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Alternative phase-integral approximations

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Abstract. Phase-integral approximations of a new kind are obtained. They are closely related to the phase-integral approximations generated from an unspecified base function $Q(z)$, due to Professor N Fröman and Professor P O Fröman. In the search for an optimal base function, a sequence of successively improved base functions $Q_N(z)$ are derived ($N=0,1,2,\ldots$) together with a concise recurrence formula for these functions that is suitable for computer calculations. (The function $Q_N(z)$ is an approximate solution to the nonlinear q-equation, equivalent to the Schrödinger equation). The proposed approximation, which is immediately obtained from $Q_N(z)$, is expected to be somewhat more accurate (for $N\geqslant 2$) than the corresponding phase-integral approximation of order $2N+1$, obtained from the function $q_N(z)$ given by

$$q_N(z)Q(z)\sum_{n=0}^{N} Y_{2n}(z).$$

A detailed comparison is made between $Q_N(z)$ and $q_N(z)$ for $N=0$, 1, 2, and 3. The proposed approximations have the correct form required to combine them with the F-matrix technique for solving connection problems.

1. Introduction

The author has previously treated one-dimensional problems concerning transmission (tunnelling) and bound states [1–3] by means of the well-known phase-integral method due to Fröman and Fröman and developed by them in [4–6]. The method combines arbitrary-order phase-integral approximations generated from an unspecified base function, derived in [4] and [5], with the F-matrix technique for solving connection problems, constructed in [6]. The advantages of using higher-order phase-integral approximations instead of the related higher-order JWKB approximations, as documented in [7], are connected with the fact that the expressions for the phase-integral functions have the same simple structure as displayed by $\Psi(z)$ in equation (2). For a short introduction to the phase-integral method the reader is referred to appendix A of [1], where some key facts about the method are given. A more recent review article [8], containing an extensive reference list, is published in a book in commemoration of the article *Ramifications, Old and New, of the Eigenvalue Problem* by Hermann Weyl [9]. Further, in section 2 of the present paper, the main steps in the derivation of the phase-integral approximations are described.

In section 3 the new alternative phase-integral approximations are obtained. These approximations have a simple structure making them suitable for computer calculations. The recurrence formulas for the functions $Q_N(z)$ and $\varepsilon_N(z)$, given by (42) and (43), constitute the principal result of this article. Appendix 1 and appendix 2 give mathematical support to the reasoning in sections 2 and 3 as well as to appendix 3 where (for $N=0$, 1, 2, and 3) a detailed comparison is made between the expression for the base function $Q_N(z)$, on one hand, and the phase-integral expression of order $2N+1$, i.e.

$$Q(z)\sum_{n=0}^{N} Y_{2n}(z)$$

on the other hand, indicating that the new approximations should be somewhat more accurate for $N\geqslant 2$. However, this question must be investigated by means of numerical calculations on model potentials before anything definite could be said about this point.

The phase-integral method has been successfully applied to various physical problems in the past two decades. Simple formulas admitting accurate evaluation have been obtained for a number of physical quantities such as energy eigenvalues, level densities, normalization factors, quantal expectation values, quantal matrix elements, dispersion relations, phase shifts, and transmission and reflection coefficients. Problems concerning, for instance, an unharmonic oscillator, a compressed atom, screened Coulomb potentials, Regge poles, scattering by complex potentials, complex angular momentum analysis of scattering, and black holes have been treated. For information, a number of pertinent papers [10]–[25] have been included in the reference list. By using in the phase-integral method, for $N=2, 3, \ldots$, the base function $Q_N(z)$ instead of the original phase-integral expression of order $2N+1$, we expect to gain some improvements in the numerical results due to a faster 'convergence' of the successive expressions. In the first place, this improvement is expected to show in those successive approximate solutions of the Schrödinger equation which are obtained (for $N=2, 3, \ldots$) if one replaces the function $q(z)$, occurring in the expression (2) for the wavefunction, by the base function $Q_N(z)$ instead of replacing it by the original phase-integral expression of order $2N+1$. We remark that the functions $Q_N(z)$ are constructed as successively improved approximate solutions of the nonlinear q-equation (3) that is equivalent to the Schrödinger equation.

2. Phase-integral approximations generated from an unspecified base function

We begin by giving a short account of the main steps in the derivation of the Fröman phase-integral expressions for the function $q(z)$. In doing so we shall slightly change the notation in order to make it more suited to the treatment later in this article.

We consider the Schrödinger equation

$$\frac{d^2\Psi}{dz^2}+R(z)\Psi(z)=0 \tag{1}$$

where $R(z)$ is assumed to be a single-valued analytical function in some region of the complex z-plane.

Inserting in (1)

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

we obtain the equation

$$R(z) - q^{2}(z) + q^{+1/2}(z)\frac{\mathrm{d}^{2}}{\mathrm{d}z^{2}}q^{-1/2}(z) = 0 \tag{3}$$

called the q-equation, which is equivalent to the original Schrödinger equation. The quantity $\varepsilon(q)$ occurring in the theory is defined by

$$\varepsilon(q) = \frac{R(z) - q^{2}(z)}{q^{2}(z)} + q^{-3/2}(z)\frac{\mathrm{d}^{2}}{\mathrm{d}z^{2}}q^{-1/2}(z). \tag{4}$$

From (3) and (4) we realize that $\varepsilon(q) \equiv 0$, if q is an exact solution of the q-equation. In the case that we cannot find an exact solution, we shall try to find a function $q(z)$ which makes $\varepsilon(q)$ as small as possible, i.e. a function $q(z)$ that is the best approximate solution of (3) that we are able to attain.

Inserting in (4),

$$q(z) = Q(z)g(z) \tag{5}$$

where $Q(z)$ is called the base function (not yet specified), we can write (4) in the form

$$\varepsilon(Qg) = \frac{1 + \varepsilon(Q) - g^{2}}{g^{2}} + g^{-3/2}\frac{\mathrm{d}^{2}}{\mathrm{d}\zeta^{2}}g^{-1/2} \tag{6}$$

where the variable ζ is defined by

$$\zeta = \int^{z} Q(z)\,\mathrm{d}z \tag{7}$$

and where the explicit expression for $\varepsilon(Q)$ is given by

$$\varepsilon(Q) = \frac{R(z) - Q^{2}(z)}{Q^{2}(z)} + Q^{-3/2}(z)\frac{\mathrm{d}^{2}}{\mathrm{d}z^{2}}Q^{-1/2}(z) \tag{8}$$

according to the definition (4). The relation (6) is originally derived in [1] and given there by (A27) in appendix A. The quantity $\varepsilon(Q)$ is identical with ε_0 occurring in the phase-integral theory. Inserting (5) in the q-equation (3), we obtain an equation for $g(z)$ instead, which reads

$$1 + \varepsilon(Q) - g^{2} + g^{+1/2}\frac{\mathrm{d}^{2}}{\mathrm{d}\zeta^{2}}g^{-1/2} = 0. \tag{9}$$

If the base function $Q(z)$ is chosen such that $\varepsilon(Q) \equiv 0$, we realize that $g(z) \equiv 1$ is an exact solution of (9). However, if we have succeeded in finding a base function $Q(z)$ that makes $\varepsilon(Q)$ very small (even though not exactly equal to zero), we expect to find a solution of the g-equation (9) having the form $g(z) = 1 +$ some small function.

We shall now assume that $R(z)$ is very large. We introduce a small local parameter p defined by the equation $|R(z)| = p^{-2}$. The function $R(z)$ at the point z and in the neighbourhood of z is thus of the order of magnitude of p^{-2}. Being a local parameter,

p is different in different regions of the complex z-plane. We shall visibly display the largeness of $R(z)$, expressed in terms of the parameter p, by writing $R(z)\cdot\lambda^{-2}$, where λ is a new parameter having the numerical value $\lambda=1$. The symbol λ is intended to appear merely as a sign giving information about the term to which it is multiplied. One can delete λ at any moment, thereby destroying a certain information about the term to which it is multiplied, but nothing else would be changed. Instead of deleting λ, one can achieve the same result by putting λ equal to unity.

