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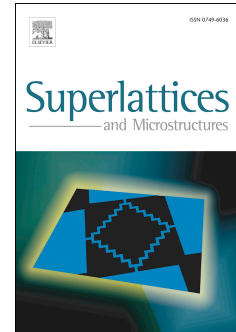
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# A New Approximation of Fermi-Dirac Integrals of Order $1/2$ for Degenerate Semiconductor Devices

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## Abstract

There had been tremendous growth in the field of Integrated circuits (ICs) in the past fifty years. Scaling laws mandated both lateral and vertical dimensions to be reduced and a steady increase in doping densities. Most of the modern semiconductor devices have invariably heavily doped regions where Fermi-Dirac Integrals are required. Several attempts have been devoted to developing analytical approximations for Fermi-Dirac Integrals since numerical computations of Fermi-Dirac Integrals are difficult to use in semiconductor devices, although there are several highly accurate tabulated functions available. Most of these analytical expressions are not sufficiently suitable to be employed in semiconductor device applications due to their poor accuracy, the requirement of complicated calculations, and difficulties in differentiating and integrating. A new approximation has been developed for the Fermi-Dirac integrals of the order  $1/2$  by using Prony's method and discussed in this paper. The approximation is accurate enough (Mean Absolute Error (MAE) = 0.38%) and easy enough to be used in semiconductor device equations. The new approximation of Fermi-Dirac Integrals is applied to a more generalized Einstein Relation which is an important relation in semiconductor devices.

*Keywords:* Fermi-Dirac, Prony's method, Einstein's Relation

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## 1. Introduction

One of the most important fundamental set of quantities needed to study semiconductor devices is the density of electrons and holes. The thermal equilibrium electron density in the Conduction band is obtained by knowing the density of available states and the Fermi-Dirac Distribution Law as follows:

$$n = 2 \left( \frac{2\pi m_n^* kT}{h^2} \right)^{3/2} \int_0^\infty \frac{t^{1/2}}{1 + \exp(t - \eta)} dt \quad (1)$$

where  $m_n^*$  is the effective mass of an electron,  $k$  is the Boltzmann's constant,  $h$  is the Planck's constant,  $T$  is the temperature and the integral is called Fermi-Dirac integral of order 1/2,  $F_{\frac{1}{2}}(\eta)$  [1].

The constant  $\eta$  in this case is equal to  $\frac{E_f - E_c}{kT}$ , which is the normalized Fermi level referenced to the Conduction band edge  $E_C$ . The Fermi-Dirac Integrals have a general form [1], which is expressed as follows for any order  $j$ :

$$F_j(x) = \int_0^\infty \frac{t^j}{1 + \exp(t - x)} dt \quad (2)$$

### 1.1. Boltzmann's Approximation of FDI

Instead of the direct use of Fermi-Dirac Integrals often, an exponential function, which is the result of Boltzmann's approximation, is used to express the electron density as follows:

$$n = N_C \exp\left(\frac{E_f - E_c}{kT}\right) \quad (3)$$

where  $N_C = 2 \left( \frac{2\pi m_n^* kT}{h^2} \right)^{3/2}$  is the effective density of states in the conduction band.

Boltzmann's approximation is an excellent one when the Fermi-level is more than  $3kT$  away from the majority carrier band. However, when the Fermi level is less than  $3kT$  away from the majority carrier band, serious errors result in carrier densities. For degenerate semiconductors, the Boltzmann's approximation is not adequate [2]. Thus, we are required to use  $F_{\frac{1}{2}}(\eta)$ , and it has an important role in determining other significant quantities in semiconductor devices along with the electron density, hole density, and the Einstein relation. Despite such

25 requirements, FDIs are at present either numerically evaluated or analytically approximated.

### 1.2. Numerical Evaluations

While the FDI does not have a closed form solution, there have been many attempts made to compute the FDI. Numerical evaluations have been typically developed with high accuracies by using different numerical integration methods or programming approaches. To obtain accurate values of FDI, there have been many numerical evaluations performed by using numerical integration of the general form of FDI [3, 4], using a pair of extrapolation procedures [5], or with quadratures of the integrand [6, 7, 8, 9], FDI has been numerically evaluated by applying Chebyshev approximations for different ranges [10] and different orders [11].

