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Two classes of special functions for the phase-integral approximation

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Abstract. Two classes of functions obtainable from the special function Y_{2n} for the phase-integral approximation are computed symbolically. The first class is that of functions Z_{2n} and U_{2n}, where $Y_{2n} = Z_{2n} + \mathrm{D}U_{2n}$, and D is a differential operator. It has the advantage of simplifying the evaluation of integrals involving Y_{2n}. The second class, of functions A_{2n} and B_{2n-2} which are derived from Z_{2n}, is associated with an important integral identity in the phase-integral approximation.

1. Introduction

The phase-integral approximation provides a means of solving with high accuracy the equation

$$\frac{\mathrm{d}^2\psi}{\mathrm{d}z^2} + \frac{Q^2(z)}{\lambda^2}\psi = 0 \tag{1}$$

where λ is small. The approximate solutions for ψ are

$$q^{-1/2}(z)\exp\left(\pm\mathrm{i}\int q(z)\,\mathrm{d}z\right), \tag{2}$$

where

$$q(z) = \frac{Q(z)}{\lambda}\sum_{n=0}^{N} Y_{2n}(z). \tag{3}$$

The expressions (2) and (3) define the phase-integral approximation of order $2N+1$. The special functions $Y_{2n}(z)$ for $n > 1$ are determined from the equation which follows when (2) and (3) are substituted into (1), each Y_{2n} being of order λ^{2n}. From the same substitution it is easy to find that $Y_0(z) = 1$ and $Y_2(z) = \frac{1}{2}\epsilon_0(z) = \frac{1}{2}\epsilon_0$, where

$$\epsilon_0 = \left(\frac{\lambda}{Q(z)}\right)^{3/2}\frac{\mathrm{d}^2}{\mathrm{d}z^2}\left(\frac{\lambda}{Q(z)}\right)^{1/2}.$$

The higher Y functions are given in terms of ϵ_0 and quantities which may be written as

$$\epsilon_m = \left(\frac{\lambda}{Q(z)}\frac{\mathrm{d}}{\mathrm{d}z}\right)^m\epsilon_0 = \frac{\lambda}{Q(z)}\frac{\mathrm{d}}{\mathrm{d}z}\epsilon_{m-1} = \frac{\mathrm{d}}{\mathrm{d}\zeta}\epsilon_{m-1}. \tag{4}$$

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For example (Fröman 1966, Fröman and Fröman 1970),

$$Y_4 = -\tfrac{1}{8}(\epsilon_0^2 + \epsilon_2), \qquad Y_6 = \tfrac{1}{32}(2\epsilon_0^3 + 6\epsilon_0\epsilon_2 + 5\epsilon_1^2 + \epsilon_4)$$

and

$$Y_8 = -\tfrac{1}{128}(5\epsilon_0^4 + 30\epsilon_0^2\epsilon_2 + 50\epsilon_0\epsilon_1^2 + 10\epsilon_0\epsilon_4 + 28\epsilon_1\epsilon_3 + 19\epsilon_2^2 + \epsilon_6).$$

Expressions for the functions through Y_{20} have already been published (Campbell 1972).

Although (1), (2) and (3) set out a complete scheme for approximation, there are circumstances in which different methods of calculation from those that use the Y functions directly may be preferable, e.g. to draw attention to some particular property of the calculation, or because evaluation of $q(z)$ is merely a step in the evaluation of something else. These considerations lead to the introduction of two other pairs of special functions (U, Z) and (A, B) which can be obtained from the Y functions, order by order. Their overall purpose is to make common practical computations with the phase-integral approximation shorter and more efficient.

Section 3 refers to the functions $A_{2n}(z)$ and $B_{2n}(z)$, which are formed from Z_{2n} and Z_{2n+2}. The main use of the A and B functions at present is in connection with the approximation scheme

$$\frac{\partial}{\partial E}\int_\Gamma q(z;E)\,\mathrm{d}z = \int_\Gamma \frac{1}{2}\frac{\partial Q^2(z;E)}{\partial E}\frac{\mathrm{d}z}{q(z;E)} \tag{5}$$

of Fröman (1974a) and Fröman (1974b). The scheme (5) simplifies greatly the calculation of the integral on its left-hand side over a closed contour of integration Γ, and is general in the sense that E can be any parameter other than z appearing in q.

