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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 $F_\sigma(\alpha)$ for $-10\leqslant\alpha\leqslant-1$. We give values of $F_\sigma(\alpha)$ for $\sigma=n+\frac{1}{2}$ $(n=0,1,\cdots,6)$ with α in the same range.

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I. INTRODUCTION

The Fermi–Dirac functions $F_\sigma(\alpha)$, where σ is a positive real parameter, is defined for all real numbers α by

$$F_\sigma(\alpha)=\frac{1}{\Gamma(\sigma)}\int_0^\infty\frac{x^{\sigma-1}}{e^{x+\alpha}+1}\,dx.$$

When σ 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 σ, there are several expansions depending on the range of values of α.[2–4] The calculation of $F_\sigma(\alpha)$ 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 $-10\leqslant\alpha\leqslant-1$. Previous evaluations of $F_\sigma(\alpha)$ for this range were made by numerical integration[4,5] or by polynomial approximation.[6] In this paper we obtain a fast convergent series expansion of $F_\sigma(\alpha)$ for $-10\leqslant\alpha\leqslant-1$.

II. SERIES EXPANSION FOR $-10\leqslant\alpha\leqslant-1$

For simplicity, let us define

$$I=I_\sigma(\alpha)=\Gamma(\sigma)F_\sigma(\alpha)=\int_0^\infty\frac{x^{\sigma-1}}{e^{x+\alpha}+1}\,dx.$$

Substituting $y=x+\alpha$ in this integral gives

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

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.

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A. Evaluation of I_1

First we expand the integrand denominator of

$$I_1=\int_{-|\alpha|}^{-p}\frac{(y+|\alpha|)^{\sigma-1}}{e^y+1}\,dy \tag{1}$$

in a series of powers of e^y

$$\frac{1}{e^y+1}=\sum_{n\geqslant0}(-1)^n e^{ny}.$$

This series converges uniformly for $|e^y|<1$, that is, for $y<0$. Now, by expanding e^{ny} at a convenient point y_0, we obtain

$$e^{ny}=e^{ny_0}\sum_{k\geqslant0}\frac{n^k(y-y_0)^k}{k!}.$$

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

$$I_1=\sum_{n\geqslant0}(-1)^n e^{ny_0}\sum_{k\geqslant0}\frac{n^k}{k!}\times\int_{-|\alpha|}^{-p}(y+|\alpha|)^{\sigma-1}(y-y_0)^k\,dy.$$

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

$$\int(a+bx)^{\sigma-1}x^k\,dx=\frac{(a+bx)^\sigma}{b^{k+1}}\times\sum_{0\leqslant j\leqslant k}\frac{(-1)^j\binom{k}{j}(a+bx)^{k-j}a^j}{k-j+\sigma}.$$

Thus,

$$I_1=(|\alpha|-p)^\sigma\sum_{n\geqslant0}(-1)^n e^{ny_0}\sum_{k\geqslant0}\frac{n^k}{k!}A_k,$$

where

$$A_k=\sum_{0\leqslant j\leqslant k}\frac{(-1)^j\binom{k}{j}(|\alpha|-p)^{k-j}(y_0+|\alpha|)^j}{k-j+\sigma}.$$

B. Evaluation of I_2

We notice that

$$I_2 = |\alpha|^{\sigma-1} \int_{-p}^{p} \frac{(y/|\alpha| + 1)^{\sigma-1}}{e^y + 1}\, dy.$$

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

$$\left(\frac{y}{|\alpha|} + 1\right)^{\sigma-1} = \sum_{n\geqslant 0} \binom{\sigma-1}{n} \left(\frac{y}{|\alpha|}\right)^n$$

converges uniformly. The same statement holds[7] for the series

$$\frac{1}{e^y + 1} = \frac{1}{2} + \frac{1}{2} \sum_{k\geqslant 1} \frac{(1-4^k)B_k y^{2k-1}}{k(2k-1)!}$$

