Reality and Complexity in Asymptotic Expansions for Eigenvalues and Eigenfunctions, with Application to the JWKB Connection-Formula Problem

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Abstract

Asymptotic expansions occur widely in quantum physics. The Rayleigh–Schrödinger perturbation theory for hydrogen in an electrostatic field (the LoSurdo–Stark effect) is one example. The $1/R$ expansion for the hydrogen molecule ion $H_2^+$ is a second. The quantum defect theory and the JWKB method are two more. It is not so widely known that the sum of such real asymptotic expansions may be complex, while the sum of complex asymptotic expansions may be real. The key to this nonintuitive behavior is Borel summation. By examining a simple example related to the exponential integral, the nature of this real-is-complex, complex-is-real phenomenon is made simple. Then special application is made to derive and clarify the connection formulas (to all orders) in the JWKB method.

1. Introduction

Asymptotic expansions have broad usefulness in quantum physics. Familiar series that are divergent and asymptotic include the Rayleigh–Schrödinger perturbation theory (RSPT) [1–3] for the hydrogen atom in an electric field (the LoSurdo–Stark effect) [4–9], RSPT for hydrogen in the field of a proton (the hydrogen-molecule ion, $H_2^+$ [10–13], the electronic wave function in the quantum-defect model [14], and the Jeffreys–Wentzel–Kramers–Brillouin (JWKB) expansion [15, 16]. It is not generally realized, however, that the sum of such real asymptotic expansions may be complex, while the sum of complex asymptotic expansions may be real [11, 12, 17–20].

For example, the hydrogen atom in an electric field $F$, has resonance eigenvalues, for which the ground state has the RSPT expansion [8],

$$E \sim -0.5 - 2.25F^2 - 55.546875F^4 - \ldots.$$  (1)

It is also known that the imaginary part of the ground-state resonance eigenvalue is given by [21–23]

$$\text{Im } E \sim -2F^{-1}e^{-2(3F)^{1/2}}[1 - (107/12)F + (7363/288)F^2 + \ldots],$$  (2)

and partial sums of these combined series for small-enough $F$ agree well with exact resonance eigenvalues. Nevertheless, the imaginary information is already contained in the real RSPT series (1), since the Borel sum of the real series alone is complex and equal to the exact resonance eigenvalue [24].

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A second example is provided by $H_2^+$ whose ground state has the expansion
\[
E \sim -0.5 - 2.25 R^{-4} - \ldots - 2 R e^{-R^{-1}} [1 + 0.5 R^{-1} + \ldots] \\
\pm 4 \pi i R^2 e^{-2 R^{-1}} [1 + R^{-1} + \ldots],
\]
where $R$ is the internuclear distance. For $H_2^+$ the expansion is explicitly complex, but the eigenvalue is real [11, 12].

The key to understanding this real-is-complex, complex-is-real paradox is Borel summation [17]. (See also Refs. 11–13, 18–20, and 25). The purposes of this brief paper are, first, to show by simple example how the Borel sum of real series can be complex and how thereby to understand the above-mentioned perturbation-theory expansions, and, second, to apply these ideas to the usual JWKB method, which in turn needs some revision in interpretation, but which consequently becomes much clearer and unambiguous.

2. Asymptotic Power Series in the Sense of Poincaré

Poincaré [26] in 1886 formalized the definition, that $\sum_{n=0}^N c_n x^{-n}$ is an asymptotic power series for the function $f(x)$ if
\[
\lim_{x \to 0^+} x^N |f(x) - \sum_{n=0}^N c_n x^{-n}| = 0, \quad \text{for all } N \geq 0.
\]
(4)
The “standard example” of a divergent asymptotic power series is the $1/x$ series for the integral (see, e.g., Ref. 16),
\[
f(x) = \int_0^x \frac{e^{-t}}{1 + t} dt = x e^{x} E_1(x),
\]
(5)
\[
\sim \sum_{n=0}^\infty n! (-x)^{-n},
\]
(6) where $E_1(x)$ is the usual exponential-type integral [27]. In this standard example, the error in the $N$th partial sum is bounded by the $N + 1$st term,
\[
\left| f(x) - \sum_{n=0}^N n! (-x)^{-n} \right| < (N + 1)! x^{-N-1}.
\]
(7) which both shows that the expansion, indeed, satisfies Poincaré’s definition (1), and also illustrates the “rule of thumb” for using asymptotic expansions: that the error of a given partial sum is usually the order of magnitude of the first omitted term. That is, in practice one should truncate the expansion just before the smallest term.

