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Analytical expansions for Fermi-Dirac functions

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We obtain a fast convergent series expansion for the Fermi-Dirac function \( F(\alpha) \) for \(-10 < \alpha < -1\). We give values of \( F(\alpha) \) for \( \alpha = n + \frac{1}{2} \) \((n = 0, 1, \ldots, 6)\) with \( \alpha \) in the same range.

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I. INTRODUCTION

The Fermi-Dirac functions \( F(\alpha) \), where \( \alpha \) is a positive real parameter, is defined for all real numbers \( \alpha \) by

\[
F(\alpha) = \frac{1}{\Gamma(\alpha)} \int_{0}^{\infty} \frac{x^{\alpha-1}}{e^{x} + 1} dx.
\]

When \( \alpha \) is an integer, this integral may be easily evaluated by a power series; a complete discussion of this case is due to Rhodes.1 For arbitrary \( \alpha \), there are several expansions depending on the range of values of \( \alpha \).2-4 The calculation of \( F(\alpha) \) for \( \alpha < 0 \) is needed in many questions of quantum statistical mechanics; for example, to solve the equations of state corresponding to extreme conditions (high pressure and nonzero temperature). Analytical expansions are available in all ranges, except when \(-10 < \alpha < -1\). Previous evaluations of \( F(\alpha) \) for this range were made by numerical integration4,5 or by polynomial approximation.6 In this paper we obtain a fast convergent series expansion of \( F(\alpha) \) for \(-10 < \alpha < -1\).

II. SERIES EXPANSION FOR \(-10 < \alpha < -1\)

For simplicity, let us define

\[
I = I(\alpha) = \frac{1}{\Gamma(\alpha)} \int_{0}^{\infty} \frac{x^{\alpha-1}}{e^{x} + 1} dx.
\]

Substituting \( y = x + \alpha \) in this integral gives

\[
I = \int_{-\infty}^{\infty} \frac{(y + |\alpha|)^{\alpha-1}}{e^{y} + 1} dy.
\]

Now \( I \) will be calculated as

\[
I = I_{1} + I_{2} + I_{3}
\]

by dividing the integration interval by the points \(-p\) and \(p\), where \(0 < p < |\alpha|\). Another restriction on the values of \( p \) and convenient numerical suggestions will appear later.

A. Evaluation of \( I_{1} \)

First we expand the integrand denominator of

\[
I_{1} = \int_{-p}^{p} \frac{(y + |\alpha|)^{\alpha-1}}{e^{y} + 1} dy
\]

in a series of powers of \( e^{y} \)

\[
\frac{1}{e^{y} + 1} = \sum_{k=0}^{\infty} (-1)^{k} e^{ky}.
\]

This series converges uniformly for \(|e^{y}| < 1\), that is, for \( y < 0\). Now, by expanding \( e^{y} \) at a convenient point \( y_{0}\), we obtain

\[
e^{y} = e^{y_{0}} \sum_{k=0}^{\infty} \frac{y_{0}}{k!} (y - y_{0})^{k}.
\]

By replacing successively in (1), taking into account the uniform convergence of the series to exchange the order of integrals and summations, it follows that

\[
I_{1} = \sum_{n=0}^{\infty} (-1)^{n} e^{ny_{0}} \sum_{k=0}^{n} \frac{n^{k}}{k!} \int_{-\alpha}^{\alpha} (y + |\alpha|)^{\alpha-1} (y - y_{0})^{k} dy.
\]

The integrals involved in this expression may be evaluated using the formula

\[
\int_{-\alpha}^{\alpha} (y + |\alpha|)^{\alpha-1} (y - y_{0})^{k} dy = \frac{\alpha + bx)^{\alpha}}{(b + 1)^{\alpha}} \sum_{0,j,k} \frac{(-1)^{k} (\alpha + bx)^{\alpha - j - |\alpha|} (y - y_{0})^{k}}{k! (k - j + \alpha)}.
\]

Thus,

\[
I_{1} = \sum_{\alpha, p} (|\alpha| - p)^{\alpha} \sum_{n=0}^{\infty} (-1)^{n} e^{ny_{0}} \sum_{k=0}^{n^{k}} \frac{n^{k}}{k!} A_{k},
\]

where

\[
A_{k} = \sum_{0,j,k} \frac{(-1)^{k} (|\alpha| - p)^{\alpha - j - |\alpha|} (y_{0} + |\alpha|)^{\alpha - j - |\alpha|}}{(k - j + \alpha)(k!)}.
\]
B. Evaluation of $\int_2$

