APPROXIMATION OF FERMI-DIRAC INTEGRALS OF DIFFERENT ORDERS USED TO DETERMINE THE THERMAL PROPERTIES OF METALS AND SEMICONDUCTORS

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Summary. In this paper, we obtain a continuous analytical expressions approximating the Fermi-Dirac integrals of orders *j=-1/2, 1/2, 1, 3/2, 2, 5/2, 3* and *7/2* in a convenient form for calculation with reasonable accuracy *(1÷3)%* over a wide range of degeneration. For approximation was used the approach based on the method of least squares. Requirements for the approximation of integrals, the range of variation of order j and η adduced Fermi level are considered in terms of the use of Fermi-Dirac integrals to determine the properties of metals and semiconductors.

1 INTRODUCTION

Fermi-Dirac statistics are widely used in many of the problems associated with semiconductors and metals [1-3]. Interest in the use and calculation of the Fermi-Dirac integrals of different orders originated in the 20s of XX century. By this time the first work done by Sommerfeld and his co-workers [4,5], and Pauli [6] who has investigated problems of electron theory of metals. In these papers to describe degenerate electron gas of metals was used a family of functions, called Fermi-Dirac integrals. Because of the substantial differences in metals and semiconductors in determining its properties the same family of integrals calculated and used differently. First of all, significant differences has the electron gas in metals and semiconductors [2,3,7].

In metals at low temperatures electron gas is degenerate and obeys quantum Fermi-Dirac statistics. The number of valence electrons in the metal, taking part in the electrical conductivity, is almost independent of the temperature, so the carrier concentration is constant and can be characterized by a specific value of the electrochemical potential, called the Fermi energy E_F. As the temperature increases in metals and when $E>E_F$ degeneracy is lifted, and the electron gas of metals obeys the classical Maxwell-Boltzmann statistics and becomes non-degenerate.

Quite different situation is in semiconductors. The number of carriers and its mobility are dependent on temperature, the presence of impurities and defects. At low temperatures in semiconductors the valence band is completely occupied and, according to the Pauli principle, the movement within the valence band is not possible. In this regard, at low temperatures in semiconductors conduction electron concentration is so small that it behave like a gas of non-interacting particles obey the classical Maxwell-Boltzmann statistics and the electron gas is non-degenerate. To move the free carriers from the valence to the unoccupied conduction band requires additional finite energy exceeding the energy band gap, which for

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semiconductors amounts to $E_g<2\text{-}3$ eV. With increasing temperature, the hot electrons give energy to the lattice, the band gap is reduced, and the Fermi level E_F energy increases. The concentration of free charge carriers in the conduction band increases, determined by processes of generation and recombination of electrons from the conduction band and holes from the valence band, which occur continuously and parallel. In this situation, the electron gas degenerates and obeys Fermi-Dirac statistics. In the molten state semiconductors take on the properties of metals. The degeneracy of the electron gas in semiconductors, depending on the intensity of external influence can occur before the substance melts, so the description of the properties of solid-state semiconductors requires the use of both classical and quantum statistics of the electron gas [3,7,8]. The probability that the electron will be in a quantum state with energy E is expressed by the Fermi-Dirac function:

$$f(E,T) = \frac{1}{\left(1 + exp\left(\frac{E - E_F}{k_B T}\right)\right)}, \tag{1}$$

where E_F - Fermi energy, defined as the value of the energy, at which all the states of a system of particles that obey Fermi-Dirac statistics, are occupied, k_B - Boltzmann constant. When the energy is less than the Fermi energy $E<E_F$, the Fermi-Dirac function is equal to 1 ($f(E,T)=1$) and all quantum states are filled with electrons. If $E > E_F$, the Fermi-Dirac function is equal to 0 ($f(E,T)= 0$) and corresponding quantum states are not filled. In semiconductors at low temperatures, the Fermi energy level is between the valence band (E_V) and the conduction band (E_C), for a few k_BT below the conduction band ($(E_F\text{-}E_C)/k_BT<0$), the electron gas behaves like a gas of classical particles and obeys Boltzmann statistics

$$f(E,T) = exp\left(\frac{E_F - E}{k_B T}\right) \tag{2}$$

In view of the importance of location of the Fermi level relative to the bottom of the conduction band and valence band top, especially in the case of non-equilibrium, distribution function of the Fermi-Dirac (1) are in the form [4-7]

$$f(\varepsilon) = \frac{1}{\left(1 + exp(\varepsilon - \eta)\right)} \tag{3}$$

where $\varepsilon=(E\text{-}E_C)/k_BT$ - datum level of the electron (the distance to the bottom of the conduction band), $\eta=(E_F\text{-}E_C)/k_BT$ - datum Fermi level for electrons, which is an indicator of the semiconductor degeneration, E_C - the energy level of bottom of conduction band. In case of violation of thermodynamic equilibrium the Fermi level splits into electron E_{Fe} and hole E_{Fh}, which correspond to the datum Fermi level for electrons $\eta_e=(E_{Fe}\text{-}E_C)/k_BT$ and holes $\eta_h=(E_{Fh}\text{-}E_C)/k_BT$. In this work will be used the electronic component, and thus the index e in the notation will be omitted. In terms of ε and η in [4-7] Fermi-Dirac integral was defined as

$$F_j(\eta) = \int_0^\infty \frac{\varepsilon^j}{1 + exp(\varepsilon - \eta)} d\varepsilon \tag{4}$$

where j - the order of the integral.

In computational practice, usually in semiconductor physics [7-12], the integral (4) is replaced by the related function of the form

$$\mathcal{F}_j(\eta) = \frac{F_j(\eta_c)}{\Gamma(j+1)} = \frac{1}{\Gamma(j+1)} \int_0^\infty \frac{\varepsilon^j}{1+exp(\varepsilon-\eta)} d\varepsilon \,, \qquad (5)$$

where $\Gamma(x)$ – gamma function.

