

Precise and fast computation of generalized Fermi–Dirac integral by parameter polynomial approximation



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ABSTRACT

The generalized Fermi–Dirac integral, $F_k(\eta, \beta)$, is approximated by a group of polynomials of β as $F_k(\eta, \beta) \approx \sum_{j=0}^J g_j \beta^j F_{k+j}(\eta)$ where $J = 1(1)10$. Here $F_k(\eta)$ is the Fermi–Dirac integral of order k while g_j are the numerical coefficients of the single and double precision minimax polynomial approximations of the generalization factor as $\sqrt{1+x/2} \approx \sum_{j=0}^J g_j x^j$. If β is not so large, an appropriate combination of these approximations computes $F_k(\eta, \beta)$ precisely when η is too small to apply the optimally-truncated Sommerfeld expansion (Fukushima, 2014 [15]). For example, a degree 8 single precision polynomial approximation guarantees the 24 bit accuracy of $F_k(\eta, \beta)$ of the orders, $k = -1/2(1)5/2$, when $-\infty < \eta \leq 8.92$ and $\beta \leq 0.2113$. Also, a degree 7 double precision polynomial approximation assures the 15 digit accuracy of $F_k(\eta, \beta)$ of the same orders when $-\infty < \eta \leq 29.33$ and $0 \leq \beta \leq 3.999 \times 10^{-3}$. Thanks to the piecewise minimax rational approximations of $F_k(\eta)$ (Fukushima, 2015 [18]), the averaged CPU time of the new method is roughly the same as that of single evaluation of the integrand of $F_k(\eta, \beta)$. Since most of $F_k(\eta)$ are commonly used in the approximation of $F_k(\eta, \beta)$ of multiple contiguous orders, the simultaneous computation of $F_k(\eta, \beta)$ of these orders is further accelerated by the factor 2–4. As a result, the new method runs 70–450 times faster than the direct numerical integration in practical applications requiring $F_k(\eta, \beta)$.

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1. Introduction

The generalized Fermi–Dirac integral is an important special function in astrophysics [1, Section 24.4] and in solid state physics [2]. The integral is written in the form of an integral transform [3, Section 6.10] as

$$F_k(\eta, \beta) \equiv \int_0^\infty \frac{t^k \sqrt{1 + (\beta/2)t} dt}{\exp(t - \eta) + 1}. \quad (k > -1; -\infty < \eta < \infty; \beta \geq 0) \quad (1)$$

It is a generalization of $F_k(\eta)$, the Fermi–Dirac integral [2] widely used in quantum statistics, in the sense $F_k(\eta) = F_k(\eta, 0)$. There are a few other expressions of the generalized Fermi–Dirac integrals [4,5]. However, the above standard form will be treated throughout this article.

The precise and fast computation of $F_k(\eta, \beta)$ is quite difficult [3, Section 6.10]. This issue has been discussed since the early days when a Nobel laureate, Chandrasekhar, determined the limit mass of white dwarf by employing the integrals [6]. Indeed, a single chapter is fully devoted to its computation in a modern text on the stellar structure [1, Chapter 24].

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Despite that many methods have been proposed to compute the integral [5,7–12], the current standard procedure [3, Section 6.10] is the numerical quadrature by the double exponential rule [13] with a splitting of the integration interval at $t = \eta$. The method is sufficiently accurate but slow in general. In the astrophysical applications, frequently required is the simultaneous computation of $F_k(\eta, \beta)$ of three contiguous half integer orders, $k = 1/2, 3/2$, and $5/2$. As a result, the standard method requires 150–1800 evaluations of the integrand for each combination of η and β [3, Section 6.10].

This is quite time-consuming if considering their frequent utilization. For example, the evaluation of the integrals must be conducted at all locations inside the stars at every step of their evolution tracking. Thus, the evolution computation of a three-dimensional star with even a small number of spatial grids as 128 for just 1000 time steps would require the number of the simultaneous evaluation of the three integrals as many as $128^3 \times 1000 \approx 2.1 \times 10^9$. Even if each computation costs only $50 \mu\text{s}$, the total CPU time would be of the order of day.