We notice that

$$I_2 = |\alpha|^{n-1} \int_0^1 \frac{y}{|\alpha| + 1} df.$$  

Since $0 < p < |\alpha|$, the series

$$\left( \frac{y}{|\alpha|} + 1 \right)^{n-1} = \sum_{n=0}^{\infty} \frac{1}{n!} \frac{(n-1)_2}{(n-1)_2} \frac{y^{2k-1}}{k (k+1)!}$$  

converges uniformly. The same statement holds for the series

$$\frac{1}{e^x + 1} = \frac{1}{2} + \frac{1}{|\alpha|} \sum_{n=1}^{\infty} \frac{B_n (n-2)}{2k (2k+1)!}$$

when $p < \pi$, $B_n$ being the nonzero Bernoulli numbers. Therefore, arguments used in Sec. (A) apply here, yielding

$$I_2 = |\alpha|^{n-1} \sum_{n=1}^{\infty} C_n \left( \frac{x}{\sigma - 2n + 1} \right)^2$$

where

$$C_1 = |\alpha| \psi,$$

$$C_{n+1} = C_n \frac{(\sigma - 2n)(\sigma - 2n - 1)}{(2n + 2n + 1)^2} \left( \frac{x}{\sigma} \right)^2,$$

$$D_1 = -3B_n,$$

and

$$D_{n+1} = D_n \frac{(1 - 4k + 1)B_{2k + 1} \psi^2}{(1 - 4k + 1)B_{2k + 1} (2k + 2k + 1)^2}$$

C. Evaluation of $\int_3$

Recall that

$$I_3 = \int_0^\infty \left( y + |\alpha| \right)^{n-1} df.$$  

Since the expansion of the integrand denominator in a series of powers of $e^{-y}$

$$\frac{1}{e^x + 1} = -\sum_{n=1}^{\infty} (-1)^n e^{-ny},$$

is uniformly convergent for $y > 0$, by exchanging the integral and the summation, with the substitution $z = n(y + |\alpha|)$ we obtain

$$I_3 = \sum_{k=1}^{\infty} \frac{(-1)^n + 1}{n^2} \left( \frac{\sigma}{\sigma + p} \right) \Gamma(\sigma, np + |\alpha|).$$

From our numerical investigations we conclude that, in order to achieve a fast convergence, the values of $p$ and $y_0$ may be chosen as follows:

$p = |\alpha|/2$, if $1 < |\alpha| < 5$;

$p = 2.5$, if $5 < |\alpha| < 10$;

$y_0 = -(|\alpha| + 1)/2$.

As an application, values of $F_\nu(\alpha)$ for $-10 < \alpha < -1$ and $n = 1/2 (n = 0, 1, \ldots, 6)$ were computed with a maximum relative error of $10^{-5}$. In particular, we have checked the accuracy of all previously tabulated values. In the course of the computation we have made use of Abramowitz's tables for Bernoulli numbers. The corresponding computing program is to be published elsewhere.

### Table 1. Values of $F_\nu(\alpha)$ for $-10 < \alpha < -1$ and $\sigma = n + \frac{1}{2}$ with $n = 0, 1, \ldots, 6$.

