Notes on Fermi-Dirac Integrals

2nd edition

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1. Introduction

Fermi-Dirac integrals appear frequently in semiconductor problems, so an understanding of their properties is essential. The purpose of these notes is to collect in one place, some basic information about Fermi-Dirac integrals and their properties. To see how they arise, consider computing the equilibrium electron concentration per unit volume in a three-dimensional semiconductor with a parabolic conduction band from the expression,

\[ n = \int_{E_C}^{\infty} g(E) f_0(E) dE = \int_{E_C}^{\infty} \frac{g(E) dE}{1 + e^{(E-E_F)/k_B T}} , \]

(1)

where \( g(E) \) is the density of states, \( f_0(E) \) is the Fermi function, and \( E_C \) is the conduction band edge. For three dimensional electrons,

\[ g_{3D}(E) = \frac{(2m^*)^{3/2}}{2\pi^2 \hbar^3} \sqrt{E - E_C} \]

(2)

which can be used in (1) to write

\[ n = \frac{(2m^*)^{3/2}}{2\pi^2 \hbar^3} \int_{E_C}^{\infty} \frac{\sqrt{E - E_C} dE}{1 + e^{(E-E_F)/k_B T}}. \]

(3)

By making the substitution,

\[ \epsilon = (E - E_C)/k_B T \]

(4)

eqn. (3) becomes

\[ n = \frac{(2m^* k_B T)^{3/2}}{2\pi^2 \hbar^3} \int_{0}^{\infty} \frac{\epsilon^{1/2} d\epsilon}{1 + e^{\epsilon/k_B T}}, \]

(5)
where we have defined

$$\eta_F \equiv (E_F - E_C)/k_B T. \quad (6)$$

By collecting up parameters, we can express the electron concentration as

$$n_0 = N_{3D} \frac{2}{\sqrt{\pi}} F_{1/2}(\eta_F) \quad (7)$$

where

$$N_{3D} = 2 \left( \frac{2\pi m^* k_B T}{\hbar^2} \right)^{3/2} \quad (8)$$

is the so-called effective density-of-states and

$$F_{1/2}(\eta_F) \equiv \int_0^\infty \frac{\varepsilon^{1/2} d\varepsilon}{1 + \exp(\varepsilon - \eta_F)} \quad (9)$$

is the Fermi-Dirac integral of order 1/2. This integral can only be done numerically. Note that its value depends on $\eta_F$, which measures the location of the Fermi level with respect to the conduction band edge. It is more convenient to define a related integral,

$$\mathcal{F}_{1/2}(\eta_F) \equiv \frac{2}{\sqrt{\pi}} \int_0^\infty \frac{\varepsilon^{1/2} d\varepsilon}{1 + \exp(\varepsilon - \eta_F)} \quad (10)$$

so that eqn. (7) can be written as

$$n = N_{3D} \mathcal{F}_{1/2}(\eta_F). \quad (11)$$

It is important to recognize whether you are dealing with the “Roman” Fermi-Dirac integral or the “script” Fermi-Dirac integral.

There are many kinds of Fermi-Dirac integrals. For example, in two dimensions, the density-of-states is

$$g_{2D}(E) = \frac{m^*}{\pi \hbar^2}, \quad (12)$$

and by following a procedure like that one we used in three dimensions, one can show that the electron density per unit area is
\[ n_s = N_{2D} F_0(\eta_F) \]  

(13)

where

\[ N_{2D} = \frac{m^* k_B T}{\pi \hbar^2}, \]  

(14)

and

\[ F_0(\eta_F) = \int_0^\infty \frac{d\varepsilon}{1 + e^{\varepsilon - \eta_F}} = \ln \left(1 + e^{\eta_F}\right) \]  

(15)

is the Fermi-Dirac integral of order 0, which can be integrated analytically.

Finally, in one dimension, the density-of-states is

\[ g_{1D}(E) = \sqrt{\frac{2m^*}{\pi \hbar^2}} \frac{1}{\sqrt{E - E_C}} \]  

(16)

and the equilibrium electron density per unit length is

\[ n_L = N_{1D} F_{-1/2}(\eta_F) \]  

(17)

where

\[ N_{1D} = \frac{1}{\hbar} \sqrt{\frac{2m^* k_B T}{\pi}} \]  

(18)

and

\[ F_{-1/2}(\eta_F) = \int_0^\infty \frac{d\varepsilon}{\sqrt{\pi}} \frac{1}{1 + e^{\varepsilon - \eta_F}} \]  

(19)

is the Fermi-Dirac integral of order \(-1/2\), which must be integrated numerically.

