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Uniform asymptotic approximation of Fermi–Dirac integrals

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Abstract: The Fermi–Dirac integral

$$F_q(x)=\frac{1}{\Gamma(q+1)}\int_0^\infty \frac{t^q}{1+e^{t-x}}\,dt,\quad q>-1,$$

is considered for large positive values of x and q. The results are obtained from a contour integral in the complex plane. The approximation contains a finite sum of simple terms, an incomplete gamma function and an infinite asymptotic series. As follows from earlier results, the incomplete gamma function can be approximated in terms of an error function.

Keywords: Uniform asymptotic expansions of integrals, incomplete gamma function, error function, saddle point method.

1. Introduction

In a recent paper of Schell [5], several new asymptotic expansions of the Fermi–Dirac integral

$$F_q(x)=\frac{1}{\Gamma(q+1)}\int_0^\infty \frac{t^q}{1+e^{t-x}}\,dt,\quad q>-1,\tag{1.1}$$

are derived. Schell considered the following combinations of parameters.

(i) $x\to\infty$, q fixed. In this case the approximation is given in terms of $F_q(-x)$ and an asymptotic series. A discussion on estimation of the remainder is included. The expansion follows from [2].

(ii) $x\to\infty$, $q\sim x$. Again $F_q(-x)$ is used, but the essential part in the approximation is an incomplete gamma function $\Gamma(q+2, x)$, which in turn is approximated in terms of the error function.

(iii) $x\to\infty$, $q=ax$, $0<a<2$. Again an incomplete gamma function is used and $F_q(-x)$.

(iv) $x\to\infty$, $\sqrt{q}=o(q-x)$ (that is, $x\ll q$). In this case elementary approximations based on the saddle point method are obtained.

From (2.2) it follows that $F_q(-x)$ can be easily computed when x is large.

In the present paper we obtain a single asymptotic approximation, which covers the above four cases. The function $F_q(-x)$ is not needed in our expansion. Again, an essential term is an incomplete gamma function.

2. Representation as a contour integral

We show that $F_q(x)$ equals the following integral [2, p.39]

$$\Phi_q(x) := \frac{1}{2\mathrm{i}} \int_{\gamma-\mathrm{i}\infty}^{\gamma+\mathrm{i}\infty} \frac{\mathrm{e}^{xs}}{s^{q+1}\,\sin(\pi s)}\,\mathrm{d}s, \quad 0<\gamma<1, \quad |\mathrm{Im}(x)|<\pi. \tag{2.1}$$

First let $\mathrm{Re}(x)<0$. Then the expansion

$$\frac{1}{1+\mathrm{e}^{t-x}} = \sum_{n=1}^{\infty} (-1)^{n-1}\,\mathrm{e}^{n(x-t)}, \quad \mathrm{Re}(x-t)<0,$$

can be substituted in (1.1), giving

$$F_q(x) = \sum_{n=1}^{\infty} \frac{(-1)^{n-1}\,\mathrm{e}^{xn}}{n^{q+1}}, \quad \mathrm{Re}(x)<0. \tag{2.2}$$

Next we shift the contour in (2.1) to the right, picking up the residues at $s=1, 2,\ldots,$ with the result

$$\Phi_q(x) = -\frac{2\pi\mathrm{i}}{2\mathrm{i}} \sum_{n=1}^{\infty} \frac{\mathrm{e}^{xn}}{n^{q+1}} \left[\lim_{s\to n} \frac{s-n}{\sin(\pi s)}\right] = -\sum_{n=1}^{\infty} \frac{\mathrm{e}^{xn}}{n^{q+1}}(-1)^n = F_q(x),$$

under the condition that the remainder integral vanishes for $\gamma \to +\infty$. If $q>0$, this is easily verified.

It follows that the right-hand sides of (2.1) and (2.2) are equal and analytic functions of x when $\mathrm{Re}(x)<0$, $|\mathrm{Im}(x)|<\pi$. But (2.1) and (1.1) are analytic functions of x in the full strip $|\mathrm{Im}(x)|<\pi$. So, $\Phi_q(x)$ of (2.1) equals $F_q(x)$ of (1.1) in the same strip. In the remaining part of the paper we write $p=q+1$, and we consider

$$F_{p-1}(x) = \frac{1}{2\mathrm{i}} \int_L \frac{\mathrm{e}^{xs}}{s^p\,\sin(\pi s)}\,\mathrm{d}s, \quad p>0, \quad x>0, \tag{2.3}$$

where, initially, L is a vertical contour that cuts the real s-axis between 0 and 1. In the asymptotic analysis L will be deformed into a different contour.

