1. Introduction

Fermi-Dirac integrals appear frequently in semiconductor problems, so a basic 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. We also present Matlab functions (see Appendix and [1]) that calculate Fermi-Dirac integrals (the “script F” defined by Dingle [2] and reviewed by Blakemore [3]) in three different ways.

To see how they arise, consider computing the equilibrium electron concentration per unit volume in a three-dimensional (3D) semiconductor with a parabolic conduction band from the expression,

\[ n = \int_{E_c}^{\infty} g(E)f_0(E)dE = \int_{E_c}^{\infty} \frac{g(E)dE}{1 + e^{(E-E_f)/k_BT}}, \]  

(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 3D electrons with a parabolic band structure,

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

(2)

which can be used in Eq. (1) to write

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

(3)

By making the substitution,

\[ \varepsilon = (E - E_C)/k_BT, \]  

(4)

Eq. (3) becomes
\[
n = \frac{(2m^* k_B T)^{3/2}}{2\pi^2 \hbar^3} \int_{0}^{\infty} \frac{\xi^{1/2} d\xi}{1 + e^{\xi - \eta_F}}, \tag{5}
\]

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
\[
n = N_{3D} \frac{2}{\sqrt{\pi}} F_{1/2}(\eta_F), \tag{7}
\]

where
\[
N_{3D} = 2 \left( \frac{2m^* k_B T}{\hbar^2} \right)^{3/2} \tag{8}
\]
is the so-called effective density-of-states and
\[
F_{1/2}(\eta_F) \equiv \int_{0}^{\infty} \frac{\xi^{1/2} d\xi}{1 + \exp(\xi - \eta_F)} \tag{9}
\]
is the Fermi-Dirac integral of order 1/2. This integral can only be evaluated 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,
\[
\tilde{F}_{1/2}(\eta_F) \equiv \frac{2}{\sqrt{\pi}} \int_{0}^{\infty} \frac{\xi^{1/2} d\xi}{1 + \exp(\xi - \eta_F)}, \tag{10}
\]
so that Eq. (7) can be written as
\[
n = N_{3D} \tilde{F}_{1/2}(\eta_F). \tag{11}
\]

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 dimensional (2D) semiconductors with a single parabolic band, the density-of-states is
\[
g_{2D}(E) = \frac{m^*}{\pi \hbar^2}, \tag{12}
\]

\text{2}
and by following a procedure like that one we used in three dimensions, one can show that the electron density per unit area is

$$n_s = N_{2D} \tilde{\mathcal{F}}_0 (\eta_F),$$

(13)

where

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

(14)

and

$$\tilde{\mathcal{F}}_0 (\eta_F) = \int_0^\infty \frac{e^{\eta_F} d\varepsilon}{1 + e^{\eta_F}} = \ln (1 + e^{\eta_F})$$

(15)

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

Finally, in one-dimensional (1D) semiconductors with a parabolic band, 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

$$n_e = N_{1D} \tilde{\mathcal{F}}_{-1/2} (\eta_F),$$

(17)

where

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

(18)

and

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

(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
\[ J_j(\eta_F) \equiv \frac{1}{\Gamma(j+1)} \int_0^\infty \frac{\epsilon^j d\epsilon}{1 + \exp(\epsilon - \eta_F)}, \quad (20) \]

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 \( J_{1/2}(\eta_F) \) from Eq. (20):

\[ J_{1/2}(\eta_F) \equiv \frac{1}{\Gamma(1/2+1)} \int_0^\infty \frac{\epsilon^{1/2} d\epsilon}{1 + e^{\epsilon - \eta_F}}, \quad (22a) \]

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

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

so \( J_{1/2}(\eta_F) \) is evaluated as

\[ J_{1/2}(\eta_F) = \frac{2}{\sqrt{\pi}} \int_0^\infty \frac{\epsilon^{1/2} d\epsilon}{1 + e^{\epsilon - \eta_F}}, \quad (22c) \]

which agrees with Eq. (10). For more practice, use the general definition, Eq. (20) and Eqs. (21a-c) to show that the results for \( J_0(\eta_F) \) and \( J_{-1/2}(\eta_F) \) agree with Eqs. (15) and (19).