The main weakness of the Poincaré definition is that the relationship between function and asymptotic series is not unique. For any $a > 0$, both $f(x)$ and $f(x) + e^{-ax}$ have the same asymptotic power series in $1/x$.

3. Borel Sum

A. Definition

In contrast with Poincaré definition, the Borel summation method [28, 29], when applicable, associates a unique function to a given asymptotic power series $\sum_{n=0}^\infty c_n x^{-n}$.
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The method consists of the following three steps:

1. Sum the associated power series,

   \[ B(x) = \sum_{n=0}^{\infty} c_n x^{-n}/n! . \]  

   (8)

2. Analytically continue \( B(x) \) beyond the radius of convergence of the power series in Eq. (8) to all of \( x^{-1} \geq 0 \).

3. Calculate the integral,

   \[ F(x) = \int_0^\infty B(xt^{-1})e^{-t} \, dt . \]  

   (9)

If \( B(x) \) and \( F(x) \) exist, then \( B(x) \) is called the Borel transform, and \( F(x) \) is called the Borel sum of the series. One can easily see that the Borel transform of the asymptotic series (6) of the standard example above is just the sum \( (1 + x^{-1})^{-1} \) of the geometric series \( \sum_{n=0}^{\infty} (-x)^{-n} \). Then Eq. (9) recovers the integral representation given in Eq. (5). That is, \( F(x) \) is identical with \( f(x) \). Remember that \( F(x) \) was obtained by starting only with the divergent power series.

B. Cut in the Borel Sum and Complex Sum of the Real Series \( \sum_{n=0}^{\infty} x^{-n} n! \)

If \( x = -x' \) is real and negative, then the integration path in Eq. (5) passes through a zero of the denominator and is invalid. The limit of \( f(x) \) as \( x \) approaches the negative real axis from above or below is

\[ f(e^{\pm i\pi} x') = \lim_{e \to 0} \int_0^{\infty} \frac{1}{1 + (-x' \pm i e)^{-1} t} e^{-t} \, dt \]

\[ = P \int_0^{\infty} \frac{1}{1 - x'^{-1} t} e^{-t} \, dt \pm i \pi x' e^{-x'}, \quad (x' > 0) , \]  

(10)

where \( P \) denotes the principal value. Thus the Borel sum of the series (6), which for this example is precisely the same as the integral representation (5), has a cut on the negative real axis.

Now consider the series (6) with \( -x' \) put for \( x \): \( \sum_{n=0}^{\infty} x'^{-n} n! \). What is its sum for \( x' \) real and positive? Since \( x \) falls on the cut of the Borel sum, the question has a unique answer only after it is specified from which side the real axis is to be included by analytic continuation. The two possible answers are given by Eq. (10) and in either case are complex. It is in this sense that the sum of a real asymptotic expansion is complex — when \( x \) lies on the cut of the Borel sum, and the value of the Borel sum on the cut is obtained by analytic continuation from either above or below.

It is typical to find such cuts coming from the Borel-sum formula. However, unlike the present case, it frequently happens that the Borel-sum formula leads to a cut where the underlying function has none, as we see next.

C. Slightly Modified Standard Example: Complex Expansion with a Real Sum

In this section we make a minor modification to the standard example \( f(x) \) to construct a function \( g(x') \) that is real and analytic where the Borel sum has a cut. In this
example the sum of a complex series turns out to be real, and the cut in the Borel sum turns out to be a "Stokes line."

We define \( g(x') \) by

\[
g(x') = \begin{cases} 
  f(e^{-i\pi} x') + i\pi x' e^{-x'}, & (0 < \arg x' < \pi), \\
  f(e^{+i\pi} x') - i\pi x' e^{-x'}, & (-\pi < \arg x' < 0).
\end{cases}
\]  

We remark in passing that \( g(x') \) is \( x' e^{-x} Ei(x') \), where \( Ei(x') \) is the usual exponential integral. Let us focus on the behavior of \( g(x') \) near \( x' > 0 \). It is clear from Eq. (10) that \( g(x') \) is real and continuous on the positive real \( x' \) axis. The analytic properties are even more transparent if we invoke the convergent, ascending series [30] for \( f(x) \) and \( g(x') \) by using Eqs. (5.1.11) and (5.1.10) of Ref. 27:

\[
f(x) = xe^x \left[ -\gamma - \ln x - \sum_{n=1}^{\infty} (-1)^n x^n/(n!) \right],
\]

\[
g(x') = x'e^{-x} \left[ \gamma + \ln x' + \sum_{n=1}^{\infty} x'^n/(n!) \right].
\]