3. Saddle point analysis

We write $p=ax$. Then the saddle point of the integrand in (2.3), that is, of $\exp(xs - p\ln s)$, is located at $s=p/x=a$. We shift the contour L of (2.3) towards this point, and we may pass the poles located at $s=1, 2,\ldots$. First we assume that $a \neq 1, 2,\ldots$. Let the positive integer N satisfy $N-1<a<N$. Then (2.3) becomes

$$F_{p-1}(x) = \sum_{n=1}^{N-1} \frac{(-1)^{n-1}\,\mathrm{e}^{xn}}{n^p} + \frac{1}{2\mathrm{i}} \int_L \frac{\mathrm{e}^{xs}}{s^p\,\sin(\pi s)}\,\mathrm{d}s, \tag{3.1}$$

where L cuts the real positive s-axis at $s=a$, the saddle point. When $N=1$, the sum in (3.1) is empty.

It is not difficult to verify (use the graph of $\exp(xs-p\ln s)$ for $s>0$) that the terms in the finite sum of (3.1) decrease (in absolute value) as n increases. Therefore, the main contribution to

$F_{p-1}(x)$ comes from the term with $n=1$. Moreover, the integral in (3.1) is not dominating any term of the finite sum.

When the sum in (3.1) contains more than one term (i.e., $N>2$), the terms generate an asymptotic sequence. (For the definition of asymptotic sequences see [3, p.25].) This follows from

$$\frac{e^{x(n+1)}}{(n+1)^p} \leqslant \frac{e^{xn}}{n^p}\left(1+\frac{1}{n(n+2)^2}\right)^{-x} = o\left(\frac{e^{xn}}{n^p}\right), \quad p,\ x \to \infty,$$

which is easily verified (we assume that for n the relation $n+1<a=p/x$ holds).

When a assumes an integer value, the saddle point of the integral in (3.1) coincides with a pole of $1/\sin(\pi s)$. This is a well-known phenomenon in asymptotics, and the case can be handled by using an error function. However, by introducing an incomplete gamma function, the analysis is more transparent.

When $a \uparrow N$, we proceed as follows. Introduce a function h_N by writing

$$\frac{\pi}{\sin(\pi s)} = \frac{(-1)^N}{s-N} + h_N(s). \tag{3.2}$$

Then $h_N(s)$ is regular at $s=N$, and (3.1) becomes

$$F_{p-1}(x) = \sum_{n=1}^{N-1} \frac{(-1)^{n-1}\,e^{xn}}{n^p} + G_{p-1}(x) + H_{p-1}(x), \tag{3.3}$$

where

$$G_{p-1}(x) = \frac{(-1)^N}{2\pi i}\int_L \frac{e^{xs}}{s^p(s-N)}\,ds, \tag{3.4}$$

$$H_{p-1}(x) = \frac{1}{2\pi i}\int_L \frac{e^{xs}}{s^p} h_N(s)\,ds, \tag{3.5}$$

where the vertical L cuts the real s-axis between $N-1$ and a.

The function $G_{p-1}(x)$ can be written in terms of an incomplete gamma function. Differentiating $e^{-xN}G_{p-1}(x)$ with respect to x, we obtain by inverse Laplace transformation of s^{-p}

$$G_{p-1}(x) = \frac{(-1)^{N-1}\,e^{xN}}{\Gamma(p)}\int_x^\infty t^{p-1}\,e^{-tN}\,dt = \frac{(-1)^{N-1}\,e^{xN}}{N^p} Q(p,\ xN), \tag{3.6}$$

where $Q(p,\ z)$ is the complete gamma function ratio

$$Q(p,\ z) = \frac{1}{\Gamma(p)}\int_z^\infty t^{p-1}\,e^{-t}\,dt. \tag{3.7}$$

The asymptotics of this function is considered in [6]. Especially when p and z both are large, and nearly equal, an error function is needed for a uniform expansion. Observe that in (3.6) $Q(p,\ xN) = Q(ax,\ xN)$, and that we assumed that $a \uparrow N$.

The asymptotic expansion of (3.5) can be obtained by integrating along the steepest descent path through the saddle point $s=a$. This path is given by the equation $\mathrm{Im}(s - a\ln s) = 0$ or $\rho(\theta) = a\theta/\sin\theta$, where $s=\rho e^{i\theta}$. We proceed differently, and we expand

$$h_N(s) = \sum_{n=0}^{\infty} c_n(a)(s-a)^n, \tag{3.8}$$

where $c_n(a) = h_N^{(n)}(a)/n!$ and the series is defined and convergent on $s \in (a-\delta,\ a+\delta)$, where $\delta = \min(a-N+1,\ N+1-a)$. Thus, when $a \in [N-\rho,\ N+\rho]$, where $0<\rho<1$, ρ fixed, the coefficients $|c_n(a)|$ are uniformly bounded.

