# Notes on Fermi-Dirac Integrals 2<sup>nd</sup> edition

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# 1. Introduction

Fermi-Dirac integrals appear frequently in semiconductor problems, so a 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,

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

which can be used in (1) to write

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

By making the substitution,

$$\varepsilon = \left(E - E_C\right) / k_B T \tag{4}$$

eqn. (3) becomes

$$n = \frac{\left(2m^*k_BT\right)^{3/2}}{2\pi^2\hbar^3} \int_0^\infty \frac{\varepsilon^{1/2}d\varepsilon}{1+e^{\varepsilon-\eta_F}},$$
(5)

where we have defined

$$\eta_F \equiv \left(E_F - E_C\right) / k_B T \,. \tag{6}$$

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

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

where

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

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

$$F_{1/2}(\eta_F) \equiv \int_{0}^{\infty} \frac{\varepsilon^{1/2} d\varepsilon}{1 + \exp(\varepsilon - \eta_F)}$$
(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,

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

so that eqn. (7) can be written as

$$n = N_{3D} \mathcal{F}_{1/2}(\boldsymbol{\eta}_F). \tag{11}$$

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

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

$$n_{s} = N_{2D} \mathcal{F}_{0} \left( \boldsymbol{\eta}_{F} \right) \tag{13}$$

where

$$N_{2D} = \frac{m^* k_B T}{\pi \hbar^2},\tag{14}$$

and

$$F_{0}(\eta_{F}) = \int_{0}^{\infty} \frac{\varepsilon^{0} d\varepsilon}{1 + e^{\varepsilon - \eta_{F}}} = \ln\left(1 + e^{\eta_{F}}\right)$$
(15)

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

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

$$g_{1D}(E) = \frac{\sqrt{2m^*}}{\pi\hbar} \sqrt{\frac{1}{E - E_C}}$$
(16)

and the equilibrium electron density per unit length is

$$n_L = N_{1D} \mathcal{F}_{-1/2} \left( \eta_F \right) \tag{17}$$

where

$$N_{1D} = \frac{1}{\hbar} \sqrt{\frac{2m^* k_B T}{\pi}}$$
(18)

and

$$\mathcal{F}_{-1/2}(\eta_F) = \frac{1}{\sqrt{\pi}} \int_0^\infty \frac{\varepsilon^{-1/2} d\varepsilon}{1 + e^{\varepsilon - \eta_F}}$$
(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

$$\mathcal{F}_{j}(\eta_{F}) \equiv \frac{1}{\Gamma(j+1)} \int_{0}^{\infty} \frac{\varepsilon^{j} d\varepsilon}{1 + \exp(\varepsilon - \eta_{F})}, \qquad (20)$$

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

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

Also

$$\Gamma(1/2) = \sqrt{\pi} \tag{21b}$$

and

$$\Gamma(p+1) = p\Gamma(p) \tag{21c}$$

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

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

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

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

so  $\mathcal{F}_{_{1/2}}(\eta_{_F})$  is evaluated as

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

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

$$\frac{d\mathcal{F}_{j}}{d\eta_{F}} = \mathcal{F}_{j-1},\tag{23}$$

which often comes in useful. For example, we have an analytical expression for  $\mathcal{F}_0(\eta_F)$ , which means that we have an analytical expression for  $\mathcal{F}_{-1}(\eta_F)$ ,

$$\mathcal{F}_{-1} = \frac{d\mathcal{F}_0}{d\eta_F} = \frac{1}{1 + e^{-\eta_F}}.$$
(24)

Similarly, we can show that there is an analytic expression for any Fermi-Dirac integral of integer order, *j*, for  $j \le -2$ ,

$$\mathcal{F}_{j}(\eta_{F}) = \frac{e^{\eta_{F}}}{\left(1 + e^{\eta_{F}}\right)^{-j}} P_{-j-2}(e^{\eta_{F}})$$
(25)

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

$$p_{k,0} = 1$$
 (26a)

$$p_{k,i} = (1+i)p_{k-1,i} - (k+1-i)p_{k-1,i-1} \qquad i = 1, \dots, k.$$
(26b)

#### 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,

$$\mathcal{F}_{i}(\eta_{F}) \to e^{\eta_{F}} \tag{27}$$

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]

$$\mathcal{F}_{j}(\eta_{F}) = 2\eta_{F}^{j+1} \sum_{n=0}^{\infty} \frac{t_{2n}}{\Gamma(j+2-2n)\eta_{F}^{2n}} + \cos(\pi j) \sum_{n=1}^{\infty} \frac{(-1)^{n-1} e^{-n\eta_{F}}}{n^{j+1}}$$
(28)

where  $t_0 = 1/2$ ,  $t_n = \sum_{\mu=1}^{\infty} (-1)^{\mu-1} / \mu^n = (1 - 2^{1-n}) \zeta(n)$ , and  $\zeta(n)$  is the Riemann zeta function. The expressions for the Fermi-Dirac integrals in the degenerate limit ( $\eta_F >> 0$ ) come from (28) as  $\mathcal{F}_j(\eta_F) \to \eta_F^{j+1} / \Gamma(j+2)$  [4]. Specific results for several Fermi-Dirac integrals are shown below.

$$\mathcal{F}_{-1/2}(\eta_F) \to \frac{2\eta_F^{1/2}}{\sqrt{\pi}} \tag{29a}$$

$$\mathcal{F}_{1/2}(\eta_F) \to \frac{4\eta_F^{3/2}}{3\sqrt{\pi}} \tag{29b}$$

$$\mathcal{F}_{1}(\eta_{F}) \to \frac{1}{2}\eta_{F}^{2} \tag{29c}$$

$$\mathcal{F}_{3/2}(\eta_F) \to \frac{8\eta_F^{5/2}}{15\sqrt{\pi}} \tag{29d}$$

$$\mathcal{F}_2(\eta_F) \to \frac{1}{6} \eta_F^3 \tag{29e}$$

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

$$\int_{0}^{\infty} H(\varepsilon) f_{0}(\varepsilon) d\varepsilon = \int_{0}^{\eta_{F}} H(\varepsilon) d\varepsilon + \sum_{n=1}^{\infty} a_{n} \frac{d^{2n-1}}{d\varepsilon^{2n-1}} H(\varepsilon) \Big|_{\varepsilon = \eta_{F}}$$
(30)

where

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

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

$$\mathcal{F}_{j}(\eta_{F}) = 2\eta_{F}^{j+1} \sum_{n=0}^{\infty} \frac{t_{2n}}{\Gamma(j+2-2n)\eta_{F}^{2n}}.$$
(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 *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  $j \ge -1/2$  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  $-1/2 \le j \le 7/2$  [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 *et al.* for generalized Fermi-Dirac integrals with order j > -1 [15]. In this approach, the composite trapezoidal rule with variable transformation  $\varepsilon = \exp(t - e^{-t})$  is used for  $\eta_F \le 15$ , and the double exponential (DE) rule is used for larger  $\eta_F$ . The double precision (eps, ~  $2.2 \times 10^{-16}$ ) 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

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