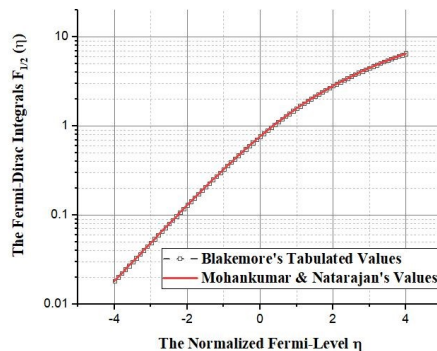


Fig. 1: The Numerical Evaluations of FDI by Mohankumar and Natarajan compared to Blakemore's Tabulated Values.

A few of the recent numerical evaluations with high accuracies have been proposed by Fukushima [12, 13, 14, 15]. The four papers of Fukushima between 2014 and 2015 have aimed to accomplish numerical evaluations of FDI that can achieve high precisions (16 to 20 digits) with different orders. Mohankumar and Natarajan [16] proposed one of the highest precision numerical evaluations, using an algorithm which uses Double Exponential, Trapezoidal and GaussLegendre quadratures. Unlike these numerical evaluations, a few of the earlier

computations of FDI have been tabulated to be used as reference values for  
 45 analytical expressions [17, 18, 19]. A set of computations of FDI, proposed and  
 tabulated by Blakemore [20], are the ones employed in this paper as a reference.  
 Fig. 1 shows the FDI values tabulated by Blakemore and compared with the  
 values of FDI by Mohankumar and Natarajan.

### 1.3. Analytical Approximations

50 The numerical evaluations, although they offer very high accuracies, they  
 do not have a convenient and insightful form to be employed in semiconductor  
 device calculations. Thus there have been a few attempts devoted to developing  
 an analytical approximation that holds good accuracy [21, 22, 23, 24]. However  
 those expressions are not sufficiently useful for implementation in semiconduc-  
 55 tor device equations because they have complicated forms and are not easy to  
 differentiate or to integrate. In order to avoid the numerical evaluations of FDI,  
 a few researchers have developed analytical approximations of the normalized  
 Fermi-Level instead of FDI [25, 26]. Seeking a simple approximation to be im-  
 plemented in semiconductor device analyses, a few researchers have developed  
 60 analytical expressions of FDI [27, 28, 29, 30, 31, 32, 33, 34]. Most of these ap-  
 proximations cannot be easily differentiated or integrated and further they are  
 not sufficiently accurate.

We are presenting in this paper a *closed-form* analytical approximation of  
 FDI that is accurate enough and simple enough to be used in semiconductor  
 65 device calculations. The form we are trying to approach is similar to Boltzmanns  
 approximation which is an exponential function. We develop a summation of  
 exponential functions as an approximation for FDI.

In order to compare the approximations, a suitable error estimation measure  
 is to be chosen. Two of the common methods used in evaluating the accuracies  
 70 of the models in these studies are Relative Root Mean Square Error (RMSE)  
 and Mean Absolute Error (MAE). Since the number of the tried points is large,  
 Mean Absolute Error gives smaller error than Relative Root Mean Square Error  
 (RMSE) [35]. The two ways of determining the error are shown in Eg.(4) and

Eq.(5).

$$MAE = \frac{1}{m} \sum_{i=1}^m \left| \frac{(Actual)_i - (Approximated)_i}{(Actual)_i} \right| \quad (4)$$

75

$$RMSE = \sqrt{\frac{1}{m} \sum_{i=1}^m \left( \frac{(Actual)_i - (Approximated)_i}{(Actual)_i} \right)^2} \quad (5)$$

## 2. Prony's Method

The Prony's method is a systematic way to approximate a function with a sum of a series of exponential functions [36]. The Prony's method lends itself to approximate certain functions in the field of semiconductor such as the Two-  
80 Step Diffusion Profiles [37] and in the digital communication field for the average probability of transmission error instead of Fourier series [38].