Recently, an extension of the numerical integration method of [14, Section 3] is developed to compute a general integral of the Fermi–Dirac distribution including $F_k(\eta, \beta)$ [15]. This method significantly reduces the number of integrand evaluations when $\eta > 4$ by the factor 1.2–120 [15, Fig. 3]. Nevertheless, the extended method is not effective for negative and small positive values of η . On the other hand, when η is sufficiently large, applicable is the Sommerfeld expansion [16] to compute a general integral of the Fermi–Dirac distribution. Although the expansion is of asymptotic nature, its appropriate truncations compute $F_k(\eta, \beta)$ with the single and double precision accuracies, respectively [17]. However, still challenging is the precise and fast computation of $F_k(\eta, \beta)$ for not so large values of η .

In order to overcome this situation, by using newly-developed procedures to compute $F_k(\eta)$ [18], a new method is developed to compute $F_k(\eta, \beta)$ in this article. Below, Section 2 explains the new method of computation, and Section 3 shows the results of numerical experiments.

2. Method

2.1. Series expansion of $F_k(\eta, \beta)$ with respect to β

Consider the computation of $F_k(\eta, \beta)$ of the half integer orders, $-1/2(1)5/2$, when η is less than η_S , the threshold values of the truncated Sommerfeld expansion [17], which ranges 8.9–13.4 and 29.3–38.8 in the single and the double precision environments, respectively. In many practical applications, the parameter β is relatively small. In the astrophysical cases, for example, the maximum value of β of electrons in ordinary stars like the Sun is of the order of 10^{-3} [7]. Meanwhile, that of protons as well as neutrons is less than 0.1 for all cases. On the other hand, also small are β of typical semiconductors including that of InSb being around 0.3 [8].

Therefore, examined is the series expansion of $F_k(\eta, \beta)$ with respect to β . The key function here is the generalization factor, $g(x) \equiv \sqrt{1+x/2}$, where $x \equiv \beta t$. If it is well approximated as a polynomial of x as $g(x) \approx \sum_{j=0}^J g_j x^j$, then an approximation of $F_k(\eta, \beta)$ is obtained by the termwise integration as

$$F_k(\eta, \beta) \approx F_k^{(J)}(\eta, \beta) \equiv \sum_{j=0}^J g_j \beta^j F_{k+j}(\eta). \quad (2)$$

Notice that the coefficients g_j are independent on the order k , and therefore, they can be commonly used for the approximation of $F_k(\eta, \beta)$ of different orders in general.

2.2. Approximation of generalization factor

Consider an approximation of the generalization factor, $g(x)$. Since the effectiveness of the Maclaurin series expansion [21, Formula 15.4.6] is limited by an algebraic singularity of $g(x)$ at $x = -2$, developed are the minimax polynomial approximations. Assume that both of J , the degree of the approximation polynomial, and X , the length of the approximation interval, are specified. Then, a set of the polynomial coefficients, g_j for $j = 0, 1, \dots, J$, are determined so as to minimize the relative approximation error in the interval $0 \leq x \leq X$. In practice, the process is reversed. Namely, when the required error tolerance is specified, X is maximized under the condition the maximum relative error of approximation does not exceed the tolerance. The reversed procedure implemented by Mathematica Version 10 [19] determined the coefficients as listed in Tables 1–3.

