Notes on Fermi-Dirac Integrals

Article · November 2008

Source: arXiv

2 authors:

Raseong Kim
Intel

M.s. Lundstrom
Purdue University

Notes on Fermi-Dirac Integrals
2nd edition

Raseong Kim and Mark Lundstrom
Network for Computational Nanotechnology
Purdue University

June 27, 2008

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,

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

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,

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

which can be used in (1) to write

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

By making the substitution,

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

eqn. (3) becomes

$$n = \frac{\left(2m^* k_B T\right)^{3/2}}{2\pi^2\hbar^3} \int_{0}^{\infty} \frac{\varepsilon^{1/2} d\varepsilon}{1 + e^{\varepsilon - \eta_F}} , \tag{5}$$

where we have defined

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

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

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

where

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

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

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

is the Fermi-Dirac integral of order 1/2. This integral can only be done numerically. Note that its value depends on η_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,

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

so that eqn. (7) can be written as

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

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

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

and by following a procedure like that one we used in three dimensions, one can show that the electron density per unit area is

$$n_S = N_{2D}\mathcal{F}_0\left(\eta_F\right) \tag{13}$$

where

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

and

$$\mathcal{F}_0\left(\eta_F\right) = \int_0^\infty \frac{\varepsilon^0 d\varepsilon}{1+e^{\varepsilon-\eta_F}} = \ln\left(1+e^{\eta_F}\right) \tag{15}$$

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

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

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

and the equilibrium electron density per unit length is

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

where

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

and

$$\mathcal{F}_{-1/2}\left(\eta_F\right) = \frac{1}{\sqrt{\pi}}\int_0^\infty \frac{\varepsilon^{-1/2} d\varepsilon}{1+e^{\varepsilon-\eta_F}} \tag{19}$$

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

$$\mathcal{F}_j(\eta_F) \equiv \frac{1}{\Gamma(j+1)} \int_0^\infty \frac{\varepsilon^j d\varepsilon}{1+\exp(\varepsilon-\eta_F)}, \tag{20}$$

where Γ is the gamma function. The Γ 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):

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

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

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

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

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

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 $\mathcal{F}_{-1}(\eta_F)$,

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

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

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

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

$$p_{k,0} = 1 \tag{26a}$$

$$p_{k,i} = \left(1+i\right) p_{k-1,i} - \left(k+1-i\right) p_{k-1,i-1} \qquad i = 1,\ldots,k . \tag{26b}$$

4. Asymptotic Expansions for Fermi-Dirac Integrals

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

$$\mathcal{F}_j(\eta_F) \to e^{\eta_F} \tag{27}$$

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]

$$\mathcal{F}_j(\eta_F) = 2\eta_F^{j+1} \sum_{n=0}^{\infty} \frac{t_{2n}}{\Gamma\left(j+2-2n\right)\eta_F^{2n}} + \cos\left(\pi j\right) \sum_{n=1}^{\infty} \frac{\left(-1\right)^{n-1} e^{-n\eta_F}}{n^{j+1}} \tag{28}$$

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

$$\int_0^\infty H(\varepsilon) f_0(\varepsilon) d\varepsilon = \int_0^{\eta_F} H(\varepsilon) d\varepsilon + \sum_{n=1}^{\infty} a_n \frac{d^{2n-1}}{d\varepsilon^{2n-1}} H(\varepsilon)\Big|_{\varepsilon=\eta_F} \tag{30}$$

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

$$\mathcal{F}_j(\eta_F) = 2\eta_F^{j+1} \sum_{n=0}^{\infty} \frac{t_{2n}}{\Gamma(j+2-2n)\eta_F^{2n}} . \tag{32}$$

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 $j \geq -1/2$ 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 *et al.* for generalized Fermi-Dirac integrals with order $j > -1$ [15]. In this approach, the composite trapezoidal rule with variable transformation $\varepsilon = \exp\left(t - e^{-t}\right)$ is used for $\eta_F \leq 15$, and the double exponential (DE) rule is used for larger η_F. The double precision (eps, $\sim 2.2\times10^{-16}$) 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

[1] G. Michele, "Algorithm 745: computation of the complete and incomplete Fermi-Dirac integral," *ACM Trans. Math. Softw.,* vol. 21, pp. 221-232, 1995.

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

[3] R. B. Dingle, *Asymptotic Expansions: Their Derivation and Interpretation*. London: Academic Press, 1973.

[4] J. McDougall and E. C. Stoner, "The computation of Fermi-Dirac functions," *Philosophical Transactions of the Royal Society of London. Series A, Mathematical and Physical Sciences,* vol. 237, pp. 67-104, 1938.

[5] A. Sommerfeld, "Zur Elektronentheorie der Metalle auf Grund der Fermischen Statistik," *Zeitschrift für Physik A Hadrons and Nuclei,* vol. 47, pp. 1-32, 1928.

[6] N. W. Ashcroft and N. D. Mermin, *Solid State Physics*. Philadelphia: Saunders College Publishing, 1976.

[7] A. C. Beer, M. N. Chase, and P. F. Choquard, "Extension of McDougall-Stoner tables of the Fermi-Dirac functions," *Helvetica Physica Acta,* vol. 28, pp. 529-42, 1955.

[8] P. Rhodes, "Fermi-Dirac functions of integral order," *Proceedings of the Royal Society of London. Series A, Mathematical and Physical Sciences,* vol. 204, pp. 396-405, 1950.

[9] D. Bednarczyk and J. Bednarczyk, "The approximation of the Fermi-Dirac integral $\mathcal{F}_{1/2}(\eta)$," *Physics Letters A,* vol. 64, pp. 409-410, 1978.

[10] X. Aymerich-Humet, F. Serra-Mestres, and J. Millán, "An analytical approximation for the Fermi-Dirac integral $F_{3/2}(\eta)$," *Solid-State Electronics,* vol. 24, pp. 981-982, 1981.

[11] X. Aymerich-Humet, F. Serra-Mestres, and J. Millan, "A generalized approximation of the Fermi--Dirac integrals," *Journal of Applied Physics,* vol. 54, pp. 2850-2851, 1983.

[12] J. S. Blakemore, "Approximations for Fermi-Dirac integrals, especially the function $\mathcal{F}_{1/2}(\eta)$ used to describe electron density in a semiconductor," *Solid-State Electronics,* vol. 25, pp. 1067-1076, 1982.

[13] P. V. Halen and D. L. Pulfrey, "Accurate, short series approximations to Fermi-Dirac integrals of order -1/2, 1/2, 1, 3/2, 2, 5/2, 3, and 7/2," *Journal of Applied Physics,* vol. 57, pp. 5271-5274, 1985.

[14] P. Van Halen and D. L. Pulfrey, "Erratum: "Accurate, short series approximation to Fermi-Dirac integrals of order -1/2, 1/2, 1, 3/2, 2, 5/2, 3, and 7/2" [J. Appl. Phys. 57, 5271 (1985)]," *Journal of Applied Physics,* vol. 59, p. 2264, 1986.

[15] W. H. Press, S. A. Teukolsky, W. T. Vetterling, and B. P. Flannery, *Numerical Recipes: The Art of Scientific Computing*, 3rd ed. New York: Cambridge University Press, 2007.