Fermi-Dirac Integrals in terms of Zeta Functions

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Abstract
This paper shows the Fermi-Dirac Integrals $F_{\frac{1}{2}}(\eta)$ and $F_{\frac{3}{2}}(\eta)$ expressed in terms of Riemann and Hurwitz Zeta functions. This is done by defining an auxiliary function that permits rewrite the Fermi-Dirac integral in terms of simpler and known integrals resulting in the Zeta functions mentioned. The approach used here evades the use of iterative methods for the integrals and presents a clever procedure for around $\eta \leq 5$, complementing Sommerfeld lemma, one that can be generalized for any integer $k$ in $F_{\frac{k}{2}}(\eta)$ in the refereed interval.

1 Introduction.

The motivation of this paper is to find expressions in order to calculate the Fermi-Dirac integrals specifically for $\eta \leq 5$, values that so far had been calculated using iterative methods as the trapezoidal method, [5]. This integrals appears in partial degenerate stars, [2], thermal conductions by electrons [4], and condensed matter physics. The Fermi-Dirac integral $F_{\frac{k}{2}}(\eta)$ is defined by

$$F_{\frac{k}{2}}(\eta) = \int_0^\infty \frac{\xi^{\frac{k}{2}}}{1 + e^{\xi - \eta}} d\xi$$

(1)

Where $\eta = \frac{\mu}{k_B T}$, $k_B$ is the Boltzmann constant and $\mu$ the chemical potential.

In this paper we focus on the Fermi-Dirac integral $F_{\frac{1}{2}}(\eta)$, and the procedure and result can be extended to the $F_{\frac{k}{2}}(\eta)$ and generalized for any integer $k$ in equation (1). This procedure involves an auxiliary function that relates $F_{\frac{k}{2}}(\eta)$ with $F_{\frac{1}{2}}(0)$, and based on their (graphical) relation will permit to write the auxiliary function in simple terms and make the integral $F_{\frac{1}{2}}(\eta)$ easier to calculate obtaining Riemann and Hurwitz Zeta functions. That is, with almost no need for iterative methods.

2 Fermi-Dirac $F_{\frac{1}{2}}(\eta)$ and the auxiliary function

As we mentioned, we work on the Fermi-Dirac integral $F_{\frac{1}{2}}(\eta)$, defined by
\( F_{\frac{1}{2}}(\eta) = \int_{0}^{\infty} \frac{\xi^{\frac{1}{2}}}{1 + e^{\xi - \eta}} d\xi \) \hspace{1cm} (2)

Actually, we focus on the term defined here by \( f_{\frac{1}{2}}(\xi, \eta) \):

\[ f_{\frac{1}{2}}(\xi, \eta) = \frac{\xi^{\frac{1}{2}}}{1 + e^{\xi - \eta}} \] \hspace{1cm} (3)

and define the function \( f_{\frac{1}{2}}(\xi) \):

\[ f_{\frac{1}{2}}(\xi) = \frac{\xi^{\frac{1}{2}}}{1 + e^{\xi}} \] \hspace{1cm} (4)

We define a function, denoted as \( f(\xi, \eta) \), that is the ratio of both functions:

\[ f(\xi, \eta) = \frac{f_{\frac{1}{2}}(\eta)}{f_{\frac{1}{2}}(0)} = \frac{1 + e^{\xi}}{1 + e^{\xi - \eta}} \] \hspace{1cm} (5)

this function, graphically, behaves as \( a - be^{-c\xi} \) for \( \eta \leq 5 \). That is, we assume that we can model and define the function \( f(\xi, \eta) \) as:

\[ f(\xi, \eta) = a - be^{-c\xi} \] \hspace{1cm} (6)

where \( a, b, \) and \( c \) are constants. The \( a \) and \( b \) can be found considering some aspects of equation (5):

\[ f(0, \eta) = \frac{2}{1 + e^{\eta}} \]

