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Analytical Approximation of the Fermi-Dirac Integrals of Half-Integer and Integer Orders[1]

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Abstract—We have obtained continuous analytical expressions approximating the Fermi-Dirac (F-D) 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 (1–4)% in a wide degeneration range in this paper. An approach based on the least squares method for approximation was used. The demands for the approximation of integrals, the range of variation of order j, and the definitional domain are considered in terms of the use of F-D integrals to determine the properties of metals and semiconductors.

Keywords: Fermi-Dirac integrals, analytical approximation

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1. INTRODUCTION

The Fermi-Dirac (F-D) integrals are widely used in the field of statistical physics [1]. Their application is also widely known in condensed matter physics [2], in particular, in the simulation of properties and processes in semiconductors and metals [3]. F-D integrals started being used in the 1920s in classic articles by Pauli [4] and Sommerfeld [5], in which, for the first time, a family of functions called F-D integrals was used to describe the degenerate electron gas of metals. Methods of calculating F-D integrals of various orders and their use remains relevant and widely used today.

An F-D integral is defined [4] as

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

where j is the order (index) of the integral, $\varepsilon = (E - E_C)/(k_B T)$ is the reduced electron energy (the distance to the bottom of the conduction band), $\eta = (E_F - E_C)/(k_B T)$ is the reduced Fermi level for electrons, and E_C is the energy level of the bottom of the conduction band.

In computational practice a different form of the F-D integral is used [6, 7]:

$$\mathscr{F}_j(\eta) = \frac{F_j(\eta)}{\Gamma(j+1)} = \frac{1}{\Gamma(j+1)}\int_0^\infty \frac{\varepsilon^j}{1+\exp(\varepsilon-\eta)}d\varepsilon, \tag{2}$$

where $\Gamma(x)$ is the gamma function. Integral (2) has a number of advantages over integral (1), [6, 7]:

1. Functions $\mathscr{F}_j$ exist for negative integer orders in contrast to F_j.

2. Simplified search for integral values with half-integer orders j, and also interpolation of arguments η using $\mathscr{F}_j$. The relationship between a function and its derivative is also simplified; thus, it is easier to interpolate by Taylor series

$$\mathscr{F}'_j(\eta) = \frac{d}{d\eta}\mathscr{F}_j(\eta) = \mathscr{F}_{j-1}(\eta). \tag{3}$$

[1] The article was translated by the authors.

3. In the nondegenerate limits $\eta \ll 0$, all members of the family $\mathcal{F}_j(\eta)$ reduced to $\mathcal{F}(\eta) \to e^{\eta}$ independent of order j.

For physical applications, the important F-D integrals with integer and half-integer subscripts are usually not high: $-1/2 \le j \le 7/2$ and $-1 \le j \le 3$ [8]. Integral (2), with the exception of the integral with order $j = 0$, cannot be calculated analytically. A variety of methods for approximate calculation and approximation of Fermi integrals [7], including the following methods, are connected with this: expansion in series [9–11], numerical quadrature [12, 13], recurrence relations and interpolation of table values [8, 14–17], and piecewise polynomial and rational functions [18, 19].

Methods for the numerical solution of F-D integrals with the further tabulation of results for orders $j = -1/2$, 1/2, 1, 3/2, 2, 5/2, 3, and 7/2 in the range of changes of η, covering the area of the nondegeneracy and degeneracy of the electron gas, have been presented in [6, 14, 15]. However, in the problems of mathematical modeling, tabular representation of F-D integrals is difficult to use. It is desirable to have some efficient algorithm for computing the integrals based on the use of relatively simple approximation functions.

Taking into account that it is required to approximate the function on an infinite interval $-\infty < \eta < +\infty$, it is difficult to specify such an approximating function which could comply with both the requirements for asymptotic behavior. As a result, the original interval $-\infty < \eta < +\infty$ has to broken into at least two parts and in the best options for each part have to be selected. Therefore, for the construction of acceptable approximation formulas in the defined range split into several intervals, in order to achieve the required accuracy, the number of terms (usually not exceeding 10) have to be varied in each interval.