Integral (5) has a number of advantages over the integral (4) described in detail in [9,15], namely:

1. In contrast with Fj, $\mathcal{F}_j$ functions exist for negative integer orders.
2. When using $\mathcal{F}_j$ easier to find integral values with half-integer orders j, and also interpolation of η arguments. The relationships between the function and its derivative are also simplified

$$\mathcal{F}_j'(\eta) = \frac{d}{d\eta}\mathcal{F}_j(\eta) = \mathcal{F}_{j-1}[\eta] \qquad (6)$$

3. In the non-degenerate $\eta<<0$ limits all members of the family $\mathcal{F}_j(\eta)$ are reduced to $\mathcal{F}(\eta) \to e^\eta$ regardless of the order j.

Members of the family $F_j(\eta)$ and related $\mathcal{F}_j(\eta)$ are widely used in the modeling of thermo-physical properties of semiconductors and metals. For such tasks are important integrals of Fermi-Dirac with usually low integer and half-integer indexes $-1/2 \le j \le 7/2$ and $-1 \le j \le 3$ [3,7,11,13,14] and with a range of η changes from the classical Boltzmann limit (η<<0) to a degenerate Fermi-Dirac (η>0). For such a wide range of η there are table values of the integrals of all the above order j. However, when using the Fermi-Dirac statistics in modeling of problems of semiconductors and metals is more convenient not tabular but analytical representation of integrals. It is desirable to have some efficient algorithm for computing integrals, based on the use of relatively simple approximation functions.

The aim of this work is to obtain a continuous analytical expressions approximating the Fermi-Dirac integrals of orders j = -1/2, 1/2, 1, 3/2, 2, 5/2, 3 and 7/2 and in the form convenient for calculations with acceptable accuracy in a wide range of degeneration. To obtain these analytical expressions approximating the Fermi-Dirac integrals are encouraged to use an approach based on the method of least squares.

In the next section we consider briefly previously developed methods of approximation of Fermi-Dirac integrals.

2 OVERVIEW OF METHODS OF WAYS TO APPROACH THE FERMI-DIRAC INTEGRALS

The integral (5), excepting the integral with order cannot be calculated analytically. There are a variety of methods associated with it of approximate calculation of the Fermi integrals and approximations, such as: the expansion in a series [14-23], the numerical quadrature [24-28], recurrence relations and interpolation of table values [29-34], piecewise polynomials and rational functions [34-48].

Mathematical bases of calculating of the Fermi-Dirac integrals developed in the works of A. Sommerfeld [4,5], J. McDougall and E.C. Stoner [29], P. Rhodes [14], R. B. Dingle [9,15] formed the basis for various follow-up procedures of expression $F_j(\eta)$ or $\mathscr{F}_j(\eta)$ with an appropriate number of significant digits. Presentation of the results of the numerical solution of the integrals in the form of tables, beginning with the work of J. McDougall and E.C. Stoner in 1938 [29] for the orders of -1/2, 1/2 and 3/2is one of the main. In [9, 14, 15, 24-27, 29-31] presented tables of Fermi-Dirac integrals for integer and half-integer order of *j=-1/2* to *j=7/2*. The highest accuracy of calculations, less than 10-5%, has numerical integration methods [24-34]. However, in modeling of properties of semiconductors and metals is sufficient accuracy from ± 2% to ± 0,2%, commensurate with typical accuracy of the experimental data to determine the carrier densities in semiconductors [12].

An alternative to numerical methods, more convenient form for calculation is an approximation of the Fermi integrals using analytic functions. In the works of different years [16-20, 23, 38-40, 42-47] analytical representation of integrals Fermi-Dirac mainly based on the expansion of the expression (5) in series. In [12] J. S. Blakemore presented an overview of the analytical approximation methods of Fermi-Dirac integrals (5). Considered methods, primarily for the order *j=1/2*, based on asymptotic expansions of Sommerfeld [4,5]. According to the generalization of [42,43], made in [12], to approximate the integral (5) by a single expression for the range $-\infty<\eta<\infty$ proposed to use expression of the form, well reflecting the asymptotic behavior of the integral

$$\mathscr{F}_j(\eta) \approx \left[e^{-\eta} + \varphi_j(\eta)\right]^{-1} \tag{7}$$

where $\varphi_j(\eta)$ - an arbitrary fitting function. Offered in [42] fitting function for order j=1/2 with error not exceeding 0.4% has the form

$$\varphi(\eta) = 3\sqrt{\pi}/4\left(\nu(\eta)\right)^{3/8}, \tag{8}$$

where $\nu(\eta) = \eta^4 + 50 + 33.6\eta\left\{1 - 0.68\exp\left[-0.17(\eta+1)^2\right]\right\}$.

The approximating function for $\eta\to-\infty$ leads to the asymptote $\left(1/2\sqrt{\pi}\right)exp(\eta)$ and with $\eta\to+\infty$ leads to another asymptote $2/3\,\eta^{3/2}$.

