# Computation of a Class of Functions Useful in the Phase-Integral Approximation. I. Results

## J. A. CAMPBELL\*

Department of Physics, Center for Particle Theory, and Department of Computer Science, University of Texas at Austin, Austin, Texas 78712

Received November 24, 1971

Wavefunctions in the phase-integral approximation, which is closely related to the JWKB approximation, may be expressed as expansions in terms of functions  $Y_{2n}$  first defined by N. Fröman. Previously, only the functions up to  $Y_8$  have been known. This paper presents computed expressions for the functions through  $Y_{20}$ .

For the equation

$$\frac{d^2\psi}{dz^2} + \frac{Q^2(z)}{\lambda^2} \psi = 0, \qquad (1)$$

where  $\lambda$  is small and  $Q^2(z)$  is usually assumed to be real when Im z = 0, a solution of the form

$$\psi(z) = \exp\left(\frac{i}{\lambda} \int \sum_{m=0}^{M} \lambda^m y_m(z) \, dz\right) \tag{2}$$

is the JWKB approximation of order M. When (2) is substituted into (1), the functions  $y_m(z)$  are determined by the requirement that the multiplier of each power of  $\lambda$  in the resulting equation should be zero. In particular,  $y_0 = \pm Q$ . The remaining functions follow from the recurrence

$$\frac{dy_{m-1}(z)}{dz} = -i \sum_{\mu=0}^{m} y_{\mu}(z) y_{m-\mu}(z).$$
(3)

The equation (3) provides a basis for showing that there is an alternative form [1] of the approximate  $\psi$  in which all odd-order functions  $y_{2m+1}(z)$  are eliminated in favor of even-order functions. When this is done, the alternative version of  $\psi$  is

$$\psi(z) = \exp\left(\frac{i}{\lambda} \int \sum_{n=0}^{N} \lambda^{2n} y_{2n}(z) dz\right) / \left(\lambda^{-1/2} \sum_{n=0}^{N} \lambda^{2n} y_{2n}(z)\right), \tag{4}$$

\* Address after 1 September 1972: King's College, Cambridge, England.

which is the phase-integral approximation of order 2N + 1. A comparison of (2) and (4) suggests that it is easier to work with the phase-integral approximation than with the JWKB approximation for high orders.

There are two independent approximate solutions contained in (4), which are evident from (3) and from the fact that  $y_0(z)$  is two-valued. The solutions are the expressions

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

where

$$q(z) = \frac{Q(z)}{\lambda} \sum_{n=0}^{N} Y_{2n}(z), \qquad (5)$$

and  $Y_{2n}$  is a convenient abbreviation for combinations of the y functions which may be computed from (3). Explicitly, they are given [1] by the defining relation

$$Y_{2n} = \epsilon_{0}Y_{2n-2} - \frac{1}{4}Y_{2n-2}'' + \frac{1}{2}\sum_{\alpha+\beta=n}'Y_{2\alpha}Y_{2\beta} - \frac{1}{2}\sum_{\alpha+\beta+\gamma+\delta=n}'Y_{2\alpha}Y_{2\beta}Y_{2\gamma}Y_{2\delta} + \frac{1}{2}\sum_{\alpha+\beta=n-1}'[\epsilon_{0}Y_{2\alpha}Y_{2\beta} + \frac{3}{4}Y_{2\alpha}'Y_{2\beta}' - \frac{1}{4}(Y_{2\alpha}Y_{2\beta}'' + Y_{2\alpha}''Y_{2\beta})]$$
(6)

for n > 1. Since the lowest-order JWKB and phase-integral approximations are identical, it is obvious without the use of (3) that  $Y_0(z) = 1$ . With a little more effort, one finds that  $Y_2(z) = \frac{1}{2}\epsilon_0$ , where

$$\epsilon_0 = \left(rac{\lambda}{Q(z)}
ight)^{3/2} rac{d^2}{dz^2} \left(rac{Q(z)}{\lambda}
ight)^{-1/2}.$$

In (6), each prime on a Y function denotes one differentiation with the operator  $\lambda Q^{-1}(z)(d/dz)$ . The primes on the summations in (6) have a different meaning: it is required that at least two Y functions appearing in any term of each sum should have subscript indices greater than zero.

