179334496E−01 | 4.70252591891375E−01 |
| 9 ...... | ... | ... | 1.00000000000000E+00 | −2.15540156936373E−02 |
| 10 ...... | ... | ... | ... | 2.34829436438087E−03 |

TABLE 5

COEFFICIENTS OF RATIONAL FUNCTION APPROXIMATIONS FOR $F_{5/2}(x)$

| $i$ | $a_i$ | $b_i$ | $c_i$ | $d_i$ |
|---|---|---|---|---|
| | $m_1 = 2$ | $k_1 = 2$ | $m_2 = 2$ | $k_2 = 2$ |
| 0 ...... | 1.54674E+02 | 4.65428E+01 | 5.69090E−01 | 1.99168E+00 |
| 1 ...... | 4.80784E+01 | 1.85625E+01 | 7.68654E+00 | −1.71711E+00 |
| 2 ...... | 1.00000E+00 | 9.93679E−01 | 1.00000E+00 | 1.36953E+00 |
| | $m_1 = 4$ | $k_1 = 4$ | $m_2 = 6$ | $k_2 = 5$ |
| 0 ...... | 1.178194436E+04 | 3.545200171E+03 | 1.4405190262E−06 | 5.0418165971E−06 |
| 1 ...... | 1.110612718E+04 | 3.655199255E+03 | 1.5534321883E−04 | 4.7113349177E−04 |
| 2 ...... | 2.722654825E+03 | 1.066529195E+03 | 6.9564011735E−03 | 1.7503664846E−02 |
| 3 ...... | 1.645171224E+02 | 9.326993632E+01 | 1.2618111665E−01 | 1.8378232714E−01 |
| 4 ...... | 1.000000000E+00 | 1.690677494E+00 | 9.0276909572E−01 | 2.9430307063E−01 |
| 5 ...... | ... | ... | 1.9952283074E+00 | 3.2980790411E−02 |
| 6 ...... | ... | ... | 1.0000000000E+00 | ... |
| | $m_1 = 6$ | $k_1 = 7$ | $m_2 = 10$ | $k_2 = 9$ |
| 0 ...... | 6.61606300631656E+4 | 1.99078071053871E+4 | 8.42667076131315E−12 | 2.94933476646033E−11 |
| 1 ...... | 1.20132462801652E+5 | 3.79076097261066E+4 | 2.31618876821567E−09 | 7.68215783076936E−09 |
| 2 ...... | 7.67255995316812E+4 | 2.60117136841197E+4 | 3.54323824923987E−07 | 1.12919616415947E−06 |
| 3 ...... | 2.10427138842443E+4 | 7.97584657659364E+3 | 2.77981736000034E−05 | 8.09451165406274E−05 |
| 4 ...... | 2.44325236813275E+3 | 1.10886130159658E+3 | 1.14008027400645E−03 | 2.81111224925648E−03 |
| 5 ...... | 1.02589947781696E+2 | 6.35483623268093E+1 | 2.32779790773633E−02 | 3.99937801931919E−02 |
| 6 ...... | 1.00000000000000E+0 | 1.16951072617142E+0 | 2.39564845938301E−01 | 2.27132567866839E−01 |
| 7 ...... | ... | 3.31482978240026E−3 | 1.24415366126179E+00 | 5.31886045222680E−01 |
| 8 ...... | ... | ... | 3.18831203950106E+00 | 3.70866321410385E−01 |
| 9 ...... | ... | ... | 3.42040216997894E+00 | 2.27326643192516E−02 |
| 10 ...... | ... | ... | 1.00000000000000E+00 | ... |

TABLE 6

MAXIMUM ERROR IN MINIMAX APPROXIMATIONS FOR $X_n(f)$

| $n$ | $m_1$ | $k_1$ | $\mathrm{err}_{\max}$ | $m_2$ | $k_2$ | $\mathrm{err}_{\max}$ |
|---|---|---|---|---|---|---|
| −0.5 ...... | 3 | 3 | $4.17\times10^{-5}$ | 2 | 2 | $3.50\times10^{-5}$ |
| 0.5 ...... | 2 | 2 | $1.89\times10^{-5}$ | 2 | 2 | $3.02\times10^{-5}$ |
| 1.5 ...... | 2 | 2 | $4.27\times10^{-7}$ | 2 | 2 | $2.29\times10^{-5}$ |
| 2.5 ...... | 1 | 2 | $1.99\times10^{-6}$ | 2 | 2 | $7.95\times10^{-6}$ |
| −0.5 ...... | 5 | 6 | $1.10\times10^{-9}$ | 6 | 6 | $3.03\times10^{-9}$ |
| 0.5 ...... | 4 | 3 | $2.67\times10^{-10}$ | 6 | 5 | $4.19\times10^{-9}$ |
| 1.5 ...... | 3 | 4 | $2.72\times10^{-10}$ | 6 | 5 | $2.26\times10^{-9}$ |
| 2.5 ...... | 2 | 3 | $3.02\times10^{-9}$ | 6 | 6 | $6.17\times10^{-9}$ |