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

$$I_2 = |\alpha|^{\sigma-1} \sum_{n\geqslant 1} C_n \left(\frac{1}{\sigma - 2n + 1} + \frac{1}{|\alpha|} \sum_{k\geqslant 1} \frac{D_k}{2k + 2n - 1}\right),$$

where

$$C_1 = (\sigma - 1)p,$$

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

$$D_1 = -3B_1 p^2,$$

and

$$D_{k+1} = D_k \frac{(1 - 4^{k+1})B_{k+1}p^2}{(1-4^k)B_k 2(k+1)(2k+1)}.$$

C. Evaluation of I_3

Recall that

$$I_3 = \int_p^\infty \frac{(y + |\alpha|)^{\sigma-1}}{e^y + 1}\, dy.$$

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

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

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

$$I_3 = \sum_{n\geqslant 1} \frac{(-1)^{n+1} e^{n|\alpha|}}{n^\sigma} \int_{n(|\alpha| + p)}^{\infty} z^{\sigma-1} e^{-z}\, dz.$$

Thus, I_3 can be expressed in terms of incomplete Gamma functions as

$$I_3 = \sum_{n\geqslant 1} \frac{(-1)^{n+1} e^{n|\alpha|}}{n^\sigma} \Gamma(\sigma, n(p + |\alpha|)).$$

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:

$$p = |\alpha|/2, \text{ if } 1 \leqslant |\alpha| < 5;$$
$$p = 2.5, \text{ if } 5 \leqslant |\alpha| \leqslant 10$$
$$y_0 = -(|\alpha| + p)/2.$$

As an application, values of $F_\sigma(\alpha)$ for $-10 \leqslant \alpha \leqslant -1$ and $\sigma = n + \frac{1}{2}$ $(n = 0,1,...,6)$ were computed with a maximum relative error of 10^{-5}. In particular, we have checked the accuracy of all previously tabulated values.[4,6] In the course of the computation we have made use of Abramowitz's tables[7] for Bernoulli numbers. The corresponding computing program is to be published elsewhere.[8]

TABLE I. Values of $F_\sigma(\alpha)$ for $-10 \leqslant \alpha \leqslant -1$ and $\sigma = n + \frac{1}{2}$ with $n = 0,1,...,6$.

ALPHA	F1/2	F3/2	F5/2	F7/2	F9/2	F11/2	F13/2
-1.0	1.02705D 00	1.57565D 00	2.00225D 00	2.29484D 00	2.47867D 00	2.58718D 00	2.64830D 00
-1.1	1.07166D 00	1.66058D 00	2.16502D 00	2.50312D 00	2.71842D 00	2.84684D 00	2.91980D 00
-1.2	1.11628D 00	1.76997D 00	2.33852D 00	2.72820D 00	2.97986D 00	3.13158D 00	3.21849D 00
-1.3	1.16082D 00	1.90384D 00	2.52317D 00	2.97119D 00	3.26467D 00	3.44360D 00	3.54701D 00
-1.4	1.20519D 00	2.02213D 00	2.71943D 00	3.23323D 00	3.57472D 00	3.78536D 00	3.90820D 00
-1.5	1.24932D 00	2.14487D 00	2.92775D 00	3.51547D 00	3.91198D 00	4.15946D 00	4.30516D 00
-1.6	1.29315D 00	2.27199D 00	3.14855D 00	3.81918D 00	4.27855D 00	4.56872D 00	4.74127D 00
-1.7	1.33660D 00	2.40348D 00	3.38229D 00	4.14563D 00	4.67659D 00	5.01620D 00	5.22019D 00
-1.8	1.37964D 00	2.53929D 00	3.62940D 00	4.49610D 00	5.10845D 00	5.50516D 00	5.74590D 00
-1.9	1.42222D 00	2.67939D 00	3.89030D 00	4.87195D 00	5.57664D 00	6.03913D 00	6.32273D 00
-2.0	1.46429D 00	2.82373D 00	4.16541D 00	5.27462D 00	6.08374D 00	6.62181D 00	6.95534D 00
-2.1	1.50584D 00	2.97223D 00	4.45517D 00	5.70552D 00	6.63253D 00	7.25726D 00	7.64882D 00
-2.2	1.54683D 00	3.12487D 00	4.76000D 00	6.16617D 00	7.22586D 00	7.94979D 00	8.40868D 00
-2.3	1.58725D 00	3.28158D 00	5.08029D 00	6.65805D 00	7.86680D 00	8.70400D 00	9.24084D 00
-2.4	1.62708D 00	3.44230D 00	5.41645D 00	7.18275D 00	8.55855D 00	9.52483D 00	1.01517D 01
-2.5	1.66631D 00	3.60698D 00	5.76888D 00	7.74188D 00	9.30448D 00	1.04175D 01	1.11482D 01
-2.6	1.70494D 00	3.77555D 00	6.13797D 00	8.33707D 00	1.01081D 01	1.13877D 01	1.22376D 01
-2.7	1.74298D 00	3.94795D 00	6.52411D 00	8.97003D 00	1.09732D 01	1.24412D 01	1.34285D 01