Here, \( \gamma \) is Euler's constant (0.5772156649...). Note in particular that \( g(x') \) is \( x' e^{-x} \ln x' \) plus an entire function of \( x' \). Moreover, \( g(x') \) has been defined so that the cut in the \( \ln x' \) in Eq. (14) is on the negative \( x' \) axis:

\[
\ln(e^{-i\pi} x') = \ln x' \mp i\pi.
\]

Thus \( g(x') \) is not only real and analytic on the positive real axis, but it also satisfies the reflection principle

\[
g(x'^*) = [g(x')]^*,
\]

where the asterisk denotes complex conjugation.

Let us now focus on the asymptotic expansion for \( g(x') \), which can be obtained directly from Eqs. (11) and (12) by putting the asymptotic power series (6) for \( f(x) \) and taking proper account of phase

\[
g(x') \sim \begin{cases} 
  \sum_{n=0}^{\infty} x'^{-n} n! + i\pi x' e^{-x'}, & (0 < \arg x' < \pi), \\
  \sum_{n=0}^{\infty} x'^{-n} n! - i\pi x' e^{-x'}, & (-\pi < \arg x' < 0).
\end{cases}
\]

What do these last two equations mean? The function \( g(x') \) is real and analytic on \( x' > 0 \). Yet its asymptotic expansion is complex and discontinuous there. The Borel sum of the power series along with the imaginary exponential contribution in either half-plane gives exactly \( g(x') \). The positive real \( x' \) axis is a cut of the Borel sum of the series. If included by analytic continuation from either half-plane, the result on the positive real axis is exactly the real result

\[
g(x') = P \int_0^{\infty} \frac{1}{1 - x'^{-t}} e^{-t} dt, \quad (x' > 0).
\]
It is in this sense that the sum of a complex expansion is real — when \( x' \) lies on the cut of the Borel sum, and the complex value of the Borel sum on the cut is obtained by analytic continuation from either side, with the implicit imaginary contribution coming from the Borel sum being canceled by the explicit imaginary term in the expansion [17]. Since the positive real axis is a cut of the Borel sum here but not of the function \( g(x') \) itself, the form of the asymptotic expansion must change to cancel the discontinuity in the Borel sum. Again, we emphasize that the sum of the asymptotic expansion in either half-plane gives \( g(x') \) exactly. On the positive \( x' \) axis, either expression gives the correct sum by analytic continuation. The line of discontinuity in the formal asymptotic expansion is called a Stokes line [16, 29]. Here the Stokes line is identical with the cut in the Borel sum, and in this context its presence and role are quite understandable.

Contrast the above observation — which depends on taking the asymptotic power series in the sense of Borel summation — with the interpretation of Eqs. (17) and (18) based only on the Poincaré definition [16, 29]. The exponentially small terms when \( x' \) is near the positive real axis are smaller than any power as \( x' \to \infty \) and, thus, just reflect that under the Poincaré definition many functions can have the same asymptotic power series. In this sense, the exponentially small terms are tolerated but regarded as negligible. Consequently, a discontinuity in their weights is of no importance near the Stokes line. Their presence is “really” required only when \( x' \) is in the second or third quadrants, where they become exponentially large compared with the power-series terms. Moreover, according to some authors [16], they should be ignored completely on the Stokes line itself, which raises the uncomfortable question of at what values of \( x' \) should the imaginary terms be switched on. In the Borel sense, they are always on. The Poincaré point of view has greatest relevance for computations using partial summation — i.e., truncation of the asymptotic expansion. The Borel method, however, not only permits arbitrarily high computational accuracy [24], but, because of the unique association between series and function, is also by far the more powerful for analysis [11–43], as we see in the next section on the discussion of JWKB connection formulas.

4. JWKB Connection Formulas

The objective of this section is to obtain the exact connection formulas for the JWKB method at a linear classical turning point. First, the JWKB method [15] and the Langer–Cherry [31, 32] refinement of it will be briefly sketched. Then, the connection formulas [33] will be discussed.