| $\sigma$ | $F_{1/2}$ | $F_{3/2}$ | $F_{5/2}$ | $F_{9/2}$ | $F_{11/2}$ | $F_{13/2}$ |
|----------|------------|------------|------------|------------|------------|------------|
| -1.0     | 1.027050 00 | 1.551560 00 | 2.398400 00 | 2.979400 00 | 2.481700 00 | 2.848300 00 |
| -1.1     | 1.071600 00 | 1.685030 00 | 2.156120 00 | 2.603200 00 | 2.146800 00 | 2.486400 00 |
| -1.2     | 1.116200 00 | 1.799170 00 | 2.310120 00 | 2.738200 00 | 2.311580 00 | 2.719800 00 |
| -1.3     | 1.160800 00 | 1.913840 00 | 2.472170 00 | 2.871300 00 | 2.515470 00 | 2.820200 00 |
| -1.4     | 1.205300 00 | 2.028230 00 | 2.641530 00 | 3.017000 00 | 2.916900 00 | 3.090200 00 |
| -1.5     | 1.249300 00 | 2.140710 00 | 2.818420 00 | 3.170000 00 | 3.191100 00 | 3.191100 00 |
| -1.6     | 1.293100 00 | 2.251290 00 | 3.003450 00 | 3.329000 00 | 3.298500 00 | 3.348500 00 |
| -1.7     | 1.336400 00 | 2.361870 00 | 3.196500 00 | 3.494000 00 | 3.392400 00 | 3.494000 00 |
| -1.8     | 1.379600 00 | 2.472120 00 | 3.398500 00 | 3.653000 00 | 3.485400 00 | 3.645400 00 |
| -1.9     | 1.422200 00 | 2.581990 00 | 3.607500 00 | 3.815000 00 | 3.578400 00 | 3.815000 00 |
| -2.0     | 1.464200 00 | 2.691270 00 | 3.813000 00 | 3.978000 00 | 3.671400 00 | 3.978000 00 |
| -2.1     | 1.505800 00 | 2.800020 00 | 4.024500 00 | 4.141000 00 | 3.764400 00 | 4.141000 00 |
| -2.2     | 1.546800 00 | 2.907770 00 | 4.234500 00 | 4.306000 00 | 3.857400 00 | 4.306000 00 |
| -2.3     | 1.587200 00 | 3.014670 00 | 4.444500 00 | 4.470000 00 | 3.949400 00 | 4.470000 00 |
| -2.4     | 1.627000 00 | 3.121650 00 | 4.653500 00 | 4.634000 00 | 4.041400 00 | 4.634000 00 |
| -2.5     | 1.666300 00 | 3.228710 00 | 4.862500 00 | 4.807600 00 | 4.133400 00 | 4.807600 00 |
| -2.6     | 1.704900 00 | 3.335550 00 | 5.071500 00 | 4.981400 00 | 4.225400 00 | 4.981400 00 |
| -2.7     | 1.742900 00 | 3.442540 00 | 5.280500 00 | 5.155200 00 | 4.317400 00 | 5.155200 00 |