We require that the base function $Q(z)$ shall be chosen such that the expressions

$$Q^2(z)\cdot\lambda^{-2} \qquad \text{and} \qquad [R(z)-Q^2(z)]\cdot\lambda^0 \tag{10a}$$

give correct information about the largeness of the terms $Q^2(z)$ and $[R(z)-Q^2(z)]$, respectively. The information implied by (10a) is that the quantities $Q^2(z)$ and $[R(z)-Q^2(z)]$ are of the order of magnitude of p^{-2} and p^0, respectively. It is also assumed in phase-integral theory that $\varepsilon(Q)$, given by (8), can correctly be written

$$\varepsilon(Q)\cdot\lambda^2, \tag{10b}$$

That this is a new assumption which does not follow from (10a) is usually not mentioned in phase-integral literature.

Since

$$\frac{dg}{d\zeta}=\frac{dz}{d\zeta}\frac{dg}{dz}=\frac{1}{Q}\frac{dg}{dz} \tag{11}$$

we find that we can take the largeness of the different terms in (9) into account by writing the equation in the following form

$$1+\varepsilon(Q)\cdot\lambda^2-g^2+g^{+1/2}\frac{d^2}{d\zeta^2}g^{-1/2}\cdot\lambda^2=0. \tag{12}$$

Inserting in (12) the formal expansion

$$g(z)=\sum_{n=0}^{\infty} Y_{2n}(z)\cdot\lambda^{2n} \tag{13}$$

and ordering the terms according to the powers of λ, we obtain a certain coefficient expression for each λ^{2n} ($n=0, 1, 2, \ldots$) which we set equal to zero. In this way we successively obtain

$$Y_0(z)=1 \tag{14a}$$

$$Y_2(z)=\frac{1}{2}\varepsilon_0 \tag{14b}$$

$$Y_4(z)=-\frac{1}{8}\left[\varepsilon_0^2+\frac{d^2\varepsilon_0}{d\zeta^2}\right] \tag{14c}$$

$$Y_6(z)=\frac{1}{32}\left[2\varepsilon_0^3+5\left(\frac{d\varepsilon_0}{d\zeta}\right)^2+6\varepsilon_0\frac{d^2\varepsilon_0}{d\zeta^2}+\frac{d^4\varepsilon_0}{d\zeta^4}\right] \tag{14d}$$

$$Y_8(z)=-\frac{1}{128}\left[5\varepsilon_0^4+50\varepsilon_0\left(\frac{d\varepsilon_0}{d\zeta}\right)^2+30\varepsilon_0^2\frac{d^2\varepsilon_0}{d\zeta^2}+19\left(\frac{d^2\varepsilon_0}{d\zeta^2}\right)^2\right.$$
$$\left.+28\frac{d\varepsilon_0}{d\zeta}\frac{d^3\varepsilon_0}{d\zeta^3}+10\varepsilon_0\frac{d^4\varepsilon_0}{d\zeta^4}+\frac{d^6\varepsilon_0}{d\zeta^6}\right] \tag{14e}$$

etc.

The expressions (14*a*–*e*) are quoted from equations (6*a*–*e*) in [26]; for simplicity we have kept the symbol ε_0 that stands for $\varepsilon(Q)$. Equations (14*a*–*c*) were originally obtained by N. Fröman [27] together with the recurrence formula

$$\sum_{\alpha+\beta=n} Y_{2\alpha}Y_{2\beta} - \sum_{\alpha+\beta+\gamma+\delta=n} Y_{2\alpha}Y_{2\beta}Y_{2\gamma}Y_{2\delta} + \sum_{\alpha+\beta=n-1}\left[\varepsilon_0 Y_{2\alpha}Y_{2\beta} + \frac{3}{4}\frac{\mathrm{d}Y_{2\alpha}}{\mathrm{d}\zeta}\frac{\mathrm{d}Y_{2\beta}}{\mathrm{d}\zeta} - \frac{1}{4}\left(Y_{2\alpha}\frac{\mathrm{d}^2Y_{2\beta}}{\mathrm{d}\zeta^2} + \frac{\mathrm{d}^2Y_{2\alpha}}{\mathrm{d}\zeta^2}Y_{2\beta}\right)\right] = 0 \qquad n \geqslant 1. \tag{15}$$

Explicit expressions for Y_{2n} up to Y_{20} have been calculated by Campbell [28], who used a symbolic (algebraic) computation system. By cutting off the expansion (13) at N, with Y_{2n} given by (14*a*–*e*) and (15), we obtain

$$g(z) = \sum_{n=0}^{N} Y_{2n}(z) \tag{16}$$

which is an approximate solution of the g-equation (9). From (5) and (16) we realize that the function

$$q(z) = Q(z)\sum_{n=0}^{N} Y_{2n}(z) \tag{17}$$

is an approximate solution of the q-equation (3), and further that (2) will be transformed into two approximate solutions of the original Schrödinger equation if the function $q(z)$ occurring in (2) is replaced by the expression in (17). These functions, obtained by (2) and (17), are called phase-integral functions of order $2N+1$ generated from the unspecified base function $Q(z)$. By forming linear combinations of the two phase-integral functions, we obtain the corresponding phase-integral approximation of order $2N+1$.

The expression for $q(z)$ given by (17) will, in the present paper, be called the phase-integral expression of order $2N+1$ generated from the base function $Q(z)$. The third-order phase-integral expression for $q(z)$ is

$$q(z) = Q(z)\left(1 + \frac{1}{2}\varepsilon_0\right) \tag{18}$$

as we see from (17) and (14*a*, *b*).

3. The base functions $Q_N(z)$

The main idea of the present article is to use the function in (18) as a new base function $Q_1(z)$ replacing the original base function $Q(z)$, which from now on will be called $Q_0(z)$. The variable ζ that corresponds to Q_0 and is defined by (7) will now be called ζ_0. The function Q_0 will be regarded as the first one in a sequence of base functions $Q_N(z)$, where $N=0, 1, 2, 3, \ldots$ Each base function Q_N can be used as a starting point for obtaining a kind of phase-integral expression of order $2M+1$ (for $M=0, 1, 2, \ldots$) generated from Q_N. But Q_N can alternatively be used in a direct way to obtaining approximate solutions of the Schrödinger equation (1), simply by putting $q(z)=Q_N$ in formula (2). This can later be realized from the fact that the functions Q_N, for $N=0, 1, 2, \ldots$, are constructed as successively improved approximate solutions of the q-equation (3). When used in the latter direct way it becomes interesting to compare the base function Q_N with the corresponding phase-integral expression

$$Q_0 \sum_{n=0}^{N} Y_{2n}(z).$$

It will be argued that, for $N \geqslant 2$, the approximate solutions of the Schrödinger equation, obtained by using Q_N, will probably be somewhat more accurate than those obtained by using the corresponding phase-integral expression. We will come back to this point later, particularly in appendix 3.

The new alternative phase-integral approximation, proposed in the present paper, is obtained by forming linear combinations of the two functions in (2), with $q(z)$ replaced by $Q_N(z)$, where N is any integer $\geqslant 0$.

As mentioned above, we take

$$Q_1 = Q_0\left(1+\frac{1}{2}\varepsilon(Q_0)\right) \tag{19}$$

as our new base function. Using the definition

$$g_0 = 1+\frac{1}{2}\varepsilon(Q_0) \tag{20}$$

we can write $Q_1 = Q_0 g_0$. Let us in the main repeat the procedure followed in section 2, but now with Q_1 as base function (instead of Q_0). Putting

$$q = Q_1 \cdot g \tag{21}$$

in (3), we obtain the new g-equation

$$1+\varepsilon(Q_1) - g^2 + g^{+1/2}\frac{\mathrm{d}^2}{\mathrm{d}\zeta_1^2} g^{-1/2} = 0 \tag{22}$$

where now

$$\zeta_1 = \int^z Q_1\, \mathrm{d}z \tag{23}$$

and

$$\varepsilon(Q_1) = \frac{R - Q_1^2}{Q_1^2} + Q_1^{-3/2}\frac{\mathrm{d}^2}{\mathrm{d}z^2} Q_1^{-1/2}. \tag{24}$$

Proceeding formally in a similar way as before, we can write (22) in the following form, displaying the largeness of each term:

$$1+\varepsilon(Q_1)\cdot\lambda^4 - g^2 + g^{+1/2}\frac{\mathrm{d}^2}{\mathrm{d}\zeta_1^2} g^{-1/2}\cdot\lambda^2 = 0 \tag{25}$$

In order to obtain (25) we have used the fact that Q_1 can correctly be written $Q_1 \cdot \lambda^{-1}$, which follows from (19) and (10*a*, *b*). We have also used that

$$\frac{\mathrm{d}}{\mathrm{d}\zeta_1}=\frac{\mathrm{d}z}{\mathrm{d}\zeta_1}\frac{\mathrm{d}}{\mathrm{d}z}=\frac{1}{Q_1}\frac{\mathrm{d}}{\mathrm{d}z} \tag{26}$$

which follows from (23), and further that $\varepsilon(Q_1)$ is a quantity which correctly can be written $\varepsilon(Q_1)\cdot\lambda^4$, according to (A1.10) in appendix 1.