2.3. Maximum parameter

Now that the minimax polynomial approximation of $g(x)$ is established, easily constructed are the polynomial approximations of $F_k(\eta, \beta)$ by using them. Since the interval of η is as limited as $-\infty < \eta \leq \eta_S$, the maximum relative error for the given value of β is measured by setting $\eta = \eta_S$. This must be compared with δ , the given relative error tolerance. Extending the process, actually determined is β_S , the maximum value of β when $\eta \leq \eta_S$ such that the relative error does not exceed δ . The relative errors of $F_k(\eta, \beta)$ are measured by numerically comparing the approximate value with the reference values, which are prepared by the quadruple precision numerical integration by means of a quadruple precision extension of Ooura's `intde`, an adaptive numerical quadrature program in the double precision environment based on the double exponential rule [20]. Notice that, only the integrals of negative arguments are required in some applications such as the evaluation of the physical quantities of the

Table 1

Coefficients of minimax polynomial approximation of generalization factor with maximum length of approximation interval: $J = 1(1)6$. Listed are the numerical values of g_j , the polynomial coefficients of minimax polynomial approximations of the generalization factor $\sqrt{1+x/2}$ in the interval $0 \leq x \leq X$ while X is the maximum length of approximation interval. Omitted are the common zeroth coefficients, $g_0 = +1.000\,000\,06$ and $+1.000\,000\,000\,000\,000\,11$, in the single and double precision computations, respectively. A few more-than-enough digits are shown so as to avoid unnecessary information loss in the implementation.

J	j	Single precision	Double precision
1	1	+2.498 779 47 E–1	+2.499 999 947 343 752 50 E–1
2	1	+2.499 829 20 E–1	+2.499 999 999 740 136 08 E–1
	2	–3.052 442 39 E–2	–3.124 909 885 573 587 90 E–2
3	1	+2.499 921 38 E–1	+2.499 999 999 977 169 47 E–1
	2	–3.108 809 17 E–2	–3.124 999 264 796 570 38 E–2
	3	+6.728 903 04 E–3	+7.804 923 096 532 070 96 E–3
4	1	+2.499 945 79 E–1	+2.499 999 999 993 985 56 E–1
	2	–3.117 128 73 E–2	–3.124 999 947 860 719 60 E–2
	3	+7.406 429 47 E–3	+7.812 341 762 814 953 85 E–3
	4	–1.540 642 86 E–3	–2.421 787 931 468 446 82 E–3
5	1	+2.499 955 77 E–1	+2.499 999 999 997 339 28 E–1
	2	–3.119 687 79 E–2	–3.124 999 989 649 847 93 E–2
	3	+7.575 971 34 E–3	+7.812 485 270 036 438 14 E–3
	4	–1.944 547 34 E–3	–2.440 457 513 128 191 56 E–3
	5	+3.146 194 18 E–4	+8.262 274 250 209 465 31 E–4
6	1	+2.499 960 68 E–1	+2.499 999 999 998 434 56 E–1
	2	–3.120 783 33 E–2	–3.124 999 996 394 713 14 E–2
	3	+7.640 914 43 E–3	+7.812 496 884 887 274 91 E–3
	4	–2.096 350 76 E–3	–2.441 277 881 946 481 26 E–3
	5	+4.661 948 91 E–4	+8.517 666 893 749 751 45 E–4
	6	–5.410 906 77 E–5	–2.914 565 127 153 156 25 E–4

Table 2

Coefficients of minimax polynomial approximation of generalization factor with maximum length of approximation interval: $J = 7(1)9$.

