**COMPUTATION OF CHEMICAL POTENTIAL AND FERMI-DIRAC INTEGRALS APPLIED TO STUDY THE TRANSPORT PHENOMENA OF SEMICONDUCTORS**

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**Keywords:** Chemical potential, Fermi–Dirac integrals, Gauss–Legendre method

In the given paper, two methods of calculating with high precision accuracy the chemical potential and the integrals of the type called the Fermi–Dirac of different indexes are presented. Our calculations are conclusive with already existing data. These data are essential not only in the study of the theory of solids but at the explanation of the experimental results of investigated transport phenomena in solids, namely, in semiconductors.

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**Methodology**

**Gauss–Legendre method integrals solution**

Functional integral according to Gauss–Legendre method is presented as the sum of \((n-1)\) coefficients:

\[ I \approx C_0 f(x_0) + C_1 f(x_1) + C_2 f(x_1) + C_3 f(x_1) + \ldots + C_{n-1} f(x_{n-1}) \]

Let’s say, at searching of integral we foresee only 2 coefficients, then it follows from (1):

\[ I \approx C_0 f(x_0) + C_1 f(x_1) \]

This expression consists of 4 unknown coefficients \((C_0, C_1, x_0, x_1)\) and, consequently, we need 4 boundary conditions:

\[ f = \text{const} \]

\[ f = x \]

\[ f = x^2 \]

\[ f = x^3 \]

The value of integral may be taken at an arbitrary \([a,b]\) boundary. In our case, we take \([-1,1]\) interval and \(\text{const}=1\). From (3), boundary conditions follow:

\[ \int_{-1}^{1} x^0 \, dx = C_0 f(x_0) + C_1 f(x_1) = 2 \]

\[ \int_{-1}^{1} x \, dx = C_0 f(x_0) + C_1 f(x_1) = 0 \]

\[ \int_{-1}^{1} x^2 \, dx = C_0 f(x_0) + C_1 f(x_1) = \frac{2}{3} \]

\[ \int_{-1}^{1} x^3 \, dx = C_0 f(x_0) + C_1 f(x_1) = 0 \]

The solution of (4) equations gives the following values for \(C\) and \(x\) coefficients:
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\[ C_0 = 1, \quad x_0 = -\frac{1}{\sqrt{3}} \]
\[ C_1 = 1, \quad x_1 = \frac{1}{\sqrt{3}} \]  

(5)

Taking into account the value of two coefficients, the magnitude of integral is:

\[ I = f\left(-\frac{1}{\sqrt{3}}\right) + f\left(\frac{1}{\sqrt{3}}\right) \]  

(6)

Taking into account 4 coefficients, we have to add 4 boundary conditions: \( f = x^4, f = x^5, f = x^6, f = x^7 \). At these boundary conditions calculated coefficients are:

\[ C_0 = \frac{18 - \sqrt{30}}{36}, \quad C_2 = \frac{18 + \sqrt{30}}{36} \]
\[ C_1 = \frac{18 + \sqrt{30}}{36}, \quad C_3 = \frac{18 - \sqrt{30}}{36} \]
\[ x_0 = -\frac{\sqrt{525 + 70\sqrt{30}}}{35}, \quad x_2 = \frac{\sqrt{525 - 70\sqrt{30}}}{35} \]
\[ x_1 = -\frac{\sqrt{525 - 70\sqrt{30}}}{35}, \quad x_3 = \frac{\sqrt{525 + 70\sqrt{30}}}{35} \]  

(7)

These coefficients are needed to be installed into (1) for calculation of the digital value of integral. If we take into account \( n \) coefficients, we will need \( 2n \) boundary conditions.

In general, our task is to solve integral

\[ I = \int_a^b f(x)dx \]

in arbitrary boundaries. For calculation of integral, it is necessary to transfer the boundary \([a,b]\) into \([-1,1]\). Let’s say, the value of the new argument is given by:

\[ x = a_1 + a_2 x_d \]  

(8)

and we search the integral value in the form of

\[ I = \int_{-1}^1 f(x_d)dx_d \]

because integrals values are equal to each other:

\[ I = \int_{-1}^1 f(x_d)dx_d = I = \int_a^b f(x)dx \]

From this it follows new conditions:

\[ a_1 + a_2 = b \]
\[ a_1 - a_2 = a \]
\[ dx = \frac{b-a}{2}dx_d \]

Finally, for integral solved with two coefficients we obtain formula:

\[ \int_a^b f(x)dx = \frac{1}{2} \int_a^b \left[ f\left(\frac{b-a}{2} + \frac{b-a}{2} x_d\right) \right] dx_d \]  

(9)

The more terms we take into account in the formula (1), the more accurate value of integral will be. In general, taking into \( n \) coefficients:

\[ \int_a^b f(x)dx = \sum_{i=1}^n C_i \frac{b-a}{2} f\left(\frac{a+b}{2} + \frac{b-a}{2} x_i\right) \]  

(10)

where \( f(x) \) is an arbitrary function, which is continuous in \([a,b]\) interval and \( C_i \) and \( x_i \) are coefficients found from boundary conditions.

