New Phase-Integral Method Platform Function

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The phase-integral method (PIM) is an asymptotic method of the geometrical optics or semi-classical type for solving approximatively, but in many cases very accurately, a wide class of differential equations in physics. Unlike the related (J)WKB method, the higher-order corrections in the PIM can be generated from a generic, unspecified base function, providing added symmetry and flexibility. However, with the conventional approach of using the next-to-lowest (third) order correction to the integrand in the phase integral as a platform for calculating higher (fifth, seventh, ninth, . . . ) order corrections, the higher-order calculations very often become quite complicated.

We therefore introduce a new platform function, which considerably simplifies the calculation of the third-order contribution for a wide range of problems. We also present directly integrable conditions for the phase integral, which so far seem to have gone unnoticed.

For a large number of observables, our analysis makes a clearer distinction between physical and, in a sense, unphysical contributions.

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I. INTRODUCTION

In their pioneering 1936 article on the calculation of Coulomb wave functions in non-relativistic quantum mechanics, Yost, Wheeler and Breit1 commented on the fact that the WKB method in the first-order approximation sometimes has an unsatisfactory accuracy. Moreover, they found that the replacement, originally suggested by Kramers,2 of l(l + 1) by (l + 1/2)² where l is the orbital angular momentum quantum number, does not always improve the results obtained in the first-order WKB approximation. This situation can mostly be remedied by going to the next-order approximation. The phase-integral method of Fröman and Fröman3 provides a straightforward structure for calculating the contributions of order five and higher. For this, Ref. 4 introduces a platform function ε₀(z) which, apart from a factor 1/2, is the third-order contribution.

In the Fröman and Fröman PIM, the third-order contribution is the most important correction. Hence, it is desirable to find ways to simplify the calculation of this contribution. For this purpose, we here introduce a more flexible platform function Pₜ(z) which generalizes ε₀(z) in a way that depends on the number of singularities in the integrand and which has the potential to simplify the evaluation of higher-order correction terms. As a result, the choice of the so-called base function, usually denoted Q(z), becomes more transparent.

II. HIGHER-ORDER PHASE-INTEGRAL APPROXIMATIONS AND THE PLATFORM FUNCTION

Let us consider the differential equation

\[ \frac{d^2 \psi}{dz^2} + R(z) \psi = 0 \] (1)

where R(z) is a meromorphic function of the complex variable z. Following Ref. 4, we introduce into equation (1) a “small” book-keeping parameter \( \lambda \), ultimately to be set equal to unity, such that we obtain the auxiliary differential equation

\[ \frac{d^2 \psi}{dz^2} + \left( \frac{Q^2(z)}{\lambda^2} + R(z) - Q^2(z) \right) \psi = 0 \] (2)

which goes over into equation (1) when \( \lambda = 1 \). The meromorphic function \( Q(z) \) is the unspecified base which determines the phase-integral approximation of order one. The auxiliary differential equation (2) has two linearly independent solutions

\[ f_+ = q^{1/2}(z) e^{i w(z)} \] (3a)
\[ f_- = q^{1/2}(z) e^{-i w(z)} \] (3b)

where

\[ w(z) = \int^z q(z) dz \] (4)

and

\[ q^2(z) - q^{1/2}(z) \frac{d^2}{dz^2} q^{-1/2}(z) = R(z) - \left( 1 - \frac{1}{\lambda^2} \right) Q^2(z) \] (5)

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or, alternatively,

\[
\left( \frac{g(z)\lambda}{Q(z)} \right)^2 - \lambda^2 \left( \frac{1}{Q(z)} \right)^2 \left[ \frac{g(z)\lambda}{Q(z)} \right]^{\frac{1}{2}} \frac{d^2}{dz^2} \left[ \frac{g(z)\lambda}{Q(z)} \right]^{\frac{1}{2}} = 1
\]

(6)

Introducing the complex variable

\[ \zeta = \int_{z_0}^z Q(z) \, dz \]

(7)

where, typically, \( \{ z_0 : Q^2(z_0) = 0 \} \), one finds, after some calculations, that equation (6) can be rewritten

\[
\left( \frac{g(z)\lambda}{Q(z)} \right)^2 - \lambda^2 \left( \frac{1}{Q(z)} \right)^2 \left( \frac{g(z)\lambda}{Q(z)} \right) \frac{d^2}{d\zeta^2} \left( \frac{g(z)\lambda}{Q(z)} \right)^{\frac{1}{2}} - \lambda^2 \frac{R(z) - Q^2(z)}{2Q^2(z)} = 1
\]

(8)

[cf. equation (2.2.5), with (2.2.1), in Ref. 4]. Using equation (7), and the equality

\[
\frac{1}{Q(z)} \frac{d^2}{dz^2} \frac{1}{Q(z)} = \frac{1}{Q(z)} \frac{d}{dz} \left( \frac{1}{2} \frac{d}{dz} \frac{1}{Q(z)} \right) - \left( \frac{1}{2} \frac{d}{dz} \frac{1}{Q(z)} \right)^2 + \frac{s(s-2)}{4\pi^2 Q^2(z)}
\]

(9)

this can be rewritten

\[
\left( \frac{g(z)\lambda}{Q(z)} \right)^2 - \lambda^2 \left( \frac{1}{Q(z)} \right)^2 \left( \frac{g(z)\lambda}{Q(z)} \right) \frac{d^2}{d\zeta^2} \left( \frac{g(z)\lambda}{Q(z)} \right) + \lambda^2 \left( \frac{Q^2(z) - R(z) - \frac{s(s-2)}{4\pi^2}}{Q^2(z)} \right) + \frac{dP_1(z)}{d\zeta} + P_2(z) = 1
\]

(10)

where

\[ P_1(z) = \frac{1}{2} \text{e}^z \frac{d}{dz} \frac{1}{Q(z)} \]

(11)

This is our new platform function. It allows us to write the right hand member of (3.5c) in Ref. 3 as

\[
\frac{R(z) - Q^2(z)}{2Q^2(z)} + \frac{dP_1(z)}{d\zeta} - P_2(z)
\]

(12)

In practice, the choice of \( s \) in \( P_1(z) \) more or less determines the base function \( Q(z) \) as we shall show next.

