

Evaluation of the generalized Fermi-Dirac integral and its derivatives for moderate/large values of the parameters ^{☆,☆☆}

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ARTICLE INFO

Article history:

Received 8 June 2022

Received in revised form 8 October 2022

Accepted 14 October 2022

Available online 24 October 2022

Keywords:

Generalized Fermi-Dirac integral

Relativistic Fermi-Dirac integral

Asymptotic expansions

Numerical approximations

Matlab implementations

ABSTRACT

Approximations with Matlab implementations for the relativistic Fermi-Dirac integral and its partial derivatives are given in this paper. As the numerical tests show, the expansions allow to calculate the functions efficiently and with high accuracy for a large range of parameters. Therefore, our algorithms are expected to be a very useful tool, in combination with other methods, for building reliable and efficient software for computing the functions for all the parameters ranges.

Program summary

Program Title: FermiDiracExpans

CPC Library link to program files: <https://doi.org/10.17632/sk34wtcxhh.1>

Licensing provisions: GPLv3

Programming language: Matlab

Nature of problem: The evaluation of the relativistic Fermi-Dirac function and its partial derivatives is needed in different problems in applied and theoretical physics, such as stellar astrophysics, plasma physics or electronics.

Solution method: Convergent and asymptotic expansions are provided to approximate the relativistic Fermi-Dirac function and its derivatives for moderate/large values of its parameters.

Additional comments including restrictions and unusual features: The functions work in recent versions of Matlab (from version R2014b on).

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1. Introduction

The relativistic Fermi-Dirac integral $F_q(\eta, \beta)$ is defined by

$$F_q(\eta, \beta) = \int_0^{\infty} \frac{x^q \sqrt{1 + \beta x/2}}{e^{x-\eta} + 1} dx, \quad \beta \geq 0, \quad q \geq 0, \quad \eta \in \mathbb{R}. \quad (1)$$

The function (1) is crucial for computations in physical problems dominated by the degenerate fermions. Therefore, $F_q(\eta, \beta)$ is widely used in astrophysics, where a high-density hot electron gas with large values of both η and β drives many important processes during late stages of stellar evolution and explosive environments. Notable examples are the M_{\pm}^m functions given in [1], which require multiple

[☆] The review of this paper was arranged by Prof. N.S. Scott.

^{☆☆} This paper and its associated computer program are available via the Computer Physics Communications homepage on ScienceDirect (<http://www.sciencedirect.com/science/journal/00104655>).

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evaluations of $F_q(\eta, \beta)$ to compute some properties of neutrino emission from electron-positron annihilation in pre-supernovae stars [2] type Ia thermonuclear supernovae stars [3] and physical processes in Gamma-Ray Burst (GRB) engines [4,5]. Fermi-Dirac integrals are also useful for the description of weak nuclear processes (see [6], Appendix B). For these applications, the evaluation of $F_q(\eta, \beta)$ alone is enough. However, in the stellar Equation Of State (EOS) [7,8] not only the function, but also its partial derivatives with respect to η, β , are required. To achieve fully consistent EOS, precise values of the derivatives up to $m + n \leq 3$, being m, n the orders of the derivatives with respect to η and β , respectively, are needed [9,7]. To our knowledge, none of the existing methods is able to handle the third-order derivative with respect to η for large degeneracy ($\eta \gg 1$).

Derivatives are involved in changes of the Helmholtz free energy, the higher-order ones in heat capacities. The limit $\beta \rightarrow \infty$ appears to be particularly troublesome, and in physical applications it is customary to simply put the fermion mass identically zero (drop the 1 under the square root in (1)) reducing the problem to a combination of $\beta = 0$ cases. However, this is not an appropriate method and even the sign of the derivative can be wrong for some combinations of η, β . Although this happens for very large β only, such a situation is not unimaginable in a real astrophysical situation of, e.g., a hot, degenerate light neutrino gas.

For the numerical calculation of (1), an extensive number of references can be found in the literature; see for example [7,10–19]. However, only [17] provided working code for the third order derivatives. MESA, the stellar evolution software [20] uses a code based on [10] with derivatives up to $m + n \leq 2$ order. As one can infer from the reference list, the majority of the successful methods of computation are integration-based, and therefore more suitable for moderate values of the parameters.

In [21] complete asymptotic expansions for the relativistic Fermi-Dirac integral were considered. In this paper, we also give expansions for the k th-partial derivatives with respect to the parameters η and β ; Matlab implementations are provided for all the expansions. These approximations allow to calculate the functions efficiently and with high accuracy for large ranges of the parameters. Therefore, we expect that our algorithms will be a very useful ingredient, in combination with other methods, for building reliable and efficient software for computing the functions for all the parameter ranges.

2. Derivatives with respect to η

2.1. Negative values of η

For negative values of η , we have the convergent expansion for the k th-partial derivative with respect to η

$$\frac{\partial^k F_q}{\partial \eta^k}(\eta, \beta) = \Gamma(q + 1) \sum_{n=1}^{\infty} (-1)^{n-1} \frac{e^{n\eta}}{n^{q+1-k}} U_q(n, \beta), \tag{2}$$

in which $U_q(n, \beta)$ is given in terms of the Kummer confluent hypergeometric function $U(a, b, z)$ as follows

$$U_q(s, \beta) = \left(\frac{2s}{\beta}\right)^{q+1} U\left(q + 1, q + \frac{5}{2}, \frac{2s}{\beta}\right) = \left(\frac{2s}{\beta}\right)^{-\frac{1}{2}} U\left(-\frac{1}{2}, -q - \frac{1}{2}, \frac{2s}{\beta}\right), \tag{3}$$

where $s \neq 0$, $|\text{ph } s| < \pi$, $\beta > 0$, with limiting value $U_q(s, 0) = 1$.