A. JWKB Wave Function

The JWKB solution of the Schrödinger equation,

\[
-\frac{\hbar^2}{2m} \frac{d^2}{dx^2} \psi + [V(x) - E] \psi = 0,
\]

is characterized by the form [15],
\[ \psi_h = \begin{cases} (dS/dx)^{-1/2}[Ce^{is/h} + de^{-is/h}], & (E - V) > 0, \\ (-dQ/dx)^{-1/2}[Ce^{iQ/h} + De^{-iQ/h}], & (V - E) > 0. \end{cases} \]  

(21a)  

(21b)

S and Q are meant to be real in the classically allowed and forbidden regions, respectively. Formally one could set Q = ±iS, however, so that detailed discussion of just S can suffice for both. The function S(\hbar, x) satisfies the Riccati equation

\[ (dS/dx)^2 = 2m(E - V) + \hbar^2(dS/dx)^{1/2}(d/dx)^2(dS/dx)^{-1/2}. \]  

(22)

In the standard JWKB approach, S(\hbar, x) is expanded in a power series in \hbar^2:

\[ S(\hbar, x) = \sum_{N=0}^{\infty} \hbar^{2N}S^{(N)}(x). \]  

(23)

dS^{(0)}/dx is the classical momentum, and S^{(0)} the classical action:

\[ dS^{(0)}/dx = [2m(E - V)]^{1/2} = p(x), \]  

(24)

\[ S^{(0)} = \int p \, dx. \]  

(25)

The higher-order dS^{(N)}/dx for N = 1 can be found recursively from the Riccati equation (22) via

\[ dS^{(N)}/dx = \frac{1}{2}(dS^{(0)}/dx)^{-1} \left\{ -\sum_{k=1}^{N-1} (dS^{(k)}/dx)(dS^{(N-k)}/dx) \\ + [(dS/dx)^{1/2}(d/dx)^2/dS/dx)^{-1/2}]^{(N-1)} \right\}, \]  

(26)

where [\cdot]^{(N-1)} denotes the terms of [\cdot] proportional to \hbar^{2(N-1)}.

The major problem with the JWKB form (21), as is well known, is that the S^{(N)} for N = 1 are singular at classical turning points. We bring out this problem, and the related connection formula problem, by looking at S^{(0)} and S^{(1)} near the classical turning point x_0. Near x_0, 2m(E - V) is (by assumption) linear:

\[ 2m(E - V) = q(x - x_0) + O((x - x_0)^2), \]  

(27)

where for concreteness we take q > 0, which puts the classically allowed region to the right of the turning point. Near x_0, one can solve Eqs. (25) and (26) to get the following (we give the results for both x > x_0 and x < x_0):

\[ S^{(0)} \sim \frac{2}{3}q^{1/2}(x - x_0)^{3/2}, \quad Q^{(0)} \sim \frac{2}{3}q^{1/2}(x_0 - x)^{3/2}, \]  

(28)

\[ S^{(1)} \sim -\frac{4}{3q}q^{-1/2}(x - x_0)^{-3/2}, \quad Q^{(1)} \sim +\frac{4}{3q}q^{-1/2}(x_0 - x)^{-3/2}. \]  

(29)

Equation (29) displays the singular behavior of S^{(1)} at x_0. On either side of, but away from x_0, a wave function of the JWKB form (21) holds. But how are the coefficients C and D on the left-hand side connected with c and d on the right? Naively, if one set x - x_0 = e^{i\theta}(x_0 - x), then it would seem that C should equal e^{-i\theta}c. But if one set x - x_0 = e^{-i\theta}(x_0 - x), then it would seem that C should equal e^{i\theta}d. In fact, neither
is correct: $C$ is actually the sum of the two [see Eq. (30) below]. The formulas (21) and (23) for the wave function constitute an asymptotic expansion, and there are Stokes lines between $\arg(x - x_0) = 0$ and $\arg(x - x_0) = \pm \pi$. In addition, $\arg(x - x_0) = \pm \pi$ is itself another Stokes line. The problem of finding the correct relationship between the two sets of coefficients is the connection-formula problem.

We remark that there is another ambiguity, the integration constant in $S^{(N)}$, which is not determined by the Riccati equation (22). Of course, the integration constant could be absorbed into the coefficients $c$ and $d$. However, it turns out that near $x_0$, the derivative $dS^{(N)}/dx$ has the form, $(x - x_0)^{-3N + 1/2}$ times a function analytic at $x_0$, and it is convenient to take the integration constant so that $S^{(N)}$ itself has the form $(x - x_0)^{-3N + 3/2}$ times a function analytic at $x_0$. See especially the discussion in Sect. 4D below.