2. General Definition

In the previous section, we saw three examples of Fermi-Dirac integrals. More generally, we define

\[ \int_0^\infty \frac{d\varepsilon}{1 + e^{\varepsilon - \eta_F}} = \ln \left(1 + e^{\eta_F}\right) \]
\[ \mathcal{F}_j(\eta_F) = \frac{1}{\Gamma(j+1)} \int_0^\infty \frac{\varepsilon^j d\varepsilon}{1+\exp(e-\eta_F)}, \quad (20) \]

where \( \Gamma \) is the gamma function. The \( \Gamma \) function is just the factorial when its argument is a positive integer,

\[ \Gamma(n) = (n-1)! \quad \text{(for } n \text{ a positive integer)}. \quad (21a) \]

Also

\[ \Gamma(1/2) = \sqrt{\pi} \quad (21b) \]

and

\[ \Gamma(p+1) = p\Gamma(p) \quad (21c) \]

As an example, let’s evaluate \( \mathcal{F}_{1/2}(\eta_F) \) from eqn. (20):

\[ \mathcal{F}_{1/2}(\eta_F) \equiv \frac{1}{\Gamma(1/2+1)} \int_0^\infty \frac{\varepsilon^{1/2} d\varepsilon}{1+\exp(e-\eta_F)}, \quad (22a) \]

so we need to evaluate \( \Gamma(3/2) \). Using eqns. (21b) and (21c), we find,

\[ \Gamma(3/2) = \Gamma(1/2+1) = \frac{1}{2} \Gamma(1/2) = \frac{\sqrt{\pi}}{2}, \quad (22b) \]

so \( \mathcal{F}_{1/2}(\eta_F) \) is evaluated as

\[ \mathcal{F}_{1/2}(\eta_F) \equiv \frac{2}{\sqrt{\pi}} \int_0^\infty \frac{\varepsilon^{1/2} d\varepsilon}{1+\exp(e-\eta_F)}, \quad (22c) \]

which agrees with eqn. (10). For more practice, use the general definition, eqn. (20) and eqns. (21a-c) to show that the results for \( \mathcal{F}_0(\eta_F) \) and \( \mathcal{F}_{-1/2}(\eta_F) \) agree with eqns. (15) and (19).

3. Derivatives of Fermi-Dirac Integrals

Fermi-Dirac integrals have the property that

\[ \frac{d\mathcal{F}_j}{d\eta_F} = \mathcal{F}_{j-1}, \quad (23) \]
which often comes in useful. For example, we have an analytical expression for \( F_0(\eta_F) \), which means that we have an analytical expression for \( F_{-1}(\eta_F) \),

\[
F_{-1} = \frac{dF_0}{d\eta_F} = \frac{1}{1 + e^{-\eta_F}}.
\]  

Similarly, we can show that there is an analytic expression for any Fermi-Dirac integral of integer order, \( j \), for \( j \leq -2 \),

\[
F_j(\eta_F) = \frac{e^{\eta_F}}{(1 + e^{\eta_F})^{j}} P_{j-2}(e^{\eta_F})
\]

where \( P_k \) is a polynomial of degree \( k \), and the coefficients \( p_{k,i} \) are generated from a recurrence relation [1]

\[
p_{k,0} = 1
\]

\[
p_{k,i} = (1 + i)p_{k-1,i} - (k + 1 - i)p_{k-1,i-1}, \quad i = 1, \ldots, k.
\]

4. Asymptotic Expansions for Fermi-Dirac Integrals

It is useful to examine Fermi-Dirac integrals in the non-degenerate (\( \eta_F \ll 0 \)) and degenerate (\( \eta_F \gg 0 \)) limits. For the non-degenerate limit, the result is particularly simple,

\[
F_j(\eta_F) \to e^{\eta_F}
\]

which means that for all orders, \( j \), the function approaches the exponential in the non-degenerate limit. To examine Fermi-Dirac integrals in the degenerate limit, we consider the complete expansion for the Fermi-Dirac integral for \( j > -1 \) and \( \eta_F > 0 \) [2, 3]

\[
F_j(\eta_F) = 2\eta_F^{j+1} \sum_{n=0}^{\infty} \frac{t_{j,n}}{\Gamma(j + 2 - 2n)\eta_F^{2n}} + \cos(\pi j) \sum_{n=1}^{\infty} \frac{(-1)^{n-1} e^{-n\eta_F}}{n^{j+1}}
\]

where \( t_0 = 1/2 \), \( t_n = \sum_{\mu=1}^{n} (-1)^{\mu-1}/\mu^n = (1 - 2^{1-n}) \zeta(n) \), and \( \zeta(n) \) is the Riemann zeta function. The expressions for the Fermi-Dirac integrals in the degenerate limit (\( \eta_F \gg 0 \)) come from (28) as \( F_j(\eta_F) \to \eta_F^{j+1}/\Gamma(j + 2) \) [4]. Specific results for several Fermi-Dirac integrals are shown below.
\[ F_{-1/2}(\eta_F) \rightarrow \frac{2\eta_F^{1/2}}{\sqrt{\pi}} \]  
(29a)