J	j	Single precision	Double precision
7	1	+2.499 963 49 E–1	+2.499 999 999 998 915 83 E–1
	2	–3.121 357 13 E–2	–3.124 999 998 256 529 98 E–2
	3	+7.672 609 17 E–3	+7.812 498 931 424 413 22 E–3
	4	–2.168 733 32 E–3	–2.441 374 033 111 533 66 E–3
	5	+5.444 981 36 E–4	+8.539 627 267 207 382 00 E–4
	6	–9.399 442 78 E–5	–3.155 739 894 863 824 76 E–4
	7	+7.701 051 66 E–6	+1.021 479 417 062 174 78 E–4
8	1	+2.499 965 32 E–1	+2.499 999 999 999 162 61 E–1
	2	–3.121 702 40 E–2	–3.124 999 998 958 074 42 E–2
	3	+7.690 681 12 E–3	+7.812 499 500 670 424 99 E–3
	4	–2.209 108 36 E–3	–2.441 394 241 600 083 19 E–3
	5	+5.896 414 47 E–4	+8.543 293 472 401 205 72 E–4
	6	–1.204 950 81 E–4	–3.191 276 504 607 513 34 E–4
	7	+1.550 088 92 E–5	+1.196 742 377 506 852 76 E–4
	8	–9.069 763 86 E–7	–3.457 780 000 424 379 09 E–5
9	1	+2.499 966 51 E–1	+2.499 999 999 999 306 94 E–1
	2	–3.121 920 69 E–2	–3.124 999 999 285 855 02 E–2
	3	+7.701 832 58 E–3	+7.812 499 714 478 664 35 E–3
	4	–2.233 767 23 E–3	–2.441 400 442 866 540 34 E–3
	5	+6.177 721 67 E–4	+8.544 240 958 563 101 31 E–4
	6	–1.383 141 91 E–4	–3.199 451 261 061 160 00 E–4
	7	+2.182 125 74 E–5	+1.236 788 520 521 445 44 E–4
	8	–2.080 417 52 E–6	–4.496 673 003 438 536 55 E–5
	9	+8.872 074 81 E–8	+1.108 476 311 510 663 28 E–5

positron and other anti-particles in general. For this purpose, separately computed are the maximum parameter values when $-\infty < \eta \leq 0$.

Numerical examinations revealed that when $-\infty < \eta < 9.80$, the 24 bit accuracy of the integrals of the orders $k = 1/2$ and $3/2$ is guaranteed by the degree 3, 4, and 7 single precision polynomial approximations if β is less than 0.02305, 0.04966, and 0.1696, respectively. They are enough for the single precision computation of the number density of Ge, Si and GaAs, and InAs, respectively [8]. Also, the degree 7 and 8 single precision polynomial approximations are sufficient to compute $F_k(\eta, \beta)$ of

Table 3Coefficients of minimax polynomial approximation of generalization factor with maximum length of approximation interval: $J = 10$.

J	j	Single precision	Double precision
10	1	+2.499 967 34 E–1	+2.499 999 999 999 399 72 E–1
	2	–3.122 069 94 E–2	–3.124 999 999 463 355 82 E–2
	3	+7.709 280 85 E–3	+7.812 499 812 854 383 54 E–3
	4	–2.250 059 82 E–3	–2.441 402 897 425 561 26 E–3
	5	+6.365 462 02 E–4	+8.544 570 257 612 728 58 E–4
	6	–1.507 459 30 E–4	–3.202 031 799 789 860 24 E–4
	7	+2.670 975 77 E–5	+1.248 958 834 492 572 38 E–4
	8	–3.206 554 14 E–6	–4.836 688 576 571 362 02 E–5
	9	+2.289 299 17 E–7	+1.626 743 268 901 661 49 E–5
	10	–7.278 637 97 E–9	–3.320 433 997 565 375 55 E–6

Table 4

CPU time comparison. Listed are the averaged CPU time to compute $F_k(\eta, \beta)$ of a single order solely or multiple orders simultaneously by two methods; (i) the direct numerical integration, and (ii) the combined polynomial approximation described in the main text. The average is taken over (i) the values of η uniformly distributed in $-4 < \eta \leq 0$ and $0 < \eta \leq \eta_s$, respectively, and (ii) the values of β uniformly distributed in $0 < \beta \leq \beta_s$. In the case of multiple orders, β_s is chosen as the minimum value among those of different orders. The numerical integration was conducted by Ooura's `intde` [20] with two kinds of relative error tolerance, $\delta = 2^{-24} \approx 5.96 \times 10^{-8}$ and $\delta = 10^{-15}$, respectively, while the integration interval is split at $t = \eta$ if $\eta > 4$. The unit of CPU time is μs . The measurements are conducted at a PC with the Intel Core i7-4600U running at 2.10 GHz clock. All the programs are coded in Fortran 90 and compiled by the Intel Visual Fortran Composer XE 2011 update 8 with the maximum optimization. Notice that the averaged CPU time to evaluate the integrand of $F_k(\eta, \beta)$ is 0.141 in the same unit.