(continued)

TABLE I. (*Continued*).

-2.8	1.78041D 00	4.12412D 00	6.92769D 00	9.64248D 00	1.19034D 01	1.35845D 01	1.4729[illegible]D 01
-2.9	1.81724D 00	4.30401D 00	7.34906D 00	1.03562D 01	1.29030D 01	1.48242D 01	1.61486D 01
-3.0	1.85349D 00	4.48755D 00	7.78861D 00	1.11129D 01	1.39761D 01	1.61675D 01	1.76973D 01
-3.1	1.88915D 00	4.67469D 00	8.24669D 00	1.19145D 01	1.51271D 01	1.76220D 01	1.93858D 01
-3.2	1.92424D 00	4.86536D 00	8.72367D 00	1.27629D 01	1.63606D 01	1.91957D 01	2.12257D 01
-3.3	1.95877D 00	5.05952D 00	9.21988D 00	1.36599D 01	1.76813D 01	2.08970D 01	2.32292D 01
-3.4	1.99275D 00	5.25710D 00	9.73568D 00	1.46075D 01	1.90942D 01	2.27350D 01	2.54097D 01
-3.5	2.02619D 00	5.45805D 00	1.02714D 01	1.56077D 01	2.06046D 01	2.47191D 01	2.77811D 01
-3.6	2.05912D 00	5.66232D 00	1.08274D 01	1.66625D 01	2.22176D 01	2.68593D 01	3.03587D 01
-3.7	2.09153D 00	5.86986D 00	1.14040D 01	1.77739D 01	2.39389D 01	2.91662D 01	3.31585D 01
-3.8	2.12345D 00	6.08061D 00	1.20015D 01	1.89439D 01	2.57743D 01	3.16509D 01	3.61979D 01
-3.9	2.15489D 00	6.29453D 00	1.26202D 01	2.01749D 01	2.77297D 01	3.43251D 01	3.94950D 01
-4.0	2.18587D 00	6.51157D 00	1.32605D 01	2.14667D 01	2.98114D 01	3.72011D 01	4.30696D 01
-4.1	2.21639D 00	6.73169D 00	1.39226D 01	2.28277D 01	3.20257D 01	4.02918D 01	4.69424D 01
-4.2	2.24648D 00	6.95484D 00	1.46069D 01	2.42540D 01	3.43792D 01	4.36109D 01	5.11356D 01
-4.3	2.27614D 00	7.18097D 00	1.53137D 01	2.57498D 01	3.68788D 01	4.71725D 01	5.56727D 01
-4.4	2.30539D 00	7.41005D 00	1.60432D 01	2.73175D 01	3.95315D 01	5.09917D 01	6.05787D 01
-4.5	2.33425D 00	7.64204D 00	1.67958D 01	2.89592D 01	4.23447D 01	5.50842D 01	6.58801D 01
-4.6	2.36271D 00	7.87689D 00	1.75717D 01	3.06774D 01	4.53259D 01	5.94663D 01	7.16052D 01
-4.7	2.39081D 00	8.11457D 00	1.83713D 01	3.24744D 01	4.84828D 01	6.41552D 01	7.77837D 01
-4.8	2.41855D 00	8.35504D 00	1.91947D 01	3.43525D 01	5.18235D 01	6.91690D 01	8.44471D 01
-4.9	2.44594D 00	8.59827D 00	2.00424D 01	3.63141D 01	5.53561D 01	7.45263D 01	9.16289D 01
-5.0	2.47299D 00	8.84422D 00	2.09145D 01	3.83618D 01	5.90892D 01	8.02469D 01	9.93644D 01
-5.1	2.49971D 00	9.09285D 00	2.18113D 01	4.04978D 01	6.30314D 01	8.63512D 01	1.07691D 02
-5.2	2.52612D 00	9.34415D 00	2.27331D 01	4.27248D 01	6.71918D 01	9.28605D 01	1.16648D 02
-5.3	2.55222D 00	9.59807D 00	2.36802D 01	4.50453D 01	7.15795D 01	9.97971D 01	1.26277D 02
-5.4	2.57803D 00	9.85458D 00	2.46528D 01	4.74617D 01	7.62041D 01	1.07184D 02	1.36623D 02
-5.5	2.60355D 00	1.01137D 01	2.56512D 01	4.99767D 01	8.10751D 01	1.15046D 02	1.47730D 02
-5.6	2.62879D 00	1.03753D 01	2.66756D 01	5.25929D 01	8.62028D 01	1.23408D 02	1.59648D 02
-5.7	2.65376D 00	1.06394D 01	2.77264D 01	5.53127D 01	9.15972D 01	1.32296D 02	1.72429D 02
-5.8	2.67848D 00	1.09060D 01	2.88036D 01	5.81390D 01	9.72688D 01	1.41737D 02	1.86126D 02
