Accurate, short series approximations to Fermi–Dirac integrals of order 1/2, 1/2, 1, 3/2, 2, 5/2, 3, and 7/2

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Accurate, short series approximations to Fermi–Dirac integrals of order − 1/2, 1/2, 1, 3/2, 2, 5/2, 3, and 7/2

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Short series approximations based on the classical series expansions of the Fermi-Dirac integrals $F_j(x)$ are presented for the orders $-1/2$, $1/2$, 1, $3/2$, 2, $5/2$, 3, and $7/2$. The approximations are accurate to better than 1 part in 10^5 over the range $-\infty < x < \infty$.

A Fermi–Dirac (F–D) integral or order j is defined[1] as

$$F_j(x) = \frac{1}{\Gamma(j+1)} \int_0^\infty \frac{\epsilon^j d\epsilon}{1 + \exp(\epsilon - x)}. \quad (1)$$

These integrals are widely used in many problems concerned with semiconductors and metals. The evaluation, tabulation and approximation of these integrals have a long history which has recently been reviewed by Blakemore.[1] The thrust of recent work in this area has been to seek very simple approximations to Eq. (1) in order to allow calculations involving F–D integrals to proceed on small computers. For example, in work that has appeared since Blakemore's review, Aymerich-Humet *et al.*[2] have proposed a single analytical approximation to $F_j(x)$ for real j which works for $-\infty < x < \infty$ with an error of 1.2% for $-1/2 < j < 1/2$ and 0.7% for $1/2 < j < 5/2$; Selvakumar[3] has provided a single approximation expression for $j = \pm 1/2$ which is accurate to 1% over the range $-4 \leqslant x \leqslant 12$.

To justify yet another paper in this area we make use of the fact that the compromising of either the accuracy or the range of applicability of j or x, which use of a single approximation expression inevitably entails, can be avoided by using several simple approximation expressions without having to resort to a large computer to carry out the computations. The equations proposed here are easily handled by a small desktop computer, such as HP9836, and, as is shown below, provide approximations to Eq. (1) with an error that is better than 10^{-5} for $-1/2 \leqslant j \leqslant 7/2$ over the range $-\infty < x < \infty$.

The idea of using several approximations to cover a wide range of x for various orders of j is, of course, not new.[1] For example, Cody and Thatcher[4] covered the range of $-\infty < x < \infty$ using three rational Chebyshev approximations to obtain an accuracy of better than 9×10^{-5} for $j = -1/2$, and better than 3×10^{-6} for $j = -1/2$ and $j = 3/2$. The merit of the method proposed here is that high accuracy over a wide range of both x and j can be obtained by using simple approximation expressions which are very closely related to short forms of the classic series expansions to Eq. (1).[1,5] These latter expressions are

for $x \leqslant 0$,

$$F_j(x) = \sum_{r=1}^{\infty} \frac{(-1)^{r+1} \exp(rx)}{r^{j+1}}; \quad (2)$$

for $x > 0$,

$$F_j(x) = \cos(j\pi) F_j(-x) + \frac{x^{j+1}}{\Gamma(j+2)} [1 + R_j(x)], \quad (3)$$

where

$$R_j(x) = \sum_{r=1}^{\infty} \frac{\alpha_r}{x^{2r}} \frac{\Gamma(j+2)}{\Gamma(j+2-2r)}$$

and α_r is given in Ref. 6.

In the work that follows, approximate expressions based on Eqs. (2) and (3) which satisfy Eq. (1) to an accuracy of better than 10^{-5} for $-\infty < x < \infty$ and $-1/2 \leqslant j \leqslant 7/2$ are given. Accuracy is defined in terms of the error, namely

$$\text{error} = \left| \frac{\text{FD}^* - \text{FD}}{\text{FD}} \right|,$$

where FD* is the approximate value and FD is the exact value calculated by numerical integration of Eq. (1).

1. For $x \leqslant 0$, all j

The expression used in this regime approximates Eq. (2) with a finite series with $1 \leqslant r \leqslant 7$, namely

TABLE II. Coefficients used in Eq. (6) for $x \geqslant 4$ ($j = 1/2, 3/2, 5/2, 7/2$) and for $x \geqslant 5$ ($j = -1/2$).

j	$-1/2$	$1/2$	$3/2$	$5/2$	$7/2$
a_1	1.12837	0.752253	0.300901	0.085972	0.019105
a_2	0.470698	0.928195	1.85581	1.23738	0.494958
a_3	0.453108	0.680839	0.466432	1.07293	2.13722
a_4	228.975	25.7829	7.71648	0.362030	0.503902
a_5	8303.50	553.636	120.535	38.7579	6.99243
a_6	118124	3531.43	800.702	750.718	96.6031
a_7	632895	3254.65	2189.84	4378.70	426.046

TABLE II. Coefficients used in Eq. (6) for $x \geq 4$ ($j = 1/2, 3/2, 5/2, 7/2$) and for $x \geq 5$ ($j = -1/2$).