In [43] offers the fitting function for the order *j = 1/2* with accuracy of 0.53%, for the order of *j = 3/2* with an accuracy of 0.63%.

$$\varphi_j(\eta) = 2^{j+1}\Gamma(j+2)\left[(\eta+b) + \left(|\eta-b|^c + a\right)^{1/c}\right]^{j+1} \tag{9}$$

For the order *j=1/2* (i.e. for the function $F_{1/2}(\eta)$ recommended values for the parameters *a*, *b* and *c* were *a=9.60, b=2.13, c=2.40,* so

$$\varphi_{1/2}(\eta) = 3\sqrt{\pi/2}\left[(\eta+2.13) + \left(|\eta-2.13|^{2.4} + 9.6\right)^{5/12}\right]^{3/2} \tag{10}$$

For the *j= +3/2* order recommended parameter values, *a=14.9, b=2.64, c=2.25* so that

$$\varphi_{3/2}(\eta) = 15\sqrt{\pi/2}\left[(\eta+2.64) + \left(|\eta-2.64|^{2.25} + 4.9\right)^{4/9}\right]^{5/2} \tag{11}$$

Among the proposed methods of approximation in the reviews [36,37] highlighted the work of Van Halen's, and of P.D.L. Pulfrey [16], where the results of approximation of the Fermi-Dirac integrals $\mathcal{F}_j(x)$ by short series based on the classic decomposition [9, 10, 19]

$$\mathcal{F}_j(\eta) = 2\eta^{j+1}\sum_{n=0}^{\infty}\frac{t_{2n}}{\Gamma(j+2-2n)\eta^{2n}} + cos(\pi j)\sum_{n=1}^{\infty}\frac{(-1)^{n-1}e^{n\eta}}{n^{j+1}}, \qquad (12)$$

where $t_0 = 1/2, \quad t_n = \sum_{\mu=1}^{\infty}(-1)^{\mu-1}/\mu^n = (1-2^{1-n})\zeta(n)$, a $\zeta(n)$ - is Riemann zeta function.

P. Van Halen and D. L. Palfrey have presented approximations of Fermi-Dirac integrals of the form (5) of orders $j= -1/2, 1/2, 1, 3/2, 2, 5/2, 3, 7/2$. The variation range of η for each order j consists of several - from the classical limit of the Boltzmann $(\eta \le 0)$ to a degenerate Fermi-Dirac $\eta > 4$ (or 5), individually selected range of the transition from the non-degeneracy to the weak degeneration ($0 < \eta \le 4$ *or* $0 < \eta \le 5$). For each of the ranges of changes of η proposed smooth, continuous on an interval approximating expression on the basis of the expansion (12), the error is less than 10^{-5}. The advantage of the method proposed by the authors is that sufficiently high accuracy over a wide range of η and j can be obtained using a simple approximate expressions that are very closely related to the short form of the classical expansions in the series of (12). The disadvantage is the lack of a single analytic expression for the approximation of integrals on the whole interval $-\infty < \eta < \infty$.

One of the common approaches to the approximation of Fermi-Dirac integrals is the use of Chebyshev rational approximations [21,38-40]. In [40] obtained the Chebyshev approximations for $\mathcal{F}_{1/2}(\eta)$, based on the tables of J. McDougall and E.C. Stoner [29]. These approximations were used a polynomial of the fifth degree, with a relative error of less than $5\text{x}10^{-4}$. The approximating expressions formulated for 6 ranges of argument η.

In [38], were presented the Chebyshev rational approximations for Fermi-Dirac integrals $\mathcal{F}_{1/2}(\eta)$ $(j = -1/2, 1/2$ and $3/2)$. The approximating expressions were formulated for three ranges of η: $-\infty < \eta \le 1, \ 1 < \eta \le 4, \ 4 < \eta < \infty$. The maximum relative error vary depending on the function and the interval in question, but not exceed 10^{-9}. Using Chebyshev rational approximations developed in [38], in paper [39] the authors have approximated integrals of Fermi-Dirac of orders $j=0, 1/2, 1, 3/2$ and 2, breaking the range of $-4 \le \eta \le 20$ into two. The relative error of approximation is $5\text{x}10^{-6}$.

Taking into account characteristics of the electron gas in metals in [44,45] were proposed a convenient approximation for the integrals of Fermi-Dirac type (4) of the order $j = k+1/2$, which allows to express the integrals $F_{k+1/2}(\xi)$ through transcendental Gamma function $\Gamma(k+1/2)$ and dimensionless temperature $\xi = \frac{k_B T_e}{E_F} = \frac{1}{\eta}$:

$$F_{k+1/2}(\xi) = A\xi^{-3/2}\left[1+(B/\xi)^2\right]^{k/2}, \qquad (13)$$

where $A = \frac{2}{3}\frac{\Gamma(k+\frac{3}{2})}{\Gamma(\frac{3}{2})}$, $B = \left[A(k+\frac{3}{2})\right]^{-1/k}$ are the coefficients expressed through the Gamma function. In [45] by means of approximation of integrals (13) have been determined the most important thermophysical and thermodynamic characteristics of the electron Fermi gas of

metals such as specific heat, thermal diffusivity and thermal conductivity in a wide temperature range.

Despite the longstanding ongoing work in the field of approximation of Fermi-Dirac integrals you cannot build, especially for semiconductors, common expressions for all interesting orders j. Taking into account the fact that the need to approximate the function on an infinite interval $-\infty<\eta<+\infty$, it is difficult to specify such approximating function, which could meet once both asymptotic behavior (when $\eta << 0$, $\mathcal{F}(\eta) \to e^{\eta}$, when $\eta >> 0$, $\mathcal{F}(\eta) \to \eta^{3/2}$). As a result, the original interval $-\infty<\eta<+\infty$ have to divide in at least two and in each choose its best parameters. As a result, for the construction of acceptable approximation formulas in the range of definition, broken into several intervals in each of them to achieve the accuracy required have to vary the number of terms (usually not exceeding 10). Almost all proposed so far approximations were a set of formulas, each of which is used in one range of values of η. Such approximations are only piecewise smooth and even piecewise continuous. Uniform type of approximating formulas failed to pick up, because the qualitative behavior of the Fermi-Dirac functions for different values of η varies greatly.

Since the investigations of fundamental properties of materials such as metals and semiconductors undergoing various external effects are of interest in several areas of science, particularly in the development of new materials especially with new properties. Solving such problems assumes use of mathematical modeling, the basic mathematical apparatus in which is a system of equations in partial derivatives. Therefore, not only approximating functions of family of integrals (5) or (4), and its derivatives must be continuous, smooth, defined in a wide range of argument η. It is desirable to have a convenient for computing form of approximating functions and an acceptable error of approximation.