2. The functions Z and U

Both in the usual phase-integral approximation introduced above, and in the modified phase-integral approximation (Fröman and Fröman 1974), an integral of q such as the left-hand side of (5) involves a sum of integrals over the individual Y functions. This follows immediately from the substitution of (3) into (5). If

$$\zeta = \int \lambda^{-1} Q(z)\,\mathrm{d}z, \tag{6}$$

an indefinite integral, then

$$\int_\Gamma q(z)\,\mathrm{d}z = \int_\Gamma \sum_{n=0}^{N} Y_{2n}\,\mathrm{d}\zeta. \tag{7}$$

In many realistic cases, the contour Γ in the complex plane is closed. When this is so, most terms in the expanded sum in (7) contribute zero to the integral because they are in effect total derivatives with respect to ζ. Hence the use of (7) is far more efficient computationally if each Y_{2n} can be broken down into two parts, one containing these total derivatives and the other part Z_{2n} containing the significantly smaller number of terms which make finite contributions to (7) when Γ is closed.

The resultant splitting of Y_{2n} has the form

$$Y_{2n} = Z_{2n} + \frac{\mathrm{d}}{\mathrm{d}\zeta}U_{2n}, \tag{8}$$

and the choice of Z and U to satisfy (8) is made unique by the requirement that, when the symbolic content of any term is written as $\epsilon_{i_1}^{p_1}\epsilon_{i_2}^{p_2}\ldots\epsilon_{i_f}^{p_f}$, where $i_1 < i_2 < \ldots < i_f$, then p_f in each term in any Z_{2n} is strictly greater than 1. The requirement was first stated in a different way in an unpublished report by P O Fröman and W Mrazek, but was deduced in this form by the system of symbolic programs which computed the Z and U functions.

Results for Z_{2n} are:

$$Z_0 = 1, \qquad Z_2 = \tfrac{1}{2}\epsilon_0, \qquad Z_4 = -\tfrac{1}{8}\epsilon_0^2, \qquad Z_6 = \tfrac{1}{32}(2\epsilon_0^3 - \epsilon_1^2),$$

$$Z_8 = -\tfrac{1}{128}(5\epsilon_0^4 - 10\epsilon_0\epsilon_1^2 + \epsilon_2^2), \qquad Z_{10} = \tfrac{1}{512}(14\epsilon_0^5 - 70\epsilon_0^2\epsilon_1^2 + 14\epsilon_0\epsilon_2^2 - \epsilon_3^2),$$

$$Z_{12} = -\tfrac{1}{2048}(42\epsilon_0^6 - 420\epsilon_0^3\epsilon_1^2 + 126\epsilon_0^2\epsilon_2^2 - 18\epsilon_0\epsilon_3^2 - 35\epsilon_1^4 + 20\epsilon_2^3 + \epsilon_4^2),$$

$$Z_{14} = \tfrac{1}{8192}[132\epsilon_0^7 - 2310\epsilon_0^4\epsilon_1^2 + 924\epsilon_0^3\epsilon_2^2 - 198\epsilon_0^2\epsilon_3^2 + \epsilon_0(-770\epsilon_1^4 + 440\epsilon_2^3 + 22\epsilon_4^2)$$
$$+ 462\epsilon_1^2\epsilon_2^2 - 110\epsilon_2\epsilon_3^2 - \epsilon_5^2],$$

$$Z_{16} = -\tfrac{1}{32\,768}[429\epsilon_0^8 - 12\,012\epsilon_0^5\epsilon_1^2 + 6006\epsilon_0^4\epsilon_2^2 - 1716\epsilon_0^3\epsilon_3^2$$
$$+ \epsilon_0^2(-10\,010\epsilon_1^4 + 5720\epsilon_2^3 + 286\epsilon_4^2)$$
$$+ \epsilon_0(12\,012\epsilon_1^2\epsilon_2^2 - 2860\epsilon_2\epsilon_3^2 - 26\epsilon_5^2) - 858\epsilon_1^2\epsilon_3^2 + 1001\epsilon_2^4 + 182\epsilon_2\epsilon_4^2 + \epsilon_6^2].$$