Inserting in (25) a series expansion for $g(z)$,

$$g(z)=\sum_{n=0}^{\infty} Y_{2n}^{(1)}(z)\cdot\lambda^{2n} \tag{27}$$

ordering the terms according to the powers of λ and putting the coefficient expression for λ^{2n} equal to zero (for $n=0, 1, 2, \ldots$), we successively obtain in this case (disregarding the possibility $Y_0^{(1)}=-1$)

$$Y_0^{(1)}=1 \tag{28a}$$

$$Y_2^{(1)}=0 \tag{28b}$$

$$Y_4^{(1)}=\frac{1}{2}\varepsilon(Q_1) \tag{28c}$$

$$Y_6^{(1)}=-\frac{1}{8}\frac{\mathrm{d}^2\varepsilon(Q_1)}{\mathrm{d}\zeta_1^2} \tag{28d}$$

$$Y_8^{(1)}=\frac{1}{32}\left[-4\varepsilon^2(Q_1)+\frac{\mathrm{d}^4\varepsilon(Q_1)}{\mathrm{d}\zeta_1^4}\right] \tag{28e}$$

etc.

The superscript (1) in the symbol $Y_{2n}^{(1)}$ indicates that the expansion coefficient $Y_{2n}^{(1)}(z)$ is related to the base function $Q_1(z)$. We note that the function $Y_{2n}^{(1)}$ in (28*a*–*e*) indeed differs from Y_{2n} in (14*a*–*e*), for $n\neq 0$, and that $Y_{2n}^{(1)}$ given by (28) is not obtained from Y_{2n} in (14) simply by exchanging ε_0 and ζ for $\varepsilon(Q_1)$ and ζ_1, respectively. By cutting off the series expansion in (27) at N, we obtain

$$g(z)=\sum_{n=0}^{N} Y_{2n}^{(1)}(z). \tag{29}$$

From (21) and (29) we obtain in this case

$$q(z)=Q_1\sum_{n=0}^{N} Y_{2n}^{(1)}(z) \tag{30}$$

which is a kind of phase-integral expression of order $2N+1$ generated from the base function $Q_1(z)$, but which differs from the ordinary phase-integral expression of order $2N+1$ generated from the base function $Q_1(z)$. From (21), (22), and (29) we realize that the expression (30) is an approximate solution of the nonlinear q-equation (3). As before, we shall choose the first two non-zero terms in the expression (30) for $q(z)$ as our next base function $Q_2(z)$. Thus we set

$$Q_2=Q_1\sum_{n=0}^{2} Y_{2n}^{(1)}=Q_1\left(1+\frac{1}{2}\varepsilon(Q_1)\right). \tag{31}$$

It is now easy to understand how to proceed, going through one more cycle of similar reasoning, resulting in the next base function Q_3 defined by $Q_3=Q_2(1+\frac{1}{2}\varepsilon(Q_2))$. Having followed the first steps in detail leading to Q_1 and Q_2, we shall next go on to consider the general case and follow the steps leading from the base function Q_N to the base function Q_{N+1}.

Inserting in (3),

$$q(z)=Q_N(z)\cdot g(z) \tag{32}$$

we obtain the pertaining g-equation

$$1+\varepsilon(Q_N)-g^2+g^{+1/2}\frac{\mathrm{d}^2}{\mathrm{d}\zeta_N^2}g^{-1/2}=0 \tag{33}$$

where

$$\zeta_N=\int^z Q_N\,\mathrm{d}z \tag{34}$$

and

$$\varepsilon(Q_N)=\frac{R-Q_N^2}{Q_N^2}+Q_N^{-3/2}\frac{\mathrm{d}^2}{\mathrm{d}z^2}Q_N^{-1/2}. \tag{35}$$

Since, according to (A2.7) in appendix 2, the expressions $\varepsilon(Q_N)\cdot\lambda^{2N+2}$ and $Q_N^2\cdot\lambda^{-2}$ correctly display the largeness of $\varepsilon(Q_N)$ and Q_N^2, respectively, we can write the equation (33) in the following form

$$1+\varepsilon(Q_N)\cdot\lambda^{2N+2}-g^2+g^{+1/2}\frac{\mathrm{d}^2}{\mathrm{d}\zeta_N^2}g^{-1/2}\cdot\lambda^2=0. \tag{36}$$

Inserting in (36) the formal expansion

$$g(z)=\sum_{n=0}^{\infty}Y_{2n}^{(N)}(z)\cdot\lambda^{2n} \tag{37}$$

and putting the coefficient expression for each λ^{2n} equal to zero, for $n=0, 1, 2, \ldots,$ we successively obtain (disregarding the case $Y_0^{(N)}=-1$)

$$Y_0^{(N)}=1 \tag{38a}$$

$$Y_{2n}^{(N)}=0 \qquad \text{for } n=1,2,\ldots,N \tag{38b}$$

$$Y_{2N+2}^{(N)}=\frac{1}{2}\varepsilon(Q_N) \qquad \text{for } n=N+1. \tag{38c}$$

The functions $Y_{2n}^{(N)}$, for $n>N+1$, have not yet been calculated. The superscript (N) in the symbol $Y_{2N+2}^{(N)}$ signals that the symbol is related to the base function Q_N.

Cutting off the expansion (37) at $n=M$, we obtain

$$g(z)=\sum_{n=0}^{M}Y_{2n}^{(N)}(z)\cdot\lambda^{2n}. \tag{39}$$

From (32) and (39), recalling (38), we obtain

$$q(z)=Q_N\sum_{n=0}^{M}Y_{2n}^{(N)}(z)\cdot\lambda^{2n} \tag{40}$$

which is a kind of phase-integral expression of order $2M+1$ generated from the base function Q_N. From (32), (33), and (39) we realize that the expression (40) is an approximate solution of the nonlinear q-equation (3). We should observe that (40) is not equal to the ordinary phase-integral expression of order $2M+1$ generated from the base function Q_N. However, if $q(z)$ given by (40) is inserted in formula (2) one obtains a kind of phase-integral functions of order $2M+1$. And by forming linear combinations of the latter two functions one obtains a kind of phase-integral approximation of order $2M+1$, generated from the base function Q_N.

According to the main idea in this article, we choose for our next base function Q_{N+1} the expression obtained from (40) by cutting off the series expansion at $M=N+1$, thus keeping only the first two non-zero terms. We obtain

$$Q_{N+1}=Q_N\sum_{n=0}^{N+1}Y_{2n}^{(N)}(z)=Q_N\left(1+\frac{1}{2}\varepsilon(Q_N)\right). \tag{41}$$

Summarizing, the sequence of base functions $Q_N(z)$ ($N=0, 1, 2, 3, \ldots$) constructed in this way is given by the recurrence formula

$$Q_{N+1}(z)=Q_N(z)\left(1+\frac{1}{2}\varepsilon(Q_N)\right) \tag{42}$$

together with the following formula for $\varepsilon(Q_N)$

$$\varepsilon(Q_N)=\frac{R-Q_N^2}{Q_N^2}+Q_N^{-3/2}\frac{\mathrm{d}^2}{\mathrm{d}z^2}Q_N^{-1/2} \tag{43}$$

which are valid for $N=0, 1, 2, \ldots$. We note that the quantities $Q_0(z)$ and $\varepsilon(Q_0)$ occurring above should be identified with $Q(z)$ and ε_0, respectively, pertaining to the Fröman phase-integral approximations. It is assumed that $Q_0(z)$ is chosen such that the largeness of $\varepsilon(Q_0)$ is correctly displayed by the expression $\varepsilon(Q_0)\cdot\lambda^2$. Sometimes it is satisfactory to choose $Q_0=\sqrt{R(z)}$. For calculation, it is convenient to rewrite the last term in (43) by using the identity (A1.5) of appendix 1 with $q(z)$ replaced by $Q_N(z)$. From (42) we get, by iteration

$$Q_{N+1}=Q_0\prod_{n=0}^{N}\left(1+\frac{1}{2}\varepsilon(Q_N)\right). \tag{44}$$