3 A SUMMARY OF THE METHOD OF APPROXIMATION THE FERMI-DIRAC INTEGRALS

To obtain continuous analytical expressions approximating the Fermi-Dirac integrals, we used an approach consisting of two stages.

In the first stage all the integrals $\mathcal{F}_j(\eta)$ with indexes $j = -1 / 2, 1/2, 1, 3/2, 2, 5/2, 3$ and $7/2$ were solved numerically using the techniques outlined in [16,29, 30] with a step $\Delta\eta$. The results are presented in tables

$$\varphi_{j,\ell} \approx \mathcal{F}_j(\eta_\ell),\ \ell=0,\ldots,n-1 \qquad (14)$$

for all j. Because of the bulkiness tabulated values of the Fermi-Dirac integrals are omitted. Close to the used discrete integral values can be found in [29,30].

In the second stage was used the least squares method, which allows on the basis of table values to formulate analytical expressions for the approximation of the Fermi-Dirac integrals. The least squares method includes a sequence of the following: definition of the range of the degeneration parameter η, the choice of the approximating function and criteria of approximation.

The range of the degeneration parameter nin the general case should vary from non-degenerate values to strong degeneration $-\infty<\eta<+\infty$. However, the solution of specific problems does not require an infinite interval, each specific statement of characterized by

their own limitations [8, 16-21,24,42,43]. For an acceptable accuracy of determination the thermophysical characteristics of metals and semiconductors we allow limitations on n in the range of $-10 \le \eta \le 10$.

For approximating functions were specified requirements of correct asymptotic behavior in interval of approximation and the minimum error between original and approximating functions.

In accordance with the classical concepts [6], close to the original function on the asymptotic is the function

$$\mathscr{F}_j(x) \approx f_j(x) = \left[exp(P_m(x))\right]_j, \tag{15}$$

where

$$P_{j,m}(x) = ln\left(\mathscr{F}_j(x)\right) = \left[\sum_{i=0}^{m} a_i x^i\right]_j \tag{16}$$

is algebraic polynomial of degree m, where $a_0, a_1, ..., a_m$ are unknown coefficients to be determined, $j = -1/2, 1/2, 1, 3/2, 2\ 5/2, 3$ and $7/2$ - order of Fermi-Dirac integral.

As a criterion permitting one to get the best approximation of the function $P_{j,m}(x)$ given in tabular form by its approximate values, in accordance with [48, 49], was used criterion of the method of least squares.

Using tables (14), we represent function $ln(\mathscr{F}_j(\eta))$ for each order j in tabular form, with $x = \eta_\ell$, $-10 \le \eta_\ell \le 10$

$$y_{j,\ell} = ln(\mathscr{F}_j(\eta_\ell)) = ln(\varphi_{j,\ell}),\ \ell = 0,...,n.$$

According to the criterion of least squares method it is necessary to find such a polynomial $P_{j,m}(x)$ of degree $m<n$, so that value of the standard deviation of $P_{j,m}(\eta_\ell)$ from the function values $y_{j,0}, y_{j,1}, ..., y_{j,n}$ would be minimal

$$\rho\left(P_{j,m}, y_j\right) = \left[\sqrt{\frac{1}{n+1}\sum_{\ell=0}^{n}\left(P_m(\eta_\ell) - y_\ell\right)^2}\right]_j \to min \tag{17}$$

A minimum of standard deviation $\rho\left(P_{j,m}, y_j\right)$ is reached at the same values of a_i $(i= 0, ..., m)$ for each order of j, that minimum of the function [49]

$$\sigma_j(a,y) = \left[\sum_{\ell=0}^{n}\sum_{i=0}^{m}\left(a_i\eta_\ell^i - y_\ell\right)^2\right]_j = \left[\left|P_m(a) - y\right|^2\right]_j \tag{18}$$

with

$$\rho\left(P_{j,m}, y_j\right)^2 = \left[\frac{1}{n+1}\sigma(a,y)\right]_j. \tag{19}$$

Thus, using (17-19) for determining coefficients $[a_0, a_1, ..., a_m]_j$ of the polynomial (16) it is necessary to find the minimum of function (18). The simplest method of solutions is to use the necessary criterion of function extremum $\sigma_j(a,y)$

$$\left[\frac{\partial\sigma(a,y)}{\partial a_i}\right]_j = 0, \quad i = 0,\dots m \tag{20}$$

Calculating the partial derivatives (20), we obtain a system of *m+1* linear algebraic equations for each order j of Fermi-Dirac integral

$$\begin{bmatrix} S_{00}a_0 + S_{01}a_1 + \dots + S_{0m}a_m = T_0 \\ S_{10}a_0 + S_{11}a_1 + \dots + S_{1m}a_m = T_1 \\ \dots\dots\dots\dots\dots\dots\dots\dots\dots \\ S_{m0}a_0 + S_{m1}a_1 + \dots + S_{mm}a_m = T_m \end{bmatrix}_j \tag{21}$$

Where $\left[S_{i,k} = \sum_{\ell=1}^{n} \eta_\ell^{i+k}\right]_j$, $\left[T_i = \sum_{\ell=1}^{n} y_\ell \eta_\ell^{i}\right]_j$, $i = 0,\dots m, \quad k = 0,\dots m.$

Solving this system with respect to ai, we find the coefficients of desired polynomial for each order *j*. The system of equations (21) was solved by the lower relaxation method [48,49].