value of $f$, it is not possible to obtain an approximation with finite relative error over the entire region. This problem may be overcome by looking for approximations to $X_n(f)/[f - F_n(0)]$ which is nonzero for all values of $f$. However, $F_n(0)$ is not known exactly, and further, it is difficult to calculate the inverse function $X_n(f)$ very accurately near its zero. Consequently, it is difficult to ensure high relative accuracy in such approximations.

For these reasons, we divide the range into two at $f = 4$ and look for approximations of the form

$$X_n(f) \approx \begin{cases} \ln[fR^1_{m_1k_1}(f)] & \text{for } f < 4 \\ f^{1/(1+n)}R^2_{m_2k_2}(f^{-1/(1+n)}) & \text{for } f \geq 4 \,, \end{cases} \tag{6}$$

where $R^1_{m_1k_1}$ and $R^2_{m_2k_2}$ are again defined by equation (4). This form of approximation takes care of the asymptotic form of the function as $f \to \pm\infty$. Over the interval $0 \leq f \leq 4$ the minimax approximation is obtained by minimizing the maximum relative error in approximating $e^x/f$ by the rational function $R^1_{m_1k_1}(f)$. The logarithm of this translates into absolute error for $x = X_n(f)$. Hence, in the neighborhood of the zero of $X_n(f)$, the relative error in such approximations could be higher.

The results are summarized in Table 6, which gives the values of $m_1$, $k_1$, $m_2$, $k_2$, as well as the maximum relative error in these approximations. The coefficients in these approximations are listed in Tables 7–10. From Tables 1 and 6 it can be seen that for the same accuracy, approximation to the inverse function requires a smaller degree of the rational function as

TABLE 7

COEFFICIENTS OF RATIONAL FUNCTION APPROXIMATIONS FOR $X_{-1/2}(f)$

| $i$ | $a_i$ | $b_i$ | $c_i$ | $d_i$ |
|---|---|---|---|---|
| | $m_1 = 3$ | $k_1 = 3$ | $m_2 = 2$ | $k_2 = 2$ |
| 0 ...... | 7.8516685E+02 | 1.3917278E+03 | 8.9742174E−03 | 3.5898124E−02 |
| 1 ...... | −1.4034065E+02 | −8.0463066E+02 | −1.0604768E−01 | −4.2520975E−01 |
| 2 ...... | 1.3257418E+01 | 1.5854806E+02 | 1.0000000E+00 | 3.6612154E+00 |
| 3 ...... | 1.0000000E+00 | −1.0640712E+01 | ... | ... |
| | $m_1 = 5$ | $k_1 = 6$ | $m_2 = 6$ | $k_2 = 6$ |
| 0 ...... | −1.570044577033E+4 | −2.782831558471E+4 | 2.206779160034E−8 | 8.827116613576E−8 |
| 1 ...... | 1.001958278442E+4 | 2.886114034012E+4 | −1.437701234283E−6 | −5.750804196059E−6 |
| 2 ...... | −2.805343454951E+3 | −1.274243093149E+4 | 6.103116850636E−5 | 2.429627688357E−4 |
| 3 ...... | 4.121170498099E+2 | 3.063252215963E+3 | −1.169411057416E−3 | −4.601959491394E−3 |
| 4 ...... | −3.174780572961E+1 | −4.225615045074E+2 | 1.814141021608E−2 | 6.932122275919E−2 |
| 5 ...... | 1.000000000000E+0 | 3.168918168284E+1 | −9.588603457639E−2 | −3.217372489776E−1 |
| 6 ...... | ... | −1.008561571363E+0 | 1.000000000000E+0 | 3.124344749296E+0 |