Almost all the proposed approximations to date [9, 10, 18, 19] were a set of formulas, each of which was used in its range of values of η. Such approximations were piecewise smooth and even piecewise continuous. It was not possible to select a uniform class of approximating formulas because the qualitative behavior of the F-D function for different values of η varies greatly. The aim of this work is to obtain, in a form suitable for the calculation, continuous analytical expressions approximating the F-D integrals of orders $j = -1/2$, 1/2, 1, 3/2, 2, 5/2, 3, and 7/2 with reasonable accuracy over a wide range of degeneracy. The requirements for the approximation of the integrals, and the range of variation of order j and the reduced Fermi level η are considered in terms of the use of F-D integrals to determine the properties of metals and semiconductors.

2. PROBLEM STATEMENT AND ALGORITHM OF THE SOLUTION

The approach used to obtain continuous analytical expressions for the approximation of F-D integrals consists of two stages.

In the first stage, all integrals $\mathcal{F}_j(\eta)$ with indices $j = -1/2$, 1/2, 1, 3/2, 2, 5/2, 3, and 7/2 were solved numerically using the technique described in [9, 14, 15], with step $\Delta\eta$. The results are presented in tabular form:

$$\varphi_{j,\ell} \approx \mathcal{F}_j(\eta_\ell), \quad \ell = 0,\ldots,n-1 \tag{4}$$

for all j. Due to their cumbersomeness, the tabular values of the F-D integrals are omitted. Values close to the used discrete values of the integrals can be found in [14, 15].

At the second stage, we used the least squares method, which based on the table values, allowed us to formulate analytical expressions for the approximation of F-D integrals. The least squares method includes a sequence of the following operations: definition of the range of degeneracy parameter η, the choice of the approximating function, and the choice of approximation criterion. The range of degeneracy parameter η, in general, should vary from nondegenerate values to strong degeneracy $-\infty < \eta < +\infty$. However, to solve specific problems, we do not require an infinite interval; moreover, each specific statement is characterized by its own limitations [9–12, 18, 19]. For determining acceptably accurately the thermophysical characteristics of the metals and semiconductors, η is limited to $-10 \le \eta \le 10$.

For the approximating functions, the following requirements were observed: correct asymptotic behavior in the range of approximation; minimal error between the original and approximating functions.

In accordance with the classical concepts [4], function (5) is close to the original function in terms of asymptotic behavior.

$$\mathcal{F}_j(x) \approx f_j(x) = \left[\exp(P_m(x))\right]_j, \tag{5}$$

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

a_i ($i = 0, ..., m$)	F-D integral orders j		
	$-1/2$	$1/2$	1
a_0	-0.547817220021095	-0.275999786315927	-0.207827331088279
a_1	0.62180892681873	0.798663570658078	0.831283483122959
a_2	-0.0751504337606216	-0.0510854399040039	-0.0451239253185932
a_3	-0.0016030745760407	$-3.8884943669144 \times 10^{-3}$	$-3.38318007690 \times 10^{-3}$
a_4	$6.71653533828143 \times 10^{-4}$	$3.06243290502822 \times 10^{-4}$	$2.828994181929 \times 10^{-4}$
a_5	$1.78158795239303 \times 10^{-5}$	$4.25600395211334 \times 10^{-5}$	$3.494589935874 \times 10^{-5}$
a_6	$-3.0796549243596 \times 10^{-6}$	$-1.09132901271 \times 10^{-6}$	$-1.15443768474 \times 10^{-6}$
a_7	$-7.70854081325175 \times 10^{-8}$	$-1.7735539872507 \times 10^{-7}$	$-1.46571706647 \times 10^{-7}$
	$3/2$	2	$5/2$
a_0	-0.1486593579599	-0.105264307459	-0.0768619544439613
a_1	0.8719917921548592	0.9036830992850	0.919228896777874
a_2	$-3.77026823061 \times 10^{-2}$	$-3.12387208 \times 10^{-2}$	-0.0250502936462509
a_3	$-3.43676637225 \times 10^{-3}$	$-3.34505872 \times 10^{-3}$	$-2.3148638563603 \times 10^{-3}$
a_4	$1.956898356657 \times 10^{-4}$	$1.235519859 \times 10^{-4}$	$4.63301130675965 \times 10^{-5}$
a_5	$3.427979450715 \times 10^{-5}$	$3.199669205 \times 10^{-5}$	$1.02281466571666 \times 10^{-5}$
a_6	$-7.40518675978 \times 10^{-7}$	$-4.05448029 \times 10^{-7}$	
a_7	$-1.41636342802 \times 10^{-7}$	$-1.29768277 \times 10^{-7}$	
	3	$7/2$	
a_0	-0.050898937014924	-0.034692642459137	
a_1	0.947159393500044	0.961597271258725	
a_2	$-2.08140384458 \times 10^{-2}$	$-1.669792028063 \times 10^{-2}$	
a_3	$-2.89194285420 \times 10^{-3}$	$-2.593622326081 \times 10^{-3}$	
a_4	$1.812925912814 \times 10^{-5}$	$-1.80158070437 \times 10^{-5}$	
a_5	$2.471580355196 \times 10^{-5}$	$2.05290664912 \times 10^{-5}$	
a_6	$6.265497388018 \times 10^{-8}$	$2.11752277872 \times 10^{-7}$	
a_7	$-9.50514690624 \times 10^{-8}$	$-7.59153817940 \times 10^{-8}$	

