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

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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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Introduction

The physical laws of systems consisting of a huge number of particles are of a statistical nature. Statistical distribution determines the probability of having those or other defining states parameters of the particles of the system.¹ One example of systems of the huge number of particles that requires a statistical approach is the solid state, in particular, semiconductors. The distribution of electrons over energies, namely, the Fermi–Dirac distribution, is the most important. The Boltzmann distribution, which is valid for particles obeying classical mechanics, is the limiting case of the Fermi–Dirac distribution. In the state of statistical equilibrium, the ideal electrons gas in solid state obeys the Fermi–Dirac statistics.²,³ Different physical phenomena are differently sensitive to the type of statistical distribution. When considering the transport properties in a solid state, we inevitably collide with integrals of the type called the Fermi–Dirac integrals.²,³ These are certain integrals often encountered not only in the study of the theory of semiconductors but at the explanation of the experimental results of investigated transport phenomena in semiconductors.

In this case, we have to use not only the tables of values of the Fermi integral but also their approximate formulas.⁴ However, the calculation of integrals according to approximate formulas and tables gives a sufficiently high value of error, especially for large and small values of the reduced Fermi level. The error can reach approximately 25%. Using approximations is inconvenient and inaccurate. Therefore, the goal of our paper is to find an appropriate method for calculation of the Fermi–Dirac integrals for application in the study of semiconductors properties with high accuracy <<1%. The presented paper allows also determining a normalization constant, included in the Fermi–Dirac statistics, - the chemical potential with high reasonable accuracy.

Methodology

Gauss–Legendre method integrals solution

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

\[
I \approx C_0 f(x_0) + C_1 f(x_1) + C_2 f(x_2) + C_3 f(x_3) + ... + C_{n-1} f(x_{n-1})
\]  

(1)

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

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

(2)

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

\[
f = \text{const} \quad f = x \quad f = x^2 \quad f = x^3
\]  

(3)

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

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

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

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

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

(4)

The solution of (4) equations gives the following values for \(C\) and \(x\) coefficients:
Finally, for integral solved with two coefficients we obtain formula:
\[
\int_a^b f(x)dx = \frac{1}{2} f\left(\frac{b-a}{2}ight)x_d + \frac{b-a}{2} x_d \int_0^1 f\left(\frac{b-a}{2}x + \frac{b-a}{2} x_d\right)dx_d
\]  (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:
\[
\int_a^b f(x)dx = \sum_{i=0}^{n} C_i \frac{b-a}{2} f\left(\frac{a+b}{2} + \frac{b-a}{2} x_i\right)
\]  (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 equitation:
\[
P_n(x_i) = 0
\]  (11)

\[
P_n(x) = \frac{2(1-x^2)}{[nP_n(x)]^2}
\]  (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, or we can manually generate. Program (legendrePolynomials_2.m) uses polynomials properties:

\[
P_0(x) = 1
\]
\[
P_1(x) = x
\]
\[
P_2(x) = \frac{1}{2}(3x^2-1)
\]
\[
P_3(x) = \frac{1}{2}(5x^3-3x)
\]

\[
P_{n+1} = \frac{2n+1}{n+1} P_n(x) - \frac{n}{n+1} P_{n-1}(x)
\]  (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:
\[
\int_0^\infty f(x)dx = \int_0^1 f(x)dx + \int_0^\infty f(x)dx
\]  (14)

In the second part of integral, we substitute the variable:
\[
t = \frac{1}{x} \quad dx = -\frac{1}{t^2}dt \quad x = 1 \quad t = 1
\]
\[
x = \infty \quad t = 0
\]
Finally, we obtain formula (15) for approximate calculation of integral:

\[ \int_0^\infty f(x)dx = \int_0^1 f(x)dx + \int_1^\infty f(1/t)dt \] (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:

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

\[ \int_1^\infty f(1/t)dt = \sum_{i=0}^n C_i \frac{1}{0.5 + 0.5 x_i} f(0.5 + 0.5 x_i) \]

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:

\[ F_{\psi}(\xi) = \frac{1}{\Gamma(k+1)} \int_0^\infty x^k e^{-x^2 + 1} dx \] (17)

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

\[ F_{\psi}(\xi) = \int_0^\infty x^k e^{-x^2 + 1} dx \] (18)

The formula for Fermi integrals derivative is given by:

\[ \frac{dF_{\psi}(\xi)}{d\xi} = F_{\psi+1}(\xi) \] (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) \( k = 4 \)
Table 1. Fermi integrals calculated using Gauss–Legendre numerical method for different $\xi$ and $\zeta$ values.

