JWKB Connection-Formula Problem Revisited via Borel Summation

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The traditional version of the JWKB connection formula at a linear turning point is incorrect. The correct version follows from the Borel-based summability of the Airy-function asymptotic expansions. A key point is that the classically forbidden region lies on a Stokes line. The *real* exponentially growing solution has an *explicitly complex* JWKB expansion, while the *explicitly real* exponentially growing JWKB expansion represents a *complex* solution. Inconsistencies in applications of the traditional formula, such as in transmission through a barrier, are eliminated.

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The Jeffreys-Wentzel-Kramers-Brillouin (JWKB) method has been a most versatile technique for quantum mechanical applications.[1] A problem central to its formulation is the "connection formula" linking the coefficients in the classically forbidden region with the coefficients of the trigonometric components in the classically allowed region on either side of a linear classical turning point. *The traditional version of the JWKB connection formula is incorrect.* The purpose of this Letter is to derive, with the aid of Borel's method of summation, the correct connection formula [Eqs. (24) and (25) below].

By way of example, Langer[2] writes for the leading-order JWKB wave function $\psi(x)$ near the turning point x_1, to the right of which we take $E-V$ to be positive,

$$\psi(x) \sim [2m(E-V)]^{-1/4} 2\cos(\xi - \tfrac{1}{4}\pi + \eta), \quad x > x_1, \tag{1}$$

$$\sim [2m(V-E)]^{-1/4} (2\sin\eta e^{|\xi|} + \cos\eta e^{-|\xi|}), \quad x < x_1, \tag{2}$$

where η is an arbitrary constant, and $\xi = \hbar^{-1}\int_{x_1}^{x} [2m(E-V)]^{1/2} dx$. Equation (2) is incorrect: it should be

$$\psi(x) \sim [2m(V-E)]^{-1/4} (2\sin\eta e^{|\xi|} + e^{\mp i\eta - |\xi|}), \quad x < x_1, \quad \mathrm{Im} x = \pm 0. \tag{3}$$

That is, real values of x to the left of x_1 cannot be discussed in isolation from complex values of x. The JWKB function has a discontinuous change across $x < x_1$, which is a Stokes line of the JWKB expansion. The coefficient of $e^{-|\xi|}$ at $x < x_1$ depends on whether x becomes real from above or below. Moreover, the JWKB expansion is explicitly complex, even though the wave function it represents is real. These remarks may at first seem puzzling and counterintuitive to the reader. However, they can be understood and clarified via the Borel-based summability[3] of the divergent asymptotic expansions for the Airy Ai and Bi functions from which the JWKB expansion can be obtained.

Derivation of the correct JWKB connection formula begins with the Langer-Cherry form[2,4] of the wave function (here a and b are constants),

$$\psi(x) = 2\pi^{1/2}\hbar^{-1/6} (d\phi/dx)^{-1/2} [a\,\mathrm{Ai}(-\hbar^{-2/3}\phi) + b\,\mathrm{Bi}(-\hbar^{-2/3}\phi)], \tag{4}$$

$$\phi(\hbar, x) \sim \sum_{n=0}^{\infty} \hbar^{2n} \phi^{(n)}(x), \tag{5}$$

which is designed to give a uniform asymptotic expansion in the neighborhood of a linear classical turning point x_1. (The factor $2\pi^{1/2}\hbar^{-1/6}$ is for later convenience.) For definiteness, we take the classically allowed region to the right-hand side of the turning point

$$2m(E-V) = q(x-x_1) + O((x-x_1)^2), \quad q > 0. \tag{6}$$

[To avoid confusion, note that the classically allowed (forbidden) region $x > x_1$ ($x < x_1$) used in Eqs. (1)–(6) and (15)–(32) is switched to $z < 0$ ($z > 0$) in the Airy functions $\mathrm{Ai}(z)$ and $\mathrm{Bi}(z)$, whose asymptotic expansions are given in Eqs. (9)–(14).] As is "well known," ϕ is determined from a Riccati equation obtained by substitution of Eq. (4) into the Schrödinger equation, and the $\phi^{(n)}(x)$ can be found by straightforward recursive quadratures.[4] For instance,

$$\phi^{(0)}=\left\{\frac{3}{2}\int_{x_1}^{x}[2m(E-V)]^{1/2}dx\right\}^{2/3}\sim q^{1/3}(x-x_1), \tag{7}$$

$$\phi^{(1)}=\tfrac{1}{2}(\phi^{(0)})^{-1/2}\int(\phi^{(0)})^{-1/2}\left(\frac{d\phi^{(0)}}{dx}\right)^{-1/2}\left(\frac{d^2}{dx^2}\right)\left(\frac{d\phi^{(0)}}{dx}\right)^{-1/2}dx, \tag{8}$$