The function that approximates the integral (5) of the order j, according to (15,16) wil be in the form

$$\mathscr{F}_j(x) \approx f_j(x) = exp(P_{j,m}(x)) = \left[exp(\sum_{i=0}^{m} a_i x^i)\right]_j \tag{22}$$

An error estimate for approximating function (22) is calculated using the standard deviation of the table values (14)

$$\Phi_j(f_j,\varphi_j) = \sqrt{\frac{1}{n+1}\sum_{\ell=0}^{n}\left(f_j(\eta_\ell) - \varphi_{j,\ell}\right)^2} = \sqrt{\frac{1}{n+1}\sum_{\ell=0}^{n}\left(exp(P_{j,m}(\eta_\ell) - \mathscr{F}_j(\eta_\ell)\right)^2}, \tag{23}$$

In addition, also used a number of these estimates [48]:
relative error

$$\delta_\ell\left(f_j(\eta_\ell)\right) = \frac{\left|f_j(\eta_\ell) - \mathscr{F}_j(\eta_\ell)\right|}{\mathscr{F}_j(\eta_\ell)} = \frac{\left|exp\left(P_{j,m}(\eta_\ell)\right) - \mathscr{F}_j(\eta_\ell)\right|}{\mathscr{F}_j(\eta_\ell)}, \quad \ell = 0,\dots,n., \tag{24}$$

maximum relative errov on the interval of η

$$\delta_{max}(f_j) = max\frac{\left|f_j(\eta_\ell) - \mathscr{F}_j(\eta_\ell)\right|}{\mathscr{F}_j(\eta_\ell)} = max\frac{\left|exp\left(P_{j,m}(\eta_\ell)\right) - \mathscr{F}_j(\eta_\ell)\right|}{\mathscr{F}_j(\eta_\ell)}. \tag{25}$$

If the desired relative error in some area η is not reached, the integral will be calculated with step smaller a few times. Further, the procedure of construction of approximating function was repeated.

4 RESULTS OF APPROXIMATION

Using the algorithm (14-25) was performed approximation of Fermi-Dirac integrals of orders *j=-1/2, 1/2, 1, 3/2, 2, 5/2, 3, 7/2* by uniform expressions for each order in range $-10 \le \eta \le 10$. The exponential approximations of integrals were made with the indicators $P_{j,m}(x)$ for *m = 4, 5, 6, 7, 8, 9*.

$$\mathcal{F}_j(x) \approx f_j(x) = exp(P_{j,m}(x)) = \left[exp\left(\sum_{i=0}^{m} a_i x^i \right) \right]_j \qquad (26)$$

The coefficients of polynomials *ai (i=0, ..., m)* in the exponent of approximating functions (26) for *m = 4÷9*, as well as the maximum error in the approximation interval are presented in Appendix 1.

In the graphical presentation approximating functions of Fermi-Dirac integrals for integer and half-integer orders shown in Figure 1.

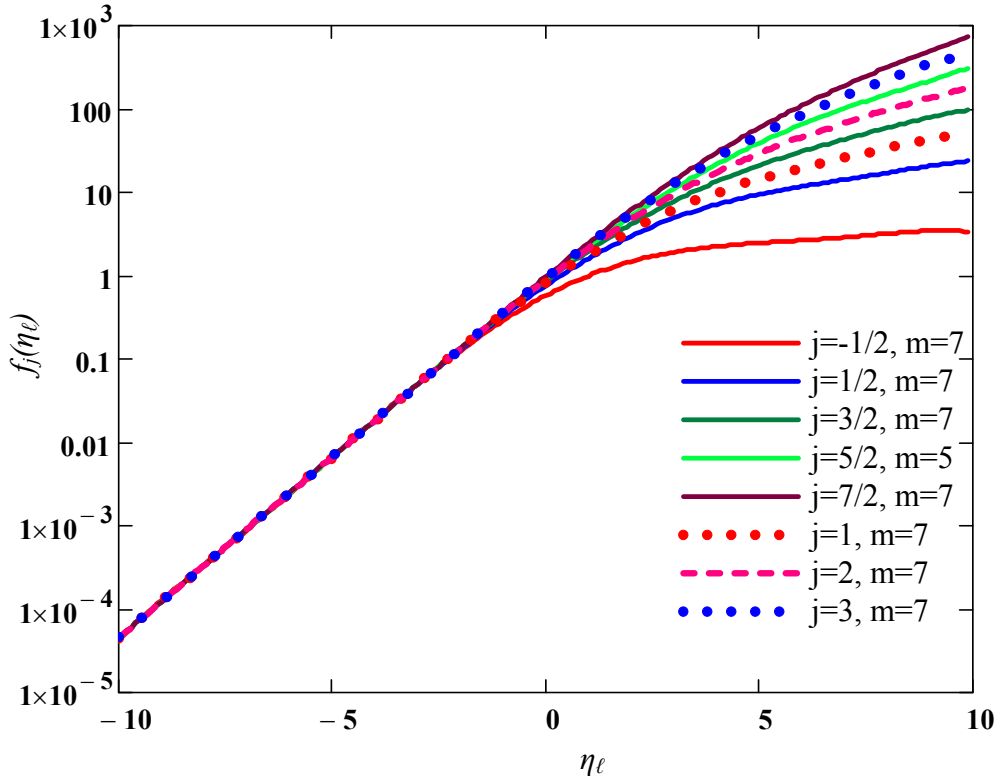

Figure 1. Approximating functions of Fermi-Dirac integrals for integer and half-integer orders.

Figure 2 shows the dependence of the maximum approximation error on the interval *[-10, +10]* on the degree of the polynomial in the exponent of approximating function. The figure shows that the error rate $2{,}0\% \le \delta_{max}(f_j) \le 3{,}0\%$ provided by approximations with polynomials of degree 5th in the exponent for integrals with orders 3/2 and 2, whereas the integrals with the order of 3, 5/2, 7/2 polynomial of the same degree in the exponent of approximation function gives an error of less than 2%. For integrals with order of 1 and 1/2 of

the error from 2% to 3% is provided by approximations with polynomials of 6th and 7th degrees in the exponent, respectively. Thus, the exponential approximation with a small number of terms gives a level of approximation error that commensurate with the accuracy of the experimental data to determine the carrier densities in semiconductors [12].