In a general determination of  $Y_{2n}$  from (6), there is no need to differentiate directly with respect to z. It is possible to write all Y functions purely in terms of  $\epsilon_0$  and quantities

$$\epsilon_m = \left(\frac{\lambda}{Q(z)} \frac{d}{dz}\right)^m \epsilon_0,$$

where  $1 \leq m \leq 2n-2$  (excluding 2n-3) for a given n.

Evaluation of  $Y_{2n}$  by hand quickly becomes rather difficult as *n* increases. For example, the number of terms in the sum over products of four Y functions [2] is (n + 1)(n + 2)(n + 3)/6. Fröman has given the values of  $Y_0$ ,  $Y_2$  and  $Y_4$  in

### CAMPBELL

the same paper in which Eq. (6) is introduced, but the expressions calculated by F. Karlsson and S. Yngve for  $Y_6$  and  $Y_8$  did not appear in print for another four years [3]. In some circumstances there is a need for the higher functions, with n > 4, to check the accuracy of certain approximations to  $Y_{2n}$  near values of z for which  $Q^2(z)$  has either a zero or a pole [2]. It is apparent that further calculations are unlikely to be either fast or rewarding without the help of a computer.

Several symbolic computing systems exist in which programming of the algorithm contained in (6), or alternative algorithms for  $Y_{2n}$ , is highly convenient. Amongst the better-known systems are CAMAL [4], SAC-2 [5], REDUCE-2 [6] and SYMBAL [7]. The exercise has been programmed in all of these systems, for use as a bench-mark problem for evaluation of performance which will be discussed in a subsequent paper. In terms of computing time, however, the winner is the dark-horse entry TRIGMAN [8], which has computed the functions through  $Y_{16}$  in 10.595 sec on a CDC 6600,  $Y_{18}$  in 17.904 sec, and  $Y_{20}$  in 30.920 sec. The programs themselves are quite short (e.g., 15–20 lines) in most of the systems, which require the user to write in ALGOL-like dialects for the symbolic computation, but up to five times longer in the systems (SAC-2, TRIGMAN) based on FORTRAN. In the bare versions of SAC-2 and TRIGMAN, pure FORTRAN statements which everyone can understand are mixed with many calls to special subroutines for the symbolic operations. Therefore, a user who wishes merely to write

$$X = Y(2)^*Y(12) + E0^*Y(14)$$
(7)

for the combination of some functions in (6) may be compelled to write

instead. This leads to alienation. The answer to the difficulty is that SNOBOL [9] translators, complete for TRIGMAN and under development for SAC-2, carry statements such as (7) for symbolic quantities automatically into subroutine calls (8) or blocks of subroutine calls before the final FORTRAN compilation. Thus they allow the user to write shorter programs and to work in a language with which he is already familiar from numerical computations without having to pick up a detailed knowledge of the interior workings of the special algebraic subsystems.

All runs of programs in different languages have generated results in agreement with each other, which is pleasing.

Independently of this reassurance, there are two other small checks on computed expressions for  $Y_{2n}$ : Skorupski [2] has pointed out that  $Y_{2n}$  must always contain the terms

$$\frac{(-1)^{n+1}(2n)! \epsilon_0^n}{2^{2n}(n!)^2(2n-1)} \quad \text{and} \quad \frac{(-1)^{n+1}\epsilon_{2n-2}}{2^{2n-1}}$$

for n > 1. As well as fulfilling these requirements, the results given below suggest some other regularities which may be regarded as propositions for eventual proof, e.g.,

(i) The coefficient of  $\epsilon_0^{n-2}\epsilon_2$  is

$$\frac{(-1)^{n+1}}{2^{2n-1}}\frac{(2n-3)!}{[(n-2)!]^2}.$$

(ii) For terms proportional to  $\epsilon_0^{n-3}$ , only terms in  $\epsilon_0^{n-3}\epsilon_{1^2}$  and  $\epsilon_0^{n-3}\epsilon_4$  enter, and the ratio of the former term to the latter is 5.