Precision	k	Numerical integration		Combined approximation	
		$-4 < \eta \leq 0$	$0 < \eta \leq \eta_s$	$-4 < \eta \leq 0$	$0 < \eta \leq \eta_s$
24 bit	–1/2	14.6	22.7	0.158	0.145
	1/2	14.2	22.3	0.163	0.139
	3/2	12.4	20.5	0.152	0.148
	5/2	12.1	21.8	0.168	0.126
	1/2, 3/2	25.1	39.8	0.171	0.147
	1/2, 3/2, 5/2	35.2	59.3	0.173	0.151
	–1/2, 1/2, 3/2, 5/2	50.8	76.2	0.195	0.169
15 digit	–1/2	15.0	23.6	0.168	0.186
	1/2	13.9	21.7	0.174	0.170
	3/2	12.2	22.0	0.168	0.162
	5/2	14.1	21.5	0.147	0.145
	1/2, 3/2	25.4	40.3	0.177	0.174
	1/2, 3/2, 5/2	35.3	60.5	0.186	0.176
	–1/2, 1/2, 3/2, 5/2	47.8	83.1	0.202	0.185

orders, $k = -1/2(1)5/2$, with the 24 bit accuracy when $-\infty < \eta \leq 0$ and $\beta < 0.2071$ and when $-\infty < \eta < 8.92$ and $\beta < 0.2113$, respectively. They are suitable for the single precision computation of the physical quantities in the stellar evolution for (i) protons/neutrons in all stages and (ii) electrons/positrons in the stages up to the neon fusion [1]. On the other hand, the degree 5 and 7 double precision polynomial approximations assure the 15 digit accuracy of $F_k(\eta, \beta)$ of orders, $k = -1/2(1)5/2$, when $-\infty < \eta \leq 0$ and $\beta < 3.827 \times 10^{-3}$ and when $-\infty < \eta < 29.33$ and $\beta < 3.999 \times 10^{-3}$, respectively. This is appropriate for the 15 digit computation of the physical quantities in normal stars including the Sun [7].

At any rate, these observations conclude that $F_k(\eta)$ of half integer orders, $-1/2(1)21/2$, are required for the approximations of $F_k(\eta, \beta)$ described in the above. Their precise and fast computation is already realized by their piecewise minimax rational approximations [18].

2.4. Combined approximation

The maximum values of β determined in the previous subsection are useful to construct a combination of the polynomial approximations of various degrees already obtained in Section 2.2 so as to realize the approximation of high cost performance. For this purpose, denote (i) by $F_k^{(J)}(\eta, \beta)$ the degree J polynomial approximation of $F_k(\eta, \beta)$, the coefficients of which are shown in Tables 1–3, (ii) by $\beta_s^{(J)}$ the maximum value of β when $\eta \leq \eta_s$, and (iii) by $\beta_0^{(J)}$ the maximum value of β when $\eta \leq 0$. Then, a

combination of the polynomial approximations is defined in a piecewise manner as

$$F_k^*(\eta, \beta) \equiv \begin{cases} F_k^{(1)}(\eta, \beta) & \text{if } [(\eta \leq 0 \text{ and } \beta \leq \beta_0^{(1)}) \text{ or } (\eta \leq \eta_s \text{ and } \beta \leq \beta_s^{(1)})] \\ F_k^{(2)}(\eta, \beta) & \text{else if } [(\eta \leq 0 \text{ and } \beta \leq \beta_0^{(2)}) \text{ or } (\eta \leq \eta_s \text{ and } \beta \leq \beta_s^{(2)})] \\ \dots & \dots \end{cases} \quad (3)$$