Although the first use of (8) is to reduce the amount of work required in the evaluation of (7) for closed contours by substituting Z_{2n} for Y_{2n}, a bonus is that the full expression (8) may make a similar reduction when Γ is not closed. Suppose that the contour connects the points ζ_0 and ζ_1. Then, in general, substitution of (8) transforms (7) into

$$\int_{\zeta_0}^{\zeta_1} \sum_{n=0}^{N} Z_{2n}\,\mathrm{d}\zeta + \sum_{n=0}^{N} (U_{2n}(\zeta_1) - U_{2n}(\zeta_0)),$$

whose evaluation involves less computing than does the right-hand side of (7). Therefore it is helpful to have on record the explicit forms for the functions U_{2n} as well as Z_{2n}. These functions are now given:

$$U_0 = 0, \qquad U_2 = 0, \qquad U_4 = -\tfrac{1}{8}\epsilon_1, \qquad U_6 = \tfrac{1}{32}(6\epsilon_0\epsilon_1 + \epsilon_3),$$

$$U_8 = -\tfrac{1}{128}(30\epsilon_0^2\epsilon_1 + 10\epsilon_0\epsilon_3 + 18\epsilon_1\epsilon_2 + \epsilon_5),$$

$$U_{10} = \tfrac{1}{512}(140\epsilon_0^3\epsilon_1 + 70\epsilon_0^2\epsilon_3 + 252\epsilon_0\epsilon_1\epsilon_2 + 14\epsilon_0\epsilon_5 + 190\epsilon_1^3/3 + 40\epsilon_1\epsilon_4 + 70\epsilon_2\epsilon_3 + \epsilon_7),$$

$$U_{12} = -\tfrac{1}{2048}[630\epsilon_0^4\epsilon_1 + 420\epsilon_0^3\epsilon_3 + 126\epsilon_0^2(18\epsilon_1\epsilon_2 + \epsilon_5)$$
$$+ \epsilon_0(1140\epsilon_1^3 + 720\epsilon_1\epsilon_4 + 1260\epsilon_2\epsilon_3 + 18\epsilon_7)$$
$$+ 910\epsilon_1^2\epsilon_3 + \epsilon_1(1242\epsilon_2^2 + 70\epsilon_6) + 168\epsilon_2\epsilon_5 + 250\epsilon_3\epsilon_4 + \epsilon_9],$$

$$U_{14} = \tfrac{1}{8192}\{2772\epsilon_0^5\epsilon_1 + 2310\epsilon_0^4\epsilon_3 + 924\epsilon_0^3(18\epsilon_1\epsilon_2 + \epsilon_5)$$
$$+ \epsilon_0^2[12\,540\epsilon_1^3 + 7920\epsilon_1\epsilon_4 + 13\,860\epsilon_2\epsilon_3 + 198\epsilon_7)$$
$$+ \epsilon_0[20\,020\epsilon_1^2\epsilon_3 + \epsilon_1(27\,324\epsilon_2^2 + 1540\epsilon_6) + 3696\epsilon_2\epsilon_5 + 5500\epsilon_3\epsilon_4 + 22\epsilon_9]$$
$$+ 13\,740\epsilon_1^3\epsilon_2 + 2730\epsilon_1^2\epsilon_5 + \epsilon_1(11\,220\epsilon_2\epsilon_4 + 7028\epsilon_3^2 + 108\epsilon_8)$$
$$+ 9702\epsilon_2^2\epsilon_3 + 330\epsilon_2\epsilon_7 + 658\epsilon_3\epsilon_6 + 924\epsilon_4\epsilon_5 + \epsilon_{11}\},$$

$$U_{16} = -\tfrac{1}{32\,768}\{12\,012\epsilon_0^6\epsilon_1 + 12\,012\epsilon_0^5\epsilon_3 + \epsilon_0^4(108\,108\epsilon_1\epsilon_2 + 6006\epsilon_5)$$
$$+ \epsilon_0^3(108\,680\epsilon_1^3 + 68\,640\epsilon_1\epsilon_4 + 120\,120\epsilon_2\epsilon_3 + 1716\epsilon_7)$$
$$+ \epsilon_0^2[260\,260\epsilon_1^2\epsilon_3 + \epsilon_1(355\,212\epsilon_2^2 + 20\,020\epsilon_6)$$
$$+ 48\,048\epsilon_2\epsilon_5 + 71\,500\epsilon_3\epsilon_4 + 286\epsilon_9] + \epsilon_0[357\,240\epsilon_1^3\epsilon_2 + 70\,980\epsilon_1^2\epsilon_5$$
$$+ \epsilon_1(291\,720\epsilon_2\epsilon_4 + 182\,728\epsilon_3^2 + 2808\epsilon_8)$$
$$+ 252\,252\epsilon_2^2\epsilon_3 + 8580\epsilon_2\epsilon_7 + 17\,108\epsilon_3\epsilon_6 + 24\,024\epsilon_4\epsilon_5 + 26\epsilon_{11}]$$
$$+ 27\,942\epsilon_1^5 + 73\,800\epsilon_1^3\epsilon_4 + \epsilon_1^2(380\,604\epsilon_2\epsilon_3 + 6402\epsilon_7)$$
$$+ \epsilon_1(173\,316\epsilon_2^3 + 34\,944\epsilon_2\epsilon_6 + 61\,404\epsilon_3\epsilon_5 + 36\,920\epsilon_4^2 + 154\epsilon_{10})$$
$$+ 42\,042\epsilon_2^2\epsilon_5 + \epsilon_2(126\,620\epsilon_3\epsilon_4 + 572\epsilon_9) + 26\,506\epsilon_3^3 + 1428\epsilon_3\epsilon_8$$
$$+ 2574\epsilon_4\epsilon_7 + 3430\epsilon_5\epsilon_6 + \epsilon_{13}\}.$$