The symbols that are used in Prony's method are now defined before introducing the steps in the Prony's method [39].  $N$  is the number of equally spaced chosen points. The quantity  $n$  is the number of terms in Prony's approxima-  
85 tion. The quantity  $C$  is the coefficient multiplying the exponential term in the function, and  $a$  is an exponent. Secondly, the general form of Prony's function is:

$$f(x_k) = \sum_{i=1}^n C_i \exp(a_i x_k) \quad (6)$$

where  $k = 1, 2, \dots, N$  and  $i = 1, 2, \dots, n$

In order to simplify the form during computations, the general form of  
90 Prony's function can be written as:

$$f(x_k) = \sum_{i=1}^n C_i \mu_i^{x_k} \quad (7)$$

where  $\mu_i = \exp(-a_i)$

The first step towards finding the coefficients  $C$ s is forming the  $N$  equations using the actual values of  $f(x_k)$  in the following order:

$$C_1 + C_2 + \dots + C_n = F_0 \quad (8a)$$

$$C_1\mu_1 + C_2\mu_2 + \dots + C_n\mu_n = F_1 \quad (8b)$$

95

$$C_1\mu_1^2 + C_2\mu_2^2 + \dots + C_n\mu_n^2 = F_2 \quad (8c)$$

$$\vdots$$

$$C_1\mu_1^{N-1} + C_2\mu_2^{N-1} + \dots + C_n\mu_n^{N-1} = F_{N-1} \quad (8.N)$$

After forming the  $N$  equations, the next step is letting  $\mu_1, \dots, \mu_n$  to be the roots of an algebraic equation as follows:

$$\mu^n + \alpha_1\mu^{n-1} + \alpha_2\mu^{n-2} + \dots + \alpha_{n-1}\mu + \alpha_n = 0 \quad (9)$$

so that it can be expressed as follows:  $(\mu - \mu_1)(\mu - \mu_2)\dots(\mu - \mu_n)$

100 In order to determine  $\alpha_1, \dots, \alpha_n$ , the first actual value  $F_0$  should be multiplied by  $\alpha_n$ , second actual value  $F_1$  should be multiplied by  $\alpha_{n-1}$ , and  $n$ th actual value should be multiplied by 1. Thus, the result is seen to be of the form:

$$F_n + \alpha_1 F_{n-1} + \alpha_2 F_{n-2} + \dots + \alpha_n F_0 = 0 \quad (10)$$

Then, a set of  $N-n-1$  additional equations of similar type is obtained in the same way by starting instead successively with the second, third, ...,  $(N-n)$ th equations. Therefore, Eq.(9) and Eq.(10) imply a set of  $N-n$  linear equations.

105

$$F_n + \alpha_1 F_{n-1} + \alpha_2 F_{n-2} + \dots + \alpha_n F_0 = 0 \quad (11a)$$

$$F_{n+1} + \alpha_1 F_n + \alpha_2 F_{n-1} + \dots + \alpha_n F_1 = 0 \quad (11b)$$

$$\vdots$$

$$F_{N-1} + \alpha_1 F_{N-2} + \alpha_2 F_{N-3} + \dots + \alpha_n F_{N-n-1} = 0 \quad (11.N-n)$$

Since the Prony's method is based on a series of exponential terms in the main case or cosine and sine terms in the particular case, it can be easily differentiated and integrated. As a result, Prony's method can be used to approximate certain functions in electronic devices which need to be differentiated

110

or integrated. This method is sometimes required in the computation of some quantities such as the use of the half integer Fermi-Dirac function in the charge density equation [2]. The first and second derivation forms of Prony's general  
 115 form can be expressed as:

$$\frac{dF(x_k)}{dx_k} = \sum_{i=1}^n C_i * a_i \exp(a_i x_k) \quad (12)$$

$$\frac{d^2 f(x_k)}{dx_k^2} = \sum_{i=1}^n C_i * a_i^2 \exp(a_i x_k) \quad (13)$$

In addition, the Prony's approximation can be integrated as shown below:

$$F_s(x_k) = \int f(x_k) dx = \sum_{i=1}^n \frac{C_i}{a_i} \exp(a_i x_k) + K_1 \quad (14)$$

$$F_{ss}(x_k) = \int F_s(x_k) dx = \sum_{i=1}^n \frac{C_i}{a_i^2} \exp(a_i x_k) + K_1 * x_k + K_2 \quad (15)$$

Furthermore, the steps of the Prony's method can be easily followed as  
 120 described in [39], and the coefficients of the Pronys method can be determined in few steps [39].