where

$$P_{j,m}(x) = \ln\left(\mathcal{F}_j(x)\right) = \left[\sum_{i=0}^{m} a_i x^i\right]_j \tag{6}$$

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

As a criterion allowing us to obtain the best approximation of the function $P_{j,m}(x)$ given in tabular form by its approximate values, in accordance with [20, 21], the criterion of the least squares method was used.

Using Tables (4), we represent the function $\ln(\mathcal{F}_j(x))$ for each order j in tabular form, with $x = \eta_\ell$, $-10 \le \eta_\ell \le 10$

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

According to the criterion of the least squares method, it is required to find a polynomial $P_{j,m}(x)$ of degree $m < n$ such that the value of the mean-square deviation $P_{j,m}(\eta_\ell)$ from the function values $y_{j,0}, y_{j,1}, \ldots, y_{j,n}$ are minimal:

$$\rho\left(P_{j,m}, y_j\right) = \left[\sqrt{\frac{1}{n+1}\sum_{\ell=0}^{n}\left(P_m(\eta_\ell) - y_\ell\right)^2}\right]_j \to \min. \tag{7}$$

The function that approximates integral (2) of order j, according to (5) and (6) has the form

$$\mathcal{F}_j(x) \approx f_j(x) = \exp\left(P_{j,m}(x)\right) = \left[\exp\left(\sum_{i=0}^{m} a_i x^i\right)\right]_j. \tag{8}$$

The error estimation of function (8) can be computed using the mean-square deviation from the values in Table (4):

$$\Phi_j\left(f_j, \varphi_j\right) = \sqrt{\frac{1}{n+1}\sum_{\ell=0}^{n}\left(f_j(\eta_\ell) - \varphi_{j,\ell}\right)^2} = \sqrt{\frac{1}{n+1}\sum_{\ell=0}^{n}\left(\exp(P_{j,m}(\eta_\ell) - \mathcal{F}_j(\eta_\ell)\right)^2}. \tag{9}$$

Moreover, the following estimates were also used [20]:

—relative error

$$\delta_\ell\left(f_j(\eta_\ell)\right) = \frac{\left|f_j(\eta_\ell) - \mathcal{F}_j(\eta_\ell)\right|}{\mathcal{F}_j(\eta_\ell)} = \frac{\left|\exp\left(P_{j,m}(\eta_\ell)\right) - \mathcal{F}_j(\eta_\ell)\right|}{\mathcal{F}_j(\eta_\ell)}, \quad \ell = 0, \ldots, n, \tag{10}$$

—the maximum relative error on the interval η,

$$\delta_{\max}(f_j) = \max\frac{\left|f_j(\eta_\ell) - \mathcal{F}_j(\eta_\ell)\right|}{\mathcal{F}_j(\eta_\ell)} = \max\frac{\left|\exp\left(P_{j,m}(\eta_\ell)\right) - \mathcal{F}_j(\eta_\ell)\right|}{\mathcal{F}_j(\eta_\ell)}. \tag{11}$$

If the required relative error in some area of η is not reached: $\delta_\ell\left(f_j(\eta_\ell)\right) \geq (1\text{–}4)\%$, the integral was calculated with a significantly smaller step. Then the construction procedure of the approximating function was repeated.