(iii) The coefficient of  $\epsilon_0^{n-3}\epsilon_4$  is

$$\frac{(-1)^{n+1}}{3\cdot 2^{2n}}\frac{(2n-3)!}{(n-2)!(n-3)!}.$$

- (iv) The coefficient of  $\epsilon_0^4 \epsilon_{2n-10}$  is  $(-1)^{n+1} 2^{2-2n} (2n-3)(2n-5)(2n-7)(2n-9)/3$ .
- (v) The coefficient of  $\epsilon_0^3 \epsilon_{2n-8}$  is  $(-1)^{n+1} 2^{3-2n} (2n-3)(2n-5)(2n-7)/3$ .
- (vi) The coefficient of  $\epsilon_0^2 \epsilon_{2n-6}$  is  $(-1)^{n+1} 2^{2-2n} (2n-3)(2n-5)$ .
- (vii) The coefficient of  $\epsilon_1 \epsilon_{2n-5}$  is  $(-1)^{n+1} 2^{2-2n}(n-2)(2n-1)$ .
- (viii) The coefficient of  $\epsilon_0 \epsilon_{2n-4}$  is  $(-1)^{n+1} 2^{2-2n}(2n-3)$ .

All of these propositions refer to  $Y_{2n}$ . They are examples of the possibility of using a symbolic computing system conversationally to discover interesting general relationships among the particular data which are either the subjects or the products of a computation.

The construction of a difference table hints that, for n larger than the values considered here,  $Y_{2n}$  will be a sum of  $(2n^3 - 30n^2 + 175n - 339)/3$  terms, or at least that this quantity will be a lower bound on the expected number of terms. The result has acted as a deterrent to the evaluation of the Y functions beyond n = 10: the project is practical as far as computing time and requirements of storage are concerned, but not necessarily practical in face of the predicted bill for the computation under the accounting system for the machine on which this work has been carried out.

The writing of a symbolic program around Eq. (6) is straightforward, except perhaps for the treatment of the sum over  $Y_{2\alpha}Y_{2\beta}Y_{2\gamma}Y_{2\delta}$ , and for the observation

## CAMPBELL

that the sum over  $Y_{2\alpha}Y_{2\beta}$  for a given *n* should be stored as soon as it is calculated because it provides the bulk of the sum over  $\epsilon_0 Y_{2\alpha}Y_{2\beta}$  in the next iteration, when *n* is increased to n + 1. For the sum whose terms are products of four *Y* functions, the fastest method of computation seems to be to arrange that  $\alpha \leq \beta \leq \gamma \leq \delta$ , and to multiply each resulting term by a weighting factor which is 24 if all indices are distinct, 12 if only two indices are equal, 6 if two distinct pairs of equal indices occur, 4 if three indices are equal, and 1 otherwise. Further, time and space are saved in some systems if each such term is written as  $F_{\alpha\beta\gamma}Y_{2\delta}$ , where  $F_{\alpha\beta\gamma} = Y_{2\alpha}Y_{2\beta}Y_{2\gamma}$  need be calculated and stored only once for each combination of indices.

The computed functions  $Y_{2n}$  are as follows:

$$\begin{split} Y_0 &= 1, \\ Y_2 &= \frac{1}{2} \epsilon_0 \,, \\ Y_4 &= -\frac{1}{8} (\epsilon_0^2 + \epsilon_2), \\ Y_6 &= \frac{1}{32} (2\epsilon_0^3 + 6\epsilon_0\epsilon_2 + 5\epsilon_1^2 + \epsilon_4), \\ Y_8 &= -\frac{1}{128} (5\epsilon_0^4 + 30\epsilon_0^2\epsilon_2 + 50\epsilon_0\epsilon_1^2 + 10\epsilon_0\epsilon_4 + 28\epsilon_1\epsilon_3 + 19\epsilon_2^2 + \epsilon_6), \\ Y_{10} &= \frac{1}{512} (14\epsilon_0^5 + 140\epsilon_0^3\epsilon_2 + 350\epsilon_0^2\epsilon_1^2 + 70\epsilon_0^2\epsilon_4 + 392\epsilon_0\epsilon_1\epsilon_3 + 266\epsilon_0\epsilon_2^2 \\ &\quad + 14\epsilon_0\epsilon_6 + 442\epsilon_1^2\epsilon_2 + 54\epsilon_1\epsilon_5 + 110\epsilon_2\epsilon_4 + 69\epsilon_3^2 + \epsilon_8), \\ Y_{12} &= -\frac{1}{2048} (42\epsilon_0^6 + 630\epsilon_0^4\epsilon_2 + 420\epsilon_0^3 [5\epsilon_1^2 + \epsilon_4] \\ &\quad + \epsilon_0^2 [3528\epsilon_1\epsilon_3 + 2394\epsilon_2^2 + 126\epsilon_6] \\ &\quad + \epsilon_0 [7956\epsilon_1^2\epsilon_2 + 972\epsilon_1\epsilon_5 + 1980\epsilon_2\epsilon_4 + 1242\epsilon_3^2 + 18\epsilon_8] \\ &\quad + 1105\epsilon_1^4 + 1630\epsilon_1^2\epsilon_4 + \epsilon_1 [5564\epsilon_2\epsilon_3 + 88\epsilon_7] + 1262\epsilon_2^3 + 238\epsilon_2\epsilon_6 \\ &\quad + 418\epsilon_3\epsilon_5 + 251\epsilon_4^3 + \epsilon_1), \end{split}$$

$$\begin{split} Y_{16} &= -\frac{1}{32\,768}\,(429\epsilon_0^3+12\,012\epsilon_0^{\,6}\epsilon_2+12\,012\epsilon_0^{\,5}[5\epsilon_1^2+\epsilon_4] \\ &+ \epsilon_0^{\,3}[168\,168\epsilon_1\epsilon_9+1114\,114\epsilon_2^{\,2}+6006\epsilon_6] \\ &+ \epsilon_0^{\,3}[758\,472\epsilon_1^{\,2}\epsilon_2+92\,664\epsilon_1\epsilon_6+188\,760\epsilon_2\epsilon_4+118\,404\epsilon_8^{\,2}+1716\epsilon_8] \\ &+ \epsilon_0^{\,3}[316\,030\epsilon_1^{\,4}+466\,180\epsilon_1^{\,2}\epsilon_4+\epsilon_1(1\,591\,304\epsilon_2\epsilon_3+25\,168\epsilon_7) \\ &+ 360\,932\epsilon_3^{\,3}+68\,068\epsilon_2\epsilon_6+119\,548\epsilon_9\epsilon_5+17\,786\epsilon_4^{\,2}+286\epsilon_{10}] \\ &+ \epsilon_0[877\,760\epsilon_3^{\,3}\epsilon_6+\epsilon_3^{\,3}(1\,794\,156\epsilon_2^{\,2}+111\,020\epsilon_6) \\ &+ \epsilon_1(529\,776\epsilon_9\epsilon_5+800\,176\epsilon_9\epsilon_5+380\epsilon_5)+543\,972\epsilon_2^{\,2}\epsilon_4 \\ &+ \epsilon_2(68\,372\epsilon_9^{\,2}+11\,388\epsilon_6)+25\,688\epsilon_3\epsilon_7+41\,132\epsilon_4\epsilon_6+23\,998\epsilon_5^{\,3}+26\epsilon_{12}] \\ &+ 496\,950\epsilon_1^{\,3}\epsilon_6+144\,780\epsilon_3^{\,3}\epsilon_5+\epsilon_3^{\,3}[893\,724\epsilon_3\epsilon_4+562\,474\epsilon_3^{\,3}+9210\epsilon_6] \\ &+ \epsilon_1[1\,533\,408\epsilon_2^{\,2}\epsilon_3+56\,328\epsilon_2\epsilon_7+113\,456\epsilon_3\epsilon_4+159\,2268\epsilon_4\epsilon_5+180\epsilon_{12}] \\ &+ 174\,317\epsilon_8^{\,4}+76\,986\epsilon_2^{\,3}\epsilon_6+\epsilon_2[272\,108\epsilon_5\epsilon_6+163\,722\epsilon_4^{\,2}+726\epsilon_{10}] \\ &+ 206\,138\epsilon_3^{\,2}\epsilon_4+2000\epsilon_3\epsilon_9+4002\epsilon_4\epsilon_8+6004\epsilon_5\epsilon_7+3431\epsilon_6^{\,2}+\epsilon_{13}), \end{split}$$