and

\[ \lim_{x \to \infty} f(0, \eta) = e^{\eta} \]

this implies that \( a = e^{\eta} \) and \( b = \frac{e^{\eta} - 1}{e^{\eta} + 1} \). This means that

\[ f(\xi, \eta) = e^{\eta} - \frac{e^{\eta} - 1}{e^{-\eta} + 1} e^{-c\xi} \] \hspace{1cm} (7)
This leaves the issue of finding \(c\). We take the following approach, perhaps the only one in this procedure that needs iterative methods: we find the maximum of \(f_2(\xi, \eta)\), equation (3). That is, after the algebra, we must solve for \(\xi\) in:

\[
e^{\eta} + e^{\xi}(1 - 2\xi) = 0
\]

and call this value \(\xi_m\), that depends on \(\eta\). Using equations (4) and (7), and substituting \(\xi_m\), we can solve for \(c\):

\[
c = -\frac{1}{\xi_m} \ln \left[ \frac{(e^{\eta} - 1) (e^{\eta} - \frac{1 + e^{\xi_m}}{1 + e^{\xi_m} - \eta})}{e^{\eta} - 1} \right]
\]

(9)

It can be shown that calculating the two maximums, of equation (3) and \(f(\xi, \eta) * f_4(\xi)\) will lead basically to the same result. Having found the constants in equation (6), we can write equation (2) as follows:

\[
\int_{0}^{\infty} \frac{\xi^\frac{3}{2}}{1 + e^{\xi}} d\xi = \int_{0}^{\infty} \left( e^{\eta} - \frac{e^{\eta} - 1}{e^{-\eta} + 1} e^{-ct} \right) \frac{\xi^\frac{3}{2}}{1 + e^{\xi}} d\xi
\]

\[
= e^{\eta} \int_{0}^{\infty} \frac{\xi^\frac{3}{2}}{1 + e^{\xi}} d\xi - \frac{e^{\eta} - 1}{e^{-\eta} + 1} \int_{0}^{\infty} e^{-ct} \xi^\frac{3}{2} \frac{1}{1 + e^{\xi}} d\xi
\]

where the first integral in the equality we know from Arfken,\[1\], can be written as:

\[
\int_{0}^{\infty} \frac{\xi^\frac{3}{2}}{1 + e^{\xi}} d\xi = \Gamma \left( \frac{3}{2} \right) \left( 1 - 2^{-\frac{3}{2}} \right) \zeta \left( 1 + \frac{1}{2} \right)
\]

where \(\zeta(p)\) is the well known Riemann Zeta function. For the second integral, after expanding some terms:

\[
\int_{0}^{\infty} e^{-ct} \xi^\frac{3}{2} \frac{1}{1 + e^{\xi}} d\xi = \Gamma \left( \frac{3}{2} \right) \sum_{n=0}^{\infty} \frac{(-1)^n}{(c + 1 + n)^{1 + \frac{3}{2}}}
\]

\[
= \Gamma \left( \frac{3}{2} \right) \left[ 2^{-\frac{3}{2}} \zeta \left( 1 + \frac{1}{2}, \frac{c+1}{2} \right) - \zeta \left( 1 + \frac{1}{2}, c + 1 \right) \right]
\]

In the last equality we recognize \(\zeta(p, q)\) as the Hurwitz Zeta function, where we used the identity as appears in Williams & Nan-yue, \[6\]. With these results, we can finally write \(F_2(\eta)\) as:

\[
F_2(\eta) = \Gamma \left( \frac{3}{2} \right) \left[ e^{\eta} \left( 1 - 2^{-\frac{3}{2}} \right) \zeta \left( 1 + \frac{1}{2} \right) - \frac{e^{\eta} - 1}{e^{-\eta} + 1} \left[ 2^{-\frac{3}{2}} \zeta \left( 1 + \frac{1}{2}, \frac{c+1}{2} \right) - \zeta \left( 1 + \frac{1}{2}, c + 1 \right) \right] \right]
\]