### 3. Derivatives of Fermi-Dirac Integrals

Fermi-Dirac integrals have the property that

\[ \frac{d}{d\eta_F} J_j = J_{j-1}, \quad (23) \]
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 \( j \leq -2 \),

\[
\mathcal{F}_j(\eta_F) = \frac{e^{\eta_F}}{(1 + e^{\eta_F})^j} P_{-j-2}(e^{\eta_F}),
\]  

(25)

where \( P_k \) is a polynomial of degree \( k \), and the coefficients \( p_{k,i} \) are generated from a recurrence relation [4] (note that the relation in Eq. (26c) is missing in p. 222 of [4])

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

(26a)

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

(26b)

\[
p_{k,k} = -p_{k-1,k-1}.
\]

(26c)

For example, to evaluate \( \mathcal{F}_4(\eta_F) = e^{\eta_F}/(1 + e^{\eta_F})^4 \times P_2(e^{\eta_F}) \), polynomial coefficients are generated from Eqs. (26a-c) as [4]

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

\[
p_{1,0} = 1, \quad p_{1,1} = -p_{0,0} = -1,
\]

\[
p_{2,0} = 1, \quad p_{2,1} = 2 p_{1,1} - 2 p_{1,0} = -4, \quad p_{2,2} = -p_{1,1} = 1,
\]

(27)

and we find

\[
\mathcal{F}_4(\eta_F) = \frac{e^{\eta_F}}{(1 + e^{\eta_F})^4} \sum_{j=0}^{2} p_{2,j} e^{\eta_F} = \frac{e^{\eta_F}}{(1 + e^{\eta_F})^4} \left(1 - 4e^{\eta_F} + e^{2\eta_F}\right).
\]

(28)

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,
\[ \mathcal{F}_j(\eta_F) \rightarrow e^{\eta_F}, \quad (29) \]

which means that for all orders, \( j \), the Fermi-Dirac integral 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 \( \eta_F > 0 \) \([2, 5, 6]\)

\[ \mathcal{F}_j(\eta_F) = 2\eta_F^{j+1} \sum_{n=0}^{\infty} \frac{t_{2n}}{\Gamma(j+2-2n)\eta_F^{2n}} + \cos(\pi j) \sum_{n=1}^{\infty} \frac{(-1)^{n-1} e^{-\eta_F}}{n^{j+1}}, \quad (30) \]

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 Eq. (30) as \( \mathcal{F}_j(\eta_F) \rightarrow \eta_F^{j+1}/\Gamma(j+2) \) \([7]\). Specific results for several Fermi-Dirac integrals are shown below.

\[ \begin{align*}
\mathcal{F}_{-1/2}(\eta_F) &\rightarrow \frac{2\eta_F^{1/2}}{\sqrt{\pi}}, \\
\mathcal{F}_{1/2}(\eta_F) &\rightarrow \frac{4\eta_F^{3/2}}{3\sqrt{\pi}}, \\
\mathcal{F}_{1}(\eta_F) &\rightarrow \frac{1}{2} \eta_F^2, \\
\mathcal{F}_{3/2}(\eta_F) &\rightarrow \frac{8\eta_F^{5/2}}{15\sqrt{\pi}}, \\
\mathcal{F}_{2}(\eta_F) &\rightarrow \frac{1}{6} \eta_F^3.
\end{align*} \quad (31) \]

The complete expansion in Eq. (30) can be related to the well-known Sommerfeld expansion \([8, 9]\). First, note that the integrals to calculate carrier densities in Eqs. (1) and (3) are all of the form

\[ \int_{-\infty}^{\infty} H(E) f_0(E) dE. \quad (32) \]