## CAMPBELL

$$\begin{split} Y_{20} &= -\frac{1}{524\,288} \left( 4862\epsilon_0^{10} + 218\,790\epsilon_0^8\epsilon_2 + 291\,720\epsilon_0^7 [5\epsilon_1^2 + \epsilon_4] \right] \\ &+ \epsilon_0^8 [5\,717\,712\epsilon_1\epsilon_8 + 15\,519\,504\epsilon_2^3 + 204\,204\epsilon_8 ] \\ &+ \epsilon_0^8 [38\,682\,072\epsilon_1^3\epsilon_2 + 4\,725\,864\epsilon_1\epsilon_5 + 9\,626\,760\epsilon_8\epsilon_4 \\ &+ 6\,038\,604\epsilon_2^3 + 87\,516\epsilon_8 ] \\ &+ \epsilon_0^8 [26\,862\,550\epsilon_1^4 + 39\,625\,300\epsilon_1^3\epsilon_4 + 135\,260\,840\epsilon_1\epsilon_8\epsilon_3 + 30\,679\,220\epsilon_8^3 \\ &+ 2\,139\,280\epsilon_1\epsilon_7 + 5\,785\,780\epsilon_2\epsilon_6 + 10\,161\,580\epsilon_3\epsilon_5 \\ &+ 6\,101\,810\epsilon_4^2 + 24\,310\epsilon_{10} \right] \\ &+ \epsilon_0^8 [149\,219\,200\epsilon_1^3\epsilon_3 + \epsilon_1^2(305\,006\,520\epsilon_2^2 + 18\,873\,400\epsilon_6) \\ &+ \epsilon_1(90\,061\,920\epsilon_8\epsilon_5 + 136\,029\,920\epsilon_8\epsilon_4 + 574\,600\epsilon_6) + 92\,475\,240\epsilon_2^3\epsilon_4 \\ &+ \epsilon_2(116\,343\,240\epsilon_3^2 + 1\,935\,960\epsilon_8) + 4\,366\,960\epsilon_3\epsilon_7 + 6\,992\,440\epsilon_4\epsilon_6 \\ &+ 4\,079\,660\epsilon_8^2 + 4420\epsilon_{12} \right] \\ &+ \epsilon_0^3 [253\,444\,500\epsilon_1^3\epsilon_2 + 73\,837\,800\epsilon_1^3\epsilon_5 \\ &+ \epsilon_1^3 (455\,799\,240\epsilon_2\epsilon_4 + 286\,861\,740\epsilon_2^3 + 4\,697\,100\epsilon_8) \\ &+ \epsilon_1(782\,038\,080\epsilon_2^3\epsilon_4 + 28\,727\,280\epsilon_2\epsilon_7 + 57\,862\,560\epsilon_3\epsilon_6 + 81\,226\,680\epsilon_4\epsilon_5 \\ &+ 91\,800\epsilon_{11} + 88\,901\,670\epsilon_4^3 + 39\,262\,860\epsilon_2^3\epsilon_6 \\ &+ \epsilon_1(782\,038\,080\epsilon_3\epsilon_4 + 349\,8220\epsilon_4^3 + 370\,260\epsilon_{10}) + 105\,130\,380\epsilon_3\epsilon_4 \\ &+ \epsilon_2^3(455\,778\,408\epsilon_2^3 + 127\,923\,096\epsilon_2\epsilon_6 + 220\,222\,536\epsilon_5 \\ &+ 136\,134\,980\epsilon_4^3 + 594\,660\epsilon_{10}) \\ &+ \epsilon_1(307\,876\,392\epsilon_2^3\epsilon_5 + \epsilon_3(934\,106\,480\epsilon_3\epsilon_4 + 4\,32\,920\epsilon_6) \\ &+ 136\,134\,980\epsilon_4^3 + 594\,660\epsilon_{10}) \\ &+ \epsilon_4^3(168\,013\,536\epsilon_3^2 + 127\,1923\,096\epsilon_2\epsilon_6 + 220\,22\,236\epsilon_5 \\ &+ 136\,134\,980\epsilon_4^3 + 594\,660\epsilon_{10}) \\ &+ \epsilon_1(307\,876\,392\epsilon_2^3\epsilon_5 + \epsilon_3(934\,106\,480\epsilon_3\epsilon_4 + 4\,32\,920\epsilon_6) \\ &+ 196\,243\,376\epsilon_3^3 + 11\,153\,904\epsilon_2\epsilon_6 + 201\,93\,94\,24\epsilon_4\epsilon_7 \\ &+ 26\,888\,152\epsilon_5\epsilon_6 + 8092\epsilon_{13}) + 121\,168\,840\epsilon_3^3\epsilon_4 \\ &+ \epsilon_2^3(10\,335\,66\epsilon_3^2 + 75\,84\,324\epsilon_2) + \epsilon_4(34\,337\,55\,26_3\epsilon_7 + 55\,208\,520\epsilon_4\epsilon_6 \\ &+ 32\,225\,876\epsilon_5^3 + 803\,802\epsilon_{13}) + 121\,168\,846\epsilon_3^3\epsilon_4 \\ &+ \epsilon_2^3(163\,03\,536\epsilon_4\epsilon_5 + 255\,034\,560\epsilon_5\epsilon_6 + 136\,26] \\ &+ \epsilon_3(12\,857\,778\,8\epsilon_5\epsilon_6 + 255\,034\,560\epsilon_5\epsilon_6 + 126\,95\,6\epsilon_6\epsilon_{10} \\ &+ 54\,44\,76\epsilon_6\epsilon_6 + 777\,852\epsilon_6\epsilon_6 + 135\,350\,68\epsilon_6\epsilon_6 + 125\,217\,88\,6\epsilon_6\epsilon_7 + 35\,227\,86\epsilon_6\epsilon_7 + 37\,31\,107\epsilon_2\epsilon_7 \\ &+ \epsilon_3(12\,857\,716\,8\epsilon_5\epsilon_6 + 801\,220\epsilon_4\epsilon_6 + 26\,67\,140\epsilon_4\epsilon_8 + 9\,140\,140\epsilon_5\epsilon_7 \\ &+ 5\,227\,602\epsilon_6^3 + 111\,$$