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$$F_j(x) = \sum_{r=1}^{7} (-1)^{r+1} a_r \exp(rx). \tag{4}$$

The coefficients a_r are computed so as to give the required accuracy. The values used are tabulated in Table I.

2. For $x > 0$, integer j

In this case $R_j(x)$ in Eq. (3) is a polynomial rather than an asymptotic expansion and the relation between $F_j(x)$ and $F_j(-x)$ can be expressed exactly,[6] e.g.,

$$\begin{aligned} j=1: &\quad F_1(x) = -F_1(-x) + \frac{x^2}{2} + \frac{\pi^2}{6}, \\ j=2: &\quad F_2(x) = F_2(-x) + \frac{x^3}{6} + \frac{\pi^2 x}{6}, \\ j=3: &\quad F_3(x) = -F_3(-x) + \frac{x^4}{24} + \frac{\pi^2 x^2}{12} + \frac{7\pi^4}{360}. \end{aligned} \tag{5}$$

Substitution of the values of $F_j(-x)$, computed from Eq. (4), in Eqs. (5) yields results for $F_j(x)$ for $j = 1,2,3$ which differ from the exact solutions by less than 10^{-5}.

TABLE III. Coefficients used in Eq. (7).

x	$j=$	$-1/2$	$1/2$	$3/2$	$5/2$	$7/2$
$0-y$[a]				0.867200	0.927560	0.961478
$0-y/2$	a_1	0.604856	0.765147			
$y/2-y$		0.638086	0.777114			
$0-y$				0.765101	0.866971	0.927751
$0-y/2$	a_2	0.380080	0.604911			
$y/2-y$		0.292266	0.581307			
$0-y$				0.302693	0.383690	0.432494
$0-y/2$	a_3	0.059320	0.189885			
$y/2-y$		0.159486	0.206132			
$0-y$				0.062718	0.098868	0.129617
$0-y/2$	a_4	0.014526	0.020307			
$y/2-y$		0.077691	0.017680			
$0-y$				0.005793	0.017398	0.023308
$0-y/2$	a_5	0.004222	0.004380			
$y/2-y$		0.018650	0.006549			
$0-y$				0.001342	0.000418	0.004067
$0-y/2$	a_6	0.001335	0.000366			
$y/2-y$		0.002736	0.000784			
$0-y$				0.953657	0.000067	0.000009
$0-y/2$	a_7	0.000291	0.000133			
$y/2-y$		0.000249	0.000036			
$0-y$						
$0-y/2$	a_8	0.000159				
$y/2-y$		0.000013				
$0-y$						
$0-y/2$	a_9	0.000018				
$y/2-y$		0.000000				

[a] $y = 4$ for $j = 1/2, 3/2, 5/2, 7/2$. $y = 5$ for $j = -1/2$.

