

Notes on Fermi-Dirac Integrals

3rd Edition

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December 10, 2008
(Last revised on August 4, 2011)

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,

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

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,

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

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

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

By making the substitution,

$$\varepsilon = (E - E_C)/k_B T, \quad (4)$$

Eq. (3) becomes

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

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

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

where

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

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 evaluated 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,

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

so that Eq. (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 dimensional (2D) semiconductors with a single parabolic band, 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

$$n_S = N_{2D} \mathcal{F}_0(\eta_F), \quad (13)$$

where

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

and

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

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

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

and the equilibrium electron density per unit length is

$$n_L = N_{1D} \mathcal{F}_{-1/2}(\eta_F), \quad (17)$$

where

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

and

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

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

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

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

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

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 Eq. (20):

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

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

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

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

3. Derivatives of Fermi-Dirac Integrals

Fermi-Dirac integrals have the property that

$$\frac{d\mathcal{F}_j}{d\eta_F} = \mathcal{F}_{j-1}, \quad (23)$$

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

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

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

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

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])

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

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

$$p_{k,k} = -p_{k-1,k-1}. \quad (26c)$$

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]

$$\begin{aligned} p_{0,0} &= 1, \\ p_{1,0} &= 1, \quad p_{1,1} = -p_{0,0} = -1, \\ p_{2,0} &= 1, \quad p_{2,1} = 2p_{1,1} - 2p_{1,0} = -4, \quad p_{2,2} = -p_{1,1} = 1, \end{aligned} \quad (27)$$

and we find

$$\mathcal{F}_{-4}(\eta_F) = \frac{e^{\eta_F}}{(1+e^{\eta_F})^4} \sum_{i=0}^2 p_{2,i} e^{i\eta_F} = \frac{e^{\eta_F}}{(1+e^{\eta_F})^4} (1 - 4e^{\eta_F} + e^{2\eta_F}). \quad (28)$$

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,

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

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]

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

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 ($\eta_F \gg 0$) 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.

$$\mathcal{F}_{-1/2}(\eta_F) \rightarrow \frac{2\eta_F^{1/2}}{\sqrt{\pi}}, \quad (31a)$$

$$\mathcal{F}_{1/2}(\eta_F) \rightarrow \frac{4\eta_F^{3/2}}{3\sqrt{\pi}}, \quad (31b)$$

$$\mathcal{F}_1(\eta_F) \rightarrow \frac{1}{2}\eta_F^2, \quad (31c)$$

$$\mathcal{F}_{3/2}(\eta_F) \rightarrow \frac{8\eta_F^{5/2}}{15\sqrt{\pi}}, \quad (31d)$$

$$\mathcal{F}_2(\eta_F) \rightarrow \frac{1}{6}\eta_F^3. \quad (31e)$$

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]

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

Using this Taylor series expansion, the integral in Eq. (32) can be written as (see [9] for a detailed derivation)

$$\int_{-\infty}^{\infty} H(E) f_0(E) dE = \int_{-\infty}^{E_F} H(E) dE + \sum_{n=1}^{\infty} (k_B T)^{2n} a_n \left. \frac{d^{2n-1}}{dE^{2n-1}} H(E) \right|_{E=E_F}, \quad (34)$$

where

$$a_n = 2 \left(1 - \frac{1}{2^{2n}} + \frac{1}{3^{2n}} - \frac{1}{4^{2n}} + \dots \right), \quad (35)$$

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

$$\int_{-\infty}^{\infty} H(E) f_0(E) dE \simeq \int_{-\infty}^{E_F} H(E) dE + \frac{\pi^2}{6} (k_B T)^2 H'(E_F). \quad (36)$$

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

$$\int_{-\infty}^{\infty} H(\varepsilon) f_0(\varepsilon) d\varepsilon = \int_{-\infty}^{\eta_F} H(\varepsilon) d\varepsilon + \sum_{n=1}^{\infty} a_n \left. \frac{d^{2n-1}}{d\varepsilon^{2n-1}} H(\varepsilon) \right|_{\varepsilon=\eta_F}. \quad (37)$$