The numerical values of η_s , $\beta_0^{(j)}$, and $\beta_s^{(j)}$ as well as the detailed implementation of this algorithm are found in the Fortran 90 programs to compute $F_k(\eta, \beta)$ listed in the author's WEB site https://www.researchgate.net/profile/Toshio_Fukushima/

3. Results

Examine the computational cost and performance of the new method. Begin with the computational errors. Fig. 1 shows the relative error curves of the combined single precision approximation of $F_k(\eta, \beta)$ of the half integer orders, $k = -1/2(1)5/2$, in an intermediate argument interval, $-2 \leq \eta \leq 8$, for 200 values of parameter, $\beta = 0.001(0.001)0.200$. The change in the relative error curves at $\eta = 0$ is due to the switch of the polynomial approximations described in the previous section. At any rate, the figure confirms that the relative errors of the combined single precision approximation is at most the single precision machine epsilon.

Next, Fig. 2 plots the relative errors of the combined double precision approximation of $F_k(\eta, \beta)$ of the same orders, $k = -1/2(1)5/2$, in a wider argument interval, $-11 \leq \eta \leq 29$, for 7 values of parameter, $\beta = 0.000(0.001)0.006$. This graph indicates that the relative errors of the combined double precision approximation are at most 8 double precision machine epsilons. Most of these errors are caused by rounding off, especially those of the computation of $F_k(\eta)$ [18].

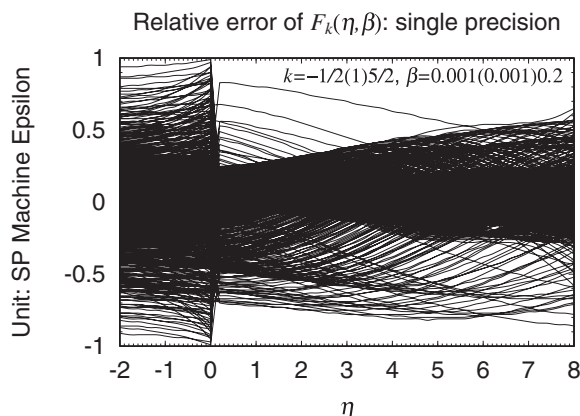


Fig. 1. Relative error of combined approximation of $F_k(\eta, \beta)$: single precision. Plotted are the relative error curves of the combined single precision polynomial approximation of $F_k(\eta, \beta)$ of orders, $k = -1/2(1)5/2$, in the argument interval, $-2 \leq \eta \leq 8$, for various values of the parameter as $\beta = 0.001(0.001)0.200$. The change of the error distributions at $\eta = 0$ is caused by the switch of policy to determine the degree of approximation polynomial, J .

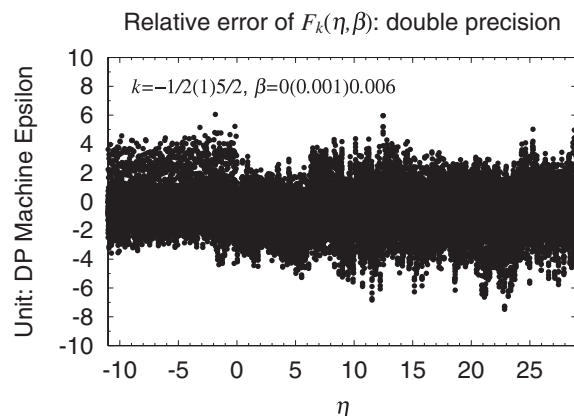


Fig. 2. Relative error of combined approximation of $F_k(\eta, \beta)$: double precision. Plotted are the relative errors of the combined double precision polynomial approximation of $F_k(\eta, \beta)$ of orders, $k = -1/2(1)5/2$, in the argument interval, $-11 \leq \eta \leq 29$, for several values of the parameter as $\beta = 0.000(0.001)0.006$. This time, no significant dependence on η nor k is seen in the error distribution since the errors are mainly due to the accumulated round-off caused by not the adopted approximation polynomials but the procedures to compute $F_k(\eta)$ [18].