Equation (2) can be used for $k \geq 0$ ($k = 0$ gives the expansion for $F_q(\eta, \beta)$).

2.2. Positive values of η

2.2.1. The case $q \neq \frac{1}{2}, \frac{3}{2}, \frac{5}{2}, \dots$

We have for $k \geq 0$

$$\frac{\partial^k F_q}{\partial \eta^k}(\eta, \beta) = \left(\frac{2}{\beta}\right)^{q+1} \frac{\Gamma\left(-q - \frac{3}{2}\right) \Gamma(q + 1)}{-2\sqrt{\pi}} \frac{\partial^k F_q^{(1)}}{\partial \eta^k}(\eta, \beta) + \left(\frac{2}{\beta}\right)^{-\frac{1}{2}} \Gamma\left(q + \frac{3}{2}\right) \frac{\partial^k F_q^{(2)}}{\partial \eta^k}(\eta, \beta), \tag{4}$$

where for fixed β and q , $q \neq \frac{1}{2}, \frac{3}{2}, \frac{5}{2}, \dots$ we have the expansions

$$F_q^{(1)}(\eta, \beta) = \sum_{n=0}^{\infty} (-1)^n e^{-n\eta} {}_1F_1\left(q + 1; \frac{-2n}{\beta}\right), \tag{5}$$

$$\frac{\partial^k F_q^{(1)}}{\partial \eta^k}(\eta, \beta) = \sum_{n=1}^{\infty} (-1)^{n+k} n^k e^{-n\eta} {}_1F_1\left(q + 1; \frac{-2n}{\beta}\right), \quad k \geq 1,$$

which converge for all $\eta > 0$, and

$$\frac{\partial^k F_q^{(2)}}{\partial \eta^k}(\eta, \beta) \sim \eta^{q+\frac{3}{2}} \sum_{n=0}^{\infty} \frac{1}{\Gamma\left(q + \frac{5}{2} - n - k\right)} \frac{a_n}{\eta^{n+k}} + \sin(\pi q) \sum_{n=1}^{\infty} (-1)^{n+k} \frac{e^{-n\eta}}{n^{q+1-k}} {}_1F_1\left(-\frac{1}{2}; \frac{-2n}{\beta}\right), \tag{6}$$

for $k \geq 0$. The first three a_n coefficients are given by

$$a_0 = 1, \quad a_1 = \frac{2}{\beta(1 + 2q)}, \quad a_2 = \frac{\tau_2 \beta^2 (4q^2 - 1) - 2}{\beta^2 (4q^2 - 1)}, \tag{7}$$

where the coefficient τ_2 is $\frac{1}{6}\pi^2$.

More a_n values can be obtained using the definition of the coefficients:

$$\frac{\pi s}{\sin(\pi s)} {}_1F_1\left(-\frac{1}{2}; \frac{2s}{\beta}; -qs\right) = \sum_{n=0}^{\infty} a_n s^n, \quad |s| < 1. \tag{8}$$

2.2.2. The case $q = \frac{1}{2}, \frac{3}{2}, \frac{5}{2}, \dots$

For the Fermi-Dirac integral, we have

$$F_q(\eta, \beta) = \Gamma\left(m - \frac{1}{2}\right) \left(\frac{2}{\beta}\right)^{m-\frac{1}{2}} \left(F_q^{(P)}(\eta, \beta) + F_q^{(Q)}(\eta, \beta)\right) + F_q^{(R)}(\eta, \beta) + F_q^{(S)}(\eta, \beta), \tag{9}$$

where for fixed β and q , $q = m - \frac{3}{2}, m = 2, 3, 4, \dots$ we have the asymptotic expansions for $\eta \rightarrow +\infty$

$$F_q^{(P)}(\eta, \beta) \sim A_m \left(-(\gamma + \ln \eta) p_{m,0} + \sum_{k=1}^{\infty} (-1)^k p_{m,k} (k-1)! \eta^{-k}\right), \tag{10}$$

$$F_q^{(Q)}(\eta, \beta) \sim A_m q_{m,0},$$

where γ is Euler's constant. The coefficients appearing in the expansions are given by

$$A_m = \frac{(-1)^{m+1}}{m! \Gamma(-\frac{1}{2})}, \quad p_{m,k} = \sum_{j=0}^k \tau_j P_{m,k-j}, \quad q_{m,k} = \sum_{j=0}^k \tau_j Q_{m,k-j}, \tag{11}$$

where

$$P_{m,k} = \left(\frac{2}{\beta}\right)^k \frac{(m - \frac{1}{2})_k}{k! (m+1)_k}, \tag{12}$$

$$Q_{m,k} = P_{m,k} \left(\ln\left(\frac{2}{\beta}\right) + \psi\left(m - \frac{1}{2} + k\right) - \psi(1+k) - \psi(m+k+1)\right),$$

and $\psi(z)$ is the digamma function $\psi(z) = \Gamma'(z)/\Gamma(z)$.