Using the definition

$$g_n=1+\frac{1}{2}\varepsilon(Q_n) \tag{45}$$

(44) can simply be written

$$Q_{N+1}=Q_0\prod_{n=0}^{N}g_n. \tag{46}$$

From the preceding text, in particular the section between (40) and (41) including these formulas, it is clear that $Q_N(z)$ by construction is an approximate solution of the

q-equation (3). The base function Q_N is to be compared with the phase-integral expression of order $2N+1$, i.e.

$$Q_0 \sum_{n=0}^{N} Y_{2n}(z)$$

in which the functions $Y_{2n}(z)$ are given by (14) and (15).

For certain model potentials and for certain physical quantities of interest, values calculated by means of phase-integral formulas (of arbitrary order) have been compared with purely numerically calculated values. It would be interesting to study the accuracy obtained by using the base function Q_N instead of the phase-integral expression of order $2N+1$. In Appendix 3, a detailed comparison is made between the analytical expressions for

$$Q_N(z) \qquad \text{and} \qquad Q_0 \sum_{n=0}^{N} Y_{2n}(z)$$

respectively, which seems to indicate that one can expect to gain some improvement of the accuracy by using the base function Q_N instead of the corresponding Fröman phase-integral expression of order $2N+1$.

Appendix 1. $\varepsilon(Q_1)$ expressed in terms of $\varepsilon(Q_0)$

We want to express $\varepsilon(Q_1)$ in terms of $\varepsilon(Q_0)$ and derivatives of $\varepsilon(Q_0)$ with respect to the variable ζ_0. From (19) and (20) we get

$$\varepsilon(Q_1) = \varepsilon(Q_0 g_0) \tag{A1.1}$$

where

$$g_0 = 1 + \frac{1}{2}\varepsilon(Q_0). \tag{A1.2}$$

From (6) and (7), replacing Q, g, and ζ by Q_0, g_0, and ζ_0, respectively, we obtain the relation

$$\varepsilon(Q_0 g_0) = \frac{1+\varepsilon(Q_0) - g_0^2}{g_0^2} + g_0^{-3/2} \frac{d^2}{d\zeta_0^2} g_0^{-1/2} \tag{A1.3}$$

where

$$\zeta_0 = \int^z Q_0 \, dz. \tag{A1.4}$$

Let us transform the last term in (A1.3). The identity (A20a) in [1] reads, for $n=1$,

$$q^{+1/2} \frac{d^2}{dz^2} q^{-1/2} = \frac{3}{4}\left(\frac{1}{q}\frac{d}{dz} q\right)^2 - \frac{1}{2q}\frac{d^2}{dz^2} q. \tag{A1.5}$$

Replacing q by g_0, and z by ζ_0, we obtain from (A1.5) the identity

$$g_0^{+1/2} \frac{d^2}{d\zeta_0^2} g_0^{-1/2} = \frac{3}{4}\left(\frac{1}{g_0}\frac{d}{d\zeta_0} g_0\right)^2 - \frac{1}{2g_0}\frac{d^2}{d\zeta_0^2} g_0. \tag{A1.6}$$

Inserting (A1.6) into (A1.3), using also (A1.2), we get from (A1.1) and (A1.3) the formula

$$\varepsilon(Q_1)=\varepsilon(Q_0g_0)=\frac{1}{g_0^2}\left(1+\varepsilon(Q_0)-\left(1+\frac{1}{2}\varepsilon(Q_0)\right)^2+g_0^{+1/2}\frac{d^2}{d\zeta_0^2}g_0^{-1/2}\right)$$

$$=\frac{1}{g_0^2}\left(-\frac{1}{4}\varepsilon^2(Q_0)+\frac{3}{16g_0^2}\left(\frac{d\varepsilon(Q_0)}{d\zeta_0}\right)^2-\frac{1}{4g_0}\frac{d^2\varepsilon(Q_0)}{d\zeta_0^2}\right). \tag{A1.7}$$

By means of the parameter λ, one can display the order of magnitude of the different terms in (A1.7). According to (10*a*, *b*), it is correct to write the functions Q_0 and $\varepsilon(Q_0)$ as $Q_0\cdot\lambda^{-1}$ and $\varepsilon(Q_0)\cdot\lambda^2$, respectively, and consequently also correct to write

$$\frac{d\varepsilon(Q_0)}{d\zeta_0}=\frac{dz}{d\zeta_0}\frac{d\varepsilon(Q_0)}{dz}=\frac{1}{Q_0}\frac{d\varepsilon(Q_0)}{dz}=\frac{1}{Q_0}\frac{d\varepsilon(Q_0)}{dz}\cdot\lambda^3. \tag{A1.8}$$

Hence, we realize that (A1.7) can be written in the following way

$$\varepsilon(Q_1)=-\frac{1}{4g_0^2}\varepsilon^2(Q_0)\cdot\lambda^4+\frac{3}{16g_0^4}\left(\frac{d\varepsilon(Q_0)}{d\zeta_0}\right)^2\cdot\lambda^6-\frac{1}{4g_0^3}\frac{d^2\varepsilon(Q_0)}{d\zeta_0^2}\cdot\lambda^4 \tag{A1.9}$$

Considered as a whole, $\varepsilon(Q_1)$ is thus a λ^4-quantity which can be exhibited by writing $\varepsilon(Q_1)$ as

$$\varepsilon(Q_1)\cdot\lambda^4 \tag{A1.10}$$

From (19) and the lines immediately above (A1.8), it follows that the largeness of Q_1 is correctly displayed by the expression

$$Q_1\cdot\lambda^{-1}. \tag{A1.11}$$

From (31), (A1.10), and (A1.11), we conclude in a similar way that the largeness of Q_2 is correctly displayed by the expression $Q_2\cdot\lambda^{-1}$.

Appendix 2. $\varepsilon(Q_{N+1})$ expressed in terms of $\varepsilon(Q_N)$

We shall now generalize the results in appendix 1. Let $Q_{N+1}(z)$ and $\varepsilon(Q_N)$ be defined by (42) and (43) for $N=0, 1, 2, \ldots$, and let us assume that $Q_0(z)$ is chosen such that the largeness of $\varepsilon(Q_0)$, and of $Q_0(z)$ itself, are correctly displayed by the expressions

$$\varepsilon(Q_0)\cdot\lambda^2 \qquad \text{and} \qquad Q_0(z)\cdot\lambda^{-1} \tag{A2.1}$$

respectively. The assumption (A2.1) originates from (10a, b). From (6) and (7), putting $Q=Q_N$ and $g=g_N$, we obtain

$$\varepsilon(Q_N g_N)=\frac{1+\varepsilon(Q_N)-g_N^2}{g_N^2}+g_N^{-3/2}\frac{\mathrm{d}^2}{\mathrm{d}\zeta_N^2}g_N^{-1/2} \tag{A2.2}$$

where

$$\zeta_N=\int^z Q_N\,\mathrm{d}z. \tag{A2.3}$$

Using (42) and (45), formula (A2.2) can be written

$$\varepsilon(Q_{N+1})=\varepsilon(Q_N g_N)=\frac{1}{g_N^2}\left(1+\varepsilon(Q_N)-\left(1+\frac{1}{2}\varepsilon(Q_N)\right)^2+g_N^{+1/2}\frac{\mathrm{d}^2}{\mathrm{d}\zeta_N^2}g_N^{-1/2}\right)$$
$$=\frac{1}{g_N^2}\left(-\frac{1}{4}\varepsilon^2(Q_N)+g_N^{+1/2}\frac{d^2}{d\zeta_N^2}g_N^{-1/2}\right). \tag{A2.4}$$