Since the sketch of the derivation of the JWKB connection formulas in Sects. 4B–4D is a bit involved, and since the main thrust of this paper is to illuminate the reality and complexity of the asymptotic expansion, we summarize in advance the correct connection formulas:

$$C = e^{-i\pi k}c + e^{i\pi k}d,$$

$$D = \begin{cases} 
e^{-i\pi k}d, & \text{Im } x > 0, \\ e^{i\pi k}c, & \text{Im } x < 0. \end{cases}$$

The significance of these formulas will be discussed in detail in Sect. 4E, but notice already that if $c = d^*$, then the wave-function expansion (21a) in the classically allowed region is explicitly a real function of $S$, but that (except when $d = e^{i\pi k}|d| = c^*$) the wave-function expansion is explicitly complex and discontinuous [Eqs. (21b), (31), and (32)] in the classically forbidden region where the wave function itself is real and continuous (when $c = d^*$). The reader interested only in the results and not the derivation may turn directly to Sect. 4E.

**B. Langer-Cherry-Type Wave Function Near the Turning Point**

One solution to the connection problem (and much more) has its roots in the work of Langer [31] and of Cherry [32] on uniform asymptotic expansions. The first step is to solve the Schrödinger equation near the turning point. Then that solution is asymptotically expanded away from the turning point and recast into JWKB form. The connection formulas fall out of the process.

Near the turning point the wave function can be written in terms of Airy functions:

$$\psi = (d\phi/dx)^{-1/2}[aAi(-\hbar^{-2/3}\phi) + bBi(-\hbar^{-2/3}\phi)].$$

$\phi(t, x)$ satisfies the Riccati equation

$$\phi(d\phi/dx)^2 = 2m(E - V) + \hbar^2(d\phi/dx)^{1/2}(d/dx)^2(d\phi/dx)^{-1/2},$$

and vanishes at $x_0$: $\phi(t, x_0) = 0$. Given Eq. (27), one can see that near $x_0$,

$$\phi \sim q^{1/3}(x - x_0).$$
As was done for $S$ in Eq. (23), $\phi$ is expanded in a power series in $\hbar^2$:

$$\phi(\hbar, x) = \sum_{N=0}^{\infty} \hbar^{2N} \phi^{(N)}(x).$$

(36)

The $\phi^{(N)}$ can be found recursively by quadrature from Eqs. (34) and (36). For instance,

$$\phi^{(0)} = \left[ \frac{1}{2} \int_{x_0}^{x} [2m(E - V)]^{1/2} dx \right]^{23}.$$

(37)

The exact formulas for the $\phi^{(N)}$ are not important here. What is important is that each $\phi^{(N)}$ is analytic and has the value 0 at $x_0$, provided only that $2m(E - V)$ is analytic and has a simple zero at $x_0$. Away from $x_0$ where $\hbar^{-3} \phi$ is large, one can use the asymptotic expansions for the Airy functions, which we discuss in the next subsection.

C. Airy Function Asymptotic Expansions

The transformation from the Airy-function–based wave function to the exponential-function–based JWKB form passes through the well-known asymptotic expansions for the Airy functions [17, 27]. We list here the expansions (for large $z$) and the domains in which they are summable in the sense of Borel summability of their constituent power series [17]:

$$\text{Ai}(z) \sim \frac{1}{2} \pi^{-1/2} z^{-1/4} e^{-i \zeta} \sum_{k=0}^{\infty} c_k (-\zeta)^{-k}, \quad [\arg(z) < 2\pi/3],$$

(38)

$$\text{Ai}(-z) \sim \frac{1}{2} \pi^{-1/2} z^{-1/4} e^{i(\zeta - \text{arg}(z))} \sum_{k=0}^{\infty} c_k (i \zeta)^{-k} + \frac{1}{2} \pi^{-1/2} z^{-1/4} e^{-i(\zeta - \text{arg}(z))} \sum_{k=0}^{\infty} c_k (-i \zeta)^{-k},$$

$$[\arg(z) < \pi/3],$$

(39)

$$\text{Bi}(z) \sim \pi^{-1/2} z^{-1/4} e^{z} \sum_{k=0}^{\infty} c_k \zeta^{-k} - i \frac{1}{2} \pi^{-1/2} z^{-1/4} e^{-i \zeta} \sum_{k=0}^{\infty} c_k (-\zeta)^{-k},$$

$$[-2\pi/3 < \arg(z) < 0],$$

(40)

$$\text{Bi}(z) \sim \pi^{-1/2} z^{-1/4} e^{z} \sum_{k=0}^{\infty} c_k \zeta^{-k} + i \frac{1}{2} \pi^{-1/2} z^{-1/4} e^{-i \zeta} \sum_{k=0}^{\infty} c_k (-\zeta)^{-k}, \quad [0 < \arg(z) < 2\pi/3],$$