If \( H(E) \) does not vary rapidly in the range of a few \( k_B T \) about \( E_F \), then we can write the Taylor expansion of \( H(E) \) about \( E_F \) as \([9]\)

\[ H(E) = \sum_{n=0}^{\infty} \frac{d^n}{dE^n} H(E) \bigg|_{E=E_F} \frac{(E-E_F)^n}{n!}. \quad (33) \]

Using this Taylor series expansion, the integral in Eq. (32) can be written as (see \([9]\) for a detailed derivation)
\[
\int_{-\infty}^{\infty} H(E) f_0(E) dE = \int_{-\infty}^{E_F} H(E) dE + \sum_{n=1}^{\infty} (k_B T)^{2n} a_n \frac{d^{2n-1}}{dE^{2n-1}} H(E) \bigg|_{E=E_F},
\]

where

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

and it is noted that \(a_n = 2t_{2n}\). Equation (34) is known as the Sommerfeld expansion [8, 9]. Typically, the first term in the sum in Eq. (34) is all that is needed, and the result is

\[
\int_{-\infty}^{\infty} H(E) f_0(E) dE = \int_{-\infty}^{E_F} H(E) dE + \frac{\pi^2}{6} (k_B T)^2 H'(E_F).
\]

If we scale \(E\) by \(k_B T\) in Eq. (34), \(\varepsilon = E/k_B T\), then Eq. (34) becomes

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

Then the Sommerfeld expansion for the Fermi-Dirac integral of order \(j\) can be evaluated by letting \(H(\varepsilon) = \varepsilon^j / \Gamma(j + 1)\) in Eq. (37), and the result is

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

Equation (38) is the same as Eq. (30) except that the second term in Eq. (30) is omitted [5]. In the degenerate limit, however, the second term in Eq. (30) vanishes, so the Eqs. (30) and (38) give the same results as Eqs. (31a-e).

5. Approximate Expressions for Common Fermi-Dirac Integrals

Fermi-Dirac integrals can be quickly evaluated by tabulation [2, 7, 10, 11] or analytic approximation [12-14]. We briefly mention some of the analytic approximations and refer the reader to a Matlab function. Bednarczyk et al. [12] proposed a single analytic approximation that evaluates the Fermi-Dirac integral of order \(j = 1/2\) with errors less than 0.4 % [3]. Aymerich-Humet et al. [13, 14] 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,” [1] calculates the Fermi-Dirac integral defined in Eq. (10) with orders \(j \geq -1/2\) using these analytic approximations. The source code of this relatively short function is listed in the Appendix.
If a better accuracy is required and a longer CPU time is allowed, then the approximations proposed by Halen and Pulfrey [15, 16] may be used. In this model, several approximate expressions are introduced based on the series expansion in Eq. (30), and the error is less than $10^{-5}$ for $-1/2 \leq j \leq 7/2$ [15]. The Matlab function, “FDjx.m,” [1] is the main function that calculates the Fermi-Dirac integrals using this model. This function includes tables of coefficients, so it is not simple enough to be shown in the Appendix, but it can be downloaded from [1].

There also have been discussions on the simple analytic calculation of the inverse Fermi-Dirac integrals of order $j = 1/2$ [3]. This has been of particular interest because it can be used to calculate the Fermi level from the known bulk charge density in Eq. (11), as $\eta_F = \sqrt[1/2]{(n/N_{5D})}$. Joyce and Dixon [17] examined a series approach that gives $|\Delta \eta_F| \leq 0.01$ for $\eta_{F\text{max}} = 5.5$ [3], and a simpler expression from Joyce [18] gives $|\Delta \eta_F| \leq 0.03$ for $\eta_{F\text{max}} = 5$ [3]. Nilsson proposed two different full-range ($-10 \leq \eta_F \leq 20$ ) expressions [19] with $|\Delta \eta_F| \leq 0.01$ and $|\Delta \eta_F| \leq 0.005$ [3]. Nilsson later presented two empirical approximations [20] that give $|\Delta \eta_F| \leq 0.01$ for $\eta_{F\text{max}} = 5.5$ and $\eta_{F\text{max}} = 20$, respectively [3].