### 3. The Results and Discussions

#### 3.1. The Proposed Approximation of FDI

The components of the approximation (the number of the chosen points and  
 125 the number of exponential terms) are selected, as Pronys method requires. The number of tested points (N) is 61 points since the exact values for the range of  $\eta$  values from -2 to +4 is 61 values as tabulated in [20]. We chose the range of  $\eta$  values from negative two to four because the Boltzmanns approximation offers less error than the proposed approximation for the values of  $\eta$  from negative  
 130 three to negative two. The exact values that are used in Pronys method steps are taken from Blakemores tabulated values [20]. The number of chosen terms of the exponentials is four. Even though a large number of terms might imply a better approximation, by using a different number of terms for this approximation (n=



6, 8, and 10) we have found that the accuracy of the approximation turns out  
 135 to be similar and not significantly improved. The general form of the proposed  
 approximation can be expressed in the following manner:

$$F_{\frac{1}{2}}(\eta) = \sum_{i=1}^4 C_i \exp(a_i \eta) = C_1 \exp(a_1 \eta) + C_2 \exp(a_2 \eta) + C_3 \exp(a_3 \eta) + C_4 \exp(a_4 \eta) \quad (16)$$

$$F_{\frac{1}{2}}(\eta) = \sum_{i=1}^4 C_i \mu_i^\eta = C_1 \mu_1^\eta + C_2 \mu_2^\eta + C_3 \mu_3^\eta + C_4 \mu_4^\eta \quad (17)$$

where  $\mu_i = \exp(a_i)$ .

The first step towards approximating the Fermi-Dirac Integral is forming  
 140 61 equations similar to equations (8) where the actual values of FDI are used.  
 Then, the  $\mu$ 's can be roots of the algebraic equation:

$$\mu^4 + \alpha_1 \mu^3 + \alpha_2 \mu^2 + \alpha_3 \mu + \alpha_4 = 0 \quad (18)$$

so, the left-hand side of this equation is identified with:

$$(\mu - \mu_1)(\mu - \mu_2)(\mu - \mu_3)(\mu - \mu_4)$$

To find  $\alpha_1, \alpha_2, \alpha_3, \alpha_4$ , we multiply  $\alpha_4$  by  $F_0$ ,  $\alpha_3$  by  $F_1$ ,  $\alpha_2$  by  $F_2$ , and  $\alpha_1$  by  $F_3$ ,  
 145 so the first equation will be formed as:

$$F_4 + \alpha_1 F_3 + \alpha_2 F_2 + \alpha_3 F_1 + \alpha_4 F_0 = 0 \quad (19)$$

By applying the same condition on the rest of the equations, 57 equations,  
 which is the difference between the number of chosen points and the number  
 of terms (N-n), are formed, and the final form can be expressed as shown in  
 Eq.(20):

$$\alpha_4 \sum_{i=0}^{56} F_i + \alpha_3 \sum_{i=0}^{56} F_{i+1} + \alpha_2 \sum_{i=0}^{56} F_{i+2} + \alpha_1 \sum_{i=0}^{56} F_{i+3} + \sum_{i=0}^{56} F_{i+4} = 0 \quad (20)$$

150 By differentiating previous equation with respect  $\alpha_1, \alpha_2, \alpha_3$ , and  $\alpha_4$ , four  
 equations are being formulated as shown in Eq.(21a):

$$\alpha_4 \sum_{i=0}^{56} F_i^2 + \alpha_3 \sum_{i=0}^{56} F_i * F_{i+1} + \alpha_2 \sum_{i=0}^{56} F_i * F_{i+2} + \alpha_1 \sum_{i=0}^{56} F_i * F_{i+3} + \sum_{i=0}^{56} F_i * F_{i+4} = 0 \quad (21a)$$

$$\alpha_4 \sum_{i=0}^{56} F_{i+1} * F_i + \alpha_3 \sum_{i=0}^{56} F_{i+1}^2 + \alpha_2 \sum_{i=0}^{56} F_{i+1} * F_{i+2} + \alpha_1 \sum_{i=0}^{56} F_{i+1} * F_{i+3} + \sum_{i=0}^{56} F_{i+1} * F_{i+4} = 0 \quad (21b)$$

