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A Note on Sommerfeld's Formula for Fermi–Dirac Integrals

I. Adawi[1]

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Sommerfeld's formula for approximate evaluation of integrals involving the Fermi–Dirac function is derived by the Laplace transform method, and its limitations are discussed.

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In his pioneering work on the electron gas problem in metals, Sommerfeld[1] considered integrals of the form

$$J \equiv \int_0^\infty g(x)(-\partial f/\partial x)\, dx \tag{1}$$

and derived the approximate formula

$$J \approx \left(1 + 2 \sum_{n=1}^{\infty} c_{2n} D^{2n}\right) g(\eta), \qquad \eta \gg 1 \tag{2}$$

where $f(x)$ is the Fermi–Dirac function, $[1 + \exp(x - \eta)]^{-1}$, x and η are the energy and chemical potential, respectively, in thermal energy units, and g is a smooth function. The constants c_{2n} are related to Bernoulli numbers, with

[1] Department of Physics, University of Missouri—Rolla, Rolla, Missouri.

$c_2 = \pi^2/12$ and $c_4 = 7\pi^4/720$. D is the differential operator $d/d\eta$. Adawi[(2)] has derived this formula by considering the residues at the poles of f in the complex energy plane. Blankenbecler[(3)] obtained Sommerfeld's formula in the closed form,

$$J \approx \pi D[\operatorname{cosec}(\pi D)]g(\eta) \tag{3}$$

but, in contrast to the other two methods,[(1,2)] his method does not give any provision for improving the approximation. In this note, formula (3) is derived by using the Laplace transform method, which clearly shows the origin of this formula and its limitation.

If $F(s)$ is the two-sided Laplace transform of $f(x)$, then $-sF(s)$ is the Laplace transform of $-\partial f/\partial x$. Since (see, e.g., Ref. 4)

$$F(s) = \int_{-\infty}^{\infty} e^{-sx}(e^{x-\eta} + 1)^{-1}\,dx$$
$$= -\pi e^{-\eta s}\operatorname{cosec}(\pi s), \qquad -1 < \operatorname{Re} s < 0$$

we have the integral representation (inversion formula)

$$-\frac{\partial f}{\partial x} = \frac{1}{2\pi i}\int_{c-i\infty}^{c+i\infty} e^{s(x-\eta)}\frac{\pi s}{\sin \pi s}\,ds, \qquad -1 < c < 0 \tag{4a}$$

$$= \frac{1}{2\pi i}\int_{a-i\infty}^{a+i\infty} e^{-s(x-\eta)}\frac{\pi s}{\sin \pi s}\,ds, \qquad 0 < a < 1 \tag{4b}$$

where (4b) is obtained from (4a) by the substitution $-s$ for s. By substituting (4b) into (1) and performing (formally) the x integration, we obtain the exact result[2]

$$J = \frac{1}{2\pi i}\int_{a-i\infty}^{a+i\infty} e^{s\eta}\frac{\pi s}{\sin \pi s}G(s)\,ds \tag{5}$$

where $G(s)$ is the one-sided Laplace transform of $g(x)$:

$$G(s) = \int_0^{\infty} e^{-sx}g(x)\,dx \tag{6}$$

The integral (5) is now studied by standard contour integration methods: Assuming $G(s)$ has no poles at $s = -n$, where n is a positive integer, the simple poles of $s\operatorname{cosec}(\pi s)$ at $s = -n$ contribute to the integral quantities of order $\exp(-n\eta)$. The Sommerfeld approximation is seen to ignore all such contributions and to concentrate on the singularities of $G(s)$ which are assumed to be near the origin. In this sense, the function $\pi s \operatorname{cosec}(\pi s)$ can be regarded as if it were analytic everywhere, and is taken outside the integral as $\pi D \operatorname{cosec}(\pi D)$, where $D = \partial/\partial\eta$; the remaining integral is the inversion

[2] An alternative way of deriving (5) is to observe that $-\partial f/\partial x$ is symmetric with respect to the variable $\eta - x$ and that the integral J is a convolution of g and f'.

formula of (6) and gives $g(\eta)$, and we have the Sommerfeld formula (3). The same result is obtained if in (4a) we ignore the poles of $\pi s \operatorname{cosec}(\pi s)$, and replace this function by $\pi D_x \operatorname{cosec}(\pi D_x)$ outside the integral, where $D_x \equiv \partial/\partial x$; the remaining integral is $\delta(x - \eta)$ and we have the approximation

$$-\partial f/\partial x \approx \pi D_x \operatorname{cosec}(\pi D_x)\, \delta(x - \eta) \tag{7}$$

from which (3) follows.

To illustrate the success and failure of the approximation (3), consider the integral J_ν corresponding to $g(x) = e^{-\nu x}$ where ν is not an integer. By inserting $G(s) = (s + \nu)^{-1}$ in (5) and integrating, we obtain

$$J_\nu = \pi\nu[\operatorname{cosec}(\pi\nu)]e^{-\nu\eta} + \sum_{n=1}^{\infty} (-1)^n[n/(n - \nu)]e^{-n\eta} \tag{8}$$

In (8) the first term is the Sommerfeld approximation (3) and forms a good approximation if $\nu \ll 1$; otherwise it fails, especially for integral values of ν, when it diverges. For $\nu = 1$ we have the exact result from (5) or (1):

$$J_1 = (\eta - 1)e^{-\eta} + e^{-2\eta}(1 + e^{-\eta})^{-1} + e^{-\eta}\ln(1 + e^{-\eta}) \tag{9}$$

By contrast, even if we ignored the divergence of the complete Sommerfeld series (2) and retained only the leading terms, we would have

$$J_1 \approx (1 + \pi^2/6)e^{-\eta} \tag{10}$$

which is quite different. For $\nu = n$, where n is an integer (and $n > 1$), $G(s) = (s + n)^{-1}$ and the leading term in J_n from (5) is $O(e^{-\eta})$ as compared to $e^{-n\eta}$ from (2). Actually the integrals J_n can be evaluated for $n > 1$ directly from (5) or by using (9) and the recursion formula,

$$J_n = (n - 1)^{-1}e^{-\eta}[(1 + e^{-\eta})^{-1} - nJ_{n-1}] \tag{11}$$

which can be derived from (1). For large η, $J_n \sim (n - 1)^{-1}e^{-\eta}$, which is the residue at $s = 1$.

Finally, in addition to illuminating the Sommerfeld approximation, formula (5) might offer advantages in evaluating integrals when, for example, $G(s)$ is simpler than the original function $g(x)$.

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