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On the very accurate numerical evaluation of the Generalized Fermi–Dirac Integrals

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ABSTRACT

We indicate a new and a very accurate algorithm for the evaluation of the Generalized Fermi–Dirac Integral with a relative error less than 10^{-20}. The method involves Double Exponential, Trapezoidal and Gauss–Legendre quadratures. For the residue correction of the Gauss–Legendre scheme, a simple and precise continued fraction algorithm is used.

1. Introduction

The Fermi–Dirac integral (FDI)

$$F_k(\eta) = \frac{1}{\Gamma(1+k)} \int_0^\infty \frac{t^k\,dt}{e^{t-\eta}+1} \tag{1}$$

is needed in a variety of problems involving the Fermi–Dirac distribution like the calculation of charge densities of semiconductor devices. A detailed account is given by Blakemore [1] for the various exact and approximate expressions available in the literature with special emphasis on $F_{1/2}(\eta)$. If the upper limit of integration is finite, the above integral is called the incomplete FDI. Goano [2] provides a large and accurate collection of algorithms to evaluate the ordinary as well as the incomplete FDI. The work in this area broadly consists of two groups. The first set deals with series expansions that are valid for small values of η and the asymptotic approximations which are valid for large values of η [3–10]. The second set consists of numerical algorithms, based either on rational approximation [11–13] that combine both high accuracy and minimum effort or they rely on numerical integration [14].

An integral related to the FDI that is needed in astrophysical problems like the stellar evolution is defined by

$$F_k(\eta,\theta) = \int_0^\infty \frac{t^k\sqrt{1+\theta\,t/2}\,dt}{e^{t-\eta}+1}. \tag{2}$$

This is the Generalized Fermi–Dirac Integral (GFDI) that depends on three parameters k, η and θ. When the parameter θ is zero, the GFDI reduces to the FDI without its gamma function term in the denominator.

As we remarked earlier, a detailed review of the asymptotic and the series expansions for the FDI is available in Blakemore [1]. For the sake of completeness, here we outline very briefly some of these approaches. Many of these expressions are derived from the classical series expansions provided by McDougall and Stoner [6] and Dingle [4,5]. The following is a typical one valid for integer and half-integer values [3].

$$F_k(\eta) = \sum_{r=1}^{\infty} (-1)^{r+1} e^{r\eta}\, r^{-(k+1)}; \quad \eta \ll 0$$

$$F_k(\eta) = \cos(k\pi) F_k(-\eta) + \frac{\eta^{k+1}}{\Gamma(k+2)}[1+R_k(\eta)]; \quad \eta > 0$$

$$R_k(\eta) = \sum_{r=1}^{\infty} \frac{\alpha_r \Gamma(k+2)}{\eta^{2r}\,\Gamma(k+2-2r)}; \quad \alpha_r = \sum_{n=1}^{\infty} (-1)^{n+1}\, 2\, n^{-2r}.$$

For evaluating the FDI, Goano [7] utilizes the fact that the term $1/[e^{t-\eta}+1]$ can be expanded in a geometric series for the cases

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$t > \eta$ and the $t < \eta$ separately. The resulting series is integrated term by term and the final quantities are expressed in terms of the Kummer confluent hypergeometric functions of the first and second kind, $M(a, b, z)$ and $U(a, b, z)$, respectively, for which efficient algorithms exist.

$$F_k(\eta) = \frac{\eta^{k+1}}{\Gamma(k+2)} \left\{ 1 + \sum_{n=1}^{\infty} (-1)^{n-1} [(k+1)\, U(1, k+2, n\eta) - M(1, k+2, -n\eta)] \right\}.$$

Bhagat et al. [13] derive series expansion for the FDI. The approach here is to expand the term $1/[e^{t-\eta}+1]$ in a series after appropriate manipulations and then integrate the resulting integrand term by term. Next, to expedite convergence, acceleration technique like the Levin transform is made use of. It must be noted that this approach works better if η is *large*. Again, for the GFDI, the term $\sqrt{1+\theta t/2}$ is also expanded in a series (possible *only for small values of* θ like 10^{-3}) and the resulting series is integrated term by term and this is followed by convergence acceleration.

The FDI can be expressed in terms of the Zeta or the Polylogarithm or the incomplete Gamma functions. Below, we indicate an *exact series expression* for $F_k(\eta)$ in terms of the incomplete Gamma function [15]. We note the Mittag-Leffler expansion of sech(z) function [16] which leads to the following modification of the denominator of the integrand of the FDI.

$$\mathrm{sech}(z) = \frac{1}{\cosh(z)} = \pi \sum_{l=0}^{\infty} \frac{(-1)^l\,(2l+1)}{z^2 + [(2l+1)\pi/2]^2}$$

$$\frac{1}{e^{t-\eta}+1} = \frac{e^{-(t-\eta)/2}}{2\,\cosh[(t-\eta)/2]}.$$

With the substitution above, we get the FDI as

$$a_l = \eta + i(2l+1)\pi; \qquad \phi_l = \tan^{-1}[(2l+1)\pi/\eta];$$
$$l = 0, 1, 2, \ldots$$

$$F_k(\eta) = \frac{2\pi e^{\eta/2}}{\Gamma(k+1)} \sum_{l=0}^{\infty} (-1)^l\,(2l+1) \int_0^{\infty} \frac{t^k\, e^{-t/2}\, dt}{(t-\eta)^2 + [(2l+1)\pi]^2}$$

$$F_k(\eta) = 2\,\mathrm{Im} \left\{ \sum_{l=0}^{\infty} e^{i[\pi(k-1/2) - k\phi_l]}\, [\eta^2 + ((2l+1)\pi)^2]^{k/2}\, \Gamma(-k, -a_l^*/2) \right\}; \quad k > (-1).$$