3. APPROXIMATION RESULTS

Using algorithm (4)–(11), we approximated the F-D integrals of orders $j = -1/2$, 1/2, 1, 3/2, 2, 5/2, 3, and 7/2 by individual expressions for each order in the range $-10 \leq \eta \leq 10$. The exponential approximations of the integral were made with factors $P_{j,m}(x)$ for $m = 4, 5, 6, 7, 8, 9$:

$$\mathcal{F}_j(x) \approx f_j(x) = \exp\left(P_{j,m}(x)\right) = \left[\exp\left(\sum_{i=0}^{m} a_i x^i\right)\right]_j. \tag{12}$$

The polynomial coefficients a_i ($i = 0, \ldots, m$) in the exponents of approximating functions (12) are shown in the table.

In the graphical display, the approximating functions of F-D integrals for integer and half-integer orders are shown in Figs. 1 and 2, respectively.

Taking into account the approximation error of the F-D integrals within 4%, the exponent factor $P_{j,m}(x)$ has eight terms ($m = 7$) for the orders $j = -1/2$, 1/2, 1, 3/2, 2, 3, and 7/2. For the order $j = 5/2$, it has six terms ($m = 5$). Increasing the degree m of the polynomial helps reduce the approximation error, but increases the volume of computation, respectively. Figures 3 and 4 show the errors (10) for integer and half-integer orders.

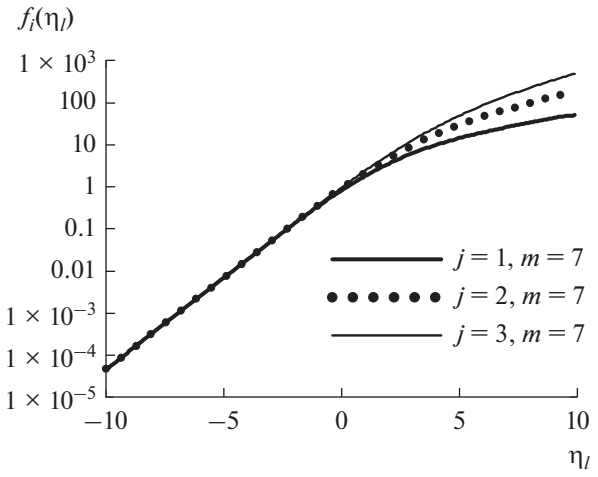

Fig. 1. Approximating functions of F-D integrals of integer orders.

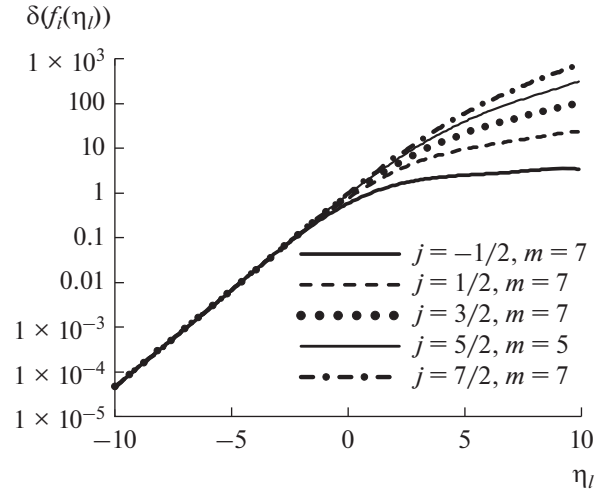

Fig. 2. Approximating functions of F-D integrals of half-integer orders.

Figure 3 shows that the level of approximation error of integrals of orders $j = 2, 3$ does not exceed one-half percent ($\delta_{max}(f_j) \le 1.5\%$) within the approximation interval $-10 \le \eta \le 10$. The integrals of these orders are approximated by analytical expressions with polynomials of degree $m = 7$ in the exponent. For the integral of order $j = 1$ to achieve such a level of approximation error, the degree of the exponent needs to be increased to $m = 8$. Approximation by exponent with a polynomial of degree $m = 7$ for the integral of this order has error $\delta_{max}(f_j) \le 3\%$.

