New Astronomy 97 (2022) 101874

Contents lists available at ScienceDirect

New Astronomy

journal homepage: www.elsevier.com/locate/newast

The general analytical expression for computation of generalized relativistic Fermi-Dirac functions

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ARTICLE INFO

Keywords:
Relativistic Fermi-Dirac (FD) functions
Semiconductor
Stellar matter physics
Thermodynamic properties

ABSTRACT

In this paper, general sufficiently analytical formulae are developed for the arbitrary order generalized relativistic Fermi-Dirac (FD) functions. Analytical assessment of relativistic FD function is very important for various fields of physics especially in the theory of relativistic nondegenerate and degenerate electron gas systems. One of the more appropriate and correct approximations is based on a binomial expansion method and incomplete Gamma functions that have been used in the calculations of the generalized relativistic FD functions. Note that, the established expression in special cases of specific values of parameters becomes the evaluation formulae of other type FD functions. Calculation results of the generalized relativistic FD functions are compared with the other approximations methods and available numerical approaches and demonstrated satisfactory agreement.

1. Introduction

The generalized relativistic FD functions are of remarkable significance in the implementation of quantum mechanics to the investigation of physical and chemical properties of gases and solids, and to the stellar matter physics (Zmmermann, 1987; Clayton, 1968; Cox and Giuli, 1968). The FD function is suitable essentially in the determination of the concentration of electrons and holes, and other related physical properties in the conduction and valence bands of semiconductors (Kovetz et al., 1972; Kovetz and Shaviv, 1973; Shaviv and Kovetz, 1972; Stolzmann and Blöker, 1996, 2000; Garoni and Frankel, 2001). Also, the calculation of generalized relativistic FD functions demonstrates the very demanding part of carrying out the evaluation of the thermodynamic properties of fully ionized stellar matter (Zmmermann, 1987; Clayton, 1968; Cox and Giuli, 1968; Kovetz et al., 1972; Kovetz and Shaviv, 1973; Shaviv and Kovetz, 1972; Stolzmann and Blöker, 1996, Garoni et al., 2001; Stolzmann and Blöker, 2000). The various efficient methods used for calculating thermodynamic properties for stellar matter can be found in works (Hubbard and DeWit, 1985; Ebeling, 1990; Baiko and Yakovlev, 2019; Fortaine and Graboske, 1977; Fehr and Kraeft, 1995; Straniero, 1988; Rosenfeld, 1980; Blinnikov et al., 1996; Apfelbaum, 2012, 2015, 2018, 2020, 2021). As far, many approaches have been proposed in the literature for the calculation of the basic FD functions (Sagar, 1991; Gautschi and Milovanovic, 1985; Goano, 1993, 1995; Guseinov and Mamedov, 2010; Aymerich-Humet et al., 1983). Unfortunately, using the method of numerical integration, some works are presented in the form of numerical values of the generalized relativistic FD functions for a limited range of parameters (Kovetz et al., 1972; Kovetz and Shaviv, 1973; Shaviv and Kovetz, 1972; Stolzmann and Blöker, 1996, Garoni et al., 2001; Stolzmann and Blöker, 2000). Therefore, the practical implementation of the generalized relativistic FD functions requires a new efficient approximation method. Analytical evaluation of FD functions is especially important for "studies of the properties of a hypothetical electron gas, consisting of electrons in a uniform neutralizing background of positive charge and understanding of the physical properties of degenerate matter" (Kovetz et al., 1972; Kovetz and Shaviv, 1973).

The objective of this work is to propose an analytical formula for the evaluation of the generalized relativistic FD functions, appearing in the calculation of thermodynamic properties of a partially degenerate, strong degeneracy, semirelativistic electron gas in the limits of weak degeneracy and nonrelativistic degeneracy of fermion gases. The availability of the approach is verified by calculating the generalized relativistic FD functions. The performance, susceptibility, and performance of the method are analyzed. As seen from the results, the proposed approach for the evaluation of the generalized relativistic FD functions has developed in a technique that permits efficient computation.

2. Definition and basic formulas

The generalized relativistic FD functions investigated in this study

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https://doi.org/10.1016/j.newast.2022.101874
Received 2 February 2022; Received in revised form 25 May 2022; Accepted 10 June 2022
Available online 11 June 2022
1384-1076/

have the following form (with $\nu > -1$) (Kovetz et al., 1972; Kovetz and Shaviv, 1973; Shaviv and Kovetz, 1972; Stolzmann and Blöker, 1996, 2000):

$$J_\nu(\psi,\lambda) = \frac{1}{\Gamma(\nu+1)} \int_0^\infty \frac{x^\nu \sqrt{1+\frac{\lambda x}{2}}}{1+e^{x-\psi}} dx, \tag{1}$$