TABLE 8

COEFFICIENTS OF RATIONAL FUNCTION APPROXIMATIONS FOR $X_{1/2}(f)$

| $i$ | $a_i$ | $b_i$ | $c_i$ | $d_i$ |
|---|---|---|---|---|
| | $m_1 = 2$ | $k_1 = 2$ | $m_2 = 2$ | $k_2 = 2$ |
| 0 ...... | 4.4593646E+01 | 3.9519346E+01 | 3.4873722E+01 | 2.6612832E+01 |
| 1 ...... | 1.1288764E+01 | −5.7517464E+00 | −2.6922515E+01 | −2.0452930E+01 |
| 2 ...... | 1.0000000E+00 | 2.6594291E−01 | 1.0000000E+00 | 1.1808945E+01 |
| | $m_1 = 4$ | $k_1 = 3$ | $m_2 = 6$ | $k_2 = 5$ |
| 0 ...... | 1.999266880833E+4 | 1.771804140488E+4 | −1.277060388085E−2 | −9.745794806288E−3 |
| 1 ...... | 5.702479099336E+3 | −2.014785161019E+3 | 7.187946804945E−2 | 5.485432756838E−2 |
| 2 ...... | 6.610132843877E+2 | 9.130355392717E+1 | −4.262314235106E−1 | −3.299466243260E−1 |
| 3 ...... | 3.818838129486E+1 | −1.670718177489E+0 | 4.997559426872E−1 | 4.077841975923E−1 |
| 4 ...... | 1.000000000000E+0 | ... | −1.285579118012E+0 | −1.145531476975E+0 |
| 5 ...... | ... | ... | −3.930805454272E−1 | −6.067091689181E−2 |
| 6 ...... | ... | ... | 1.000000000000E+0 | ... |

TABLE 9

COEFFICIENTS OF RATIONAL FUNCTION APPROXIMATIONS FOR $X_{3/2}(f)$

| $i$ | $a_i$ | $b_i$ | $c_i$ | $d_i$ |
|---|---|---|---|---|
| | $m_1 = 2$ | $k_1 = 2$ | $m_2 = 2$ | $k_2 = 2$ |
| 0 ...... | 3.5954549E+01 | 4.7795853E+01 | −9.8934493E−01 | −6.8577484E−01 |
| 1 ...... | 1.3908910E+01 | 1.2133628E+01 | 9.0731169E−02 | 6.3338994E−02 |
| 2 ...... | 1.0000000E+00 | −2.3975074E−01 | 1.0000000E+00 | −1.1635840E−01 |
| | $m_1 = 3$ | $k_1 = 4$ | $m_2 = 6$ | $k_2 = 5$ |
| 0 ...... | 1.715627994191E+2 | 2.280653583157E+2 | −6.321828169799E−3 | −4.381942605018E−3 |
| 1 ...... | 1.125926232897E+2 | 1.193456203021E+2 | −2.183147266896E−2 | −1.513236504100E−2 |
| 2 ...... | 2.056296753055E+1 | 1.167743113540E+1 | −1.057562799320E−1 | −7.850001283886E−2 |
| 3 ...... | 1.000000000000E+0 | −3.226808804038E−1 | −4.657944387545E−1 | −3.407561772612E−1 |
| 4 ...... | ... | 3.519268762788E−3 | −5.951932864088E−1 | −5.074812565486E−1 |
| 5 ...... | ... | ... | 3.684471177100E−1 | −1.387107009074E−1 |
| 6 ...... | ... | ... | 1.000000000000E+0 | ... |

TABLE 10

COEFFICIENTS OF RATIONAL FUNCTION APPROXIMATIONS FOR $X_{5/2}(f)$

| $i$ | $a_i$ | $b_i$ | $c_i$ | $d_i$ |
|---|---|---|---|---|
| | $m_1 = 1$ | $k_1 = 2$ | $m_2 = 2$ | $k_2 = 2$ |
| 0 ...... | 1.5331469E+01 | 5.0951752E+01 | −5.1891788E−01 | −3.6278896E−01 |
| 1 ...... | 1.0000000E+00 | 1.9691913E+00 | −9.1723019E−03 | −6.1502672E−03 |
| 2 ...... | ... | −2.7251177E−02 | 1.0000000E+00 | −3.3673540E−02 |
| | $m_1 = 2$ | $k_1 = 3$ | $m_2 = 6$ | $k_2 = 6$ |
| 0 ...... | 2.138969250409E+2 | 7.108545512710E+2 | −3.312041011227E−2 | −2.315515517515E−2 |
| 1 ...... | 3.539903493971E+1 | 9.873746988121E+1 | 1.315763372315E−1 | 9.198776585252E−2 |
| 2 ...... | 1.000000000000E+0 | 1.067755522895E+0 | −4.820942898296E−1 | −3.835879295548E−1 |
| 3 ...... | ... | −1.182798726503E−2 | 5.099038074944E−1 | 5.415026856351E−1 |
| 4 ...... | ... | ... | 5.495613498630E−1 | −3.847241692193E−1 |
| 5 ...... | ... | ... | −1.498867562255E+0 | 3.739781456585E−2 |
| 6 ...... | ... | ... | 1.000000000000E+0 | −3.008504449098E−2 |

compared to that for $F_n(x)$. A FORTRAN function routine FERINV for calculating $X_{1/2}(f)$ is also given in the Appendix.

