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Unified treatment for accurate and fast evaluation of the Fermi–Dirac functions

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A new analytical approach to the computation of the Fermi-Dirac (FD) functions is presented, which was suggested by previous experience with various algorithms. Using the binomial expansion theorem, these functions are expressed through the binomial coefficients and familiar incomplete Gamma functions. This simplification and the use of the memory of the computer for the calculation of binomial coefficients may extend the limits to large arguments for users and result in speedier calculation, should such limits be required in practice. Some numerical results are presented for significant mapping examples and they are briefly discussed.

Keywords: statistical, semiconductors, plasma physics, nuclear physics
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1. Introduction

The calculation of many quantities in solid state physics, nuclear physics, astrophysics and in particular the electron density and total energy, local magnetic moments and susceptibilities, is reduced to the computation of the Fermi–Dirac (FD) functions.[1−12] Also, this function appears in the plasma theory,[13] which is exploited in other work.[14−20] The FD functions determines, for instance, the charge-density distribution of nuclei and nuclear Woods–Saxson potential, in which cases ($\eta = R/a$) R denotes the nuclear radius and the 'diffuseness' of its surface.[21−23]

The different methods used by various authors to solve the problems have resulted in a wide range of different calculation methods in this category. These methods have been given in Refs. [24]–[55] and more recently in Refs. [55]–[62]. We note that, in Refs. [60]–[69] using binomial expansion theorems the FD functions have been expressed through the familiar hypergeometric functions and Bernoulli numbers in the restricted range of parameter η, respectively. In spite of the all developments of FD functions so far, analytical evaluation of the FD integrals as a function of α and μ is still one of the main problems in physics. We note that, most of the published approximations for FD functions involve many short intervals of η and different expressions are used for each of them.

As shown in the literature, the great progress of applied mathematics and powerful computer, significant progress has been made in several quarters of long standing problems of theoretical and applied physics. With this spirit in mind, an attempt is made in this paper to obtain general analytical expressions for FD functions arbitrary values of parameter α and μ. The new analytical approach method for the evaluation of FD functions is conceptually simpler than existing methods. The formulas by which the FD functions are expressed are uniform and their application to the calculation of problems arising various branches of physics presents no difficulties using a computer. Moreover the formulas can be easily implemented with an algebraic computer language. The results of this calculation have been compared with those obtained according to one of the formulas employed previously.

For the FD functions the new formulas ensure a reasonable high precision when η varies in the range $-\infty < \eta < 0$. The methods were shown to give satisfactory accuracy. Moreover, the general expressions proposed to approximate FD functions in the range $0 < \eta < \infty$ enables us to increase this accuracy.

2. General definition and binomial series expansion formulas

The FD functions are defined as

$$F_\alpha(\eta) = \int_0^\infty \frac{t^\alpha}{1 + \mathrm{e}^{t-\eta}} \mathrm{d}t, \tag{1}$$

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where η varies in the range $-\infty < \eta < \infty$ and the parameter α takes arbitrary integer and noninteger values. Normally in semiconductor physics a related function of the form

$$\bar{F}_\alpha(\eta) = \frac{1}{\Gamma(\alpha+1)} \int_0^\infty \frac{t^\alpha}{1+\mathrm{e}^{t-\eta}} \mathrm{d}t. \tag{2}$$

For the evaluation of FD function (Eq. (1)), we use the following binomial expansion theorem for an arbitrary real n and $|x| > |y|$ (see Refs. [63]–[65]):

$$(x \pm y)^n = \sum_{m=0}^{\infty} (\pm 1)^m \, f_m(n) \, x^{n-m} \, y^m, \tag{3}$$

where $f_0(n) = 1$ and

$$f_m(n) = \begin{cases} \dfrac{n(n-1)\ldots(n-m+1)}{m!}, & \text{for integer } \ n, \\ \dfrac{(-1)^m \Gamma(m-n)}{m!\Gamma(-n)}, & \text{for noninteger } \ n. \end{cases} \tag{4}$$

For $m < 0$ the binomial coefficient $f_m(n)$ occuring in Eq. (3) is zero and the positive integer n terms with negative factorials do not contribute to the summation. For fast calculations for the positive integer values of n, the binomial coefficients are stored in the memory of the computer. For the binomial coefficients we use the following recurrence relation:[64]

$$f_m(n) = f_m(n-1) + f_{m-1}(n-1). \tag{5}$$

In order to put these coefficients into or to get them back from the memory, the positions of certain coefficients $f_m(n)$ are determined by relation:[64]

$$f(n,m) = n(n+1)/2 + m + 1. \tag{6}$$

Taking into account Eq. (3) we obtain for the function $(1+\mathrm{e}^{t-\eta})^{-1}$ occurring in Eq. (1) the following series expansion relations:

$$\frac{1}{(1+\mathrm{e}^{t-\eta})} = \lim_{N\to\infty} \sum_{i=0}^{N} f_i(-1) \begin{cases} \mathrm{e}^{-(1+i)(t-\eta)}, & \text{for} \quad t \geq \eta, \\ \mathrm{e}^{(t-\eta)i}, & \text{for} \quad t \leq \eta. \end{cases} \tag{7}$$