$$\alpha_4 \sum_{i=0}^{56} F_{i+2} * F_i + \alpha_3 \sum_{i=0}^{56} F_{i+2} * F_{i+1} + \alpha_2 \sum_{i=0}^{56} F_{i+2}^2 + \alpha_1 \sum_{i=0}^{56} F_{i+2} * F_{i+3} + \sum_{i=0}^{56} F_{i+2} * F_{i+4} = 0 \quad (21c)$$

$$\alpha_4 \sum_{i=0}^{56} F_{i+3} * F_i + \alpha_3 \sum_{i=0}^{56} F_{i+3} * F_{i+1} + \alpha_2 \sum_{i=0}^{56} F_{i+3} * F_{i+2} + \alpha_1 \sum_{i=0}^{56} F_{i+3}^2 + \sum_{i=0}^{56} F_{i+3} * F_{i+4} = 0 \quad (21d)$$

155 Now, coefficients of Eq.(21a) can be solved directly to be used to determine  $\mu$ 's in Eq.(18). Next step is using  $\mu$ 's in determining C's and a's. Finally, the approximated form of Fermi-Dirac Integrals of positive half order can be written as follows:

$$F_{\frac{1}{2}}(\eta) = \sum_{i=1}^4 C_i \exp(a_i \eta) \quad (22)$$

where  $C_1 = 5.7955 * 10^3$ ,  $a_1 = -0.0992$   
 160  $C_2 = -8.3584 * 10^3$ ,  $a_2 = -0.111$   
 $C_3 = 7.0383 * 10^3$ ,  $a_3 = -0.1599$   
 $C_4 = -4.4747 * 10^3$ ,  $a_4 = -0.1728$

As shown in Fig.2, the approximated values are very close to the actual values; the Mean Absolute Error defined as  $MAE$  has been calculated to be  
 165  $MAE = 0.0038$

Our goal is not focused on exclusively achieving the smallest error but much more about achieving the simplest approximation of Fermi-Dirac Integrals with as good an accuracy as possible which can be used effectively in calculations, represented in textbooks with convenient forms and used in software programs.  
 170 The accuracy of the proposed approximation and other analytical approximations have been evaluated and depicted in Fig.3

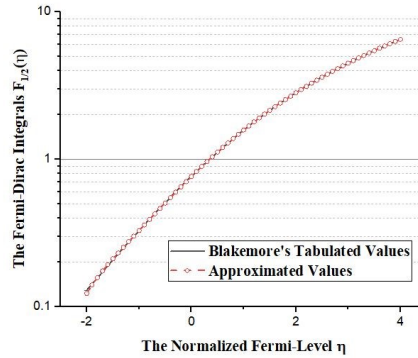


Fig. 2: Approximated and Actual Values of Fermi-Dirac Positive Half-Integral.

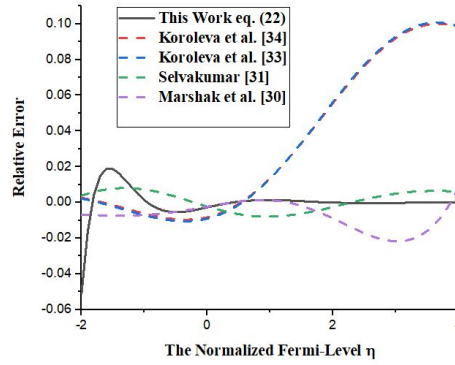


Fig. 3: The Relative Error of the Proposed Approximation and other Analytical Approximations as a function of Fermi-Level Position.

### 3.2. The lower and higher orders of FDI

We can obtain high and low orders of FDI family by integrating and differentiating the proposed approximation. By using the Prony's method we obtain the approximation in the form of a series of exponential functions. Hence it can be easily differentiated and integrated to obtain higher and lower orders of FDI. The quality of the approximation of FDI regarding absolute values can be seen from Fig.2, however what is observed is that the slope and the trend of the curve are very well approximated as well. The quality of this approximation can be assessed when the differentiated and integrated values are also compared with the actual values.