Also, we have

$$F_q^{(R)}(\eta, \beta) = \Gamma\left(m - \frac{1}{2}\right) \left(\frac{2}{\beta}\right)^{m-\frac{1}{2}} \sum_{k=1}^m \frac{R_{m,k}}{\Gamma(k)} F_{k-1}(\eta), \tag{13}$$

where

$$R_{m,k} = \left(\frac{2}{\beta}\right)^{-k} \frac{(k-1)! \left(\frac{3}{2} - m + k\right)_{m-k}}{\Gamma\left(m - \frac{1}{2}\right) (m-k)!} \tag{14}$$

and $F_q(\eta)$ is the standard Fermi-Dirac integral.

In addition, we have the convergent expansion for all $\eta > 0$

$$F_q^{(S)}(\eta, \beta) = (-1)^m \frac{\sqrt{\pi}}{2} \left(\frac{2}{\beta}\right)^{m-\frac{1}{2}} \sum_{n=1}^{\infty} (-1)^n e^{-n\eta} e^{-2n/\beta} U\left(\frac{3}{2}, m+1, \frac{2n}{\beta}\right). \tag{15}$$

For evaluating the standard Fermi-Dirac integral, we use the following expansion

$$F_q(\eta) \sim \Gamma(q+1) \eta^{q+1} \sum_{n=0}^{\infty} \frac{\tau_{2n}}{\Gamma(q+2-2n) \eta^{2n}}, \tag{16}$$

valid for $\eta \rightarrow \infty$, $|\text{ph } \eta| < \frac{1}{2}\pi$. The coefficients $\tau_0 = 1$ and τ_{2n} are given by

$$\tau_{2n} = 2 \sum_{m=1}^{\infty} \frac{(-1)^{m-1}}{m^{2n}} = 2 \left(1 - 2^{1-2n}\right) \zeta(2n) = (-1)^{n-1} \left(1 - 2^{1-2n}\right) \frac{(2\pi)^{2n}}{(2n)!} B_{2n}, \tag{17}$$

for $n \geq 1$, where B_n are the Bernoulli numbers.

For the k th derivatives ($k \geq 1$) we have

$$\frac{\partial^k F_q}{\partial \eta^k}(\eta, \beta) \sim \Gamma\left(m - \frac{1}{2}\right) \left(\frac{2}{\beta}\right)^{m-\frac{1}{2}} \frac{\partial^k F_q^{(P)}}{\partial \eta^k}(\eta, \beta) + \frac{\partial^k F_q^{(R)}}{\partial \eta^k}(\eta, \beta) + \frac{\partial^k F_q^{(S)}}{\partial \eta^k}(\eta, \beta), \tag{18}$$

where

$$\begin{aligned} \frac{\partial^k F_q^{(P)}}{\partial \eta^k}(\eta, \beta) &\sim A_m \left(\frac{(-1)^k (k-1)!}{\eta^k} p_{m,0} + \sum_{j=1}^{\infty} (-1)^j p_{m,j} (j-1)! (-j-k+1)_k \eta^{-j-k} \right), \\ \frac{\partial^k F_q^{(R)}}{\partial \eta^k}(\eta, \beta) &= \Gamma\left(m - \frac{1}{2}\right) \left(\frac{2}{\beta}\right)^{m-\frac{1}{2}} \sum_{k=1}^m \frac{R_{m,k}}{\Gamma(k)} \frac{\partial^k F_{k-1}}{\partial \eta^k}(\eta), \\ \frac{\partial^k F_q^{(S)}}{\partial \eta^k}(\eta, \beta) &= (-1)^m \frac{\sqrt{\pi}}{2} \left(\frac{2}{\beta}\right)^{m-\frac{1}{2}} \sum_{n=1}^{\infty} (-1)^{n+k} n^k e^{-n\eta} e^{-2n/\beta} U\left(\frac{3}{2}, m+1, \frac{2n}{\beta}\right), \end{aligned} \tag{19}$$

with

$$\frac{\partial^k F_q}{\partial \eta^k}(\eta) \sim \Gamma(q+1) \eta^{q+1-k} \sum_{n=0}^{\infty} \frac{\tau_{2n}}{\Gamma(q+2-2n-k) \eta^{2n}}. \tag{20}$$

3. Derivatives with respect to β

3.1. The case $q \neq \frac{1}{2}, \frac{3}{2}, \frac{5}{2}, \dots$

We have

$$\frac{\partial^k F_q}{\partial \beta^k}(\eta, \beta) = \left(\frac{2}{\beta}\right)^{q+1} \frac{\Gamma\left(-q - \frac{3}{2}\right) \Gamma(q+1)}{\Gamma\left(-\frac{1}{2}\right)} \frac{\partial^k \tilde{F}_q^{(1)}}{\partial \beta^k}(\eta, \beta) + \left(\frac{2}{\beta}\right)^{-\frac{1}{2}} \Gamma\left(q + \frac{3}{2}\right) \frac{\partial^k \tilde{F}_q^{(2)}}{\partial \beta^k}(\eta, \beta), \tag{21}$$