Above $n = 8$, the size of the expressions for these functions grows rapidly. Values of Z_{2n} and U_{2n} for $n > 8$ are available from the author on request.

3. The functions *A* and *B*

In the modified phase-integral approximation, one introduces and uses a function $Q_{\mathrm{mod}}(z;E)$ in addition to the function $Q(z;E)$ in (5). Then, as in Fröman and Fröman (1974), it is possible to write

$$\epsilon_0 = \frac{Q^2(z;E) - Q^2_{\mathrm{mod}}(z;E)}{Q^2_{\mathrm{mod}}(z;E)} + Q^{-3/2}_{\mathrm{mod}}(z;E)\frac{\mathrm{d}^2}{\mathrm{d}z^2}Q^{-1/2}_{\mathrm{mod}}(z;E) \qquad (9)$$

and

$$q(z;E) = Q_{\mathrm{mod}}(z;E)\sum_{n=0}^{N} Y_{2n}, \qquad (10)$$

analogous to (3). Here λ is set equal to 1 to agree with the notation of Fröman (1974b).

As a beginning for the discussion of the left-hand side of (5), (6) (with $Q = Q_{\mathrm{mod}}$) and (10) imply that

$$\frac{\partial}{\partial E}\int_\Gamma q(z;E)\,\mathrm{d}z = \int_\Gamma \frac{\partial \ln Q_{\mathrm{mod}}}{\partial E}\sum_{n=0}^{N} Z_{2n}\,\mathrm{d}\zeta + \int_\Gamma \sum_{n=0}^{N}\frac{\partial Z_{2n}}{\partial E}\,\mathrm{d}\zeta. \qquad (11)$$

In the first method which was used (Fröman 1974b) to obtain the approximation (5), (11) has been rewritten as

$$\frac{\partial}{\partial E}\int_\Gamma q(z;E)\,\mathrm{d}z = \int_\Gamma \frac{\partial \ln Q_{\mathrm{mod}}}{\partial E}\sum_{n=0}^{N} A_{2n}\,\mathrm{d}\zeta + \int_\Gamma \frac{1}{2}\frac{\partial \epsilon_0}{\partial E}\sum_{n=0}^{N} B_{2n-2}\,\mathrm{d}\zeta. \qquad (12)$$

Equations (11) and (12) define the *A* and *B* functions. More precisely the right-hand sides of (11) and (12) are equal for each n separately.

This initial definition is far from being algorithmic, i.e. a statement of the form '$A_{2n} = \ldots$' and '$B_{2n-2} = \ldots$' which can be turned into a computer program. The symbolic computation here has proceeded in two stages: firstly, a deduction of a possible algorithmic form for A_{2n} and B_{2n-2} which was verified by hand; and secondly, the use of the form to compute actual values.

The expressions for the A and B functions are

$$A_{2n} = Z_{2n} + \sum_{k=1}^{n-2} \sum_{j=0}^{k-1} (-1)^{j+1} T_{kn}^{(j)} \epsilon_{k-j} \tag{13}$$

and

$$B_{2n-2} = 2 \sum_{k=0}^{n-2} (-1)^k T_{kn}^{(k)}, \tag{14}$$

where

$$T_{kn}^{(j)} = \frac{\mathrm{d}}{\mathrm{d}\zeta} T_{kn}^{(j-1)} = \frac{\mathrm{d}^j}{\mathrm{d}\zeta^j} T_{kn}^{(0)}, \tag{15}$$

and the writing of $\partial Z_{2n}/\partial E$ as

$$\frac{\partial Z_{2n}}{\partial E} = \sum_{k=0}^{n-2} T_{kn}^{(0)} \frac{\partial \epsilon_k}{\partial E} \tag{16}$$

fixes $T_{kn}^{(0)}$ uniquely.