Substituting (3.8) in (3.5), we obtain, after interchanging the order of summation and integration, the formal result

$$H_{p-1}(x) \sim \frac{x^{p-1}}{\Gamma(p)} \sum_{n=0}^{\infty} c_n(a)\phi_n(p)x^{-n}, \tag{3.9}$$

where

$$\phi_n(p) = \frac{\Gamma(p)x^{n-p+1}}{2\pi i}\int_L \frac{e^{sx}(s-a)^n}{s^p}\,ds = \frac{\Gamma(p)}{2\pi i}\int_L \frac{e^t(t-p)^n}{t^p}\,dt.$$

These $\phi_n(p)$ are polynomials in p. They follow the recursion relation

$$\phi_n(p) + n\phi_{n-1}(p) + (n-1)p\phi_{n-2}(p) = 0, \quad \phi_0(p) = 1, \quad \phi_1(p) = -1.$$

The recursion is obtained by integrating by parts:

$$\begin{aligned}\phi_n(p) &= \frac{\Gamma(p)}{2\pi i}\int_L \frac{(t-p)^n}{t^p}\,d(e^t)\\ &= (p-n)\phi_{n-1}(p) + \frac{p\Gamma(p)}{2\pi i}\int_L e^t(t-p)^{n-1}\,d(t^{-p})\\ &= -n\phi_{n-1}(p) - (n-1)p\phi_{n-2}(p).\end{aligned}$$

From induction it follows that the degree of $\phi_{2n}(p)$ and $\phi_{2n+1}(p)$ equals n. It follows that the asymptotic expansion (3.9) is valid as $x \to \infty$, uniformly with respect to $a = p/x \in [N-\rho,\ N+\rho]$, where $0<\rho<1$, ρ fixed.

Remark 1. The polynomials $\phi_n(p)$ can be expressed in terms of Laguerre polynomials:

$$\phi_n(p) = n!L_n^{(p-n-1)}(p), \quad n = 0, 1, 2, \ldots .$$

These polynomials are also used in [7]; related polynomials were considered earlier in [1,4,8].

Remark 2. In the above analysis we assumed that $p = ax$, and that a is located in an interval $(N-1,\ N]$. When $p \gg x$, say $p \sim x^2$, the contribution of $G_{p-1}(x)$, $H_{p-1}(x)$ in (3.3) can be neglected (compared with the first terms of the (still finite) sum in (3.3)).

4. Series of incomplete gamma functions

The incomplete gamma function term in (3.3) is a special term in an expansion involving more incomplete gamma functions. In (2.3), we substitute

$$\frac{\pi}{\sin(\pi s)} = \sum_{n\in\mathbb{Z}} \frac{(-1)^n}{s-n},$$

and we obtain, after interchanging the order of summation and integration, which is allowed, the result

$$F_{p-1}(x)=\sum_{n\in\mathbb{Z}}\frac{(-1)^n}{2\pi i}\int_L\frac{e^{xs}}{s^p(s-n)}\,ds, \tag{4.1}$$

where the vertical L cuts the real axis between 0 and 1. We use the relations

$$\frac{1}{2\pi i}\int_L\frac{e^{xs}}{s^p(s-n)}\,ds=-\frac{e^{xn}}{n^p}Q(p,\,xn),\quad n>0,$$

$$\frac{1}{2\pi i}\int_L\frac{e^{xs}}{s^{p+1}}\,ds=\frac{x^p}{\Gamma(p+1)},$$

$$\frac{1}{2\pi i}\int_L\frac{e^{xs}}{s^p(s+n)}\,ds=e^{-xn}x^p\gamma^*(p,\,-xn),\quad n>0,$$

where $Q(p,\,z)$ is the incomplete gamma function ratio (3.7), and $\gamma^*(p,\,z)$ is the incomplete gamma function

$$\gamma^*(p,\,z)=z^{-p}P(p,\,z)=\frac{z^{-p}}{\Gamma(p)}\int_0^z t^{p-1}\,e^{-t}\,dt.$$

Substituting these relations in (4.1) we obtain

$$F_{p-1}(x)=\sum_{n=1}^{\infty}\frac{(-1)^{n-1}\,e^{xn}}{n^p}Q(p,\,xn)+\frac{x^p}{\Gamma(p+1)}+\sum_{n=1}^{\infty}(-1)^n\,e^{-xn}x^p\gamma^*(p,\,-xn). \tag{4.2}$$

From an asymptotic or numerical point of view, this expansion is not useful (when the parameters p and x are large). This follows from elementary estimates of the incomplete gamma functions occurring in (4.2).

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