where

$$\begin{aligned} \frac{\partial^k \tilde{F}_q^{(1)}}{\partial \beta^k}(\eta, \beta) &\sim \sum_{j=0}^{\infty} \frac{(-q-j-k)_k c_j}{\beta^{j+k}} \Phi_j^{(1)}(\eta), \\ \frac{\partial^k \tilde{F}_q^{(2)}}{\partial \beta^k}(\eta, \beta) &\sim \sum_{j=0}^{\infty} \frac{\left(\frac{3}{2} - j - k\right)_k d_j}{\beta^{j+k}} \Phi_j^{(2)}(\eta, q), \\ c_j &= \frac{2^j (q+1)_j}{j! \left(q + \frac{5}{2}\right)_j}, \quad d_j = \frac{2^j \left(-\frac{1}{2}\right)_j}{j! \left(-q - \frac{1}{2}\right)_j}, \end{aligned} \tag{22}$$

as $\beta \rightarrow \infty$.

The functions $\Phi_j^{(1)}(\eta)$ can be evaluated as follows

$$\Phi_{j+1}^{(1)}(\eta) = \frac{d}{d\eta} \Phi_j^{(1)}(\eta), \quad j = 0, 1, 2, \dots, \tag{23}$$

where

$$\Phi_0^{(1)}(\eta) = \sum_{n=0}^{\infty} (-1)^n e^{-n\eta} = \frac{1}{e^{-\eta} + 1}. \tag{24}$$

The function $\Phi_j^{(2)}(\eta)$ can be written as

$$\Phi_j^{(2)}(\eta) = \widehat{F}_{q+\frac{1}{2}-j}(\eta) = \frac{F_{q+\frac{1}{2}-j}(\eta)}{\Gamma\left(q + \frac{1}{2} - j\right)}. \tag{25}$$

If $j < q + \frac{3}{2}$ we can use the relation

$$\widehat{F}_q(\eta) = \frac{1}{\Gamma(q+1)} \int_0^{\infty} \frac{x^q}{e^{x-\eta} + 1} dx \tag{26}$$

to evaluate $\Phi_j^{(2)}(\eta)$. For other values of j we use

$$\widehat{F}_q(\eta) = -e^{-\pi i q} \frac{\Gamma(-q)}{2\pi i} \int_{+\infty}^{(0+)} \frac{z^q}{e^{z-\eta} + 1} dz, \quad q \neq 0, 1, 2, \dots \tag{27}$$

Equation (21) can be used for $k \geq 0$.

3.2. The case $q = \frac{1}{2}, \frac{3}{2}, \frac{5}{2}, \dots$

We have

$$\frac{\partial^k F_q}{\partial \beta^k}(\eta, \beta) \sim \Gamma\left(m - \frac{1}{2}\right) \left(\frac{2}{\beta}\right)^{m-\frac{1}{2}} \left(\frac{\partial^k F_q^{(P)}}{\partial \beta^k}(\eta, \beta) + \frac{\partial^k F_q^{(Q)}}{\partial \beta^k}(\eta, \beta) \right) + \frac{\partial^k F_q^{(R)}}{\partial \beta^k}(\eta, \beta), \tag{28}$$

where for fixed η and q , with $q = m - \frac{3}{2}$, $m = 2, 3, 4, \dots$, we have as $\beta \rightarrow \infty$

$$\begin{aligned} \frac{\partial^k F_q^{(P)}}{\partial \beta^k}(\eta, \beta) &\sim A_m \sum_{j=0}^{\infty} \frac{(-m + \frac{3}{2} - j - k)_k \tilde{P}_{m,j}}{\beta^{j+k}} \Psi_k(\eta), \\ \frac{\partial^k F_q^{(Q')}}{\partial \beta^k}(\eta, \beta) &\sim A_m (-1)^k \sum_{j=0}^{\infty} \frac{(j + m - \frac{1}{2})_k \tilde{Q}'_{m,j}}{\beta^{j+k}} \Phi_k^{(1)}(\eta), \\ \frac{\partial^k F_q^{(R)}}{\partial \beta^k}(\eta, \beta) &= \sum_{j=0}^{m-1} (-1)^j \frac{(-\frac{1}{2})_j}{j!} \left(\frac{2}{\beta}\right)^{j-\frac{1}{2}} \frac{(-j + \frac{3}{2} - k)_k}{\beta^k} F_{m-j-1}(\eta), \end{aligned} \tag{29}$$

with

$$\begin{aligned} \tilde{P}_{m,j} &= \frac{2^j (m - \frac{1}{2})_j}{j! (m + 1)_j}, \quad A_m = \frac{(-1)^{m+1}}{m! \Gamma(-\frac{1}{2})}, \\ \tilde{Q}'_{m,j} &= \tilde{P}_{m,j} \left(\ln\left(\frac{2}{\beta}\right) + \psi\left(m + k - \frac{1}{2} + j\right) - \psi(1 + j) - \psi(m + j + 1) \right). \end{aligned} \tag{30}$$