Some low-n values of the A and B functions are as follows:

$$A_0 = 1, \qquad A_2 = \tfrac{1}{2}\epsilon_0, \qquad A_4 = -\tfrac{1}{8}\epsilon_0^2, \qquad A_6 = \tfrac{1}{32}(2\epsilon_0^3 + \epsilon_1^2),$$

$$A_8 = -\tfrac{1}{128}(5\epsilon_0^4 + 10\epsilon_0\epsilon_1^2 + 2\epsilon_1\epsilon_3 - \epsilon_2^2).$$

$$A_{10} = \tfrac{1}{512}(14\epsilon_0^5 + 70\epsilon_0^2\epsilon_1^2 + 28\epsilon_0\epsilon_1\epsilon_3 - 14\epsilon_0\epsilon_2^2 + 28\epsilon_1^2\epsilon_2 + 2\epsilon_1\epsilon_5 - 2\epsilon_2\epsilon_4 + \epsilon_3^2),$$

$$A_{12} = -\tfrac{1}{2048}[42\epsilon_0^6 + 420\epsilon_0^3\epsilon_1^2 + 126\epsilon_0^2(2\epsilon_1\epsilon_3 - \epsilon_2^2) + 18\epsilon_0(28\epsilon_1^2\epsilon_2 + 2\epsilon_1\epsilon_5 - 2\epsilon_2\epsilon_4 + \epsilon_3^2)$$
$$+ 105\epsilon_1^4 + 72\epsilon_1^2\epsilon_4 + 2\epsilon_1(60\epsilon_2\epsilon_3 + \epsilon_7) - 40\epsilon_2^3 - 2\epsilon_2\epsilon_6 + 2\epsilon_3\epsilon_5 - \epsilon_4^2],$$

and

$$B_0 = 1, \qquad B_2 = -\tfrac{1}{2}\epsilon_0, \qquad B_4 = \tfrac{1}{8}(3\epsilon_0^2 + \epsilon_2), \qquad B_6 = -\tfrac{1}{32}(10\epsilon_0^3 + 10\epsilon_0\epsilon_2 + 5\epsilon_1^2 + \epsilon_4),$$

$$B_8 = \tfrac{1}{128}(35\epsilon_0^4 + 70\epsilon_0^2\epsilon_2 + 70\epsilon_0\epsilon_1^2 + 14\epsilon_0\epsilon_4 + 28\epsilon_1\epsilon_3 + 21\epsilon_2^2 + \epsilon_6),$$

$$B_{10} = -\tfrac{1}{512}[126\epsilon_0^5 + 420\epsilon_0^3\epsilon_2 + 126\epsilon_0^2(5\epsilon_1^2 + \epsilon_4) + \epsilon_0(504\epsilon_1\epsilon_3 + 378\epsilon_2^2 + 18\epsilon_6)$$
$$+ 462\epsilon_1^2\epsilon_2 + 54\epsilon_1\epsilon_5 + 114\epsilon_2\epsilon_4 + 69\epsilon_3^2 + \epsilon_8],$$

$$B_{12} = \tfrac{1}{2048}[462\epsilon_0^6 + 2310\epsilon_0^4\epsilon_2 + 924\epsilon_0^3(5\epsilon_1^2 + \epsilon_4) + \epsilon_0^2(5544\epsilon_1\epsilon_3 + 4158\epsilon_2^2 + 198\epsilon_6)$$
$$+ \epsilon_0(10\,164\epsilon_1^2\epsilon_2 + 1188\epsilon_1\epsilon_5 + 2508\epsilon_2\epsilon_4 + 1518\epsilon_3^2 + 22\epsilon_8)$$
$$+ 1155\epsilon_1^4 + 1650\epsilon_1^2\epsilon_4 + \epsilon_1(5676\epsilon_2\epsilon_3 + 88\epsilon_7)$$
$$+ 1342\epsilon_2^3 + 242\epsilon_2\epsilon_6 + 418\epsilon_3\epsilon_5 + 253\epsilon_4^2 + \epsilon_{10}].$$

Once again, higher values are available from the author on request, or they may be computed with the use of the equations (13)–(16).

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References

Campbell J A 1972 *J. Comput. Phys.* **10** 308
Fröman N 1966 *Ark. Fys.* **32** 541
—— 1974a *Phys. Lett.* A **48** 137
Fröman P O 1974b *Ann. Phys., NY* **88** 621
Fröman N and Fröman P O 1970 *Nucl. Phys.* A **147** 606
—— 1974 *Ann. Phys., NY* **83** 103