where x is dimensionless relativistic energy, ψ is degeneracy parameter, and λ is relativity parameter by the relationships:

$$x = \frac{\varepsilon}{kT} = \frac{1}{\lambda}\left(\sqrt{1+\left(\frac{p}{mc}\right)^2} - 1\right) \tag{2}$$

$$\psi = \frac{\mu}{kT} \tag{3}$$

$$\lambda = \frac{kT}{mc^2}. \tag{4}$$

Here, k is Boltzmann constant, T is absolute temperature, μ is chemical potential and p momentum. It will be seen that in the case of $\lambda = 0$, the Eq. (1) yields nonrelativistic FD functions as following:

$$I_\nu(\psi) = \frac{1}{\Gamma(\nu+1)} \int_0^\infty \frac{x^\nu}{1+e^{x-\psi}} dx. \tag{5}$$

In the studies (Zmmermann, 1987; Stolzmann and Blöker, 1996, 2000) efficient computational methods have been presented for the nonrelativistic FD functions in the case of weakly ($\psi < -5$) and strongly ($\psi > 10$) degenerate electrons by using expressions: for $\psi < -5$

$$I_\nu(\psi) = \sum_{n=0}^{5} (-1)^n \frac{e^{(n+1)\psi}}{(n+1)^{\nu+1}} \tag{7}$$

for $\psi > 10$

$$I_\nu(\psi) = \frac{\psi^{\nu+1}}{\Gamma(\nu+1)}\left[\frac{1}{\nu+1} + \sum_{n=1}^{5} 2\left(1-2^{1-2n}\right) F_{2n-1}(\nu) \frac{\Gamma(2n)\zeta(2n)}{\psi^{2n}}\right] \tag{8}$$

where $\Gamma(\nu)$ is Gamma function, $\zeta(\nu)$ is Zeta functions and $F_m(n)$ is binomial coefficients defined as respectively:

$$T_{nm}(p) = \lim_{N'\to\infty} \sum_{j=0}^{N'} F_j(1/2) \begin{cases} \dfrac{p^{n+1/2}}{n+j+1} + \dfrac{p^{n+3/2}}{n-j+3/2} & for \quad m = 0 \\ \dfrac{p^{1/2-j}\gamma(n+j+1, mp)}{m^{n+j+1}} + \dfrac{p^j \Gamma(n-j+3/2, mp)}{m^{n-j+3/2}} & for \quad m \neq 0 \end{cases} \tag{15}$$

$$\Gamma(\nu) = \int_0^\infty x^{\nu-1} e^{-x} dx \tag{9}$$

$$\zeta(\nu) = \frac{1}{\Gamma(\nu)} \int_0^\infty \frac{x^{\nu-1}}{e^x - 1} dx \tag{10}$$

$$F_m(n) = \frac{1}{m!} \prod_{i=0}^{m-1} (n-i) \tag{11}$$

Note that sufficient studies have been presented in the literature to evaluate the performance of the nonrelativistic FD functions for various values of parameters to be used directly in the study weakly and strongly degenerate electron gases and evaluating semiconductor devices and solar cells (Kovetz et al., 1972; Kovetz and Shaviv, 1973; Shaviv and Kovetz, 1972; Stolzmann and Blöker, 1996, 2000). An efficient approach has been proposed to the evaluation of the Eq.(5) for $\nu \leq -1$ in the study (Gil et al., 2022).

3. Analytical expressions for the generalized relativistic FD functions

The procedure is based on the idea split the definite integral $J_\nu(\psi,\lambda)$ up into two integrals $[0,\infty) = [0,\psi] \cup [\psi,\infty)$ for the application of the binomial expansion theorem and can be written as:

For $\psi > 0$

$$J_\nu(\psi,\lambda) = \frac{1}{\Gamma(\nu+1)}\left[\int_0^\psi \frac{x^\nu\sqrt{1+\frac{\lambda x}{2}}}{1+e^{x-\psi}} dx + \int_\psi^\infty \frac{x^\nu\sqrt{1+\frac{\lambda x}{2}}}{1+e^{x-\psi}} dx\right] \tag{12}$$

To obtain analytical formulae for the generalized relativistic FD functions we use the following binomial expansion theorem (Gradshteyn and Ryzhik, 1980):

$$(x \pm y)^n = \begin{cases} \sum_{m=0}^{\infty} (\pm 1)^m F_m(n) x^{n-m} y^m & \text{for noninteger } n \text{ and } x \geq y \\ \sum_{m=0}^{n} (\pm 1)^m F_m(n) x^{n-m} y^m & \text{for integer } n \end{cases} \tag{13}$$

Substituting the expansion Eq. (13) into Eqs. (1) and (12) we finally obtain for generalized relativistic FD functions the following formulae, respectively:

For $\psi \leq 0$

$$J_\nu(\psi,\lambda) = \frac{\sqrt{\lambda/2}}{\Gamma(\nu+1)} \lim_{N\to\infty} \sum_{i=0}^{N} F_i(-1) e^{\psi(1+i)} T_{\nu\, i+1}(2/\lambda) \tag{14}$$

where the auxiliary functions $T_{nm}(p)$ defined as:

For $\psi > 0$

$$J_\nu(\psi,\lambda) = \frac{\sqrt{\lambda/2}}{\Gamma(\nu+1)} \lim_{N\to\infty} \sum_{i=0}^{N} F_i(1/2)\left((2/\lambda)^{1/2-i} M_{\nu+i}(\psi, 2/\lambda) + (2/\lambda)^i L_{\nu-i+1/2}(\psi, 2/\lambda)\right) \tag{16}$$

The quantities $M_\nu(\mu,\eta)$ and $L_\nu(\mu,\eta)$ occurring in Eq. (16) are in terms of the special functions as:

Table 1
The comparative values of the relativistic FD functions $J_\nu(\psi,\lambda)$ for $N = N^{'} = N_1 = N_1^{'} = 150$

ν	ψ	λ	This Study	Mathematica numericalintegration results
2.5	-1.5	0.025	0.2237179260029110687[a]	0.2237179260029110704
1.5	-0.8	8.6	1.4025981914980076511[a]	1.402598481992921736
1.5	-7.8	17	0.0018486644759206604[a]	0.001848663450963744
1.5	-0.07	16.7	3.7750287672848093[a]	3.7750300171369106319
0.5	-4.5	2.1	0.017295284833615466[a]	0.017296596733596281
0.5	-0.24	0.7	0.786408567516723[a]	0.7864222006204854
-0.5	-0.24	0.07	0.52272115371472165[a]	0.522720857317506243
3.5	-5.6	11.7	0.0188409293244410194[a]	0.018840929362951098
3.5	-25.3	0.1	$1.137688876593135603.10^{-11}$[a]	$1.137688885849966991.10^{-11}$
3.5	-0.9	1.2	0.7605593834528539[a]	0.76056578940800157
3.5	0.9	0.2	2.7309173438666843[b]	2.7305222861482883
1.5	1.4	0.5	3.5710550224812874[b]	3.5674155911250818
1.5	0.06	5	2.45786903202198[b]	2.45778110225455
0.5	0.06	5	1.766117876058536[b]	1.764741162082517
0.5	4.8	2/3	12.13381922064362[b]	12.11813859612296
-0.5	0.9	1/3	1.044086787838524[b]	1.0400448326553218
-0.5	1.4	0.004	1.2077740823450194[b]	1.2062018749692764
0.5	0.98	4.2	3.356286418922865[b]	3.345713634240517
1.5	0.001	0.003	0.8697058267877301[b]	0.8697037668623195
3.5	2.7	3	15.53129202553502[b]	5.52000324917776

[a] Results obtained via Eq. (14).
[b] Results obtained via Eq. (16).

$$M_\nu(\mu,\eta) = \begin{cases} \lim\limits_{N_1\to\infty} \sum\limits_{k=0}^{N_1} F_k(-1) e^{-\mu k} K_{\nu k}(\eta) & for \quad \eta \le \mu \\ \lim\limits_{N_1\to\infty} \sum\limits_{k=0}^{N_1} F_k(-1)\left(e^{-\mu k} K_{\nu k}(\eta) + \dfrac{e^{\mu(1+k)}\gamma(\nu+1,\eta(1+k))}{(1+k)^{\nu+1}} \right) & for \quad \eta > \mu \end{cases} \tag{17}$$

and

$$L_\nu(\mu,\eta) = \begin{cases} \lim\limits_{N_1\to\infty} \sum\limits_{k=0}^{N_1} F_k(-1)\left(e^{-\mu k} E_{\nu k}(\mu,\eta) + \dfrac{e^{\mu(1+k)}\Gamma(\nu+1,\mu(1+k))}{(1+k)^{\nu+1}} \right) & for \quad \eta \le \mu \\ \lim\limits_{N_1\to\infty} \sum\limits_{k=0}^{N_1} F_k(-1) \dfrac{e^{\mu(1+k)}\Gamma(\nu+1,\eta(1+k))}{(1+k)^{\nu+1}} & for \quad \eta > \mu \end{cases}. \tag{18}$$