(41)

$$\text{Bi}(-z) \sim \frac{1}{2} \pi^{-1/2} z^{-1/4} e^{i(\zeta + \text{arg}(z))} \sum_{k=0}^{\infty} c_k (i \zeta)^{-k} + \frac{1}{2} \pi^{-1/2} z^{-1/4} e^{-i(\zeta + \text{arg}(z))} \sum_{k=0}^{\infty} c_k (-i \zeta)^{-k},$$

$$[\arg(z) < \pi/3],$$

(42)

where

$$\zeta = \frac{1}{2} z^{3/2}, \quad \text{and} \quad c_k = \frac{\Gamma(k + \frac{5}{8}) \Gamma(k + \frac{1}{8})}{\Gamma(\frac{5}{8}) \Gamma(\frac{1}{8}) 2^{8k!}}.$$

(43)
D. $S(\hbar, x)$ from $\phi(\hbar, x)$ and the Connection Formulas

The asymptotic expansion for the Airy-based $\psi$ for $x > x_0$ is obtained by putting

$$z = \hbar^{-2/3} \phi,$$
and
$$\zeta = \frac{2}{3} \phi^{3/2}/\hbar,$$

(44)

into Eqs. (39) and (42). What seems remarkable is that the explicit relationship between the JWKB $S(\hbar, x)$ and the Airy-based $\phi(\hbar, x)$ is simple [33]:

$$S \sim \frac{2}{3} \phi^{3/2} - \frac{i}{2} \hbar \ln \left[ \frac{\sum c_k(i2\phi^{3/2}/3\hbar)^{-k}}{\sum c_k(-i2\phi^{3/2}/3\hbar)^{-k}} \right].$$

(45)

$S^{(i)}$ is obtained by taking the coefficient of $\hbar^{2N}$ on both sides. To verify Eq. (45), take the derivative of $S$ [given by Eq. (45)] and use the Wronskian of $A_1$ and $B_1$ as applied to the asymptotic expansions (39) and (42), to calculate directly that

$$(dS/dx)^{-1/2} e^{iS\hbar} = \phi^{-1/4} (d\phi/dx)^{-1/2} e^{i2\phi^{3/2}/3\hbar} \sum_0^\infty c_k(\pm i2\phi^{3/2}/3\hbar)^{-k}.$$  

(46)

When $x < x_0$, the asymptotic expansion for the Airy-based $\psi$ is obtained by putting

$$z = \hbar^{-2/3} (-\phi),$$
and
$$\zeta = \frac{2}{3} (-\phi)^{3/2}/\hbar,$$

(47)

into Eq. (38) and either Eq. (40) or Eq. (41), depending whether one takes $x$ to be just above or just below the real axis, i.e., $\mp \arg(-\phi) \sim \mp \arg(x_0 - x) > 0$. As in the case of $g(\xi')$, Sect. 3C, the positive z axis is a Stokes line for $B_1(z)$ even though $B_1(z)$ is analytic there. In fact, $B_1(z)$ is an entire function. Consequently, the physical values of $x$ in the forbidden region fall on the Stokes line of the Airy-based, and by inference, of the JWKB function. The correct asymptotic expansion for the Airy-based, and consequently JWKB function, for the real wave function is then formally complex, and the real axis must be included by analytic continuation from above or below. Also, as in the case $x > x_0$, when $x < x_0$ there is again a simple, explicit relationship between the JWKB $Q(\hbar, x)$ and the Airy-based $\phi(\hbar, x)$ [in fact, one may take $Q = iS$, with the phase convention that $x - x_0 = e^{i\pi}(x_0 - x)$ when $\arg(x_0 - x) = 0$]:

$$Q \sim \frac{2}{3} (-\phi)^{3/2} + \frac{\hbar}{2} \ln \left[ \frac{\sum c_k[2(-\phi)^{3/2}/3\hbar]^{-k}}{\sum c_k[-2(-\phi)^{3/2}/3\hbar]^{-k}} \right],$$