Figure 4 shows the approximation error of the F-D integrals of half-integer orders. The approximating function (exponent degree m = 7) of the integral of order $j = -1/2$ has the greatest error within the approximation interval ($\delta_{max}(f_j) \approx 4\%$). At the end of the approximation interval, at $\eta \approx 10$ the approximation error increases to 4.5%. For the rest of the half-integer orders, the approximation error does not exceed $\delta_{max}(f_j) \le 3\%$ ($j = 1/2, 3/2, 5/2, 7/2$).

Both for the integer and for the half-integer orders (Figs. 3, 4), the level of relative error not exceeding 4% is retained only within the approximation interval; beyond the interval the error begins to increase sharply; thus, extrapolation using the obtained approximating functions leads to large errors [21]. If we are required to approximate integrals in a wider range of variation of the argument, it is necessary to use the outlined approximating approach in a modified range.

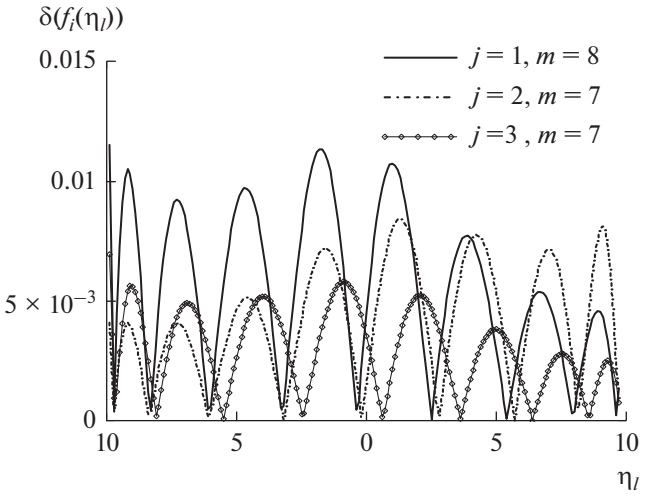

Fig. 3. Relative error in range of $\delta(f_j(\eta_\ell))$ of approximating functions (integer orders).

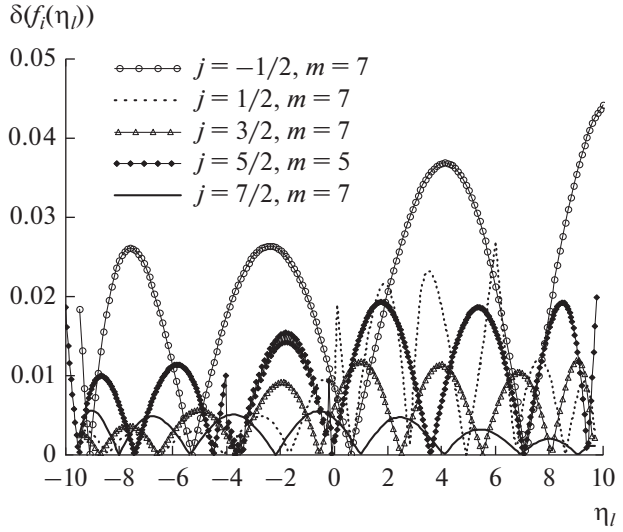

Fig. 4. Relative error in range of $\delta(f_j(\eta_\ell))$ of approximating functions (half-integer orders).

4. CONCLUSIONS

In this paper, continuous analytical expressions specific for each order in a wide range of degeneracy $-10 \le \eta \le 10$ have been obtained for F-D integrals of orders $j = -1/2$, 1/2, 1, 3/2, 2, 5/2, 3, and 7/2. The approach based on the least squares method was used for approximation. The approximating functions have the correct asymptotic behavior in the approximation range, the approximation error within which does not exceed (1–4)%. The exponential form of representation of approximating functions with algebraic polynomial in the exponent allows us to find a reasonable compromise between the approximation accuracy and computational simplicity. Increasing the terms in the exponent allows us to reduce the error, as shown in the table. Continuous analytical expressions that are specific for the entire domain of definition simplify the calculation of the properties of metals and semiconductors, and its further use in mathematical models.

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