314

#### PHASE-INTEGRAL APPROXIMATION

## ACKNOWLEDGMENTS

I thank Dr. Andrzej Skorupski for introducing me to this problem and for providing an account of his calculations prior to publication, and Dr. N. Fröman and Dr. S. R. Bourne for some helpful correspondence. The work outlined here has been supported in part by the National Science Foundation under grant No. GJ-1069 for the development of specialized algebraic programs.

## References

- 1. N. FRÖMAN, Ark. Fys. 32 (1966), 541.
- 2. A. A. SKORUPSKI, private communication.
- 3. N. FRÖMAN AND P. O. FRÖMAN, Nucl. Phys. A 147 (1970), 606.
- 4. D. BARTON, S. R. BOURNE, AND J. R. HORTON, Comp. J. 13 (1970), 243.
- G. E. COLLINS, The SAC system: An introduction and survey, in "Proceedings 2nd Symposium on Symbolic and Algebraic Manipulation," pp. 144–152, ACM Headquarters, New York, 1971.
- A. C. HEARN, REDUCE A user-oriented interactive system for algebraic simplification, in "Interactive Systems for Experimental Applied Mathematics" (M. Klerer and J. Reinfelds, Eds.), pp. 79–90, Academic Press, London/New York, 1968.
- 7. M. E. ENGELI, Adv. Inform. Systems Sci. 1 (1969), 117.
- 8. W. H. JEFFERYS, Celest. Mech. 2 (1970), 474.
- 9. R. E. GRISWOLD, J. F. POAGE, AND I. P. POLONSKY, "The SNOBOL 4 Programming Language," Prentice-Hall Inc., Englewood Cliffs, NJ, 1968.