$\phi^{(0)}$ is

and so forth. Explicit evaluation of the $\phi^{(n)}$, however, is here unimportant. What is important is that the $\phi^{(n)}(x)$ are analytic and zero at x_1, provided that $E-V$ is the same. The main role of the $\phi^{(n)}$ here is in the derivation of the connection formula, not in the practical calculation of the JWKB function itself.

The next step in the derivation is to apply the asymptotic expansions for Ai and Bi, which are valid away from x_1, where $\hbar^{-2/3}\phi$ is large. It is here—with reference to the summable asymptotic expansions of $\mathrm{Bi}(z)$—that the present derivation departs from the conventional. For conciseness in writing the Airy function expansions, we use the symbol $\beta(\zeta)$ to denote the formal asymptotic expansion,

$$\beta(\zeta)=e^{\zeta}\sum_{k=0}^{\infty}c_k\zeta^{-k}, \tag{9}$$

$$c_k=\Gamma(k+\tfrac{5}{6})\Gamma(k+\tfrac{1}{6})/\Gamma(\tfrac{5}{6})\Gamma(\tfrac{1}{6})2^k k!. \tag{10}$$

Let $\zeta=\frac{2}{3}z^{3/2}$. Then the large-z asymptotic expansions for Ai and Bi are[3,5]

$$\mathrm{Ai}(-z)\sim\tfrac{1}{2}\pi^{-1/2}z^{-1/4}[e^{-i\pi/4}\beta(i\zeta)+e^{i\pi/4}\beta(-i\zeta)],\quad |\arg z|<\pi/3, \tag{11}$$

$$\mathrm{Ai}(z)\sim\tfrac{1}{2}\pi^{-1/2}z^{-1/4}\beta(-\zeta),\quad |\arg z|<2\pi/3, \tag{12}$$

$$\mathrm{Bi}(-z)\sim\tfrac{1}{2}\pi^{-1/2}z^{-1/4}[e^{i\pi/4}\beta(i\zeta)+e^{-i\pi/4}\beta(-i\zeta)],\quad |\arg z|<\pi/3, \tag{13}$$

$$\mathrm{Bi}(z)\sim\tfrac{1}{2}\pi^{-1/2}z^{-1/4}[2\beta(\zeta)\pm i\beta(-\zeta)],\quad 0<\pm\arg z<2\pi/3. \tag{14}$$

The expansions (11)–(14) are summable[3] on the indicated domains through the Borel summability of the power series $\sum c_k(-\zeta)^{-k}$. Except for the precise specification of domain for summability,[3] Eqs. (11)–(13) are standard.[5] Equation (14), however, is not what appears in traditional JWKB derivations, and it is the key to the correct connection formula.

Equation (14) gives the expansions that are *summable uniquely* to $\mathrm{Bi}(z)$ on $0<\arg z<2\pi/3$ and on $-2\pi/3<\arg z<0$. The positive real axis, $\arg z=0$, which corresponds to the physical variable inside the classically forbidden region, is a Stokes line of the expansion across which the coefficient of the $e^{-\zeta}$ series changes discontinuously. More precisely,[3] it is a cut of the Borel sum of $\sum c_k\zeta^{-k}$. The proper way to include the positive real axis for purposes of analysis is by analytic continuation of the sum of the expansion. Consequently, the correct asymptotic expansion on $\arg z=0$ is either of the $\frac{1}{2}\pi^{-1/2}z^{-1/4}\,[2\beta(\zeta)\pm i\beta(-\zeta)]$, the sign depending on from which side the real axis is approached. The expansion for the real function $\mathrm{Bi}(z)$ $(z>0)$ is thus explicitly complex. Traditional JWKB discussions have used just the real expansion $\pi^{-1/2}z^{-1/4}\beta(\zeta)$. While satisfying the Poincaré definition[1b] and while suitable for calculation by partial summation, this expansion is not summable to $\mathrm{Bi}(z)$ near $z>0$ and is *a fortiori* not suitable for questions of analysis. That a real function is represented by an explicitly complex asymptotic expansion (albeit on a Stokes line) is a result that may require modification of naive intuition.[3,6–10]