To calculate the function $\Psi_k(\eta)$ we write

$$\Psi_k(\eta) = \Psi_k^{(1)}(\eta) + \Psi_k^{(2)}(\eta), \tag{31}$$

where

$$\Psi_k^{(1)}(\eta) = \frac{k!}{\pi} \left(\psi(k + 1) \int_0^\pi f(\theta) d\theta - \int_0^\pi g(\theta) d\theta \right), \tag{32}$$

and

$$\begin{aligned} f(\theta) &= \frac{e^{-\eta - \cos(\theta)} \cos(\mu\theta + \sin(\theta)) + \cos(\mu\theta)}{1 + 2e^{-\eta - \cos(\theta)} \cos(\sin(\theta)) + e^{-2\eta - 2\cos(\theta)}}, \\ g(\theta) &= -\theta \frac{e^{-\eta - \cos(\theta)} \sin(\mu\theta + \sin(\theta)) + \sin(\mu\theta)}{1 + 2e^{-\eta - \cos(\theta)} \cos(\sin(\theta)) + e^{-2\eta - 2\cos(\theta)}}, \end{aligned} \tag{33}$$

with $\mu = q + 1$. For $\Psi_k^{(2)}(\eta)$ we use

$$\Psi_k^{(2)}(\eta) = (-1)^{k+1} k! \int_1^\infty \frac{x^{-k-1}}{e^{x-\eta} + 1} dx, \quad k = 0, 1, 2, \dots \tag{34}$$

Equation (28) can be used for $k \geq 0$.

4. Overview of the accompanying software

The following set of Matlab functions implementing the expansions are included in the software package:

1. Fqdketaneg(k, eta, q, beta). Implementation of (2).
2. Fqdketapos1(k, eta, q, beta). Implementation of (4).
3. Fqetapos(eta, q, beta). Implementation of (9).
4. Fqdketapos2(k, eta, q, beta). Implementation of (18).
5. Fqdkbeta1(k, eta, q, beta). Implementation of (21).
6. Fqdkbeta2(k, eta, q, beta). Implementation of (28).

The input data follow the notation used in the expansions. Test files are also included in the software package. The functions work in recent versions of Matlab (from version R2014b on) but some of them are not computable in older versions of Matlab or in GNU Octave (those functions involving the use of the confluent hypergeometric functions). A Matlab/GNU Octave algorithm for the Kummer U function is currently being developed by the authors [22] and later we also plan the calculation of the Kummer M function. These two algorithms will allow the use of the whole package in GNU/Octave and will improve very significantly the efficiency of the computations.

Table 1

Test of the expansion given in (2) for $k = 0, 1, 2$. The accuracy and the number of terms n needed in the expansion to obtain such accuracy are shown.

k	η	$q = 0.8$		$q = 3.7$	
		$\beta = 5.2$		$\beta = 1000.2$	
		n	Rel. error	n	Rel. error
0	-6.3	7	1.6×10^{-14}	7	3.3×10^{-16}
0	-20.3	3	1.7×10^{-14}	4	2.9×10^{-15}
0	-100.3	2	1.7×10^{-14}	3	3.4×10^{-15}
1	-6.3	8	1.6×10^{-14}	7	3.3×10^{-16}
1	-20.3	4	1.7×10^{-14}	4	2.9×10^{-15}
1	-100.3	3	1.7×10^{-14}	3	3.4×10^{-15}
2	-6.3	8	1.6×10^{-14}	7	3.3×10^{-16}
2	-20.3	4	1.7×10^{-14}	4	2.9×10^{-15}
2	-100.3	3	1.7×10^{-14}	3	3.4×10^{-15}

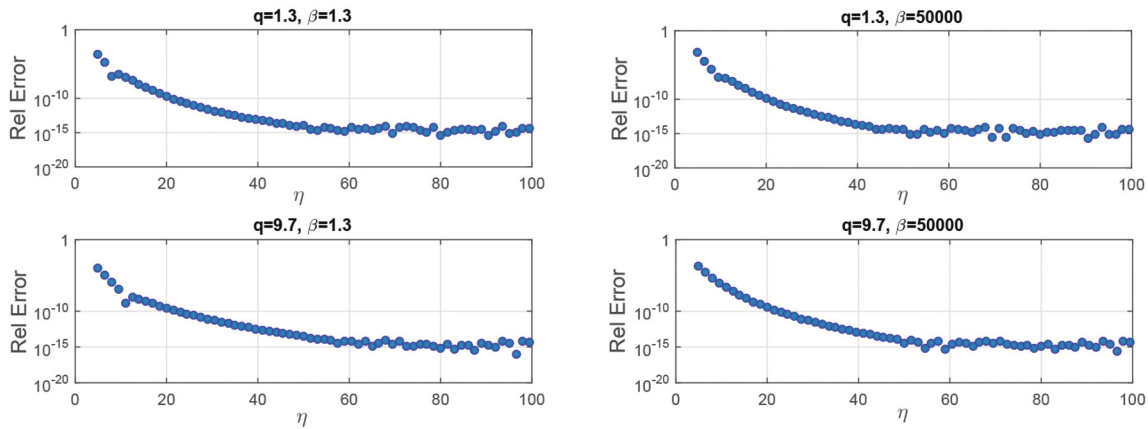


Fig. 1. Test for the first order derivative ($k = 1$) of the expansion given in Section 2.2.1.