Here the quantities $K_{\nu k}(\eta)$ and $E_{\nu k}(\mu,\eta)$are determined as follows:

$$K_{\nu k}(\eta) = \begin{cases} \dfrac{\eta^{\nu+1}}{\nu+1} & for \quad k = 0 \\ \lim\limits_{N_1^{'}\to\infty} \sum\limits_{j=0}^{N_1^{'}} \dfrac{\eta^{\nu+j+1} k^j}{(\nu+j+1)j!} & for \quad k \ne 0 \end{cases} \tag{19}$$

for $k = 0$

$$E_{\nu 0}(\mu,\eta) = \begin{cases} Ln(\mu/\eta) & for \quad \nu = -1 \\ \dfrac{\mu^{\nu+1} - \eta^{\nu+1}}{\nu+1} & for \quad \nu \ne -1 \end{cases} \tag{20}$$

for $k \ne 0$

Table 2
Convergence of derived expression for $J_\nu(\psi,\lambda)$ as a function of summation limits N

N	$\nu = 3.5; \psi = -4.8; \lambda = 20/7$
30	0.02197573987218512
40	0.021975741070351225
50	0.021975741539621032
70	0.021975741887380055
80	0.02197574196070933
90	0.02197574200752668
100	0.02197574203899109
120	0.02197574207695322
150	0.02197574210483231

$$E_{\nu k}(\mu,\eta)=\begin{cases}\lim_{N_1^{'}\to\infty}\sum_{i=0}^{N_1^{'}}\frac{Ln(\mu/\eta)k^i}{i!} & for\ \ \nu+i=-1\\ \lim_{N_1^{'}\to\infty}\sum_{i=0}^{N_1^{'}}\frac{(\mu^{\nu+i+1}-\eta^{\nu+i+1})k^i}{(\nu+i+1)i!} & for\ \ \nu+i\neq-1\end{cases} \tag{21}$$

where $\gamma(\alpha,x)$ and $\Gamma(\alpha,x)$are the well known incomplete Gamma functions defined by Gradshteyn and Ryzhik (1980):

$$\Gamma(\alpha,x)=\int_x^\infty t^{\alpha-1}e^{-t}dt \tag{22}$$

and

$$\gamma(\alpha,x)=\int_0^x t^{\alpha-1}e^{-t}dt. \tag{23}$$

Here in Eqs. (14)–(21), the indexes N, $N^{'}$, N_1 and $N^{'}{}_1$ are the upper limits of summations, respectively.

4. Numerical results and discussion

In this study, we suggest an improvement of the FD function evaluation procedure that eliminates these difficulties and essentially increases the correctness of the related physical property calculations. The new approach is successfully tested on already published literature data and can be proposed for use in future relativistic electron gas investigates. Based on the obtained formulae, we established the programs for numerical evaluations using the Mathematica 10.0 program software. The calculation results are presented in Table 1 to demonstrate the efficiency of the proposed methods in the various values of parameters. The calculation results of the present study have been checked with the Mathematica 10 numerical evaluation data. As seen from the results, the proposed theoretical approach is general and ensures useful guidance for the evaluation of the thermodynamic and other properties of electron gases.

For fast calculations of FD functions, we use the partial summations of some indices corresponding to progressively increasing upper limits appearing in the series expansion relations. As can be seen from Table 2 in the values of variable $\psi>0$ the Eq. (16) displays the slow convergence to the numerical result. For increased accuracy of results is attainable by the use of more terms in expansions (14)–(19). As seen from our investigation that for $\psi<0$, the Eq. (14) yields highly accurate results for arbitrary values of function parameters. In this paper, we have provided the comparative calculation results of relativistic FD functions for the first time.

In conclusion, we believe that the proposed analytical method for relativistic FD functions will be especially useful in accurate evaluation of thermodynamic properties of staller matter and related specific problems.

Authorship statement

Category 1

Conception and design of study: _ The objective of this work is to propose an analytical formula for the evaluation of the generalized relativistic FD functions ________, ______ acquisition of data: _Tables 1 and 2__, _________, _________, _________; analysis and/or interpretation of data: As seen from the results, the proposed approach for the evaluation of the generalized relativistic FD functions has developed in a technique that permits efficient computation.

Category 2

Drafting the manuscript: _Word file_____, __________, __________, __________; revising the manuscript critically for important intellectual content: _ According to the referee's and your comments we have done all the necessary corrections in the paper.

Category 3

Approval of the version of the manuscript to be published (the names of all authors must be listed): _B. A. Mamedov_, __________, __________, __________, __________.

Declaration of Competing Interest

No potential conflicts of interest was reported by the author.

Acknowledgments

All persons who have made substantial contributions to the work reported in the manuscript (e.g., technical help, writing and editing assistance, general support), but who do not meet the criteria for authorship, are named in the Acknowledgements and have given us their written permission to be named. If we have not included an Acknowledgements, then that indicates that we have not received substantial contributions from non-authors. This statement is signed by all the authors (a photocopy of this form may be used if there are more than 10 authors).

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