3. General expressions for the Fermi–Dirac functions

Now we move on to the determination of expressions for the FD functions in terms of binomial coefficients, and incomplete Gamma functions. Then, taking into account Eqs. (7) in Eq. (1) we obtain, for the FD functions, the following simply structured formulas:

$$\begin{aligned} F_\alpha(\eta) = {} & \frac{\eta^{\alpha+1}}{\alpha+1} + \lim_{N\to\infty} \sum_{i=1}^{N} f_i(-1) K_i(\alpha,\eta) \\ & + \lim_{N'\to\infty} \sum_{j=0}^{N'} f_j(-1) \mathrm{e}^{\eta(1+j)} \frac{\Gamma(\alpha+1, \eta(j+1))}{(j+1)^{\alpha+1}}, \quad \text{for} \ \ 0 < \eta < \infty \end{aligned} \tag{8}$$

and

$$F_\alpha(\eta) = \lim_{L\to\infty} \sum_{i=0}^{L} f_i(-1) \mathrm{e}^{-|\eta|(i+1)} \frac{\Gamma(\alpha+1)}{(i+1)^{\alpha+1}}, \quad \text{for} \quad -\infty < \eta \leq 0. \tag{9}$$

The quantities $K_i(\alpha,\eta)$ in Eq. (8) determined by the relation[68]

$$K_i(\alpha,\eta) = \int_0^\eta t^\alpha \mathrm{e}^{(t-\eta)i} \mathrm{d}t. \tag{10}$$

Using the binomial expansion theorems we can evaluate $K_i(\alpha,\eta)$ integrals. Then, we obtain finally for $K_i(\alpha,\eta)$ integrals the following relation in terms of binomial coefficients and incomplete Gamma functions:

$$K_i(\alpha,\eta)=\begin{cases}\sum\limits_{j=0}^{\alpha}(-1)^j f_j(\alpha)\eta^{\alpha-j}\dfrac{\gamma(j+1,i\eta)}{i^{j+1}}, & \text{for integer } \alpha>0,\\ \lim\limits_{M\to\infty}\sum\limits_{j=0}^{M}(-1)^j f_j(\alpha)\eta^{\alpha-j}\dfrac{\gamma(j+1,i\eta)}{i^{j+1}}, & \text{for noninteger } \alpha.\end{cases} \tag{11}$$

We can evaluate the $K_i(\alpha,\eta)$ integrals using alternative formulas:
for noninteger α

$$K_i(\alpha,\eta)=\mathrm{e}^{-\eta i}\sum_{k=0}^{\infty}\frac{\eta^{\alpha+k+1}}{(\alpha+k+1)\Gamma(k+1)}i^k; \tag{12}$$

for positive integer α

$$K_i(\alpha,\eta)=\frac{\eta^{\alpha}}{i}+\sum_{k=1}^{\alpha}(-1)^k\frac{\alpha!}{(\alpha-k)!i^{k+1}}\eta^{\alpha-k}. \tag{13}$$

In Eqs. (8), (9) and (11), the indices N, N', L and M are upper limits of summations, respectively. The quantities $\Gamma(\alpha)$, $\Gamma(\alpha,x)$ and $\gamma(\alpha,x)$ in Eqs. (8), (9) and (11) are well known familiar functions defined by[63]

$$\Gamma(\alpha)=\int_0^{\infty}t^{\alpha-1}\mathrm{e}^{-t}\mathrm{d}t, \tag{14}$$

$$\gamma(\alpha,x)=\int_0^{x}t^{\alpha-1}\mathrm{e}^{-t}\mathrm{d}t, \tag{15}$$

$$\Gamma(\alpha,x)=\int_x^{\infty}t^{\alpha-1}\mathrm{e}^{-t}\mathrm{d}t, \tag{16}$$

$$\Gamma(\alpha)=\gamma(\alpha,x)+\Gamma(\alpha,x). \tag{17}$$

These functions, Eqs. (14)–(17), have already been investigated by numerous authors with different algorithms (see, e.g., Refs. [63]–[67] and references therein). In our paper,[66] for direct calculation of the complete and incomplete Gamma functions $\Gamma(\alpha)$, $\gamma(\alpha,x)$ and $\Gamma(\alpha,x)$, the upward and downward recursion, and analytical relations were derived.