Put now $z=\hbar^{-2/3}\phi$ and $\zeta=\frac{2}{3}\phi^{3/2}/\hbar$ when $\phi>0$ into Eqs. (4), (11), and (13) to obtain for the classically allowed region,

$$\psi\sim\phi^{-1/4}(d\phi/dx)^{-1/2}[(b-ia)e^{i\pi/4}\beta(i\tfrac{2}{3}\phi^{3/2}/\hbar)+(b+ia)e^{-i\pi/4}\beta(-i\tfrac{2}{3}\phi^{3/2}/\hbar)], \tag{15}$$

$$|\arg\phi|<\pi/3,\ \text{viz.},\ \arg(x-x_1)\sim 0.$$

For the classically forbidden region, put $z=-\hbar^{-2/3}\phi$ and $\zeta=\frac{2}{3}(-\phi)^{3/2}/\hbar$ (for $-\phi>0$) into Eqs. (4), (12), and (14) to obtain

$$\psi\sim(-\phi)^{-1/4}(d\phi/dx)^{-1/2}[2b\beta(\tfrac{2}{3}(-\phi)^{3/2}/\hbar)+(a\pm ib)\beta(-\tfrac{2}{3}(-\phi)^{3/2}/\hbar)], \tag{16}$$

$$0<\pm\arg(-\phi)<\pi/3,\ \text{viz.},\ \arg(x_1-x)\sim 0,\quad \pm\mathrm{Im}\,x>0.$$

The final step in the derivation is to manipulate the asymptotic formulas (15) and (16) into JWKB form. This can be done globally and concisely. Let $S(\hbar,x)$ be defined by the asymptotic formula for the phase $\hbar\arg(\beta(i\zeta))=\frac{1}{2}\hbar\arg(\beta(i\zeta)/\beta(-i\zeta))$,

$$S\sim\tfrac{2}{3}\phi^{3/2}-\frac{i\hbar}{2}\ln\frac{\sum c_k(i2\phi^{3/2}/3\hbar)^{-k}}{\sum c_l(-i2\phi^{3/2}/3\hbar)^{-l}}. \tag{17}$$

By using the Wronskian formula,[5] $\mathrm{Ai}(d\,\mathrm{Bi}/dz)-\mathrm{Bi}(d\,\mathrm{Ai}/dz)=\pi^{-1}$, applied to the asymptotic expansions (11)–(14), one can easily calculate that

$$(dS/dx)^{-1/2}e^{\pm iS/\hbar}=\phi^{-1/4}(d\phi/dx)^{-1/2}\beta(\pm i\tfrac{2}{3}\phi^{3/2}/\hbar). \tag{18}$$

The left-hand side of Eq. (18) is the JWKB form for the classically allowed region. One need only make the expansion,[1]

$$S(\hbar,x)\sim\sum_{n=0}^{\infty}\hbar^{2n}S^{(n)}(x). \tag{19}$$

$S^{(n)}(x)$ is the coefficient of $\hbar^{2n}$ in the expansion of the right-hand side of Eq. (17) in powers of $\hbar$, after substitution of Eq. (5) for ϕ. For instance,

$$S^{(0)}=\tfrac{2}{3}(\phi^{(0)})^{3/2}\sim\tfrac{2}{3}q^{1/2}(x-x_1)^{3/2},\quad \arg(x-x_1)\sim 0. \tag{20}$$

For the classically forbidden region, we may use

$$Q(\hbar,x)=iS(\hbar,e^{\pi i}(x_1-x)+x_1),\quad Q^{(n)}(x)=iS^{(n)}(e^{\pi i}(x_1-x)+x_1). \tag{21}$$