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

$$\mathcal{F}_j(\eta_F) = 2\eta_F^{j+1} \sum_{n=0}^{\infty} \frac{t_{2n}}{\Gamma(j+2-2n)\eta_F^{2n}}. \quad (38)$$

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 $\eta_F = \mathcal{F}_{1/2}^{-1}(n/N_{3D})$. Joyce and Dixon [17] examined a series approach that gives $|\Delta\eta_F| \leq 0.01$ for $\eta_{F\max} \approx 5.5$ [3], and a simpler expression from Joyce [18] gives $|\Delta\eta_F| \leq 0.03$ for $\eta_{F\max} \approx 5$ [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 $\eta_{F\max} \approx 5.5$ and $\eta_{F\max} \approx 20$, 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 $\varepsilon = \exp(t - e^{-t})$ is used for $\eta_F \leq 15$, and the double exponential (DE) rule is used for larger η_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 $\mathcal{F}_j(\eta_F)$. The Fermi-Dirac integral of order $j = 1/2$ ($\mathcal{F}_{1/2}(\eta_F)$) is calculated for $-10 \leq \eta_F \leq 10$ with η_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 $(\mathcal{F}_{1/2,approx} - \mathcal{F}_{1/2,num}) / \mathcal{F}_{1/2,num}$, where $\mathcal{F}_{1/2,approx}$ and $\mathcal{F}_{1/2,num}$ 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.

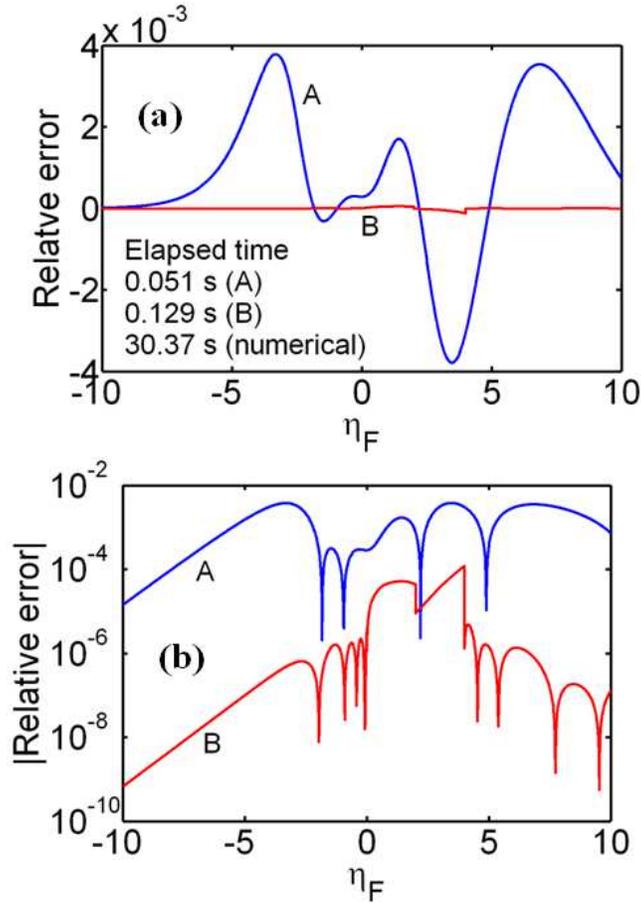


Fig. 1. (a) Relative errors from the approximate expressions for $\mathcal{F}_{1/2}(\eta_F)$ with respect to the numerical integration (“FD_int_num.m”). (A) Relative error from “FD_int_approx.m”. (B) Relative error from “FDjx.m”. All Matlab functions are available in [1].(b) The absolute values of the 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.

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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
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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]
            % The integral is divided by gamma( j + 1 ) to make it consistent with [1] and [2].
            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]
            % The integral is divided by gamma( j + 1 ) to make it consistent with [1] and [2].
            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
```

“FD_int_num.m”

```
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 ~< 15 with precision ~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
%
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% Numerical recipes: The art of scientific computing, 3rd Ed., Cambridge
% University Press, 2007.

for N = 1 : Nmax
    a = -4.5;           % limits for t
    b = 5.0;
    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 );
```