| $\xi$ | $\zeta$ | $F_0(\xi,\zeta)$ | $F_1(\xi,\zeta)$ | $F_2(\xi,\zeta)$ | $F_3(\xi,\zeta)$ | $F_4(\xi,\zeta)$ | $F_5(\xi,\zeta)$ | $F_6(\xi,\zeta)$ |
|------|--------|-----------------|-----------------|-----------------|-----------------|-----------------|-----------------|-----------------|
| -10  | -20    | 0.000000        | 0.000000        | 0.000000        | 0.000000        | 0.000000        | 0.000000        | 0.000000        |
| -9   | -19    | 0.000018        | 0.000011        | 0.000020        | 0.000028        | 0.000040        | 0.000049        | 0.000057        |
| -8   | -28    | 0.000359        | 0.000203        | 0.000257        | 0.000300        | 0.000340        | 0.000380        | 0.000421        |
| -7   | -38    | 0.000592        | 0.000335        | 0.000397        | 0.000438        | 0.000478        | 0.000518        | 0.000558        |
| -6   | -48    | 0.001167        | 0.000911        | 0.000982        | 0.001051        | 0.001110        | 0.001168        | 0.001225        |
| -5   | -58    | 0.002649        | 0.001502        | 0.001607        | 0.001708        | 0.001797        | 0.001885        | 0.001970        |
| -4   | -68    | 0.004364        | 0.002476        | 0.002743        | 0.002909        | 0.003062        | 0.003214        | 0.003363        |
| -3   | -78    | 0.011882        | 0.006275        | 0.006937        | 0.007570        | 0.008183        | 0.008792        | 0.009392        |
| -2   | -88    | 0.019442        | 0.011078        | 0.012347        | 0.013371        | 0.014384        | 0.015382        | 0.016370        |
| -1   | -98    | 0.031848        | 0.018150        | 0.021625        | 0.025171        | 0.028766        | 0.032360        | 0.035952        |
| 0    | -108   | 0.052195        | 0.029795        | 0.037311        | 0.044836        | 0.052355        | 0.059863        | 0.067364        |
| 1    | -118   | 0.084849        | 0.048587        | 0.064366        | 0.080144        | 0.095899        | 0.111630        | 0.127341        |
| 2    | -128   | 0.156919        | 0.078889        | 0.102194        | 0.125463        | 0.148690        | 0.171883        | 0.195030        |
| 3    | -138   | 0.218162        | 0.115487        | 0.148505        | 0.181224        | 0.213794        | 0.246227        | 0.278558        |
| 4    | -148   | 0.340412        | 0.183801        | 0.228210        | 0.279283        | 0.338779        | 0.398274        | 0.457770        |
| 5    | -158   | 0.518833        | 0.232603        | 0.298730        | 0.372122        | 0.453617        | 0.535112        | 0.616608        |
| 6    | -168   | 1.067828        | 0.463144        | 0.608098        | 0.754263        | 0.900427        | 1.046581        | 1.192735        |

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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):

$$
\int_a^b f(x)\,dx = \frac{\Delta x}{3} \left[ f(a) + 4(f(x_1) + f(x_3) + \ldots + f(x_{2n-1})) + 2(f(x_2) + f(x_4) + \ldots + f(x_{2n})) \right]
$$

where

$$
\Delta x = \frac{b-a}{n} \tag{20}
$$

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:

$$
\text{Error} = E \int_{\theta}^{(2n)\theta} f^2(\theta) \, d\theta
$$

where

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

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

### Table 2. Values of $E$ parameter estimated by (22) formula for different $n$

| $n$ | $E$     | $n$ | $E$     |
|-----|---------|-----|---------|
| 2   | 0.00741 | 16  | 2.73804E-45 |
| 3   | 6.34921E-5 | 17  | 6.10607E-49 |
| 4   | 2.87946E-7 | 18  | 1.21246E-52 |
| 5   | 8.07929E-10 | 19  | 2.15736E-56 |
| 6   | 1.54087E-12 | 20  | 3.54947E-60 |
| 7   | 2.12743E-15 | 21  | 5.0253E-64 |
| 8   | 2.21126E-18 | 22  | 6.64363E-68 |
| 9   | 1.21051E-21 | 23  | 8.07251E-72 |
| 10  | 6.52065E-28 | 24  | 8.89595E-76 |
| 11  | 2.95829E-31 | 25  | 9.08485E-80 |
| 12  | 1.13949E-34 | 26  | 8.56732E-84 |
| 13  | 3.77297E-38 | 27  | 7.48625E-88 |
| 14  | 1.08539E-41 | 28  | 6.07844E-92 |
| 15  | 2.73804E-45 | 29  | 4.59789E-96 |
| 16  | 3.248E-100  | 30  | 3.248E-100 |

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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