For instance,

$$Q^{(0)}(x)=\tfrac{2}{3}(-\phi^{(0)})^{3/2}\sim\tfrac{2}{3}q^{1/2}(x_1-x)^{3/2},\quad \arg(x_1-x)\sim 0. \tag{22}$$

Then one sees that

$$(-dQ/dx)^{-1/2}e^{\pm Q/\hbar}=(-\phi)^{-1/4}(d\phi/dx)^{-1/2}\beta(\pm\tfrac{2}{3}(-\phi)^{3/2}/\hbar). \tag{23}$$

That is, the connection formula is [from Eqs. (15), (16), (18), and (23)]

$$\psi\sim(dS/dx)^{-1/2}[(b-ia)e^{iS/\hbar+i\pi/4}+(b+ia)e^{-iS/\hbar-i\pi/4}],\quad \arg(x-x_1)\sim 0, \tag{24}$$

$$\sim(-dQ/dx)^{-1/2}[2be^{Q/\hbar}+(a\pm ib)e^{-Q/\hbar}],\quad \arg(x_1-x)\sim 0,\quad \mp\mathrm{Im}x>0. \tag{25}$$

Except for a few remarks, the derivation is complete.

Remark 1.—The $S^{(n)}$ (and $Q^{(n)}$) are calculated directly from equations[1] obtained by substituting $(dS/dx)^{-1/2}e^{\pm iS/\hbar}$ and Eq. (19) into the Schrödinger equation and collecting terms proportional to $\hbar^{2n}$. Nevertheless, Eq. (17) and the behavior of the $\phi^{(n)}$ at x_1, alluded to earlier, provide one crucial result not specified by the direct equations for $S^{(n)}$: namely, the integration constant C_n in $S^{(n)}=\int(dS^{(n)}/dx)dx+C_n$. The result is that C_n should be chosen[11] so that near x_1, $S^{(n)}$ has the form (where k_n is also a constant),

$$S^{(n)}\sim k_n(x-x_1)^{3/2-3n}[1+O(x-x_1)]. \tag{26}$$

Remark 2.—The connection formulas are independent of $\hbar$. That is, the coefficients of the various JWKB components are independent of the order in $\hbar$ to which S and Q have been calculated. Note, moreover, that the integration constant of each $S^{(n)}$ must first be resolved according to Eq. (26); otherwise the connection-formula coefficients would be order dependent.

Remark 3.—It is informative to look at the case of transmission through a barrier. The boundary condition to the right is purely outgoing wave, $b=-ia$ in Eq. (24). The connection formula then is

$$\psi(x)\sim 2b(dS/dx)^{-1/2}e^{iS/\hbar+i\pi/4},\quad \arg(x-x_1)\sim 0, \tag{27}$$

$$\sim 2b(-dQ/dx)^{-1/2}e^{Q/\hbar},\quad \arg(x_1-x)\sim 0,\quad \mathrm{Im}x>0. \tag{28}$$

Except for the qualification on Imx, to which we return shortly, a leading-order version of Eq. (28) is also found in texts.[1] The same texts, however, often give another connection formula with the same wave function inside the barrier, but with a standing wave in the allowed region. It is the leading-order version of

$$\psi(x)\sim b(dS/dx)^{-1/2}(e^{iS/\hbar+i\pi/4}+e^{-iS/\hbar-i\pi/4}),\quad \arg(x-x_1)\sim 0, \tag{29}$$

$$\sim 2b(-dQ/dx)^{-1/2}e^{Q/\hbar},\quad \arg(x_1-x)\sim 0, \tag{30}$$

(in texts, but incorrect). Equation (30) is clearly inconsistent with the outgoing-wave case, Eq. (28). Equations (29) and (30) are presumed to be correct by the texts, because both formulas are thought to represent real wave functions. Equation (28) is thought to be only approximate, with an imaginary exponentially small component dropped because of numerical insignificance [cf. Ref. 1b, p. 530]. In fact the interpretation and some consequent formulas in most texts are incorrect. The $e^{Q/\hbar}$ component, although formally real, represents a complex wave function, whereas the formally complex JWKB wave function,

$$\psi(x) \sim 2b(-dQ/dx)^{-1/2}(e^{Q/\hbar} \pm \tfrac{1}{2} ie^{-Q/\hbar}), \quad (31)$$

$$\arg(x_1 - x) \sim 0, \quad \mp \operatorname{Im} x > 0,$$

actually represents a real wave function.