The relative error does not exceed 3%, is maintained only within the interval of approximation for the integrals as integer and half-integer orders, outside this range the error starts to increase sharply, so extrapolation using the obtained approximating functions leads to large errors [48,49] . In case of necessary to approximate integrals in a wider range of variation of the argument must use outlined approach of approximating in the modified range.

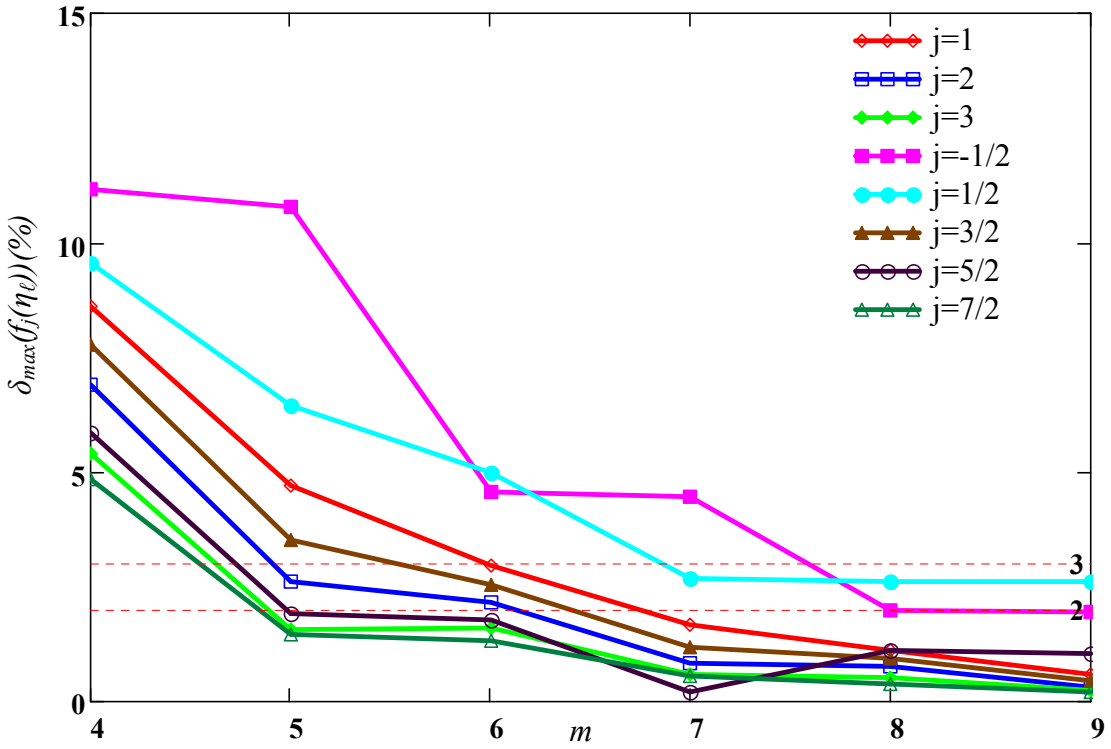

Figure 2. The dependence of the relative error of approximation on the degree of the polynomial in the exponent of approximating function for different orders *j* (in percent).

5 CONCLUSION

In this paper, for the Fermi-Dirac integrals of order *j=-1/2, 1/2, 1, 3/2, 2, 5/2, 3* and *7/2* were obtained continuous analytical expressions common for every order in a wide range of degeneration $-10 \le \eta \le 10$. For approximation was used the approach based on the least squares method. The approximating functions within the approximation interval have an error not exceeding (1÷3)%. Increasing the terms in the exponent can reduce the error, as shown in Figure 2. Common for the entire range of definition continuous analytical expressions simplify calculation of the properties of metals and semiconductors and their further use in mathematical models.

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APPENDIX 1. THE COEFFICIENTS a_i ($i=0, ..., m$) OF THE EXPONENT

$$\mathcal{F}_j(x) \approx f_j(x) = \left[exp(\sum_{i=0}^{m} a_i x^i) \right]_j$$