5. Testing

A first test of the accuracy of the expansions is given in Table 1. In the table we show examples of the accuracy obtained with the convergent expansion given in (2) and the number of terms needed to obtain such accuracy. For testing we use the integral representations of the Fermi-Dirac integral given in (1) and of the first and second order derivatives with respect to the η parameter, which are given by

$$\begin{aligned} \frac{\partial F_q}{\partial \eta}(\eta, \beta) &= \int_0^\infty \frac{x^q \sqrt{1 + \beta x/2}}{1 + e^{x-\eta}} \frac{1}{1 + e^{\eta-x}} dx, \\ \frac{\partial^2 F_q}{\partial \eta^2}(\eta, \beta) &= \int_0^\infty \frac{x^q \sqrt{1 + \beta x/2}}{1 + e^{x-\eta}} \frac{1 - e^{\eta-x}}{(1 + e^{\eta-x})^2} dx. \end{aligned} \tag{35}$$

The integrals are evaluated using the adaptive Matlab integration function. As can be seen in the table, for moderate/large values of η very few terms are needed in the expansion to obtain an accuracy close to double precision.

Additional tests of the accuracy of the expansions are shown in Figs. 1, 2, 3 and 4. The tests are considered for the first order derivatives of the Fermi-Dirac function. As before, for testing we use integral representations of the functions. For the derivative with respect to the β parameter, we use the following representation

$$\frac{\partial F_q}{\partial \beta}(\eta, \beta) = \int_0^\infty \frac{x^q \sqrt{1 + \beta x/2}}{1 + e^{x-\eta}} \frac{x}{4 + 2\beta x} dx. \tag{36}$$

The results shown in the figures are obtained by comparing the accuracy of the expansions (using the number of terms included in the Matlab implementations) with the numerical evaluation of the integrals. For very large values of η , it is convenient to use alternative high precision methods of testing because there is a loss of accuracy in the results obtained with the double precision Matlab integration function. This also applies to the testing of the higher-order derivatives even for not so large values of the parameters. In practice, we have used **NIntegrate** from Mathematica using 1024-digit arbitrary precision with a 10-minutes time limit and an Arb ball-arithmetic integrator [23] using 256-digit precision implemented as a part of [24]. In Fig. 5, we show relative errors obtained when using the expansion (4) to compute the third order partial derivative with respect to the η parameter. An integral representation of the function is given by

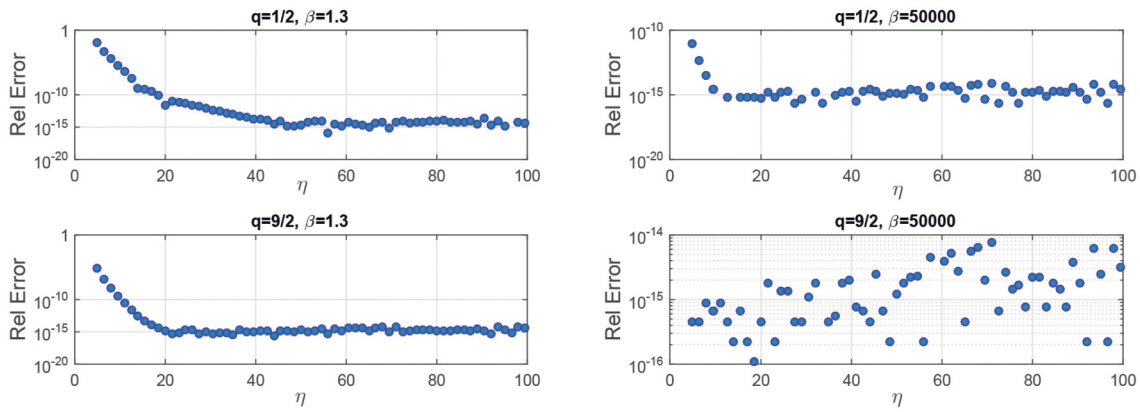


Fig. 2. Test for the first order derivative ($k = 1$) of the expansion given in Section 2.2.2.

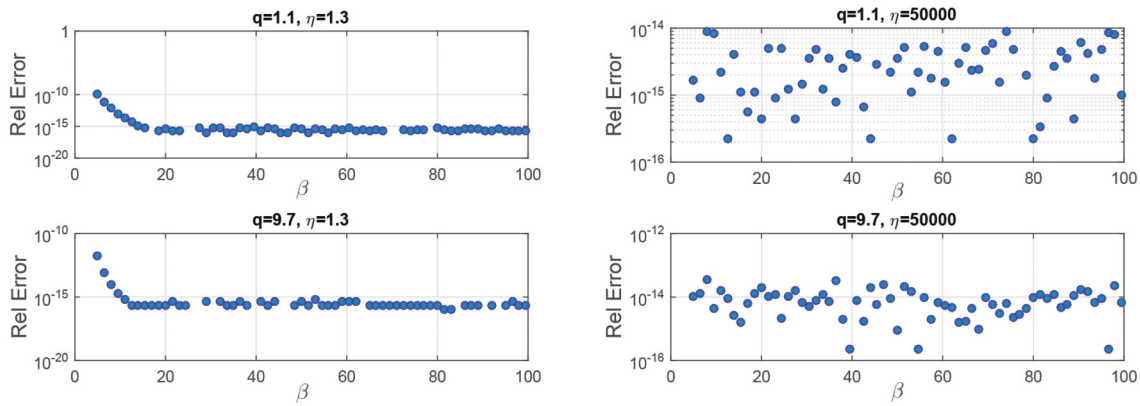


Fig. 3. Test for the first order derivative ($k = 1$) of the expansion given in Section 3.1.