Let us rewrite the last term in (A2.4). Putting $q=g_N$ and $z=\zeta_N$ in the identity (A1.5), we obtain the identity

$$g_N^{+1/2}\frac{\mathrm{d}^2}{\mathrm{d}\zeta_N^2}g_N^{-1/2}=\frac{3}{4}\left(\frac{1}{g_N}\frac{\mathrm{d}}{\mathrm{d}\zeta_N}g_N\right)^2-\frac{1}{2g_N}\frac{\mathrm{d}^2}{\mathrm{d}\zeta_N^2}g_N. \tag{A2.5}$$

From (A2.4), inserting the expression given by (A2.5), and using again that $g_N=1+\frac{1}{2}\varepsilon(Q_N)$, we obtain

$$\varepsilon(Q_{N+1})=\frac{1}{g_N^2}\left(-\frac{1}{4}\varepsilon^2(Q_N)+\frac{3}{16g_N^2}\left(\frac{\mathrm{d}\varepsilon(Q_N)}{\mathrm{d}\zeta_N}\right)^2-\frac{1}{4g_N}\frac{\mathrm{d}^2\varepsilon(Q_N)}{\mathrm{d}\zeta_N^2}\right). \tag{A2.6}$$

We shall now prove by means of complete mathematical induction that the expressions

$$\varepsilon(Q_N)\cdot\lambda^{2N+2} \qquad \text{and} \qquad Q_N\cdot\lambda^{-1}, \tag{A2.7}$$

for all $N\geqslant 0$, in a correct way display the largeness of the quantities $\varepsilon(Q_N)$ and Q_N, respectively, expressed in terms of powers of the small parameter p. Therefore, let us first assume that (A2.7), for some N, actually displays the correct expressions for $\varepsilon(Q_N)$ and Q_N. Observing that (cf. (A2.3))

$$\frac{\mathrm{d}\varepsilon(Q_N)}{\mathrm{d}\zeta_N}=\frac{\mathrm{d}z}{\mathrm{d}\zeta_N}\frac{\mathrm{d}\varepsilon(Q_N)}{\mathrm{d}z}=\frac{1}{Q_N}\frac{\mathrm{d}\varepsilon(Q_N)}{\mathrm{d}z}=\frac{1}{Q_N}\frac{\mathrm{d}\varepsilon(Q_N)}{\mathrm{d}z}\cdot\lambda^{2N+3} \tag{A2.8}$$

we realize that (A2.6) can be written in the following way

$$\varepsilon(Q_{N+1})=\frac{1}{g_N^2}\left(-\frac{1}{4}\varepsilon^2(Q_N)\cdot\lambda^{4N+4}+\frac{3}{16g_N^2}\left(\frac{\mathrm{d}\varepsilon(Q_N)}{\mathrm{d}\zeta_N}\right)^2\cdot\lambda^{4N+6}-\frac{1}{4g_N}\frac{\mathrm{d}^2\varepsilon(Q_N)}{\mathrm{d}\zeta_N^2}\cdot\lambda^{2N+4}\right) \tag{A2.9}$$

Since λ^{2N+4} is the lowest power of λ that occurs in (A2.9), we conclude that $\varepsilon(Q_{N+1})$, considered as a whole, is a λ^{2N+4}-quantity. From (42) and (A2.7) it follows that Q_{N+1} is a λ^{-1}-quantity. We have thus proved that the expressions

$$\varepsilon(Q_{N+1})\cdot\lambda^{2N+4} \qquad \text{and} \qquad Q_{N+1}\cdot\lambda^{-1} \tag{A2.10}$$

correctly display the largeness of $\varepsilon(Q_{N+1})$ and Q_{N+1}, respectively, on the assumption that (A2.7) correctly displays the largeness of $\varepsilon(Q_N)$ and Q_N, respectively. Noting next that (A2.7) is in fact correct for $N=0$, since the expressions given by (A2.1) correctly display the largeness of $\varepsilon(Q_0)$ and Q_0, we finally conclude that the assertion (A2.7), for $N \geqslant 0$, has been proved by complete induction. In addition, we conclude that (A2.9) gives a correct expression for $\varepsilon(Q_{N+1})$, for $N \geqslant 0$.

Appendix 3. The base function Q_N compared with $Q_0 \sum_{n=0}^{N} Y_{2n}(z)$

We shall denote the phase-integral expression of order $2N+1$ generated from the unspecified base function $Q_0(z)$ by the short symbol q_N. Thus we write

$$q_N = Q_0 \sum_{n=0}^{N} Y_{2n}(z) \cdot \lambda^{2n} \tag{A3.1}$$

remembering that the λ-factor can always be eliminated by putting $\lambda = 1$ (cf (17), (5) and (13)). The reader is reminded that the base function $Q(z)$ and the function $\varepsilon_0(z)$ occurring in the Fröman phase-integral approximations should be identified with $Q_0(z)$ and $\varepsilon(Q_0)$, respectively, in the present article.

We shall compare the base function Q_N with q_N, i.e. the phase-integral expression of order $2N+1$. For $N=0$ and 1, this is very easy, because Q_0 is simply equal to q_0, and from (19) together with (A3.1) and (14*a*, *b*), we see that $Q_1 = q_1$. That is, we obtain

$$Q_0 = q_0 \tag{A3.2a}$$

$$Q_1 = q_1 = Q_0\left(1 + \frac{1}{2}\varepsilon(Q_0)\right). \tag{A3.2b}$$

For $N \geqslant 2$ the comparison becomes more difficult. From (45) and (46), we obtain

$$Q_2 = Q_0 g_0 g_1 = Q_0\left(1 + \frac{1}{2}\varepsilon(Q_0) + \frac{1}{2}\varepsilon(Q_1) g_0\right) \tag{A3.3}$$

and from (A3.1) and (14*a*–*c*)

$$q_2 = Q_0\left(1 + \frac{1}{2}\varepsilon(Q_0) - \frac{1}{8}\varepsilon_0^2(Q_0) - \frac{1}{8}\frac{\mathrm{d}^2\varepsilon(Q_0)}{\mathrm{d}\zeta_0^2}\right). \tag{A3.4}$$

1. *Comparison for N=2*

In order to compare the expressions for Q_2 and q_2 given by (A3.3) and (A3.4), we should express $\varepsilon(Q_1)g_0$, occurring in (A3.3), in terms of $\varepsilon(Q_0)$ and derivatives of $\varepsilon(Q_0)$ with respect to ζ_0. To simplify the expressions in appendix 3, we shall in the following write ε_0 instead of $\varepsilon(Q_0)$.

From (A1.7) we immediately obtain

$$\frac{1}{2}\varepsilon(Q_1)\cdot g_0=-\frac{1}{8g_0}\varepsilon_0^2+\frac{3}{32g_0^3}\left(\frac{d\varepsilon_0}{d\zeta_0}\right)^2-\frac{1}{8g_0^2}\frac{d^2\varepsilon_0}{d\zeta_0^2} \tag{A3.5}$$

where, quoting (A1.2)

$$g_0=1+\frac{1}{2}\varepsilon_0. \tag{A3.6}$$

We shall also display the largeness of the different terms by means of the parameter λ. From (A2.1) and (A1.8) it follows that the expressions

$$\varepsilon_0\cdot\lambda^2 \qquad \frac{d\varepsilon_0}{d\zeta_0}\cdot\lambda^3 \qquad \frac{d^2\varepsilon_0}{d\zeta_0^2}\cdot\lambda^4$$

correctly display the largeness of the quantities

$$\varepsilon_0 \qquad \frac{d\varepsilon_0}{d\zeta_0} \qquad \frac{d^2\varepsilon_0}{d\zeta_0^2},$$

respectively, why (A3.5) correctly can be written in the following way

$$\frac{1}{2}\varepsilon(Q_1)\cdot g_0=-\frac{1}{8g_0}\varepsilon_0^2\cdot\lambda^4+\frac{3}{32g_0^3}\left(\frac{d\varepsilon_0}{d\zeta_0}\right)^2\cdot\lambda^6-\frac{1}{8g_0^2}\frac{d^2\varepsilon_0}{d\zeta_0^2}\cdot\lambda^4 \tag{A3.7}$$