a_i $(i=0,...,m)$	The order of the Fermi-Dirac integral $j = -1/2$		
	m = 4	m = 5	m = 6
a_0	-0.61546784826395	-0.615467848263953	-0.547817220021095
a_1	0.602676584217057	0.615426846473623	0.615426846473625
a_2	-0.0610134265391913	-0.0610134265391913	-0.0751504337606228
a_3	-0.00043940913385450 8	-0.00103148811525877	-0.0010314881152587
a_4	0.00024962532213125 9	0.00024962532213125 8	0.00067163553382814 3
a_5		$5.30239768412911\times10^{-6}$	$5.30239768412867\times10^{-6}$
a_6			$-3.07965492435977\times10^{-6}$
$\delta_{max}(f_j)$	11,2%	10,8%	4,6%
	m = 7	m = 8	m = 9
a_0	-0.547817220021095	-0.522116216472	-0.520853982328172
a_1	0.62180892681873	0.6218089268187	0.62538029600023
a_2	-0.0751504337606216	-0.0843580232437304	-0.0849911513781025
a_3	-0.0016030745760407	-0.00160307457603949	-0.00222978780816163
a_4	$6.71653533828143\times10^{-4}$	0.00117561624161588	0.00120165913801942
a_5	$1.78158795239303\times10^{-5}$	$1.78158795239198\times10^{-5}$	$4.25661892462514\times10^{-5}$
a_6	$-3.0796549243596\times10^{-6}$	$-1.177259427073\times10^{-5}$	$-1.2129242467151\times10^{-5}$
a_7	$-7.70854081325175\times10^{-8}$	$-7.70854081325727\times10^{-8}$	$-4.26709221627158\times10^{-7}$
a_8		$4.63428174069414\times10^{-8}$	$4.79331492203198\times10^{-8}$
a_9			$1.62622326417778\times10^{-9}$
$\delta_{max}(f_j)$	4,5%	2,0%	1,9%
a_i $(i=0,...,m)$	$j = 1/2$		
	m = 4	m = 5	m = 6
a_0	-0.30031811734647	-0.300318117346469	-0.275999786315936
a_1	0.750669866250104	0.783771806756508	0.783771806756508
a_2	-0.0460276506527707	-0.0460276506527708	-0.0510854399040026
a_3	-0.00103123932933865	-0.00256097963187296	-0.0025609796318731
a_4	0.000155972246039082	0.000155972246039082	0.0003062432905028
a_5		$1.36333739890211\times10^{-5}$	$1.36333739890214\times10^{-5}$
a_6			$-1.09132901270981\times10^{-6}$
$\delta_{max}(f_j)$	9,5%	6,5%	4,98%
	m = 7	m = 8	m = 9
a_0	-0.275999786315927	-0.276775359016042	-0.276775359016034
a_1	0.798663570658078	0.798663570658095	0.799100538145126
a_2	-0.0510854399040039	-0.050808847478201	-0.050808847478213
a_3	-0.00388849436691441	-0.003888494366913	-0.003951991369661
a_4	0.000306243290502822	0.000291173615654	0.000291173615654
a_5	$4.25600395211334\times10^{-5}$	0.000042560039521	0.000045013483446
a_6	$-1.09132901271\times10^{-6}$	-0.000000832583687	-0.000000832583687
a_7	$-1.77355398725066\times10^{-7}$	-0.000000177355399	-0.000000212078781
a_8		-0.000000001373023	-0.000000001373023
a_9			$1.624418649316369\times10^{-10}$
$\delta_{max}(f_j)$	2,7%	2,63%	2,62%

a_i (i=0,…,m)	The order of the Fermi-Dirac integral **j = 3/2**		
	m = 4	m = 5	m = 6
a_0	-0.165160502970019	-0.165160502970019	-0.148659357955996
a_1	0.832956727391009	0.86009920251184	0.860099202511838
a_2	-0.034270731578089	-0.034270731578089	-0.0377026823061288
a_3	-0.00112227522930316	-0.00237661069929918	-0.00237661069929911
a_4	$9.37237799774546\times10^{-5}$	$9.37237799774557\times10^{-5}$	0.000195689835665688
a_5		$1.11789069960535\times10^{-5}$	$1.11789069960533\times10^{-5}$
a_6			$-7.40518675978303\times10^{-7}$
$\delta_{max}(f_j)$	7,8%	3,5%	2,5%
	m = 7	m = 8	m = 9
a_0	-0.14865935795599	-0.144360069633876	-0.144360069633868
a_1	0.871991792148592	0.871991792148618	0.877424534200941
a_2	-0.0377026823061285	-0.0392359371305346	-0.0392359371305399
a_3	-0.00343676637225343	-0.00343676637225409	-0.00422621374149657
a_4	0.000195689835665719	0.000279226655571119	0.00027922665557153
a_5	$3.42797945071527\times10^{-5}$	$3.42797945071525\times10^{-5}$	$6.47830429367779\times10^{-5}$
a_6	$-7.40518675978359\times10^{-7}$	$-2.17484037670981\times10^{-6}$	$-2.17484037670917\times10^{-6}$
a_7	$-1.41636342802288\times10^{-7}$	$-1.41636342802187\times10^{-7}$	$-5.73346207590614\times10^{-7}$
a_8		$7.61117948971013\times10^{-9}$	$7.6111794897629\times10^{-9}$
a_9			$1.624418649316369\times10^{-10}$
$\delta_{max}(f_j)$	1,17%	0,94%	0,44%
a_i (i=0,…,m)	**j = 5/2**		
	m = 4	m = 5	m = 6
a_0	-0.0768619544439604	-0.0768619544439613	-0.0730704871698116
a_1	0.894634070051121	0.919228896777874	0.919228896777872
a_2	-0.025050293646251	-0.0250502936462509	-0.0258425996695149
a_3	-0.00117276343025441	-0.00231486385636026	-0.00231486385636046
a_4	4.63301130675959e-005	4.63301130675965e-005	6.99826081733829e-005
a_5		1.02281466571666e-005	1.02281466571665e-005
a_6			-1.72598705506176e-007
$\delta_{max}(f_j)$	5,9%	1,9%	1,8%
	m = 7	m = 8	m = 9
a_0	-0.0730704871698169	-0.0733183068334995	-0.0733183068335204
a_1	0.928304012988676	0.928304012988668	0.93148132960755
a_2	-0.0258425996695147	-0.0257538162991899	-0.0257538162991905
a_3	-0.00312764170866409	-0.00312764170866535	-0.00359140854603623
a_4	6.99826081733871e-005	6.51231921667828e-005	6.51231921667551e-005
a_5	2.80219216894084e-005	2.80219216894125e-005	4.60217543878372e-005
a_6	-1.72598705506065e-007	-8.87778037750309e-008	-8.87778037731255e-008
a_7	-1.09613010042557e-007	-1.0961301004269e-007	-3.65513428284697e-007
a_8		-4.46856533641514e-010	-4.46856533638775e-010
a_9			1.20258111247753e-009
$\delta_{max}(f_j)$	0,2%	1,1%	1%