4. Numerical calculations and discussion

In this paper a series analytical approach to evaluation of the FD functions have been presented. The numerical implementation of the algorithms was also discussed. On the basis of formulas obtained in this study we constructed a program for computation of the FD functions using Maple 7.0 international mathematical software.

The examples of computer calculation for the FD functions are shown in Tables 1, 2 and 3. As can be seen in Tables 1, 2 and 3, the calculated values of FD functions show a good rate of convergence with literature in the range of parameters $-\infty<\eta\leq 0$ and arbitrary real values α. As will be clear from our tests that for $0<\eta\leq\infty$, the formulas (Eq. (8)) obtained yield low accuracy for arbitrary values of integral parameter α. Greater accuracy is attainable by the use of more terms of expansion Eq. (9). Moreover, the general expression proposed to approximate FD functions in the range $-\infty<\eta\leq 0$ enables us to high accuracy.

Table 1. The comparative values of the FD functions for $\alpha\leq 0$.

α	η	Eqs. (8) and (9)	Ref. [43]
0.5	−4	$1.61277379439837770554415 4\times10^{-2}$	$1.61277379439837771\times10^{-2}$
–0.5	−4	$3.20493740378828291545290 1\times10^{-2}$	$3.20493740378828291\times10^{-2}$
1.0	−4	$1.82324489699830256703316 8\times10^{-2}$	$1.82324489699830257\times10^{-2}$
1.5	−4	$2.42694053348685870238157 4\times10^{-2}$	$2.42694053348685870\times10^{-2}$
2.0	−4	$3.65478637632424012686148 9\times10^{-2}$	$3.65478637632424013\times10^{-2}$
4.5	−4	$9.58304173823797922249170 3\times10^{-1}$	$9.58304173823797922\times10^{-1}$
5.0	−4	2.19724868233256871266 7	2.19724868233256871
0.5	−3	$4.33663675504155648413078 2\times10^{-2}$	$4.33663675504155648\times10^{-2}$
−0.5	−3	$8.52597012332688621959556 2\times10^{-2}$	$8.52597012332688622\times10^{-2}$
1.0	−3	$4.91807203388242266310615 6\times10^{-2}$	$4.91807203388242266\times10^{-2}$
1.5	−3	$6.56117388063754437141550 8\times10^{-2}$	$6.56117388063754437\times10^{-2}$
2.0	−3	$9.89634029095922634644110 0\times10^{-2}$	$9.89634029095922635\times10^{-2}$

Table 1. (*Continued*).

α	η	Eqs. (8) and (9)	Ref. [43]
4.5	−3	2.603141667351258155728957	2.60314166735125816
5.0	−3	5.969820680488160124924906	5.96982068048816012
0.5	−2	$1.14587823925263069890484 7\times10^{-1}$	$1.14587823925263070\times10^{-1}$
−0.5	−2	$2.19191607586179700098312 3\times10^{-1}$	$2.19191607586179700\times10^{-1}$
1.5	−2	$1.75800988854012886371579 3\times10^{-1}$	$1.75800988854012886\times10^{-1}$
4.5	−2	7.06294038379063542422481	7.06294038379063354
0.5	−1	$2.90500896169917553439244 4\times10^{-1}$	$2.90500896169917553\times10^{-1}$
−0.5	−1	$5.21150383107991239577683 1\times10^{-1}$	$5.21150383107991240\times10^{-1}$
1.5	−1	$4.60848806290101658548012 3\times10^{-1}$	$4.60848806290101659\times10^{-1}$
4.5	−1	$1.91050680652288268476424 2\times10^{1}$	$1.91050680652288268\times10^{1}$
0.5	0	$6.78527202571147595120930 8\times10^{-1}$	$6.78093895153101007\times10^{-1}$
1.5	0	1.15281024025788902202040 2	1.15280383708836140
2	0	1.80308631091718833262435 0	1.80308535473939143
4.5	0	$5.12905053034445306850184 8\times10^{1}$	$5.12905053032034984\times10^{1}$

Table 2. The comparative values of the FD functions for $-\infty < \eta \leq 0$.