and (A3.6) as

$$g_0=1+\frac{1}{2}\varepsilon_0\cdot\lambda^2. \tag{A3.8}$$

Expanding $1/g_0$ in the series

$$\frac{1}{g_0}=1-\frac{1}{2}\varepsilon_0\cdot\lambda^2+\frac{1}{4}\varepsilon_0^2\cdot\lambda^4-\frac{1}{8}\varepsilon_0^3\cdot\lambda^6+\cdots \tag{A3.9}$$

and expanding also $1/g_0^2$ and $1/g_0^3$ in a similar way, inserting the expansions in (A3.7), and arranging the terms according to the powers of λ, we arrive at the following expression for $\frac{1}{2}\varepsilon(Q_1)\cdot g_0$:

$$\begin{aligned}\frac{1}{2}\varepsilon(Q_1)\cdot g_0=&-\frac{1}{8}\left[\varepsilon_0^2+\frac{d^2\varepsilon_0}{d\zeta_0^2}\right]\cdot\lambda^4+\frac{1}{32}\left[2\varepsilon_0^3+3\left(\frac{d\varepsilon_0}{d\zeta_0}\right)^2+4\varepsilon_0\frac{d^2\varepsilon_0}{d\zeta_0^2}\right]\cdot\lambda^6\\&-\frac{1}{128}\left[4\varepsilon_0^4+18\varepsilon_0\left(\frac{d\varepsilon_0}{d\zeta_0}\right)^2+12\varepsilon_0^2\frac{d^2\varepsilon_0}{d\zeta_0^2}\right]\cdot\lambda^8\\&+\frac{1}{512}\left[8\varepsilon_0^5+72\varepsilon_0^2\left(\frac{d\varepsilon_0}{d\zeta_0}\right)^2+32\varepsilon_0^3\frac{d^2\varepsilon_0}{d\zeta_0^2}\right]\cdot\lambda^{10}+\cdots\end{aligned} \tag{A3.10}$$

Writing (A3.4) in the following form (cf also (A3.1))

$$q_2=Q_0(Y_0\cdot\lambda^0+Y_2\cdot\lambda^2+Y_4\cdot\lambda^4)=Q_0\left(1+\frac{1}{2}\varepsilon_0\cdot\lambda^2-\frac{1}{8}\left[\varepsilon_0^2+\frac{d^2\varepsilon_0}{d\zeta_0^2}\right]\cdot\lambda^4\right) \tag{A3.11}$$

it is now possible to compare q_2, given by (A3.11), with Q_2 given by the expression below, obtained by inserting (A3.10) in (A3.3)

$$Q_2=Q_0\left(1+\frac{1}{2}\varepsilon_0\cdot\lambda^2-\frac{1}{8}\left[\varepsilon_0^2+\frac{d^2\varepsilon_0}{d\zeta_0^2}\right]\cdot\lambda^4+\frac{1}{32}\left[2\varepsilon_0^3+3\left(\frac{d\varepsilon_0}{d\zeta_0}\right)^2+4\varepsilon_0\frac{d^2\varepsilon_0}{d\zeta_0^2}\right]\cdot\lambda^6\right.$$
$$-\frac{1}{128}\left[4\varepsilon_0^4+18\varepsilon_0\left(\frac{d\varepsilon_0}{d\zeta_0}\right)^2+12\varepsilon_0^2\frac{d^2\varepsilon_0}{d\zeta_0^2}\right]\cdot\lambda^8$$
$$\left.+\frac{1}{512}\left[8\varepsilon_0^5+72\varepsilon_0^2\left(\frac{d\varepsilon_0}{d\zeta_0}\right)^2+32\varepsilon_0^3\frac{d^2\varepsilon_0}{d\zeta_0^2}\right]\cdot\lambda^{10}+\cdots\right). \quad \text{(A3.12)}$$

First of all, we find that the expression for Q_2 includes q_2, i.e. the fifth-order phase-integral expression. The expressions for Q_2 and q_2 are identical as concerns the λ^{2n}-terms for $n=0$, 1, and 2. But the expression for Q_2 contains, in addition, higher-order terms. Do these λ^{2n}-terms, for $n>2$, improve the accuracy of the approximate solution of the Schrödinger equation that is obtained from (2) by exchanging $q(z)$ for $Q_2(z)$? Do these terms appear in the higher-order phase-integral expressions, i.e. in q_3, q_4, ... and so forth? Maybe it is the case that the λ^{2n}-contribution to Q_2, for $n>2$, is part of the λ^{2n}-contribution to the higher-order phase-integral expressions q_3, q_4, ... etc.? We shall try to answer these questions to some extent by comparing the λ^{2n}-contribution to Q_2, given by (A3.12), with the corresponding λ^{2n}-contribution to q_3, q_4, ... etc. We shall limit our task to the λ^6- and λ^8-contributions only, since the difficulty strongly increases with increasing n. We see from (A3.1) that Y_6 is the λ^6-contribution, not only to the phase-integral expression q_3 but in fact to every phase-integral expression q_N, for $N\geq 3$, and generally that Y_{2n} is the λ^{2n}-contribution to every phase-integral expression q_N, for $N\geq n$.

Let us first compare the λ^6-terms in the expression for Q_2, given by (A3.12), with the λ^6-terms in the phase-integral expression q_3, which are given by Y_6 (as mentioned above). Quoting (14*d*), we have

$$Y_6=\frac{1}{32}\left[2\varepsilon_0^3+5\left(\frac{d\varepsilon_0}{d\zeta_0}\right)^2+6\varepsilon_0\frac{d^2\varepsilon_0}{d\zeta_0^2}+\frac{d^4\varepsilon_0}{d\zeta_0^4}\right] \quad \text{(A3.13)}$$

We find that the λ^6-terms in (A3.12) reproduce a good part of the first three terms in (A3.13). But there is no λ^6-term in (A3.12) that corresponds to the fourth term in (A3.13). Summarizing the results, so far, we have found that the expression for Q_2 includes the fifth-order phase-integral expression q_2, but also that it includes a good part of those terms which constitute the difference between q_2 and the next higher-order phase-integral expression, that is q_3.

Let us go on to compare the three λ^8-terms in the expression for Q_2, given by (A3.12), with the λ^8-terms occurring in the succeeding phase-integral expression q_4, which are given by (quoting (14*e*))

$$Y_8=-\frac{1}{128}\left[5\varepsilon_0^4+50\varepsilon_0\left(\frac{d\varepsilon_0}{d\zeta_0}\right)^2+30\varepsilon_0^2\frac{d^2\varepsilon_0}{d\zeta_0^2}+\text{four additional terms}\right]. \quad \text{(A3.14)}$$

It should be observed that the terms of Y_8 form the λ^8-contribution to every higher-order phase-integral expression q_n, for $n\geq 4$. We observe that the three λ^8-terms occurring in (A3.12) have the same sign as the corresponding terms in (A3.14), and that they reproduce a good part of the latter terms. One could in principle go on to compare, also for $n>4$, the λ^{2n}-terms occurring in (A3.12) with the corresponding terms appearing in the expression for Y_{2n} in order to see how much of the expression for Y_{2n} that is covered by the λ^{2n}-terms already in the expression (A3.12) for Q_2. We shall refrain from doing so, but still want to remark that it seems probable that the λ^{2n}-terms in (A3.12) will continue to cover at least some small part of Y_{2n} also in the following, i.e. for $n>4$.