a_i (i=0,…,m)	The order of the Fermi-Dirac integral **j = 7/2**		
	m = 4	m = 5	m = 6
a_0	-0.02997411859528	-0.0299741185952794	-0.0346926424591381
a_1	0.93544135494087	0.955222985782662	0.955222985782661
a_2	-0.0176792910519343	-0.0176792910519343	-0.0166979202806328
a_3	-0.00111122289375512	-0.00202539159461124	-0.00202539159461129
a_4	1.11415191089538e-005	1.11415191089541e-005	-1.80158070437197e-005
a_5		8.14726772065816e-006	8.14726772065664e-006
a_6			2.11752277872335e-007
$\delta_{max}(f_j)$	4,9%	1,5%	1,3%
	m = 7	m = 8	m = 9
a_0	-0.0346926424591368	-0.0373504596918224	-0.0373504596918069
a_1	0.961597271258725	0.961597271258719	0.963706845501861
a_2	-0.0166979202806329	-0.015750063149218	-0.0157500631492198
a_3	-0.00259362232608051	-0.00259362232608126	-0.00290017062601322
a_4	-1.80158070437e-005	-6.96582145708335e-005	-6.96582145707411e-005
a_5	2.05290664912205e-005	2.05290664912336e-005	3.23737053040674e-005
a_6	2.11752277872376e-007	1.09844901684079e-006	1.09844901684007e-006
a_7	-7.59153817940072e-008	-7.59153817937321e-008	-2.4355154135472e-007
a_8		-4.70522619149915e-009	-4.70522619148937e-009
a_9			7.84230362046263e-010
$\delta_{max}(f_j)$	0,56%	0,39%	0,22%
a_i (i=0,…,m)	**j = 1**		
	m = 4	m = 5	m = 6
a_0	-0.23355192692012	-0.23355192692012	-0.207827331088282
a_1	0.792171153428796	0.818976492381555	0.818976492381556
a_2	-0.0397736574845399	-0.0397736574845399	-0.0451239253185927
a_3	-0.00104732754616124	-0.00228608293910271	-0.00228608293910271
a_4	0.000123938596448891	0.000123938596448891	0.000282899418192845
a_5		1.10400540045295e-005	1.10400540045283e-005
a_6			-1.15443768473466e-006
$\delta_{max}(f_j)$	8,6%	4,7%	2,9%
	m = 7	m = 8	m = 9
a_0	-0.207827331088279	-0.19995024794072	-0.19995024794071
a_1	0.831283483122959	0.831283483122962	0.837135515120167
a_2	-0.0451239253185932	-0.0479331288039901	-0.0479331288039997
a_3	-0.0033831800769013	-0.00338318007690159	-0.004233555673572
a_4	0.000282899418192857	0.000435954162848029	0.000435954162848
a_5	3.49458993587348e-005	3.49458993587577e-005	0.000067803337479
a_6	-1.15443768473472e-006	-3.78237757884398e-006	-0.000003782377579
a_7	-1.46571706647323e-007	-1.46571706647527e-007	-0.000000611600217
a_8		1.39450739762592e-008	0.000000013945074
a_9			0.000000002175482
$\delta_{max}(f_j)$	1,66%	1,13%	0,64%

a_i (i=0,…,m)	The order of the Fermi-Dirac integral **j = 2**		
	m = 4	m = 5	m = 6
a_0	-0.114298997515236	-0.114298997515235	-0.105264307458867
a_1	0.866488085382162	0.892787019661956	0.892787019661958
a_2	-0.0293596626824282	-0.0293596626824282	-0.0312387208381031
a_3	-0.00115838324848193	-0.00237373615728598	-0.00237373615728595
a_4	6.77236352648342e-005	6.77236352648336e-005	0.000123551985881182
a_5		1.08314860417262e-005	1.08314860417263e-005
a_6			-4.05448028772157e-007
$\delta_{max}(f_j)$	6,9%	2,6%	2,2%
	m = 7	m = 8	m = 9
a0	-0.105264307458862	-0.103707515355261	-0.103707515355258
a1	0.903683099285018	0.903683099285027	0.90840706100056
a2	-0.0312387208381033	-0.031793919471891	-0.031793919471895
a3	-0.00334505871848734	-0.003345058718487	-0.004031511179107
a4	0.000123551985881213	0.000153801053123	0.000153801053123
a5	3.19966920541703e-005	0.000031996692054	0.000058520347408
a6	-4.05448028772211e-007	-0.000000924822523	-0.000000924822523
a7	-1.29768277206364e-007	-0.000000129768277	-0.000000505155302
a8		0.000000002756043	0.000000002756043
a9			0.000000001756124
$\delta_{max}(f_j)$	0,84%	0,78%	0,30%
a_i (i=0,…,m)	**j = 3**		
	m = 4	m = 5	m = 6
a0	-0.114298997515236	-0.114298997515235	-0.105264307458867
a1	0.866488085382162	0.892787019661956	0.892787019661958
a2	-0.0293596626824282	-0.0293596626824282	-0.0312387208381031
a3	-0.00115838324848193	-0.00237373615728598	-0.00237373615728595
a4	6.77236352648342e-005	6.77236352648336e-005	0.000123551985881182
a5		1.08314860417262e-005	1.08314860417263e-005
a6			-4.05448028772157e-007
$\delta_{max}(f_j)$	5,4%	1,56%	1,6%
	m = 7	m = 8	m = 9
a0	-0.105264307458862	-0.052712156661734	-0.052712156661728
a1	0.903683099285018	0.947159393500042	0.95013151782922
a2	-0.0312387208381033	-0.020167390078839	-0.020167390078846
a3	-0.00334505871848734	-0.002891942854199	-0.003323830787203
a4	0.000123551985881213	-0.000017102293591	-0.000017102293591
a5	3.19966920541703e-005	0.000024715803552	0.000041403407348
a6	-4.05448028772211e-007	0.000000667578416	0.000000667578416
a7	-1.29768277206364e-007	-0.000000095051469	-0.000000331229698
a8		-0.000000003210006	-0.000000003210006
a9			0.000000001104882
$\delta_{max}(f_j)$	0,58%	0,51%	0,23%

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