\[ F_{1/2}(\eta_F) \rightarrow \frac{4\eta_F^{3/2}}{3\sqrt{\pi}} \]  
(29b)

\[ F_j(\eta_F) \rightarrow \frac{1}{2} \eta_F^2 \]  
(29c)

\[ F_{3/2}(\eta_F) \rightarrow \frac{8\eta_F^{5/2}}{15\sqrt{\pi}} \]  
(29d)

\[ F_2(\eta_F) \rightarrow \frac{1}{6} \eta_F^3 \]  
(29e)

Now we relate the complete expansion in (28) to the Sommerfeld expansion \[5, 6\]. The Sommerfeld expansion for a function \( H(\varepsilon) \) is expressed as

\[ \int_0^\infty H(\varepsilon) f_0(\varepsilon) d\varepsilon = \int_0^\eta F(\varepsilon) d\varepsilon + \sum_{n=1}^\infty a_n \frac{d^{2n-1}}{d\varepsilon^{2n-1}} H(\varepsilon) \bigg|_{\varepsilon=\eta_F} \]  
(30)

where

\[ a_n = 2 \left( 1 - \frac{1}{2^n} + \frac{1}{3^n} - \frac{1}{4^n} + \cdots \right), \]  
(31)

and it is noted that \( a_n = 2t_{2n} \). Then the Sommerfeld expansion for the Fermi-Dirac integral of order \( j \) can be evaluated by letting \( H(\varepsilon) = \varepsilon^j / \Gamma(j+1) \), and the result is

\[ F_j(\eta_F) = 2\eta_F^{j+1} \sum_{n=0}^\infty \frac{t_{2n}}{\Gamma(j+2-2n)\eta_F^{2n}}. \]  
(32)

Equation (32) is the same as the (28) except that the second term in (28) is omitted [3]. In the degenerate limit, however, the second term in (28) vanishes, so the (28) and (32) give the same results as (29a-e).

5. Approximate Expressions for Common Fermi-Dirac Integrals

The Fermi-Dirac integral can be quickly evaluated by tabulation [2, 4, 7, 8] or analytic approximation [9-11]. We briefly mention some of the analytic approximations and refer a Matlab script. Bednarczyk et al. [9] proposed a single analytic approximation which evaluates
the Fermi-Dirac integral of order \( j = 1/2 \) with errors less than 0.4% \([12]\). Aymerich-Humet \textit{et al.} \([10, 11]\) introduced an analytic approximation for a general \( j \), and it gives an error of 1.2\% for \(-1/2 < j < 1/2\) and 0.7\% for \(1/2 < j < 5/2\), and the error increases with larger \( j \). The Matlab function, “FD_int_approx.m,” calculates the Fermi-Dirac integral defined in (10) with orders \( j \geq -1/2 \) using these analytic approximations.

If a better accuracy is required while keeping the calculation relatively simple, the approximations proposed by Halen and Pulfrey \([13, 14]\) may be used. In this model, several approximate expressions are introduced based on the series expansion in (28), and the error is less than \(10^{-5}\) for \(-1/2 \leq j \leq 7/2\) \([13]\). The Matlab function, “FDjx.m,” is the main function which calculates the Fermi-Dirac integrals using this model.

6. Numerical Evaluation of Fermi-Dirac Integrals

The Fermi-Dirac integrals can be evaluated accurately by numerical integration. Here we briefly review the approach by Press \textit{et al.} for generalized Fermi-Dirac integrals with order \( j > -1 \) \([15]\).

In this approach, the composite trapezoidal rule with variable transformation \( \varepsilon = \exp(\frac{1}{2} - e^{-t}) \) is used for \( \eta_F \leq 15 \), and the double exponential (DE) rule is used for larger \( \eta_F \). The double precision (eps, \( \approx 2.2 \times 10^{-16} \)) can be achieved after 60 to 500 iterations \([15]\). The Matlab function, “FD_int_num.m,” evaluates the Fermi-Dirac integral numerically using the composite trapezoidal rule following the approach in \([15]\).

7. References

[2] R. Dingle, "The Fermi-Dirac integrals \( F_p(\eta) = \left( p! \right)^{-1} \int_0^{\infty} e^p \left( e^{-\eta} + 1 \right)^{-1} d\varepsilon \)," \textit{Applied Scientific Research}, vol. 6, pp. 225-239, 1957.