The second way to calculate \( C_i \) and \( x_i \) coefficients is to solve Legendre polynomial equitations:

\[ P_n(x_i) = 0 \]  

(11)

\[ C_i = \frac{2(1-x^2)}{nP_n(x)^2} \]  

(12)

To obtain \( C_i \) and \( x_i \) coefficients, first, we have to generate Legendre polynomials and solve them. We can use MATLAB’s built-in functions to generate polynomials and solve them (legendrePolynomials_1.m), or we can manually generate. Program (legendrePolynomials_2.m) uses polynomials properties:

\[ P_1(x) = 1 \]
\[ P_2(x) = \frac{1}{2}(3x^2 - 1) \]
\[ P_3(x) = \frac{1}{2}(5x^3 - 3x) \]

\[ P_{n+1} = \frac{2n+1}{n+1} x P_n(x) - \frac{n}{n+1} P_{n-1}(x) \]  

(13)

These values are uploaded on the repository (roots_2, weights_2).

Method of undefined integrals solution

Let’s say the integral is not given in limited \([a,b]\) interval, but in \([0,\infty]\) range. We can decompose integral into two parts:

\[ \int_0^\infty f(x)dx = \int_0^1 f(x)dx + \int_1^\infty f(x)dx \]  

(14)

In the second part of integral, we substitute the variable:

\[ t = \frac{1}{x}, \quad dx = -\frac{1}{t^2}dt \]

| \( x = 1 \) | \( t = 1 \) |
| \( x = \infty \) | \( t = 0 \) |
Finally, we obtain formula (15) for approximate calculation of integral:

\[ \int_0^1 f(x)dx = \int_0^1 f(x)dx + \int_0^1 \frac{1}{t} f\left( \frac{1}{t} \right)dt \]  (15)

We can apply (10) formula to the two parts of this integral and solve any integral, which is defined in this range. Taking into account (14) and (15) formulas, we obtain:

\[ \int_0^1 f(x)dx = \sum_{i=1}^{\infty} C_i 0.5 f(0.5 + 0.5x_i) \]  (16)

\[ \int_0^1 \frac{1}{t} f\left( \frac{1}{t} \right)dt = \sum_{i=1}^{\infty} C_i 0.5 \frac{1}{0.5 + 0.5x_i} f\left( \frac{1}{0.5 + 0.5x_i} \right) \]

Calculation of integrals by (16) formulas and their summation give the final meaning of (14) integral.

**Integral Fermi and its derivative**

The general view of integrals of Fermi is given by the formula:

\[ F_{(k)}(\xi) = \frac{1}{\Gamma(k+1)} \int_0^\infty x^k e^{-x} dx \]  (17)

where \( \xi \) is the chemical potential. Many authors do not take into account \( \Gamma(k+1) \) member and introduce integral Fermi as:

\[ F_{(k)}(\xi) = \int_0^\infty x^k e^{-x} dx \]  (18)

The formula for Fermi integrals derivative is given by:

\[ \frac{dF_{(k)}(\xi)}{d\xi} = F_{(k+1)}(\xi) \]  (19)

For gamma function, given in (17) formula, it can be written:

\[ \Gamma(n) = (n-1)! \]

If \( n \) is a natural number,

\[ \Gamma(n+1) = n\Gamma(n) \]

It is also known, that

\[ \Gamma\left( \frac{1}{2} \right) = \sqrt{\pi} \]

\[ \Gamma\left( \frac{3}{2} \right) = \frac{\sqrt{\pi}}{2} \]

The graphics of integrand function in (18) formula for different values of \( k \) and \( \xi \) are given in Fig.1. It is clear from Fig.1 that these functions are decomposable and it is possible to integrate them in certain approximation.

**Figure 1.** Dependence of integrand functions of Fermi integrals of different indexes \((k)\) on \( x \) coefficient (parameter in Gauss–Legendre decomposition) for different values of chemical potential \((\xi)\) according (18) formula.a) \( k = 1 \); b) \( k = 2 \); c) \( k = 3 \); d) \( k = 4 \)
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Finally, the Fermi integrals values have been calculated by the Gauss–Legendre method, where $C_i$ and $x_i$ coefficients have been found from (11) and (12) formulas. The Program has been written in Matlab programming language (Fermi_integral_calculator_1.m) and it uses 100 points of Gauss–Legendre coefficients. The values of calculated Fermi integrals for different parameters $k$ and $\zeta$ are given in Table 1.

Simson’s integral calculation method

Another way to calculate integrals of function $f(x)$, which are defined in $[a, b]$ range, is Simson’s integration method, the general formula of which is given in (20):

$$\int_a^b f(x)dx = \frac{\Delta x}{3} \left[ f(a) + f(b) + 4\sum f(x_i) + f(x_{n}) + \ldots \right]$$

$$\Delta x = \frac{b - a}{n} \quad (20)$$

Results for Simson’s rule are in good agreement with the Gauss–Legendre method.

Error estimation

Finally, we show the advantages of the method presented in the article by calculating the error of implemented calculations.

Gauss–Legendre method error estimation has been done by using (21) formula:

$$\text{Error} = Ef^{(2n)}(\theta)$$

where

$$E = \frac{2^{(2n+1)}(n!)^4}{(2n+1)(2n)!} \quad (22)$$

and $a \leq \theta \leq b$.

The values of $E$ parameter estimated by (22) formula are given for different $n$ in Table 2.

### Table 2. Values of $E$ according to (22) formula for different $n$

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It is clear that the increase of $n$-value decreases the value of $E$ and error goes to nearly zero.

### Conclusion

The chemical potential and Fermi–Dirac integrals are essential for a basic understanding of semiconductors properties. In this paper, there have been calculated Fermi–Dirac integrals by two different ways – Gauss–Legendre and Simson’s methods. Both methods are in good agreement with each other. Our data let reduce the error of calculation of Fermi–Dirac integrals up to $<<1\%$.

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### References


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