## 4. SUMMARY

Rational function minimax approximations to Fermi-Dirac integrals $F_{-1/2}(x)$, $F_{1/2}(x)$, $F_{3/2}(x)$, and $F_{5/2}(x)$ are obtained with varying accuracy. Three sets of approximations with maximum relative error of approximately $10^{-4}$, $10^{-8}$ and $10^{-12}$ are obtained for each of these integrals. These approximations can be used to compute the value of the integrals efficiently over the entire range of the argument $x$. Rational function minimax approximations to the corresponding inverse function $X_n(f)$ with an accuracy of approximately $10^{-4}$ and $10^{-8}$ are also obtained. For the inverse function the relative error could be larger in the neighborhood of its zero.

## APPENDIX

### A1. FERMI: FUNCTION ROUTINE TO CALCULATE $F_{1/2}(x)$

```
      DOUBLE PRECISION FUNCTION FERMI(X)
      IMPLICIT REAL*8(A-H,O-Z)
      DIMENSION A1(12),b1(12),A2(12),B2(12)

C     Initializing the degree and coefficients of rational function approximation.

      DATA AN,M1,K1,M2,K2/0.5D0,2,3,2,2/
```

```
      DATA (A1(I),I=1,3)/2.18168D+01,1.31693D+01,1.00000D+00/
      DATA (B1(I),I=1,4)/2.46180D+1,2.35546D+1,4.76290D+0,1.34481D-1/
      DATA (A2(I),I=1,3)/4.73011D-02,5.48433D-01,1.00000D+00/
      DATA (B2(I),I=1,3)/7.09478D-02,7.37041D-01,3.82065D-01/

      IF(X.LT.2.D0) THEN
        XX=DEXP(X)
        RN=XX+A1(M1)
        DO 100 I=M1-1,1,-1
100     RN=RN*XX+A1(I)
        DEN=B1(K1+1)
        DO 200 I=K1,1,-1
200     DEN=DEN*XX+B1(I)
        FERMI=XX*RN/DEN

      ELSE

        XX=1.D0/X**2
        RN=XX+A2(M2)
        DO 300 I=M2-1,1,-1
300     RN=RN*XX+A2(I)
        DEN=B2(K2+1)
        DO 400 I=K2,1,-1
400     DEN=DEN*XX+B2(I)
        FERMI=(X**(AN+1.D0))*RN/DEN
      ENDIF

      RETURN
      END
C     ------------------------------------------------------------------------------
```

## A2. FERINV: FUNCTION ROUTINE TO CALCULATE $X_{1/2}(f)$

```
      DOUBLE PRECISION FUNCTION FERINV(F)
      IMPLICIT REAL*8(A-H,O-Z)
      DIMENSION A1(9),B1(9),A2(9),B2(9)

C       Initializing the degree and coefficients of rational function approximation.

      DATA AN,M1,K1,M2,K2/0.5D0,2,2,2,2/
      DATA (A1(I),I=1,3)/4.4593646D+01,1.1288764D+01,1.0000000D+00/
      DATA (B1(I),I=1,3)/3.9519346D+01,-5.7517464D+00,2.6594291D-01/
      DATA (A2(I),I=1,3)/3.4873722D+01,-2.6922515D+01,1.0000000D+00/
      DATA (B2(I),I=1,3)/2.6612832D+01,-2.0452930D+01,1.1808945D+01/

      IF(F.LT.4.D0) THEN
        RN=F+A1(M1)
        DO 100 I=M1-1,1,-1
100     RN=RN*F+A1(I)
        DEN=B1(K1+1)
        DO 200 I=K1,1,-1
200     DEN=DEN*F+B1(I)
        FERINV=DLOG(F*RN/DEN)

      ELSE

        FF=1.D0/F**(1.D0/1.D0+AN))
        RN=FF+A2(M2)
        DO 300 I=M2-1,1,-1
300     RN=RN*FF+A2(I)
        DEN=B2(K2+1)
        DO 400 I=K2,1,-1
```

```
400     DEN=DEN*FF+B2(I)
        FERINV=RN/(DEN*FF)
      ENDIF

      RETURN
      END
```

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