6. Numerical Evaluation of Fermi-Dirac Integrals

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 $j > -1$ [21]. 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 $\eta_F$. Double precision (eps, $\sim 2.2 \times 10^{-16}$ ) can be achieved after 60 to 500 iterations [21]. The Matlab function, “FD_int_num.m,” [1] evaluates the Fermi-Dirac integral numerically using the composite trapezoidal rule following the approach in [21]. The source code is listed in the Appendix. This approach provides very high accuracy, but the CPU time is considerably longer. An online simulation tool that calculates the Fermi-Dirac integrals using this source code has been deployed at nanoHUB.org [22]. Note that the numerical approach we consider in this note is relatively simple, and there are other advanced numerical integration algorithms [23] suggested to improve the calculation speed.

In Fig. 1, we compare the accuracy and the timing of the three approaches that calculate $\varepsilon_j(\eta_F)$. The Fermi-Dirac integral of order $j = 1/2$ ($\varepsilon_{1/2}(\eta_F)$) is calculated for $-10 \leq \eta_F \leq 10$ with $\eta_F$ spacing = 0.01 using approximate expressions (“FD_int_approx.m” and “FDjx.m”) and the rigorous numerical integration (“FD_int_num.m”) with double-precision. The relative errors of the approximate expressions are calculated as $(\varepsilon_{1/2,\text{approx}} - \varepsilon_{1/2,\text{num}})/\varepsilon_{1/2,\text{num}}$, where $\varepsilon_{1/2,\text{approx}}$ and $\varepsilon_{1/2,\text{num}}$ represent the results from the approximate expression and the numerical integration respectively. The elapsed time measured for each approach (using Matlab commands “tic/toc” for Pentium 4 CPU 3.4 GHz and 2.0 GB RAM) clearly shows the compromise between the accuracy and the CPU time.
Fig. 1. (a) Relative errors from the approximate expressions for $\frac{1}{\eta_F}$ with respect to the numerical integration (“FD_int_num.m”). (A) Relative error from “FD_int_approx.m”. (B) Relative error from “FD_jx.m”. All Matlab functions are available in [1]. (b) The absolute values of the relative errors in the log scale. The elapsed time measured for the three approaches clearly shows the trade-off between the accuracy and the CPU time.
References


[2] R. Dingle, "The Fermi-Dirac integrals \( \Phi_p(\eta) = (p!)^{-1} \int_0^{\infty} e^{\eta} \left( e^{\varepsilon - \eta} + 1 \right)^{-1} d\varepsilon \)," \textit{Applied Scientific Research}, vol. 6, no. 1, pp. 225-239, 1957.


[6] T. M. Garoni, N. E. Frankel, and M. L. Glasser, "Complete asymptotic expansions of the Fermi--Dirac integrals \( \Phi_p(\eta) = \frac{\Gamma(p+1)}{\Gamma(p)} \int_0^{\infty} \frac{\varepsilon^p}{\left( 1 + e^{\varepsilon - \eta} \right)} d\varepsilon \)," \textit{J. Math. Phys.}, vol. 42, no. 4, pp. 1860-1868, 2001.