-5.9	2.70294D 00	1.11751D 01	2.99076D 01	6.10744D 01	1.03229D 02	1.51759D 02	2.00796D 02
-6.0	2.72715D 00	1.14466D 01	3.10387D 01	6.41214D 01	1.09487D 02	1.62392D 02	2.16498D 02
-6.1	2.75112D 00	1.17205D 01	3.21970D 01	6.72830D 01	1.16057D 02	1.73667D 02	2.33296D 02
-6.2	2.77487D 00	1.19968D 01	3.33829D 01	7.05618D 01	1.22948D 02	1.85614D 02	2.51254D 02
-6.3	2.79839D 00	1.22755D 01	3.45965D 01	7.39605D 01	1.30173D 02	1.98267D 02	2.70442D 02
-6.4	2.82169D 00	1.25565D 01	3.58381D 01	7.74820D 01	1.37744D 02	2.11660D 02	2.90932D 02
-6.5	2.84477D 00	1.28398D 01	3.71079D 01	8.11291D 01	1.45674D 02	2.25828D 02	3.12800D 02
-6.6	2.86766D 00	1.31254D 01	3.84061D 01	8.49045D 01	1.53974D 02	2.40808D 02	3.36125D 02
-6.7	2.89034D 00	1.34133D 01	3.97330D 01	8.88112D 01	1.62659D 02	2.56636D 02	3.60990D 02
-6.8	2.91282D 00	1.37035D 01	4.10888D 01	9.28521D 01	1.71741D 02	2.73353D 02	3.87482D 02
-6.9	2.93512D 00	1.39959D 01	4.24738D 01	9.70300D 01	1.81234D 02	2.90998D 02	4.15691D 02
-7.0	2.95723D 00	1.42905D 01	4.38881D 01	1.01348D 02	1.91152D 02	3.09613D 02	4.45714D 02
-7.1	2.97916D 00	1.45873D 01	4.53320D 01	1.05809D 02	2.01508D 02	3.29243D 02	4.77648D 02
-7.2	3.00092D 00	1.48863D 01	4.68056D 01	1.10415D 02	2.12318D 02	3.49930D 02	5.11597D 02
-7.3	3.02250D 00	1.51875D 01	4.83093D 01	1.15171D 02	2.23596D 02	3.71722D 02	5.47671D 02
-7.4	3.04392D 00	1.54908D 01	4.98432D 01	1.20078D 02	2.35357D 02	3.94666D 02	5.85980D 02
-7.5	3.06517D 00	1.57963D 01	5.14076D 01	1.25140D 02	2.47617D 02	4.18810D 02	6.26644D 02
-7.6	3.08627D 00	1.61039D 01	5.30025D 01	1.30361D 02	2.60391D 02	4.44206D 02	6.69784D 02
-7.7	3.10720D 00	1.64135D 01	5.46284D 01	1.35742D 02	2.73695D 02	4.70906D 02	7.15528D 02
-7.8	3.12799D 00	1.67253D 01	5.62853D 01	1.41287D 02	2.87545D 02	4.98963D 02	7.64010D 02
-7.9	3.14863D 00	1.7[illegible]391D 01	5.79735D 01	1.47000D 02	3.01958D 02	5.28434D 02	8.15368D 02
-8.0	3.16912D 00	1.73550D 01	5.96932D 01	1.52883D 02	3.16950D 02	5.59374D 02	8.69746D 02
-8.1	3.18948D 00	1.76730D 01	6.14446D 01	1.58940D 02	3.32540D 02	5.91844D 02	9.27294D 02
-8.2	3.20969D 00	1.79929D 01	6.32279D 01	1.65173D 02	3.48744D 02	6.25903D 02	9.88168D 02
-8.3	3.22977D 00	1.83149D 01	6.50432D 01	1.71586D 02	3.65581D 02	6.61613D 02	1.05253D 03
-8.4	3.24971D 00	1.86389D 01	6.68909D 01	1.78183D 02	3.83067D 02	6.99040D 02	1.12055D 03
-8.5	3.26953D 00	1.89648D 01	6.87711D 01	1.84966D 02	4.01223D 02	7.38249D 02	1.19240D 03
-8.6	3.28922D 00	1.92928D 01	7.06839D 01	1.91938D 02	4.20067D 02	7.79308D 02	1.26826D 03
-8.7	3.30878D 00	1.96227D 01	7.26297D 01	1.99104D 02	4.39617D 02	8.22286D 02	1.34832D 03
-8.8	3.32822D 00	1.99545D 01	7.46085D 01	2.06465D 02	4.59894D 02	8.67256D 02	1.43278D 03
-8.9	3.34754D 00	2.02883D 01	7.66207D 01	2.14026D 02	4.80917D 02	9.14290D 02	1.52184D 03
-9.0	3.36675D 00	2.06240D 01	7.86663D 01	2.21790D 02	5.02706D 02	9.63465D 02	1.61571D 03