### III. BASE FUNCTION

To obtain a solution of equation (10), we make the formal Ansatz

\[
\frac{g(z)\lambda}{Q(z)} = \sum_{n}^{\infty} Y_{2n}(z) \lambda^{2n}
\]

(13)

| TABLE I. Properties of the platform function \( P_n(z) \). equation (11), for various choices of \( s \) |
|---|---|---|
| \( s \) | Platform function | Base function | Typical \( z \) range |
| 0 | \( \frac{d}{dz} \frac{1}{Q(z)} \) | \( Q^2(z) = R(z) \) | \(-\infty < z < \infty \) |
| 1 | \( \frac{\lambda^2}{2} \frac{d}{dz} \frac{1}{Q(z)} \) | \( Q^2(z) = R(z) - \frac{1}{2} \) | \( 0 < z < \infty \) |
| \(-2\lambda \) | \( \frac{\lambda^2}{2} \frac{d}{dz} \frac{1}{Q(z)} \) | \( Q^2(z) = R(z) + \frac{l(l+1)}{z^2} \) | \( 0 < z < \infty \) |

and find that

\[
Y_0 = 1
\]

(14a)

\[
Y_2 = -\frac{1}{2} P_2 + \frac{1}{2} \frac{dP_3}{d\zeta} - \frac{Q^2(z) - R(z) - \frac{s(s-2)}{4\pi^2}}{2Q^2(z)}
\]

(14b)

Using equations (3) and (13) with \( \lambda = 1 \), and truncating after \( n = 2 \), we obtain the approximate local solutions of the original differential equation (1) as

\[
\psi_{\pm} = \left[ Q(z) \left( 1 + Y_2(z) \right) \right]^{1/2} \text{e}^{\pm \frac{i}{2} \int Q(z) \, dz}
\]

(15)

It should be noted that the integrands of these solutions contain the total derivative

\[
\frac{1}{2} Q(z) \frac{dP_3(z)}{d\zeta} = \frac{1}{2} \frac{dP_3(z)}{dz}
\]

(16)

which is integrable irrespective of the expression for \( R(z) \) in the original differential equation (1) and of the choice of the base function \( Q(z) \). Hence, we can write

\[
\psi_{\pm} = \left( \frac{1}{2} \frac{dP_3}{dz} + \left( 1 - \frac{1}{2} P_2 \right) Q - \frac{Q^2 - R - \frac{s(s-2)}{4\pi^2}}{2Q^2} \right)^{-\frac{1}{2}} \times \text{e}^{\pm \int \frac{i}{2} P_3 \, dz}
\]

(17)

From this we conclude that an obvious choice for the (square of the) base function is

\[
Q^2(z) = R(z) + \frac{s(s-2)}{4\pi^2}
\]

(18)

For the new platform function (11), three cases can be discerned (see also Table I):

1. \( s = 0 \). This corresponds to the case of an unmodified base function, \( Q^2(z) = R(z) \). One can show that the use of the platform function \( P_0(z) \) simplifies the calculation of phase-integral approximations, e.g., for the Weber functions.

2. \( s = 1 \). This corresponds to the well-known Kramers-Langer modification for obtaining the base function \( Q^2(z) = R(z) - 1/(4\pi^2) \). One can show that the use of the platform function \( P_1(z) \) simplifies the calculation of phase-integral approximations, e.g., for the Coulomb wave functions.
3. $s = -2l$. This corresponds to the omission of the centrifugal barrier in the base function, i.e., the choice $Q_2(z) = R(z) + l(l + 1)/z^2$. This is (for $l \neq 0$) a less known alternative; see, e.g., Chapter 7 in Ref. 3. One can show that the use of the platform function $P_{-2l}(z)$ simplifies the calculation of phase-integral approximations for spherically and cylindrically symmetric problems.

In all the three above cases, the third-order solution becomes

$$\psi_{\pm} = \left( \frac{1}{2} \left[ \frac{dP_{2l}}{dz} + \left( 1 - \frac{1}{2} P_{2l}^2 \right) Q \right] \right)^{-\frac{1}{2}} \times e^{\pm \frac{i}{2} P_{2l} + \frac{i}{2} \int \left( 1 - \frac{1}{2} P_{2l}^2 \right) Q dz}$$

which exhibits the simplification attainable if the new platform function $P_{s}(z)$ is used.

IV. CONCLUSIONS

We have derived a platform function $P_{s}(z)$ for the third-order correction of the phase-integral method. Since $P_{s}(z)$ is readily generalized to problems involving more than one singular point in $R(z)$ and makes computational simplifications possible, this new platform function is in many cases preferable to the conventional PIM platform function $\varepsilon_0(z)$.

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