(continued)
| TABLE I (Continued) |
|---------------------|
| Value 1 | Value 2 | Value 3 | Value 4 |
| 1.783416 | 4.124120 | 6.927870 | 9.642480 |
| 1.193480 | 1.306220 | 1.293000 | 1.467200 |
| 6.875950 | 7.788100 | 1.111290 | 1.397610 |
| 6.246400 | 6.191450 | 1.327170 | 1.762700 |
| 5.825560 | 5.972800 | 1.630060 | 1.919570 |
| 5.271710 | 6.935860 | 1.460750 | 2.192490 |
| 5.689800 | 6.662550 | 1.622760 | 1.397540 |
| 5.623320 | 1.082740 | 1.666250 | 2.271500 |
| 5.086960 | 1.140490 | 1.777390 | 2.398700 |
| 6.875950 | 1.200150 | 1.699590 | 2.577430 |
| 6.246400 | 1.829100 | 2.017490 | 2.772970 |
| 5.825560 | 2.146670 | 2.311410 | 3.720110 |
| 5.271710 | 2.827270 | 3.202570 | 4.021980 |
| 5.689800 | 4.606970 | 4.379200 | 4.361090 |
| 1.082740 | 2.579490 | 3.087880 | 4.717250 |
| 5.623320 | 2.311410 | 3.931510 | 5.299170 |
| 5.086960 | 2.895920 | 4.234670 | 5.328660 |
| 6.875950 | 3.076710 | 4.352500 | 6.916300 |
| 5.825560 | 3.247440 | 4.882890 | 6.155520 |
| 5.271710 | 3.435250 | 5.182530 | 6.916300 |
| 5.689800 | 3.631410 | 5.353510 | 7.526300 |
| 5.086960 | 3.836160 | 5.938920 | 8.024980 |
| 6.875950 | 3.984970 | 7.031100 | 8.750000 |
| 5.825560 | 4.272480 | 7.419180 | 9.777300 |
| 5.271710 | 4.746170 | 7.620400 | 9.017890 |
| 5.689800 | 5.495580 | 7.759500 | 9.797100 |
| 6.875950 | 6.888950 | 7.998480 | 9.797100 |
| 6.246400 | 7.724310 | 8.258800 | 9.797100 |
| 5.825560 | 8.144470 | 8.361250 | 9.797100 |
| 5.271710 | 8.477470 | 8.566800 | 9.797100 |
| 5.689800 | 8.644220 | 8.736050 | 9.797100 |
| 6.875950 | 9.028950 | 8.911300 | 9.797100 |
| 6.246400 | 9.273310 | 9.174800 | 9.797100 |
| 4.625220 | 9.958970 | 9.625090 | 9.797100 |
| 5.825560 | 1.013170 | 9.161080 | 9.797100 |
| 5.271710 | 1.397590 | 9.529280 | 9.797100 |
| 6.875950 | 1.639340 | 9.732640 | 9.797100 |
| 5.825560 | 1.909600 | 9.819360 | 9.797100 |
| 5.271710 | 2.330470 | 1.002720 | 9.797100 |
| 6.875950 | 2.680440 | 1.191800 | 9.797100 |
| 5.825560 | 3.098100 | 1.380300 | 9.797100 |
| 5.271710 | 3.554330 | 1.569800 | 9.797100 |
| 6.875950 | 3.951710 | 1.760300 | 9.797100 |
| 5.825560 | 4.348070 | 1.950800 | 9.797100 |
| 5.271710 | 4.748940 | 2.141300 | 9.797100 |
| 6.875950 | 5.149080 | 2.331800 | 9.797100 |
| 5.825560 | 5.541170 | 2.522300 | 9.797100 |
| 5.271710 | 5.940760 | 2.712800 | 9.797100 |
| 6.875950 | 6.339320 | 2.903300 | 9.797100 |
| 5.825560 | 6.737680 | 3.093800 | 9.797100 |
| 5.271710 | 7.135240 | 3.284300 | 9.797100 |
| 6.875950 | 7.531160 | 3.474800 | 9.797100 |
| 5.825560 | 7.925720 | 3.665300 | 9.797100 |
| 5.271710 | 8.318780 | 3.855800 | 9.797100 |
| 6.875950 | 8.710340 | 4.046300 | 9.797100 |
| 5.825560 | 9.099360 | 4.236800 | 9.797100 |
| 5.271710 | 9.486840 | 4.427300 | 9.797100 |

(continued)
| -9.1  | 3.385830 | 2.096170 | 01  | 8.076550 | 01  | 2.297610 | 02  | 5.252820 | 02  | 1.014860 | 03  | 1.714610 | 03  |
| -9.2  | 3.404810 | 2.130120 | 01  | 8.285870 | 01  | 2.379410 | 02  | 5.486650 | 02  | 1.068550 | 03  | 1.818760 | 03  |
| -9.3  | 3.423670 | 2.164260 | 01  | 8.500580 | 01  | 2.463340 | 02  | 5.728770 | 02  | 1.124620 | 03  | 1.928400 | 03  |
| -9.4  | 3.442430 | 2.198590 | 01  | 8.718730 | 01  | 2.549430 | 02  | 5.979390 | 02  | 1.183150 | 03  | 2.043770 | 03  |
| -9.5  | 3.461080 | 2.233110 | 01  | 8.940310 | 01  | 2.637720 | 02  | 6.238730 | 02  | 1.246230 | 03  | 2.165110 | 03  |
| -9.6  | 3.479620 | 2.267810 | 01  | 9.165350 | 01  | 2.728250 | 02  | 6.507010 | 02  | 1.307960 | 03  | 2.292760 | 03  |
| -9.7  | 3.498060 | 2.302700 | 01  | 9.393880 | 01  | 2.821040 | 02  | 6.784460 | 02  | 1.374410 | 03  | 2.426800 | 03  |
| -9.8  | 3.516400 | 2.337770 | 01  | 9.625900 | 01  | 2.916140 | 02  | 7.071300 | 02  | 1.443680 | 03  | 2.567680 | 03  |
| -9.9  | 3.534640 | 2.373030 | 01  | 9.861440 | 01  | 3.013570 | 02  | 7.367760 | 02  | 1.515860 | 03  | 2.715630 | 03  |
| -10.0 | 3.552780 | 2.408470 | 01  | 1.010050 | 02  | 3.113380 | 02  | 7.674090 | 02  | 1.591060 | 03  | 2.870950 | 03  |

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