(*continued*)

Cont. from Table I.

-9.1	3.38583D 00	2.09617D 01	8.07455D 01	2.29761D 02	5.25282D 02	1.01486D 03	1.71461D 03
-9.2	3.40481D 00	2.13012D 01	8.28587D 01	2.37941D 02	5.48665D 02	1.06855D 03	1.81876D 03
-9.3	3.42367D 00	2.16426D 01	8.50058D 01	2.46334D 02	5.72877D 02	1.12462D 03	1.92840D 03
-9.4	3.44243D 00	2.19859D 01	8.71873D 01	2.54943D 02	5.97939D 02	1.18315D 03	2.04377D 03
-9.5	3.46108D 00	2.23311D 01	8.94031D 01	2.63772D 02	6.23873D 02	1.24423D 03	2.16511D 03
-9.6	3.47962D 00	2.26781D 01	9.16535D 01	2.72825D 02	6.50701D 02	1.30796D 03	2.29270D 03
-9.7	3.49806D 00	2.30270D 01	9.39388D 01	2.82104D 02	6.78446D 02	1.37441D 03	2.42680D 03
-9.8	3.51640D 00	2.33777D 01	9.62590D 01	2.91614D 02	7.07130D 02	1.44368D 03	2.56768D 03
-9.9	3.53464D 00	2.37303D 01	9.86144D 01	3.01357D 02	7.36776D 02	1.51586D 03	2.71563D 03
-10.0	3.55278D 00	2.40847D 01	1.01005D 02	3.11338D 02	7.67409D 02	1.59106D 03	2.87095D 03

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