(10)
3 Some results

Using equation (10), we elaborate in Table 1, for some \( \eta \), a comparison with values taken from [2], which were based on McDougall & Stoner, *Phil. Trans. Roy. Soc.*, 237:67(1938), including some values for positive \( \eta < 1 \), used in electron conduction opacity, [4], showing how reliable and potentially applicable this method is.

| \( \eta \) | \( F_{\frac{1}{2}} \) | \( F_{\frac{1}{2}} \) | error (%) |
|---------|-------------|-------------|-----------|
| eq. (10) | Clayton     |             |           |
| -4      | 0.0161393   | 0.0161277   | 0.0715548 |
| -3      | 0.0434453   | 0.0433664   | 0.181969  |
| -2      | 0.11506     | 0.114588    | 0.411671  |
| -1      | 0.292405    | 0.290501    | 0.655385  |
| 0       | 0.678094    | 0.678094    | 6.95512E-11 |
| .1      | 0.732034    | .733403     | 0.18664   |
| .5      | 0.977945    | .990209     | 1.23858   |
| 1       | 1.35129     | 1.39638     | 3.22903   |
| 2       | 2.30003     | 2.50246     | 8.08906   |
| 3       | 3.58315     | 3.97699     | 9.90297   |
| 4       | 5.5495      | 5.77073     | 3.83358   |
| 5       | 8.99919     | 7.83798     | 14.8152   |

4 Observations

For \( \eta = 1 \), the approach here presented is an improvement for the Trapezoidal scheme, [5], where their method gives an 6.4% error. The model according to equation (6) is reliable for \( \eta \leq 5 \), specially with negative \( \eta \). Yet, as the ratio of the functions in equation (5) shows a higher inflexion point, for \( \eta > 5 \), the model needs an improvement. The reason for the limitation around this value appears when analyzing the equation (10), where a simple examination shows a dependency of order \( e^\eta \), as it happens in Sommerfeld lemma.

5 Conclusion

The equation (10) gives an expression for calculating the Fermi-Dirac integrals \( F_{\frac{1}{2}}(\eta) \) in terms of the Riemann and Hurwitz Zeta functions. Using the same procedure we find expressions for \( F_{\frac{k}{2}}(\eta) \) and \( F_{\frac{k}{2}}(\eta) \), for general integer \( k \), valid for \( \eta \leq 5 \). This approach complements that of Sommerfeld lemma, giving a nearly complete expression for Fermi-Dirac integrals.
\[ F_2(\eta) = \Gamma \left( \frac{5}{2} \right) \left[ e^\eta \left( 1 - 2^{-\frac{3}{2}} \right) \zeta \left( 1 + \frac{3}{2} \right) - \frac{e^\eta - 1}{e^{-\eta} + 1} \left[ 2^{\frac{5}{2}} \zeta \left( 1 + \frac{3}{2}, \frac{c + 1}{2} \right) - \zeta \left( 1 + \frac{3}{2}, c + 1 \right) \right] \right] \] (11)

and for general \( k \):

\[ F_2(\eta) = \Gamma \left( 1 + \frac{k}{2} \right) \left[ e^\eta \left( 1 - 2^{-\frac{k}{2}} \right) \zeta \left( 1 + \frac{k}{2} \right) - \frac{e^\eta - 1}{e^{-\eta} + 1} \left[ 2^{\frac{k}{2}} \zeta \left( 1 + \frac{k}{2}, \frac{c + 1}{2} \right) - \zeta \left( 1 + \frac{k}{2}, c + 1 \right) \right] \right] \] (12)

with the remark that \( \xi_m \), equation (8), in order to find \( c \) (notice that \( c \) and \( f(\xi, \eta) \) are \( k \)-independent), must be generalized too:

\[ ke^\eta + e^\xi(k - 2\xi) = 0 \] (13)

**References**

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