Appendix

"FD_int_approx.m"

function y = FD_int_approx( eta, j )

% Analytic approximations for Fermi-Dirac integrals of order j > -1/2
% Date: September 29, 2008
% Author: Raseong Kim (Purdue University)
%
% Inputs
% eta: eta_F
% j: FD integral order
%
% Outputs
% y: value of FD integral (the "script F" defined by Blakemore (1982))
%
% For more information in Fermi-Dirac integrals, see:
% "Notes on Fermi-Dirac Integrals (3rd Edition)" by Raseong Kim and Mark
% Lundstrom at http://nanohub.org/resources/5475
%
% References

if j < -1/2
    error('The order should be equal to or larger than -1/2.');
else
    x = eta;
    switch j
        case 0
            y = log( 1 + exp( x ) );    % analytic expression
        case 1/2
            % Model proposed in [1]
            % Expressions from eqs. (22)-(24) of [2]
            mu = x .* 4 + 50 + 33.6 * x .* ( 1 - 0.68 * exp( -0.17 * ( x + 1 ) .^ 2 ) );
            xi = 3 * sqrt( pi ) ./ ( 4 * mu .^ ( 3 / 8 ) );
            y = ( exp( - x ) + xi ) .^ -1;
        case 3/2
            % Model proposed in [3]
            % Expressions from eq. (5) of [3]
            a = 14.9;
            b = 2.64;
            c = 9 / 4;
            y = ( ( j + 1 ) .^ 2 .^ ( j + 1 ) ) .^ ( b + x + ( abs( x - b ) .^ c + a ) .^ ( 1 / c ) ) .^ ( j + 1 ) ... + exp( -x ) ./ gamma( j + 1 ) .^ -1 ./ gamma( j + 1 );
        otherwise
            % Model proposed in [4]
            % Expressions from eqs. (6)-(7) of [4]
            a = ( 1 + 15 / 4 .^ ( j + 1 ) + 1 / 40 .^ ( j + 1 ) .^ 2 ) .^ ( 1 / 2 );
            b = 1.8 + 0.61 .^ j;
            c = 2 + ( 2 - sqrt( 2 ) ) .* 2 .^ ( - j );
            y = ( ( j + 1 ) .^ 2 .^ ( j + 1 ) ) .^ ( b + x + ( abs( x - b ) .^ c + a .^ c ) .^ ( 1 / c ) ) .^ ( j + 1 ) ... + exp( -x ) ./ gamma( j + 1 ) .^ -1 ./ gamma( j + 1 );
    end
end
function [ y, N, err ] = FD_int_num( eta, j, tol, Nmax )

% Numerical integration of Fermi-Dirac integrals for order j > -1.
% Author: Raseong Kim (Purdue University)
% Date: September 29, 2008
% Extended (composite) trapezoidal quadrature rule with variable
% transformation, \( x = \exp(t - \exp(t)) \)
% Valid for \( \eta \sim < 15 \) with precision \( \sim \text{eps} \) with 60~500 evaluations.

% Inputs
% eta: \( \eta_F \)
% j: FD integral order
% tol: tolerance
% Nmax: number of iterations limit
% %
% % Note: When "eta" is an array, this function should be executed
% % repeatedly for each component.
% %
% % Outputs
% % y: value of FD integral (the "script F" defined by Blakemore (1982))
% % N: number of iterations
% % err: error
% %
% % For more information in Fermi-Dirac integrals, see:
% % "Notes on Fermi-Dirac Integrals (3rd Edition)" by Raseong Kim and Mark
% % Lundstrom at http://nanohub.org/resources/5475
% %
% % Reference
% % Numerical recipies: The art of scientific computing, 3rd Ed., Cambridge
% % University Press, 2007.

for N = 1 : Nmax
    a = -4.5;                       % limits for t
    b = 0.5;
    t = linspace( a, b, N + 1 );    % generate intervals
    x = exp( t - exp( -t ));
    f = x .* ( 1 + exp( -t ) ) .* x.^j ./ ( 1 + exp( x - eta ) );
    y = trapz( t, f );

    if N > 1                        % test for convergence
        err = abs( y - y_old );
        if err < tol
            break;
        end
    end
    y_old = y;
end

if N == Nmax
    error( 'Increase the maximum number of iterations.' )
end

y = y ./ gamma( j + 1 );