α	η	Eq. (9)	Ref. [51]
−5.5	−5.0	$5.75254456916562216291629 3\times10^{-3}$	5.75254457×10^{-3}
−5.5	–50	$1.92874984796391778298156 8\times10^{-22}$	1.92874985×10^{-22}
−0.5	−50	$1.92874984796391778297627 9\times10^{-22}$	1.92874985×10^{-22}
−0.5	−0.5	$4.31231441926397086871103 5\times10^{-1}$	4.31231442×10^{-1}
1.5	−50	$1.92874984796391778303269 7\times10^{-22}$	1.92874985×10^{-22}
10.5	−5.0	$6.73793132498542830616933 8\times10^{-3}$	6.73793132×10^{-3}
10.5	−50	$1.92874984796391778297379 9\times10^{-22}$	1.92874985×10^{-22}
10.5	−0.5	$6.06404354872261498855909 2\times10^{-1}$	6.06404355×10^{-1}
0.5	−50	$1.92874984796391778303269 7\times10^{-22}$	1.92874985×10^{-22}
0	−1	$3.32616875182228340489950\times10^{-1}$	3.3261687×10^{-1}
0	−0.1	$6.443966600779669385297\times10^{-1}$	6.44396660×10^{-1}
55.5	−70	$3.75449735908646807656774\times10^{-31}$	
75.5	−86.4	$2.99886395047261930128471 3\times10^{-38}$	
−85.5	−94.6	$8.23648689858066523409706 0\times10^{-42}$	
−7.5	−114.6	$1.69766648071772644344670 2\times10^{-50}$	
−107.5	−135.2	$1.92037501378830856958289 8\times10^{-59}$	

Table 3. The comparative values of the FD functions.

α	η	Eqs. (8) and (9)	Refs. [39] and [41]
−0.5	1.5	2.25794	2.21436
0.5	5.0	7.86004	7.837976
1	5.0	1.41482×10^{1}	1.4138208×10^{1}
2	5.0	5.83771×10^{1}	5.8129472×10^{1}
1	10	5.16648×10^{1}	5.1644889×10^{1}
5	5.0	1.08276×10^{4}	1.0821408×10^{4}
2	10	3.66431×10^{2}	3.6623211×10^{2}

Table 4 lists partial summations corresponding to progressively increasing upper summation limit (denoted L) for this expression. As can be seen from Table 4, Eq. (9) displays the most rapid convergence to the numerical result, with twenty fourth digits stable and correct by the thirteenth terms in the infinite summation.

Table 4. Convergence of derived expression for $F_{-11/2}(-5.0)$ as a function of summation limits L.

L	Eq. (9)
5	–3.45265431267226116696147 0$\times 10^{-4}$
7	–3.45265431504668161412023 2$\times 10^{-4}$
8	–3.45265431504701978227907 3$\times 10^{-4}$
9	–3.45265431504701612153800 8$\times 10^{-4}$
10	–3.45265431504701615941397 1$\times 10^{-4}$
11	–3.45265431504701615903645 1$\times 10^{-4}$
12	–3.45265431504701615904009 8$\times 10^{-4}$
13	–3.45265431504701615904006 4$\times 10^{-4}$
14	–3.45265431504701615904006 4$\times 10^{-4}$
15	–3.45265431504701615904006 4$\times 10^{-4}$

In Fig. 1, we present the convergence of the series, in Eq. (9) for $L' < L$. Here L is upper limit of the indice i. The series accuracy $\Delta f = f_L - f'_L$ is shown in Fig.1, where the quantities $f = f_L$ are the values of integral for $L = L'$. We see that the convergence series of our established formulas with respect to α and η is rapid. It is demonstrated that the general analytical relations derived in Section 3, present a simple and precise tool for calculating the FD functions.

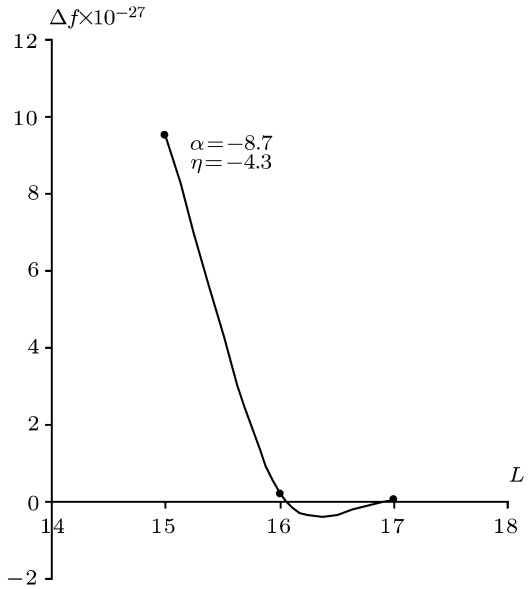


Fig. 1. The convergence of series in Eq. (9) for the FD function.

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