### 3.2.1. The Differentiation

To get lower orders of FDI such as  $F_{-\frac{1}{2}}(\eta)$  and  $F_{-\frac{3}{2}}(\eta)$ , the expression of  $F_{\frac{1}{2}}(\eta)$  needs to be differentiated successively twice. Then the evaluation of the differentiated functions are compared to the actual tabulated values based on the following equation:

$$F_{j-1}(\eta) = \frac{dF_j}{d\eta} \quad (23)$$

The first differentiated function of the approximation is  $F_{-\frac{1}{2}}(\eta) = \frac{dF_{\frac{1}{2}}}{d\eta}$  and can be expressed as shown in the following equation:

$$F_{-\frac{1}{2}}(\eta) = \sum_{i=1}^4 D_i \exp(d_i * \eta) \quad (24)$$

where  $D_1 = -1.1253 * 10^3$ ,  $d_1 = -0.0992$   
 $D_2 = 773.2507$ ,  $d_2 = -0.111$   
 $D_3 = 927.5932$ ,  $d_3 = -0.1599$   
 $D_4 = -574.9186$ ,  $d_4 = -0.1728$

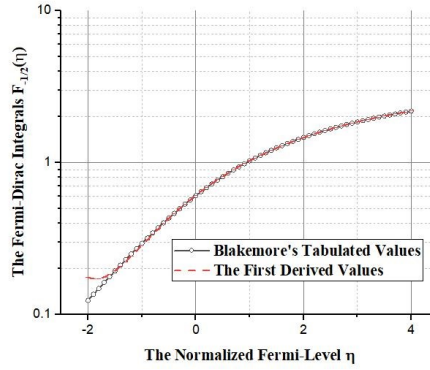


Fig. 4: The First Derivative Function and the Actual Values of Fermi-Dirac Negative Half-Integral ( $-\frac{1}{2}$ ).

The results of using Eq.(24) is then compared to another tabulated function given by Blakemore,  $F_{-\frac{1}{2}}(\eta)$ , as seen in Fig.4. It can be noticed that the differentiated function has very small errors except for the values of  $\eta$  around negative two, which also has occurred for the original approximation for  $F_{\frac{1}{2}}(\eta)$ . It should

be stated that the Mean Absolute Error of differentiated function is still good but somewhat larger than the relative mean absolute error of the original  $F_{\frac{1}{2}}(\eta)$  approximation because of differentiation. The Mean Absolute Error ( $MAE$ ) is 0.0215

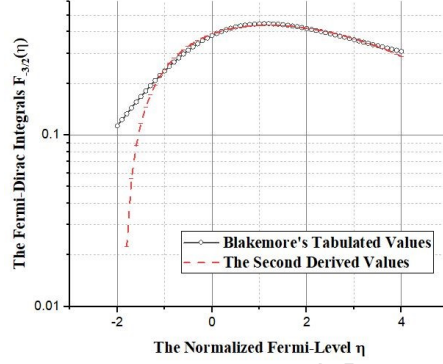


Fig. 5: The Twice Differentiated Approximation and the Actual Values of Fermi-Dirac Negative One and Half-Integral ( $\frac{-3}{2}$ ).

200

The second derivative function can be analytically derived and calculated by differentiating the approximation of the  $F_{\frac{1}{2}}(\eta)$  twice ( $F_{\frac{-3}{2}}(x_k) = \frac{d^2 F_{\frac{1}{2}}}{d\eta^2}$ ). The results can be compared to tabulated  $F_{\frac{-3}{2}}(\eta)$  as shown graphically in Fig.5. The twice-differentiated function can be written as follows:

$$F_{\frac{-3}{2}}(\eta) = \sum_{i=1}^4 B_i \exp(b_i * \eta) \quad (25)$$

205 where  $B_1 = 179.9299$ ,  $b_1 = -0.0992$   
 $B_2 = -1.336301$ ,  $b_2 = -0.111$   
 $B_3 = -102.9464$ ,  $b_3 = -0.1599$   
 $B_4 = 57.0347$ ,  $b_4 = -0.1728$

The values of the twice-differentiated function compared to the actual tabu-  
 210 lated values for the whole range have the Mean Absolute Error to be ( $MAE$ ) = 0.1019 Fig.4 and Fig.5 show the limitations of the differentiation of the proposed approximation for the values of  $\eta$  from -2 to -1