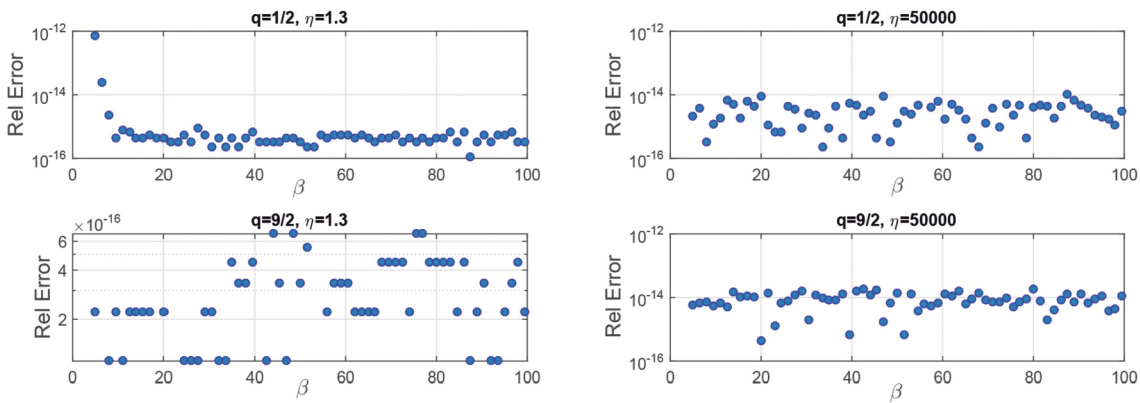


Fig. 4. Test for the first order derivative ($k = 1$) of the expansion given in Section 3.2.

$$\frac{\partial^3 F_q}{\partial \eta^3}(\eta, \beta) = \int_0^\infty \frac{x^q \sqrt{1 + \beta x/2} ((1 - e^{\eta-x})^2 - 2e^{\eta-x})}{1 + e^{x-\eta} (1 + e^{\eta-x})^3} dx. \tag{37}$$

As mentioned before, the computation of the third order derivative is an interesting example because the existing double precision software fails for very large values of η . The accuracy obtained for two choices of q and β for a very large range of η values are shown in the figure. The additional two plots in the same figure show the relative accuracy obtained using a linear scale on the horizontal axis zoomed into the range $0 < \eta < 100$. In all cases, the numerical tests show that an accuracy close to double precision can be obtained with the asymptotic expansions even for moderate values of the parameters.

Finally, in Table 2 we provide few reference values for testing the derivatives $\partial^k F_q / \partial \eta^k(\eta, \beta)$ and $\partial^k F_q / \partial \beta^k(\eta, \beta)$ for $k = 1, 2, 3$.

Declaration of competing interest

The authors declare the following financial interests/personal relationships which may be considered as potential competing interests: Amparo Gil reports financial support was provided by Spain Ministry of Science and Innovation.

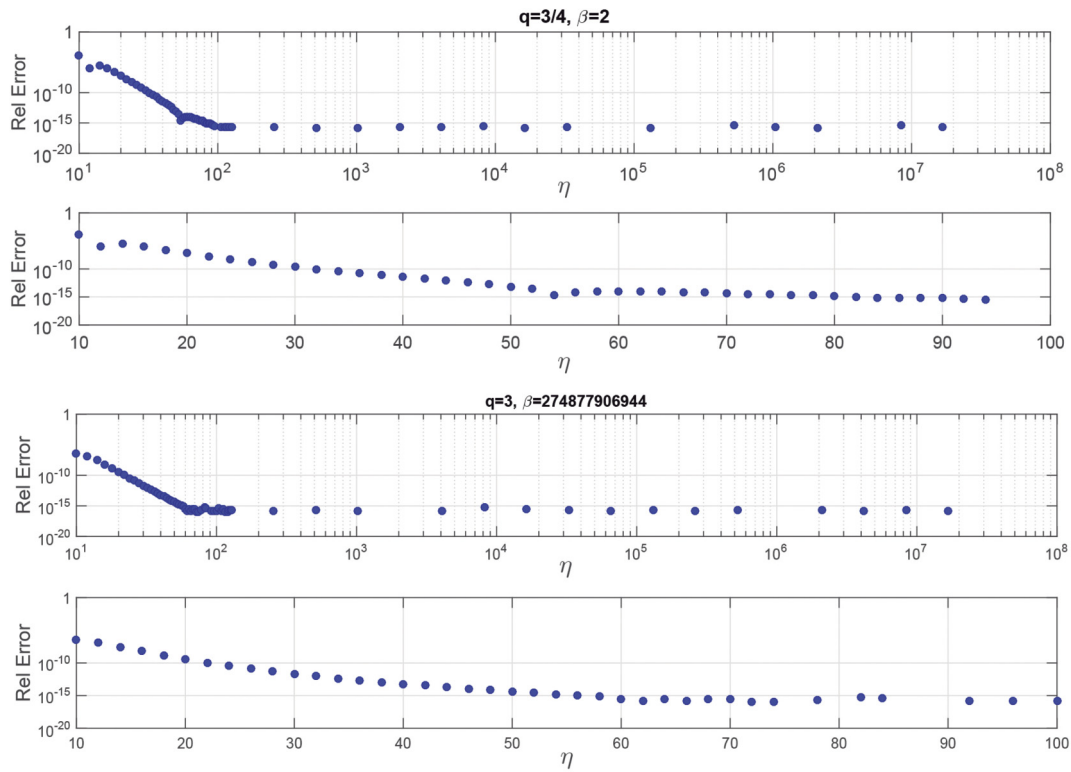


Fig. 5. Test for the third order derivative ($k = 3$) of the expansion given in Section 2.2.1.