Move to the aspect of the computational speed. Table 4 compares the averaged CPU times to compute $F_k(\eta, \beta)$ of (i) the direct numerical quadrature using Ooura's program to execute the double exponential rule [20] with the splitting of the integration interval at $t = \eta$ when $\eta > 4$, and (ii) the combined polynomial approximation. Thanks to the piecewise minimax rational approximations of $F_k(\eta)$ [18], the combined polynomial approximation runs dramatically fast.

Indeed, its averaged CPU time for individual order amounts to 0.13–0.17 μs at a PC with the Intel Core i7-4600U running at 2.10 GHz clock. Considering that the averaged CPU time of a single evaluation of the integrand of $F_k(\eta, \beta)$ is 0.14 μs at the same PC, it is concluded that these CPU times are fairly small. Consequently, the new method runs greatly faster than the numerical integration, say 40–140 times faster in the individual evaluation of $F_k(\eta, \beta)$ of orders, $k = -1/2(1)5/2$.

If required is the simultaneous computation of $F_k(\eta, \beta)$ of multiple contiguous orders such as (i) $k = 1/2$ and $3/2$, (ii) $k = 1/2$, $3/2$, and $5/2$, or (iii) $k = -1/2$, $1/2$, $3/2$, and $5/2$, this speed up ratio becomes roughly 2–4 times larger. In fact, Table 4 illustrates that the new method runs 70–450 times faster than the direct numerical integrations in such cases.

4. Conclusion

By using the minimax polynomial approximations of the generalization factor, the generalized Fermi–Dirac integrals, $F_k(\eta, \beta)$, of half integer orders, $k = -1/2(1)5/2$, are approximated by the degree 1 to 10 polynomials of β with the j th polynomial coefficients being in proportion to $F_{k+j}(\eta)$, the Fermi–Dirac integral of order $k + j$. If η is less than the threshold values of the optimally truncated Sommerfeld expansion [17], and if β is less than a certain value spanning from 0.006251 up to 0.3265, these polynomial expressions provide the approximation of $F_k(\eta, \beta)$ with the 7–15 digits accuracies. For example, a degree 8 single precision polynomial approximation guarantees the 24 bit accuracy of $F_k(\eta, \beta)$ of the orders, $k = -1/2(1)5/2$, when $-\infty < \eta \leq 8.92$ and $\beta \leq 0.2113$. Also, a degree 7 double precision polynomial approximation assures the 15 digit accuracy of $F_k(\eta, \beta)$ of the same orders when $-\infty < \eta \leq 29.33$ and $0 \leq \beta \leq 3.999 \times 10^{-3}$. These approximations cover almost all the cases of practical needs except the electrons at extremely high temperatures as 10^{10} K or more. Thanks to the precise and fast procedures to compute $F_k(\eta)$ [18] and to the fact that the most of $F_k(\eta)$ are commonly used in approximating $F_k(\eta, \beta)$ of multiple contiguous orders, the obtained approximations run so fast that their averaged CPU time is 70–450 times smaller than that of the direct numerical integrations.

The Fortran 90 programs to compute the combined single and double precision approximations of $F_k(\eta, \beta)$ of orders, $k = -1/2(1)5/2$, as well as their sample outputs are freely available from the following WEB site. https://www.researchgate.net/profile/Toshio_Fukushima/ It will be straightforward to translate these Fortran programs into other computer languages such as C, C++, and MATLAB.

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