### 3.2.2. The Integration

In order to obtain higher order FDI, we can integrate the expression for  $F_{\frac{1}{2}}(\eta)$ . By integrating the expression twice successively we can obtain  $F_{\frac{3}{2}}(\eta)$  and  $F_{\frac{5}{2}}(\eta)$ . The integration of the approximation can be done based on the following equation:

$$\int F_j(\eta)d\eta = F_{j+1}(\eta) \quad (26)$$

Thus, the first integrated function can be compared to tabulated  $F_{\frac{3}{2}}(\eta)$  as shown in Fig.6, and the resulting expression is:

$$F_{\frac{3}{2}}(\eta) = \sum_{i=1}^4 M_i \exp(m_i * \eta) + K_1 \quad (27)$$

where  $M_1 = -4.4017 * 10^4$ ,  $m_1 = -0.0992$   
 $M_2 = 2.5891 * 10^4$ ,  $m_2 = -0.111$   
 $M_3 = 7.5310 * 10^4$ ,  $m_3 = -0.1599$   
 $M_4 = -5.8417 * 10^4$ ,  $m_4 = -0.1728$

$K_1$  is the constant of the integration

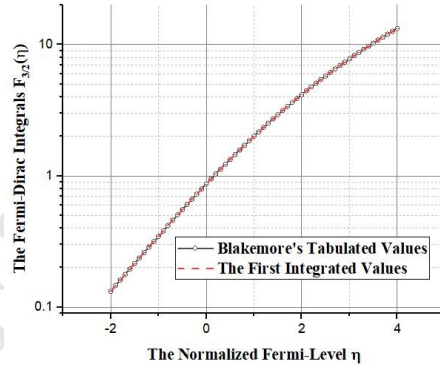


Fig. 6: The First Integrated and Actual Values of Fermi-Dirac Positive One and Half-Integral ( $\frac{+3}{2}$ ).

The appearance of the constant is normal since it appears in the general form of the integration, so the values of the integration without counting the constant were compared to the actual values in order to determine the best choice of the constant. Thus, the constant is the median of the sum of the

differences between the actual values and the integrated values which is equal to  
 230 1233.8648 Additionally, the Mean Absolute Error of the first integrated function  
 $MAE = 9.5425 * 10^{-4}$ .

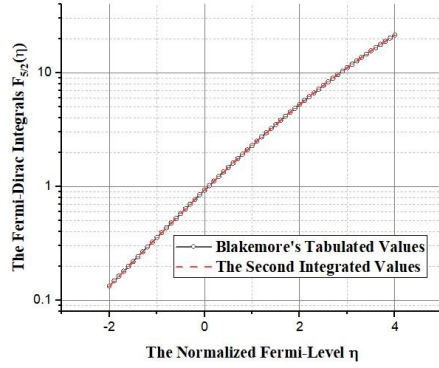


Fig. 7: The Second Integrated Function of the Approximation and the Actual Values of the Fermi-Dirac Positive Two and Half-Integral ( $\frac{+5}{2}$ ).

By twice integrating the approximate function for  $F_{\frac{1}{2}}(\eta)$ , one can assess how good the original approximation is. The twice second integrated function can be expressed as follows:

$$F_{\frac{5}{2}}(\eta) = \sum_{i=1}^4 G_i \exp(g_i * \eta) + K_1 * \eta + K_2 \quad (28)$$

235 where  $G_1 = 2.7529 * 10^5$ ,  $g_1 = -0.0992$   
 $G_2 = -1.4982 * 10^5$ ,  $g_2 = -0.111$   
 $G_3 = -6.7857 * 10^5$ ,  $g_3 = -0.1599$   
 $G_4 = 5.8885 * 10^5$ ,  $g_4 = -0.1728$   
 $K_1 = 1233.8648$

240  $K_2$  is the constant of the integration

By using the same criteria which were used with the first integrated function, the constant can be determined as equal to -35748.68618 Fig.6 depicts how close the twice integrated function is to the tabulated  $F_{\frac{5}{2}}(\eta)$ . The Mean Absolute Error is being calculated to be  $MAE = 9.3129 * 10^{-4}$