2. Comparison for $N=3$

We shall now proceed to compare the next base function Q_3 with q_3, i.e. the seventh-order phase-integral expression for $q(z)$, according to (A3.1) and the surrounding text. From (45) and (46), we obtain

$$Q_3=Q_0g_0g_1g_2=Q_0\left(g_0g_1+\frac{1}{2}\varepsilon(Q_2)\cdot g_0g_1\right)=Q_2+Q_0\cdot\frac{1}{2}\varepsilon(Q_2)\cdot g_0g_1. \tag{A3.15}$$

For Q_2 appearing in (A3.15) we have the suitable expression (A3.12). Let us also express the function $\varepsilon(Q_2)g_0g_1$, occurring in the second term of (A3.15), in terms of ε_0 and derivatives of ε_0 with respect to ζ_0. Formula (A2.9) yields for $N=1$

$$\varepsilon(Q_2)=\frac{1}{g_1^2}\left(-\frac{1}{4}\varepsilon^2(Q_1)\cdot\lambda^8+\frac{3}{16g_1^2}\left(\frac{d\varepsilon(Q_1)}{d\zeta_1}\right)^2\cdot\lambda^{10}-\frac{1}{4g_1}\frac{d^2\varepsilon(Q_1)}{d\zeta_1^2}\cdot\lambda^6\right) \tag{A3.16}$$

from which we immediately obtain

$$\frac{1}{2}\varepsilon(Q_2)g_0g_1=-\frac{g_0}{8g_1}\varepsilon^2(Q_1)\cdot\lambda^8+\frac{3g_0}{32g_1^3}\left(\frac{d\varepsilon(Q_1)}{d\zeta_1}\right)^2\cdot\lambda^{10}-\frac{g_0}{8g_1^2}\frac{d^2\varepsilon(Q_1)}{d\zeta_1^2}\cdot\lambda^6. \tag{A3.17}$$

With a view to using the suitable expression for $\frac{1}{2}\varepsilon(Q_1)g_0$, given by (A3.10), we shall first rewrite (A3.17), expressing $\frac{1}{2}\varepsilon(Q_2)g_0g_1$ as a function of $\frac{1}{2}\varepsilon(Q_1)g_0$ and derivatives of the same quantity with respect to ζ_0. Putting, to this end,

$$G=\frac{1}{2}\varepsilon(Q_1)\cdot g_0 \tag{A3.18}$$

and using that

$$\frac{d}{d\zeta_1}=\frac{1}{g_0}\frac{d}{d\zeta_0} \tag{A3.19}$$

which follows from (34), (42) and (45), we find after some calculations that the first term in the expression (A3.17) for $\frac{1}{2}\varepsilon(Q_2)g_0g_1$ can be written as

$$-\frac{1}{2g_0g_1}G^2\cdot\lambda^8 \tag{A3.20a}$$

the second term as

$$+\frac{3}{32(g_0g_1)^3}\left(\frac{1}{g_0^2}\left(\frac{d\varepsilon_0}{d\zeta_0}\right)^2G^2\cdot\lambda^{14}+4\left(\frac{dG}{d\zeta_0}\right)^2\cdot\lambda^{10}-\frac{4}{g_0}\frac{d\varepsilon_0}{d\zeta_0}G\frac{dG}{d\zeta_0}\cdot\lambda^{12}\right) \tag{A3.20b}$$

and, finally, the third term as

$$+\frac{1}{8(g_0g_1)^2}\left(\frac{3}{g_0}\frac{d\varepsilon_0}{d\zeta_0}\frac{dG}{d\zeta_0}\cdot\lambda^8-\frac{3}{2g_0^2}\left(\frac{d\varepsilon_0}{d\zeta_0}\right)^2G\cdot\lambda^{10}+\frac{1}{g_0}\frac{d^2\varepsilon_0}{d\zeta_0^2}G\cdot\lambda^8-2\frac{d^2G}{d\zeta_0^2}\cdot\lambda^6\right). \tag{A3.20c}$$

Inserting (A3.20*a*–*c*) in (A3.17), expanding g_0 and g_1 in formal series in the parameter λ, similarly as done in (A3.9), and then using the expression for G given by (A3.18) together with (A3.10), we can arrange all terms in (A3.17) according to their powers of λ. We see from (A3.20*a*–*c*) that the terms with the lowest power of λ that occur in (A3.17) are the λ^6-terms. This is to be expected, since we know from (A2.7) and (45) that, considered as a whole, $\varepsilon(Q_2)$ is a λ^6-quantity while g_0 and g_1 are both λ^0–quantities. Let us limit our interest to the λ^6- and λ^8-terms of (A3.17). The λ^6-terms are found exclusively in the last term of (A3.20*c*), and with the help of (A3.18) combined with (A3.10), we find that the λ^6-contribution to the quantity $\frac{1}{2}\varepsilon(Q_2)g_0g_1$, as given by (A3.17), is

$$+\frac{1}{32}\left[2\left(\frac{d\varepsilon_0}{d\zeta_0}\right)^2+2\varepsilon_0\frac{d^2\varepsilon_0}{d\zeta_0^2}+\frac{d^4\varepsilon_0}{d\zeta_0^4}\right]\cdot\lambda^6. \tag{A3.21}$$

The λ^8-terms occurring in (A3.17) originate from (A3.20*a*) and from all the terms in (A3.20*c*) except for the second one. The λ^8-contribution to (A3.17), calculated similarly as the λ^6-contribution, is given by

$$-\frac{1}{128}\left[\varepsilon_0^4+32\varepsilon_0\left(\frac{d\varepsilon_0}{d\zeta_0}\right)^2+18\varepsilon_0^2\frac{d^2\varepsilon_0}{d\zeta_0^2}+13\left(\frac{d^2\varepsilon_0}{d\zeta_0^2}\right)^2+20\frac{d\varepsilon_0}{d\zeta_0}\frac{d^3\varepsilon_0}{d\zeta_0^3}+8\varepsilon_0\frac{d^4\varepsilon_0}{d\zeta_0^4}\right]\cdot\lambda^8. \tag{A3.22}$$

According to (A3.15), we obtain Q_3 by adding the expression for Q_2, given by (A3.12), to the expression for $Q_0\frac{1}{2}\varepsilon(Q_2)g_0g_1$, which is given by (A3.17) together with (A3.20*a*–*c*). Restricting ourselves to λ^{2n}-terms for $0\leqslant n\leqslant 4$, and using (A3.21) and (A3.22) for the λ^6- and λ^8-contributions to (A3.17), we get the following expression for Q_3:

$$\begin{aligned}Q_3=Q_0\Bigg(1&+\frac{1}{2}\varepsilon_0\cdot\lambda^2-\frac{1}{8}\left[\varepsilon_0^2+\frac{d^2\varepsilon_0}{d\zeta_0^2}\right]\cdot\lambda^4+\frac{1}{32}\left[2\varepsilon_0^3+5\left(\frac{d\varepsilon_0}{d\zeta_0}\right)^2+6\varepsilon_0\frac{d^2\varepsilon_0}{d\zeta_0^2}+\frac{d^4\varepsilon_0}{d\zeta_0^4}\right]\cdot\lambda^6\\&-\frac{1}{128}\left[5\varepsilon_0^4+50\varepsilon_0\left(\frac{d\varepsilon_0}{d\zeta_0}\right)^2+30\varepsilon_0^2\frac{d^2\varepsilon_0}{d\zeta_0^2}+13\left(\frac{d^2\varepsilon_0}{d\zeta_0^2}\right)^2\right.\\&\left.+20\frac{d\varepsilon_0}{d\zeta_0}\frac{d^3\varepsilon_0}{d\zeta_0^3}+8\varepsilon_0\frac{d^4\varepsilon_0}{d\zeta_0^4}\right]\cdot\lambda^8+\cdots\Bigg)\end{aligned} \tag{A3.23}$$

suitable for comparison with q_3, i.e. the seventh-order phase-integral expression for $q(z)$. In (A3.23), Q_3 is thus given as a formal series expansion in the parameter λ^2. From (A3.1) and (14*a*–*d*), we obtain

$$\begin{aligned}q_3&=Q_0(Y_0\cdot\lambda^0+Y_2\cdot\lambda^2+Y_4\cdot\lambda^4+Y_6\cdot\lambda^6)\\&=Q_0\Bigg(1+\frac{1}{2}\varepsilon_0\cdot\lambda^2-\frac{1}{8}\left[\varepsilon_0^2+\frac{d^2\varepsilon_0}{d\zeta_0^2}\right]\cdot\lambda^4\\&\quad+\frac{1}{32}\left[2\varepsilon_0^3+5\left(\frac{d\varepsilon_0}{d\zeta_0}\right)^2+6\varepsilon_0\frac{d^2\varepsilon_0}{d\zeta_0^2}+\frac{d^4\varepsilon_0}{d\zeta_0^4}\right]\cdot\lambda^6\Bigg).\end{aligned} \tag{A3.24}$$