(48)

$$(-dQ/dx)^{-1/2} e^{-iQ\hbar} = (-\phi)^{-1/4} (d\phi/dx)^{-1/2} e^{i2(-\phi)^{3/2}/3\hbar} \sum_0^\infty c_k[\pm 2(-\phi)^{3/2}/3\hbar]^{-k}.$$  

(49)

Thus, for the classically allowed region, one puts together Eq. (33) for the Airy-based $\psi$, Eqs. (39) and (42) for the Airy-function asymptotic expansions, and Eqs. (44) and (46) connecting the Airy asymptotics with the JWKB function, and finds that

$$(d\phi/dx)^{-1/2}[aAi(-\hbar^{-2/3} \phi) + bBi(-\hbar^{-2/3} \phi)]$$

$\sim \frac{1}{2\pi} \hbar^{1/6} e^{i\pi/4} (b - ia) (dS/dx)^{-1/2} e^{iS\hbar} + e^{-i\pi/4} (b + ia) (dS/dx)^{-1/2} e^{-iS\hbar}.$

(50)
For the classically forbidden region, one puts together Eq. (33) for the Airy-based $\psi$, Eqs. (38), (40), and (41) for the Airy-function asymptotic expansions, and Eqs. (47) and (49) connecting the Airy asymptotics with the JWKB function, and finds that

$$
\left(\frac{d\phi}{dx}\right)^{-1/2}[aAi(-\hbar^{-2/3}\phi) + bBi(-\hbar^{-2/3}\phi)] \\
\sim \frac{1}{2\pi} \hbar^{1/6} [2b(-dQ/dx)^{-1/2}e^{iQ/\hbar} \pm i(b \pm ia)(-dQ/dx)^{-1/2}e^{-iQ/\hbar}], \quad \pm \text{Im } x > 0.
$$

(51)

Finally, by comparing Eqs. (50) and (51) with Eqs. (21), one sees that

$$
c = \frac{1}{2\pi} \hbar^{1/6} \cdot e^{im/4}(b - ia),
$$

(52)

$$
d = \frac{1}{2\pi} \hbar^{1/6} \cdot e^{-im/4}(b + ia),
$$

(53)

$$
C = \frac{1}{2\pi} \hbar^{-1/6} \cdot 2b,
$$

(54)

$$
D = \frac{1}{2\pi} \hbar^{1/6} \cdot [\mp i(b \pm ia)], \quad \pm \text{Im } x > 0.
$$

(55)

That is, the result is the above Eqs. (30)--(32).

**E. Remarks on JWKB Connection Formulas (30)--(32)**

The exact JWKB connection formulas are given by Eqs. (21) and (30)--(32). They hold for the JWKB expansion to arbitrary order. They hold in either direction (assertions in the literature of unidirectionality of JWKB connection formulas are erroneous and are best forgotten [16]), since the expansions on the left-hand side and right-hand side are uniquely connected by the procedure involving the Airy-function representation described above. Implicit in the connection formulas are the conventions (i) that $S(0,x) \sim \frac{3}{2}(x - x_0)^{3/2}$ for $x - x_0$ small and positive, (ii) that $Q(0,x) \sim \frac{3}{2}(x_0 - x)^{3/2}$ for $x_0 - x$ small and positive, (iii) that $S^{(N)} \sim (x - x_0)^{-3N+3/2}$ times a function analytic at $x_0$, and (iv) that $Q^{(N)} \sim (x_0 - x)^{-3N+3/2}$ times a function analytic at $x_0$. Points (iii) and (iv) pertain to the choice of integration constant for $S^{(N)} = \int (dS^{(N)}/dx) \, dx$.

There is a significant difference between the connection formulas here and those that appear in textbooks [15, 16]. We examine three examples—one that agrees and two that differ with standard texts.

One fundamental case, $(a \neq 0, b = 0)$, corresponds to exponential decrease away from $x_0$ in the classically forbidden region, and trigonometric behavior in the classically allowed region. The connection formulas [cf. also Eqs. (52)--(55)] give $C = 0$, $c = e^{-im/4}D$, and $d = e^{im/4}D$, which are consistent with the textbooks.