After this brief outline of the series expansions, we turn to the numerical evaluations based on quadrature. Both Pichon and Sagar [17,18] use the modified Gauss–Laguerre schemes to achieve a better accuracy. Gautschi also constructs modified Gaussian schemes [19]. But these three methods [17–19] need a lot of computational effort since the weight and the node generation is a non-trivial task and also the weights and nodes change with the parameters k, η and θ. The GFDI and its derivative with respect to its parameters were evaluated by Gong et al. [20] by splitting $(0, \infty)$ into four intervals. The Gauss–Legendre scheme is used in the first three intervals and the Gauss–Laguerre scheme is used in the last interval. Here, the choice of break points is by trial and error.

The convergence of any quadrature scheme for the evaluation of the integrals defined by Eqs. (1,2) is impaired by the singularities of the integrands. If k takes half-integer values (as in the case of the semiconductor device modeling) like $k = -(1/2), (1/2), (3/2), (5/2), \ldots$, then the origin $t = 0$ is a branch point. In addition, the integrands of both the GFDI and the FDI have a countable infinity of simple poles at t_j defined by $t_j = \eta + i(2j+1)\pi;\ j = 0, \pm1, \pm2, \ldots$. When k is a half-integer, the branch point singularity can be removed by setting $t = x^2$. Natarajan and Mohankumar employed a variety of quadrature schemes that took care of the singularities which resulted in reduced number of quadrature terms. Trapezoidal and Gauss–Legendre schemes with the correction terms for the poles were employed [14,21,22]. The clustering of the quadrature nodes that is inherent in numerical integration methods like the TANH, the IMT and the DE schemes was also profitably exploited to handle the singularities of these integrands [23,24].

2. Existing methods for the FDI and the GFDI evaluation

In this section, we discuss our earlier methods for the evaluation of the FDI and the GFDI. This will help us to identify the improvements that are needed for our earlier algorithms. In addition, it provides the necessary background for the new algorithms that are presented in the next two sections.

For the FDI needed in semiconductor applications, typical k values belong to the set $\{-(1/2), (1/2), (3/2), (5/2)\}$ and typical η values lie in the range $[-10, 50]$. For this range of parameters, we first make a change of the integration variable from t to x defined by $t = x^2$ and this has the positive effect of removing the branch point singularity at the origin. The resulting FDI (with an integrand that is even) and its new singularities $\{z_j\}$ are given below and for the sake of simplicity, we omit the factor $\frac{1}{\Gamma(1+k)}$.

$$F_k(\eta) = \int_{-\infty}^{\infty} \frac{x^{2k+1}\, dx}{e^{x^2-\eta}+1} \tag{3}$$

$$z_j = \pm\sqrt{\eta + i(2j+1)\pi}; \quad j = 0, \pm1, \pm2, \ldots. \tag{4}$$

A simple trapezoidal scheme with residue correction for the poles $\{z_j\}$ of this integrand can yield a double precision accuracy (i.e a minimum of 14 digit accuracy) with a maximum of 29 quadrature terms and 7 residue correction terms with η in the range $[-10, 50]$ and for half-integer k values. This accuracy stemming from this very modest computational requirements must be sufficient for routine estimation of the FDI. These results were reported in Mohankumar et al. [14]. Table 1 gives sample values of the FDI without its gamma function term. An algorithm based on this scheme is available as a matlab routine called fermi.m that can be freely downloaded by users [25]. For the sake of completion, a brief derivation of this trapezoidal scheme, the residue correction and its discretization error are outlined in Appendix A.

For the above mentioned scheme, it must be noted that the number of trapezoidal terms is proportional to $\eta^{1/2}$. Hence, for large η values, this implies more computational cost. To overcome this aspect, the recent quadrature methods, namely, the TANH, the IMT and the Double Exponential (DE) schemes were employed. Essentially, all the three methods are just trapezoidal schemes *after* a specific change of integration variable. We only outline the DE scheme since it is superior to the other two methods. The details of the TANH and the IMT methods can be found in Natarajan et al. [23]. With t and u as the old and the new variables, the DE transformation introduced by Takahasi and Mori [26,27] is defined as follows.

$$t \in (a, b); \quad u \in (-\infty, \infty) \tag{5}$$

$$t_k = \phi(u_k) = (1/2)(b+a) + (1/2)(b-a)\tanh\left(\frac{\pi}{2}\sinh(u_k)\right) \tag{6}$$

$$\frac{dt}{du} = \phi'(u) = \frac{\pi(b-a)}{4}\,\mathrm{sech}^2\left[\frac{\pi}{2}\sinh(u)\right]\cosh(u) \tag{7}$$

$$u_k = kh, \quad k = 0, \pm1, \pm2, \ldots. \tag{8}$$

t_k, the images of the equi-spaced nodes u_k get clustered at the ends $t = a$ and $t = b$ of the old interval (a, b). This specific