Comparing (A3.23) with (A3.24) we find that the expression for the base function Q_3 includes q_3, the seventh-order phase-integral expression for $q(z)$. But in addition, the expression for Q_3 contains λ^{2n}-terms also for $n>3$. Are these terms part of q_4, q_5, q_6, Inserting (A3.20*a*–*c*) in (A3.17), expanding g_0 and g_1 in formal series in the parameter λ, similarly as done in (A3.9), and then using the expression for G given by (A3.18) together with (A3.10), we can arrange all terms in (A3.17) according to their powers of λ. We see from (A3.20*a*–*c*) that the terms with the lowest power of λ that occur in (A3.17) are the λ^6-terms. This is to be expected, since we know from (A2.7) and (45) that, considered as a whole, $\varepsilon(Q_2)$ is a λ^6-quantity while g_0 and g_1 are both λ^0–quantities. Let us limit our interest to the λ^6- and λ^8-terms of (A3.17). The λ^6-terms are found exclusively in the last term of (A3.20*c*), and with the help of (A3.18) combined with (A3.10), we find that the λ^6-contribution to the quantity $\frac{1}{2}\varepsilon(Q_2)g_0g_1$, as given by (A3.17), is

$$+\frac{1}{32}\left[2\left(\frac{d\varepsilon_0}{d\zeta_0}\right)^2+2\varepsilon_0\frac{d^2\varepsilon_0}{d\zeta_0^2}+\frac{d^4\varepsilon_0}{d\zeta_0^4}\right]\cdot\lambda^6. \tag{A3.21}$$

The λ^8-terms occurring in (A3.17) originate from (A3.20*a*) and from all the terms in (A3.20*c*) except for the second one. The λ^8-contribution to (A3.17), calculated similarly as the λ^6-contribution, is given by

$$-\frac{1}{128}\left[\varepsilon_0^4+32\varepsilon_0\left(\frac{d\varepsilon_0}{d\zeta_0}\right)^2+18\varepsilon_0^2\frac{d^2\varepsilon_0}{d\zeta_0^2}+13\left(\frac{d^2\varepsilon_0}{d\zeta_0^2}\right)^2+20\frac{d\varepsilon_0}{d\zeta_0}\frac{d^3\varepsilon_0}{d\zeta_0^3}+8\varepsilon_0\frac{d^4\varepsilon_0}{d\zeta_0^4}\right]\cdot\lambda^8. \tag{A3.22}$$

According to (A3.15), we obtain Q_3 by adding the expression for Q_2, given by (A3.12), to the expression for $Q_0\frac{1}{2}\varepsilon(Q_2)g_0g_1$, which is given by (A3.17) together with (A3.20*a*–*c*). Restricting ourselves to λ^{2n}-terms for $0\leqslant n\leqslant 4$, and using (A3.21) and (A3.22) for the λ^6- and λ^8-contributions to (A3.17), we get the following expression for Q_3:

$$\begin{aligned}Q_3=Q_0\Bigg(1&+\frac{1}{2}\varepsilon_0\cdot\lambda^2-\frac{1}{8}\left[\varepsilon_0^2+\frac{d^2\varepsilon_0}{d\zeta_0^2}\right]\cdot\lambda^4+\frac{1}{32}\left[2\varepsilon_0^3+5\left(\frac{d\varepsilon_0}{d\zeta_0}\right)^2+6\varepsilon_0\frac{d^2\varepsilon_0}{d\zeta_0^2}+\frac{d^4\varepsilon_0}{d\zeta_0^4}\right]\cdot\lambda^6\\&-\frac{1}{128}\left[5\varepsilon_0^4+50\varepsilon_0\left(\frac{d\varepsilon_0}{d\zeta_0}\right)^2+30\varepsilon_0^2\frac{d^2\varepsilon_0}{d\zeta_0^2}+13\left(\frac{d^2\varepsilon_0}{d\zeta_0^2}\right)^2\right.\\&\left.+20\frac{d\varepsilon_0}{d\zeta_0}\frac{d^3\varepsilon_0}{d\zeta_0^3}+8\varepsilon_0\frac{d^4\varepsilon_0}{d\zeta_0^4}\right]\cdot\lambda^8+\cdots\Bigg)\end{aligned} \tag{A3.23}$$

suitable for comparison with q_3, i.e. the seventh-order phase-integral expression for $q(z)$. In (A3.23), Q_3 is thus given as a formal series expansion in the parameter λ^2. From (A3.1) and (14*a*–*d*), we obtain

$$\begin{aligned}q_3&=Q_0(Y_0\cdot\lambda^0+Y_2\cdot\lambda^2+Y_4\cdot\lambda^4+Y_6\cdot\lambda^6)\\&=Q_0\Bigg(1+\frac{1}{2}\varepsilon_0\cdot\lambda^2-\frac{1}{8}\left[\varepsilon_0^2+\frac{d^2\varepsilon_0}{d\zeta_0^2}\right]\cdot\lambda^4\\&\quad+\frac{1}{32}\left[2\varepsilon_0^3+5\left(\frac{d\varepsilon_0}{d\zeta_0}\right)^2+6\varepsilon_0\frac{d^2\varepsilon_0}{d\zeta_0^2}+\frac{d^4\varepsilon_0}{d\zeta_0^4}\right]\cdot\lambda^6\Bigg).\end{aligned} \tag{A3.24}$$

Comparing (A3.23) with (A3.24) we find that the expression for the base function Q_3 includes q_3, the seventh-order phase-integral expression for $q(z)$. But in addition, the expression for Q_3 contains λ^{2n}-terms also for $n>3$. Are these terms part of q_4, q_5, q_6,

. . . , i.e. the higher-order phase-integral expressions? To be concrete, let us consider q_4 given by (A3.1) and (14*a*–*e*):

$$q_4 = Q_0(Y_0\cdot\lambda^0 + Y_2\cdot\lambda^2 + Y_4\cdot\lambda^4 + Y_6\cdot\lambda^6 + Y_8\cdot\lambda^8) \tag{A3.25}$$

where

$$Y_8 = -\frac{1}{128}\left[5\varepsilon_0^4 + 50\varepsilon_0\left(\frac{d\varepsilon_0}{d\zeta_0}\right)^2 + 30\varepsilon_0^2\frac{d^2\varepsilon_0}{d\zeta_0^2} + 19\left(\frac{d^2\varepsilon_0}{d\zeta_0^2}\right)^2 \right.$$
$$\left. + 28\frac{d\varepsilon_0}{d\zeta_0}\frac{d^3\varepsilon_0}{d\zeta_0^3} + 10\varepsilon_0\frac{d^4\varepsilon_0}{d\zeta_0^4} + \frac{d^6\varepsilon_0}{d\zeta_0^6}\right]\cdot\lambda^8. \tag{A3.26}$$

Comparison between the λ^8-contribution to q_4 that is given by the expression for Y_8 in (A3.26), on one hand, and the λ^8-contribution to Q_3, which can be found in (A3.23), on the other hand, shows that the first three terms of the two expressions are completely identical, while the succeeding three terms in the expression for Y_8 are mainly covered by the remaining three λ^8-terms in (A3.23). But to the last term in (A3.26), i.e.

$$-\frac{1}{128}\frac{d^6\varepsilon_0}{d\zeta_0^6}\cdot\lambda^8,$$

there is no corresponding λ^8-term in (A3.23). In the region around a first-order pole or an arbitrary-order zero of Q_0^2, the term

$$-\frac{1}{128}\frac{d^6\varepsilon_0}{d\zeta_0^6}$$

is the dominant term in the expression for Y_8, at least for the choice $Q^2(z) = R(z)$, according to the analysis given in [29, 30]. But on the other hand, in this region the phase-integral approximations cease to be good.

Summarizing, the expression for the base function Q_3 includes not only q_3, i.e. the seventh-order phase integral expression, but also a good part of those terms which form the difference between q_3 and q_4, i.e. the ninth-order phase-integral expression. As concerns the rest of the terms in the expression (A3.23) for Q_3, we expect that the λ^{2n}-contribution to Q_3, occurring in the infinite series given by (A3.23), will continue, also for $n > 4$, to cover at least some small part of the expression for Y_{2n}, i.e. the λ^{2n}-contribution to q_n. We note that Y_{2n} is in fact the λ^{2n}-part of every phase-integral expression q_N, for $N \geqslant n$.

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