A second fundamental case, $(a = 0, b \neq 0)$, corresponds to exponential increase away from $x_0$ in the classically forbidden region, and trigonometric behavior in the classically allowed region. The connection formulas give $c = \frac{1}{2}e^{im/4}C$, $d = \frac{1}{2}e^{-im/4}C$, and $D = \mp iC$. The textbooks give $D = 0$. Here the difference is that the coefficient of the exponentially small component, $e^{-Q/\hbar}$ is imaginary and does not vanish: Real values of $x < x_0$ lie on a Stokes line of the asymptotic expansion of the $Bi$ function, and the explicit imaginary subseries is necessary to cancel the implicit imaginary contribution that comes from the Borel sum of the real series in $(-dQ/dx)^{-1/2}e^{iQ/\hbar}$ so that the composite sum is real.
A third fundamental case \((a = ib)\) is connected with penetration through a barrier. The connection formulas give \(d = 0\), \(C = e^{-j\mu \delta c}\), and \(D = 0\) for \(\text{Im} \, x > 0\). This case corresponds to the linear combination \(\text{Bi}(-z) + i \text{Ai}(-z)\), whose asymptotic expansion is just the \(e^{iz}\) series of Eqs. (39) and (42). With \(x\) in the upper half-plane, no Stokes line (of the \(e^{iz}\) series) is crossed in moving from \(\text{arg}(x - x_0) = +0\) to \(\text{arg}(x - x_0) = \pi - 0\), and a single JWKB-type expansion is valid in both the forbidden and allowed regions. Contrast this with what is usually found in textbooks. On one hand, \(D = 0\) in the texts is normally taken for the Bi case (the preceding paragraph), which corresponds to real trigonometric behavior outside the barrier. On the other hand, in discussing penetration through a barrier with outgoing-wave (vs. real) trigonometric behavior, it would then seem necessary to have \(D \neq 0\) for consistency. Nevertheless, that term (with \(D \neq 0\)) is generally (if not universally) discarded as being numerically unimportant, although usually no careful justification is given that it is negligible. In fact, the argument as usually presented is incorrect: There is no term to throw away; it is just not there in the first place.

5. Concluding Remarks

The Borel summation method is a powerful tool for understanding and using divergent asymptotic expansions. In descriptive, nonrigorous language, when the \(n\)th term of the divergent series grows like \(n! x^{-n}\), then the associated series for the Borel transform is like the geometric series, \(\Sigma x^{-n}\), which has a pole at \(x = 1\). The integral of the Borel transform, which gives the Borel sum, then has a cut where the pole falls on the integration path. The cuts of the Borel sum turn out to be the Stokes lines of the asymptotic expansions, the lines across which the coefficients of the “small” subseries change discontinuously. On the cuts, the Borel sum is obtained by analytic continuation. This mechanism associates a complex value to the sum of a real series, as seen by the standard example of Sect. 3.

For the RSPT examples mentioned in the introduction, the physical values of the parameters lie on Stokes lines. Consequently, the real RSPT for the LoSurdo–Stark effect has for its sum the complex, resonance eigenvalue. For \(H^+_2\), the sum of the real RSPT is complex, but there are additional exponentially small subseries that are explicitly imaginary and that are counterterms to cancel the imaginary contribution from the Borel sum of RSPT, so that the sum of the complex expansion is real.

The JWKB expansion is a double asymptotic expansion in small \(\hbar\) and large \(|x - x_0|\). The JWKB expansion can be based on Airy functions, by which one obtains an expansion valid for small, as well as large \(|x - x_0|\). The summable asymptotic expansions for the Airy function, plus algebraic rearrangement of the terms, result in the JWKB form. The connection formulas that fall out, and which are valid to all orders in \(\hbar\), agree with textbook versions for the Ai part of the wave function, but not the Bi part. The reason for the discrepancy is that the coordinate in the forbidden region lies on the Stokes line of the Bi function, and the real Bi function should be represented there by a complex asymptotic expansion. The form of the connection formula appropriate for an outgoing wave in the classically allowed region that comes up in barrier penetration and tunneling problems is particularly simple and is the result usually obtained.
in the texts with some difficulty by discarding a term speciously present from an incorrect connect formula.

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Bibliography


[30] The straightforward but nontrivial derivation of these series is not important here and should be of no concern to the reader. We introduce Eqs. (13) and (14) to make clear the analytic behavior of \( f(x) \) and \( g(x') \) at the origin.

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