245 **4. Applications**

The new approximation can have a significant impact on semiconductor device calculations where the degeneracy plays a key role. One of the fundamental quantities in semiconductor devices is Einstein Relation which is the ratio of diffusivity to the mobility and one can write it as follows:

$$\frac{D_{n,p}}{\mu_{n,p}} = \frac{1}{q} \frac{n,p}{\frac{d_{n,p}}{dE_f}} \quad (29)$$

250 where  $D$  is the Diffusion Coefficient,  $\mu$  is the mobility,  $q$  is the electron charge,  $n$  is the electron carrier density,  $p$  is the hole carrier density, and  $E_f$  is the Fermi-Level.

Eq.(29) is the general form of diffusivity-mobility ratio and can be rewritten based on the Fermi-Dirac Integrals as shown in equation (30) [40]:

$$\frac{D_{n,p}}{\mu_{n,p}} = \frac{kT}{q} \frac{F_{\frac{1}{2}}(\eta)}{F_{-\frac{1}{2}}(\eta)} \quad (30)$$

255 One of the most common approaches uses Boltzmanns distribution to calculate the Einstein relation. The form of the relation can be written as:

$$\frac{D_{n,p}}{\mu_{n,p}} = \frac{kT}{q} \quad (31)$$

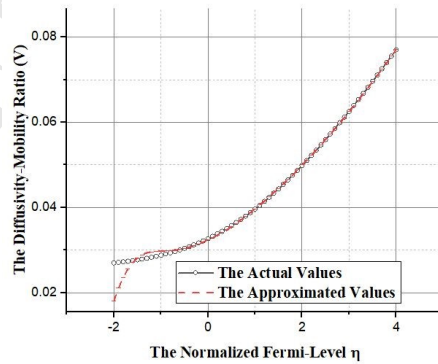


Fig. 8: Einstein Relation Calculated by the New Proposed Approximation and Actual Values.



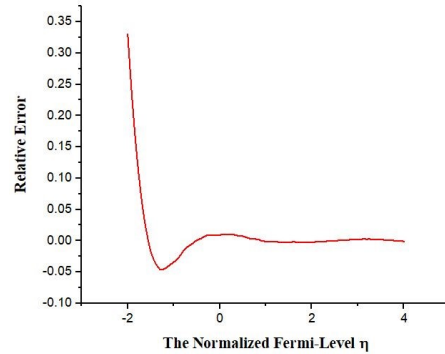


Fig. 9: Relative Error of Einstein Relation Calculated by the Proposed Approximation compared to the Actual Values as a Function of Fermi-Level Position.

With Boltzmann approximation, Eq.(31) shows that the ratio is independent of doping. However the doping concentrations have a significant effect on Einstein relation, and thus Eq.(31) is not useful in heavily doped regions. The accuracy of Einstein Relation by using Eq.(31) will be poorer as we increase the doping and the Fermi-Level comes closer to the conduction band. Without considering bandgap narrowing, an accurate and simple approximation of diffusivity-mobility ratio is required. Therefore, the proposed approximation of Fermi-Dirac Integrals and its first derivative function will be used to calculate the diffusivity-mobility ratio. Using the equation of Li and Lindholm [40], the diffusion-mobility ratio can be computed as shown in Fig.8.

As seen in Fig.8, the Einstein Relation using the new approximation closely matches Li and Lindholms results except for around  $\eta$  values of negative two. The Mean Absolute Error of the Einstein relation calculated by the new approximation is 0.0194. Fig.9 shows the relative error of each normalized Fermi-level position.

## 5. Conclusion

In summary, in this paper, we have presented a new approximation of Fermi-Dirac Integrals which has an excellent accuracy ( $MAE = 0.38\%$ ) and is simple enough to be used in simulations of semiconductor devices. The nature of the

approximation is such that it can be easily differentiated and integrated retaining good accuracy. Apart from testing the accuracy of the differentiated and the integrated functions, they have been employed for the more accurate evaluation of Einstein Relation, especially for degenerate regions. The attractiveness of the approximation is its simplicity and accuracy. It can be applied to many degenerate regions of several modern semiconductor devices. Other semiconductor device quantities such as current density and Quasi-Fermi levels would be impacted by using the new approximation of FDI.

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