Table 2

Table with reference values for testing the derivatives of the relativistic Fermi-Dirac integral up to third order. The values shown, which were obtained using the Matlab implementations of the expansions, have been truncated.

η	$\partial F_q / \partial \eta(\eta, \beta)$	$\partial^2 F_q / \partial \eta^2(\eta, \beta)$	$\partial^3 F_q / \partial \eta^3(\eta, \beta)$
	$(q = \frac{1}{2}, \beta = 3.5)$	$(q = \frac{1}{2}, \beta = 3.5)$	$(q = \frac{1}{2}, \beta = 3.5)$
10^2	$1.32664991437848 \times 10^2$	1.32288102961577	$-1.07281666575692 \times 10^{-7}$
10^3	$1.32325356602562 \times 10^3$	1.32287570949691	$-1.07899481441055 \times 10^{-10}$
10^4	$1.32291345143966 \times 10^4$	1.32287565607221	$-1.07980615132822 \times 10^{-13}$
10^5	$1.32287943517162 \times 10^5$	1.32287565553769	$-1.07988924023698 \times 10^{-16}$
10^6	$1.32287603349671 \times 10^6$	1.32287565553234	$-1.07989756870677 \times 10^{-19}$
	$(q = \frac{3}{2}, \beta = 500)$	$(q = \frac{3}{2}, \beta = 500)$	$(q = \frac{3}{2}, \beta = 500)$
10^2	$1.58113886222714 \times 10^{11}$	$3.16227769179115 \times 10^6$	$3.16227766016837 \times 10^1$
10^3	$1.58114719409694 \times 10^7$	$3.16228082244603 \times 10^4$	$3.16227766016837 \times 10^1$
10^4	$1.58113919832930 \times 10^9$	$3.16227797639614 \times 10^5$	$3.16227766016837 \times 10^1$
10^5	$1.58113886222714 \times 10^{11}$	$3.16227769179115 \times 10^6$	$3.16227766016837 \times 10^1$
10^6	$1.58113883325166 \times 10^{13}$	$3.16227766333065 \times 10^7$	$3.16227766016837 \times 10^1$
η	$\partial F_q / \partial \beta(\eta, \beta)$	$\partial^2 F_q / \partial \beta^2(\eta, \beta)$	$\partial^3 F_q / \partial \beta^3(\eta, \beta)$
	$(q = \frac{1}{2}, \beta = 30)$	$(q = \frac{1}{2}, \beta = 30)$	$(q = \frac{1}{2}, \beta = 30)$
10^0	$1.14024291003471 \times 10^{-1}$	$-1.82075022140818 \times 10^{-3}$	$8.73807158176577 \times 10^{-5}$
10^1	3.31270791969451	$-5.45284351205580 \times 10^{-2}$	$2.69314520075724 \times 10^{-3}$
10^2	$3.22640436927420 \times 10^2$	-5.37021886980341	$2.68156298857859 \times 10^{-1}$
10^3	$3.22728167991479 \times 10^4$	$-5.37808625028079 \times 10^2$	$2.68868504963348 \times 10^1$
10^4	$3.22746471275123 \times 10^6$	$-5.37903614101859 \times 10^4$	$2.68948221626916 \times 10^3$
	$(q = \frac{3}{2}, \beta = 3000)$	$(q = \frac{3}{2}, \beta = 3000)$	$(q = \frac{3}{2}, \beta = 3000)$
10^0	$2.79353728235266 \times 10^{-2}$	$-4.65460090632796 \times 10^{-6}$	$2.32665348299996 \times 10^{-9}$
10^1	2.36390696419555	$-3.93947460496645 \times 10^{-4}$	$1.96955215867537 \times 10^{-7}$
10^2	$2.15377025358968 \times 10^3$	$-3.58958121727859 \times 10^{-1}$	$1.79477267285955 \times 10^{-4}$
10^3	$2.15167757473599 \times 10^6$	$-3.58612570512633 \times 10^2$	$1.79306105951540 \times 10^{-1}$
10^4	$2.15165751933687 \times 10^9$	$-3.58609550695194 \times 10^5$	$1.79304757417124 \times 10^2$

Data availability

No data was used for the research described in the article.

Acknowledgements

We thank the referees for their constructive and helpful remarks. AG, JS and NMT thank financial support from projects PGC2018-098279-B-I00 funded by MCIN/AEI/10.13039/501100011033/ FEDER “Una manera de hacer Europa” and PID2021-127252NB-I00 funded by MCIN/AEI/10.13039/501100011033/ FEDER, UE. NMT thanks CWI Amsterdam for scientific support.

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