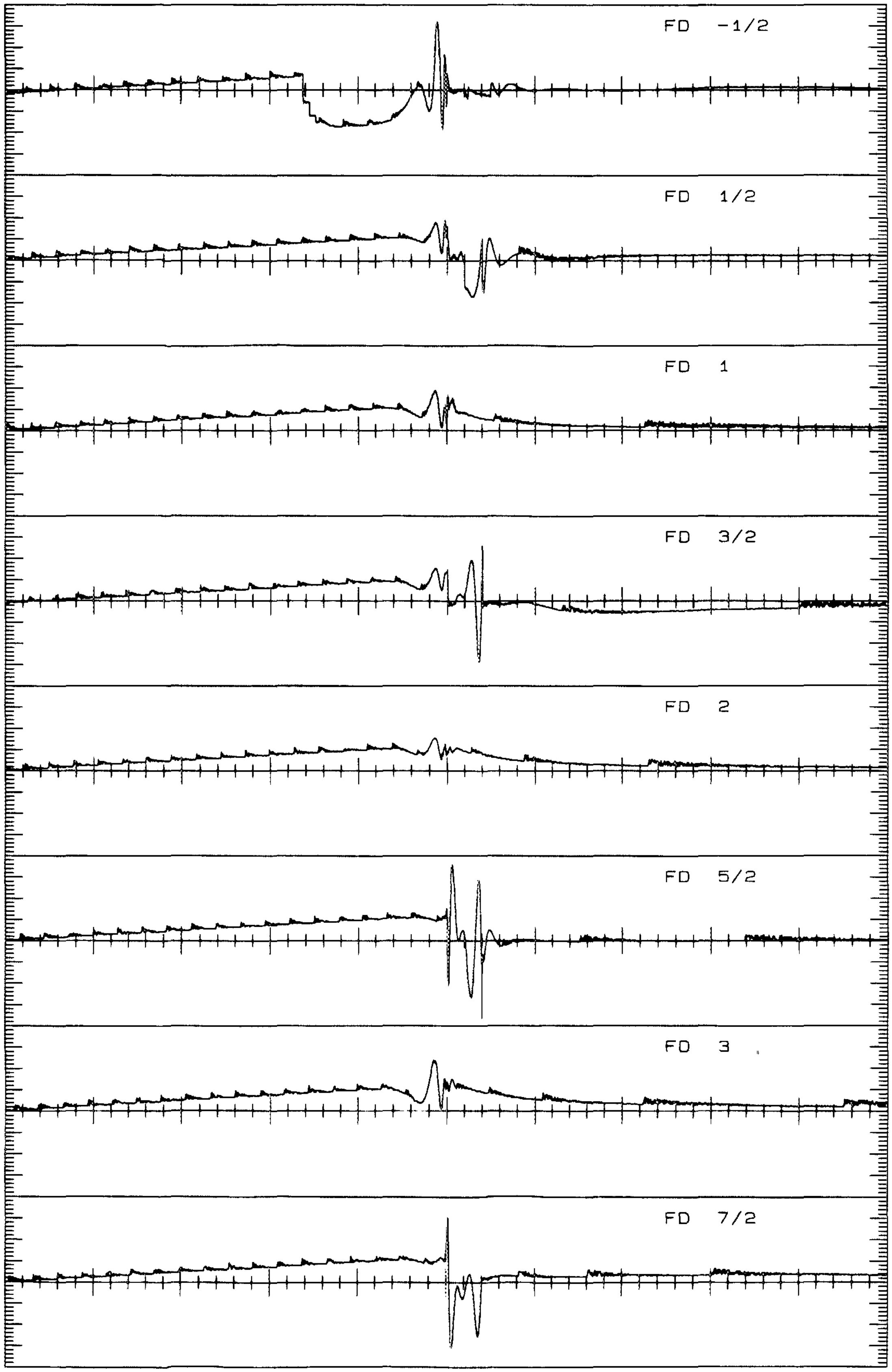

FIG. 1. Relative error profiles for the various Fermi–Dirac integrals. x on the x axis covers the range -50 to $+50$. The relative error on the y axis covers the range -1×10^{-5}–$+1\times10^{-5}$ on a linear scale for each individual case.

3. For $x > 0$, half-integer j

In this case the expansion to Eq. (3) can be written in the form

$$F_j(x) = x^{j+1} \sum_r \frac{a_r}{x^{2(r-1)}}. \tag{6}$$

For the case of $x \geqslant 4$, it was found that only seven terms in Eq. (6) need be taken to give the required accuracy for the orders $j = 1/2$, $3/2$, $5/2$, $7/2$. The appropriate coefficients are listed in Table II. For $j = -1/2$, Eq. (6) gives satisfactory results for $x \geqslant 5$ with the coefficients listed in Table II.

For the region $0 < x \leqslant 4$ (or $0 < x \leqslant 5$ for $j = -1/2$) it is not possible to choose coefficients for a short form of Eq. (6) and get the required accuracy. In these cases, therefore, the approximation expressions used were not directly related to the classic expansion forms of Eqs. (2) and (3). Instead a finite polynomial series of the form

$$F_j(x) = \sum_r a_r x^{r-1} \tag{7}$$

was used. For $j = 3/2$, $5/2$, $7/2$ one approximation with $1 \leqslant r \leqslant 7$ was sufficient to cover the range $0 < x \leqslant 4$. For $j = -1/2$ and $1/2$ two approximations were required to cover the ranges $0 < x \leqslant 5$ (with $1 \leqslant r \leqslant 9$) and $0 < x \leqslant 4$ (with $1 \leqslant r \leqslant 7$), respectively. The coefficients for all these cases are listed in Table III.

The results for all the cases discussed above are shown in Fig. 1 for the range $-50 < x < 50$. The error improves for values of x outside this range due to the asymptotic nature of the approximation expressions. It can be seen that the error incurred by use of the approximation expressions derived here is never worse than 1×10^{-5}.

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