Note that if we take $\operatorname{Im} x < 0$, then instead of Eq. (28), we get

$$\psi(x) \sim 2b(-dQ/dx)^{-1/2}(e^{Q/\hbar} + ie^{-Q/\hbar}), \quad (32)$$

$$\arg(x_1 - x) \sim 0, \quad \operatorname{Im} x < 0.$$

The Borel sum of the $e^{Q/\hbar}$ series is now appropriate for the underside of the cut, and the $ie^{-Q/\hbar}$ serves to cancel its discontinuity across the cut. That is, a different asymptotic formula is needed to represent the direct analytic continuation of the branch from above the real axis to below it.

For transmission through a barrier, there is a second classically allowed region to the left, with turning point $x_0 < x_1$. *Three* connection formulas are required: one each at x_0 and x_1, and a long-range one, not discussed in this Letter, *that connects the JWKB solution at* x_0 *with that at* x_1. If Q_0 and Q_1 denote the Q's associated with x_0 and x_1, then naive assumption of overlapping domains of validity implies

$$\left(\frac{dQ_0}{dx}\right)^{-1/2} e^{-Q_0/\hbar} = e^{-(Q_0+Q_1)/\hbar}\left(\frac{-dQ_1}{dx}\right)^{-1/2} e^{Q_1/\hbar},$$

and leads to the transmission coefficient $e^{-2(Q_0+Q_1)/\hbar}$, which is correct to all orders of $\hbar$. However, terms $O(e^{-4(Q_0+Q_1)/\hbar})$ are missing. In fact, $(-dQ_1/dx)^{-1/2}e^{Q_1/\hbar}$, near x_1 corresponds to a V-dependent linear combination of $(dQ_0/dx)^{-1/2}e^{\pm Q_0/\hbar}$ near x_0, as can be illustrated by exact solution of the simple example $V = -k|x|$ and the more subtle example $V = -kx^2$.

Remark 4.—The connection formula is bidirectional.[12] It is possible that assertions of unidirectionality have some roots in the inconsistency illustrated in Remark 3. Insofar as the correct JWKB connection formula is concerned, claims of unidirectionality are incorrect and ignorable.

Remark 5.—The relationships derived in this paper are purely formal; no attempt has been made to obtain mathematically rigorous error estimates for the applicability of the expansions.

Remark 6.—The treatment here of the JWKB expansion in $\hbar$ is quite similar to treatments of the LoSurdo-Stark effect in hydrogen as a function of field strength,[8] of the hydrogen molecule ion as a function of inverse internuclear distance,[6,7] and of the one-dimensional anharmonic oscillator.[9] In those problems, Borel summability, coupled with the recognition that on a Stokes line a real series can represent a complex-valued function while a complex expansion can represent a real-valued function, has been a powerful analytical as well as numerical tool.

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[1]See, for instance, (a) A. Messiah, *Quantum Mechanics* (Wiley, New York, 1965); or (b) C. M. Bender and S. A. Orszag, *Advanced Mathematical Methods for Scientists and Engineers* (McGraw-Hill, New York, 1978).

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[9]H. J. Silverstone, J. G. Harris, J. Čížek, and J. Paldus, Phys. Rev. A **32**, 1965 (1985).

[10]A transparent example of a real function represented by a complex asymptotic expansion is

$$g(x) = xe^{-x}\operatorname{Ei}(x) \sim \sum_{n=0}^{\infty} n!x^{-n} \pm i\pi xe^{-x},$$

where $\operatorname{Ei}(x)$ is the exponential integral. For real $x > 0$, $g(x)$ is the principal value, $P\int_0^\infty (1-x^{-1}t)^{-1}e^{-t}dt$. See H. J. Silverstone, Int. J. Quantum Chem. (to be published).

[11]In practice, $dS^{(n)}/dx$ can be integrated on a path starting and ending at x while encircling x_1.

[12]Bidirectionality has been pointed out by several authors. See, for example, R. B. Dingle, *Asymptotic Expansions: Their Derivation and Interpretation* (Academic, New York, 1973).