

ON THE BIDIRECTIONALITY OF THE JWKB CONNECTION FORMULA AT A LINEAR TURNING POINT

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Dedicated to Professor Josef Paldus on the occasion of his 70th birthday.

The bidirectionality of the Jeffreys–Wentzel–Kramers–Brillouin (JWKB) connection formula is demonstrated by a simple numerical example constructed from a linear potential and a box.

Keywords: JWKB; Connection formula; Borel sum; Asymptotic expansion; Tunneling; Jeffreys–Wentzel–Kramers–Brillouin method; Wave function; Quantum chemistry.

I. INTRODUCTION

The Jeffreys–Wentzel–Kramers–Brillouin (JWKB) method is often the technique of choice in the study of some effectively one-dimensional phenomena in chemistry, like tunneling through potential barriers or the exponentially small splitting of quasi-degenerate energy levels in double wells (see, for example, the review by Benderskii, Goldanskii and Makarov¹). A key ingredient for the application of the JWKB method to these problems is the connection formula between JWKB wavefunctions defined in regions of space separated by a linear turning point. This connection process usually has to be carried out through a sequence of consecutive turning points: to calculate the splitting of levels in a double well one would start with a decreasing JWKB wavefunction (say, to the far left), connect it through a turning point into the first well, then below the barrier, next into the second well and finally to a decreasing JWKB function in the far right. Whether this sequence of connections can always be carried out is known as the “directionality problem” of the JWKB connection formulas.

As instructively and entertainingly pointed out by Dingle² there is a “bewildering diversity of views recorded in the literature” on the direction-

ality of JWKB connection formulas at a linear turning point. For recent diversity, compare Fröman and Fröman³ and Silverstone⁴. The connection formula problem was in fact solved via the Borel summability of Airy functions⁴, and the solution is bidirectional. The purpose of this paper is to demonstrate by a clear, simple, single-linear-turning-point, concrete numerical example the sense in which the connection formula is bidirectional. The example is a particle in a box with a linear external field. Two different sets of boundary conditions are imposed: finite box (the particle being constrained by the linear potential and two walls); and semi-infinite (the particle being constrained by the linear potential and one wall). The present example is significantly simpler than the two-turning-point examples discussed elsewhere⁵.

Before proceeding, we wish to clarify the term “JWKB wave function” as used in this paper: we mean the complete, Borel-summable asymptotic expansion of the wave function in powers of \hbar according to Eqs (2)–(5) below, including exponentially small terms. Any exact wave function is in unique, one-to-one correspondence with a JWKB wave function, which is in general a linear combination of two exponentially different JWKB subseries. The linear coefficients themselves are, in general, asymptotic expansions with respect to \hbar . They may also involve exponentially small terms and are unique up to normalization. The connection problem is how the asymptotic expansion on the left is to be matched with the asymptotic expansion on the right of a classical turning point, where the expansions are singular.

II. BASICS

Consider the JWKB wave functions for the Schrödinger equation

$$\left(-\frac{\hbar^2}{2m} \frac{d^2}{dx^2} + kx - E\right) \psi(x) = 0 \quad (0 \leq x \leq x_1) \quad (1)$$

with a classical turning point $x_0 = E/k$ lying between 0 and x_1 , as illustrated in Fig. 1.

In the classically allowed Region I ($0 \leq x < x_0$) the JWKB wave function has the form

$$\psi_I(x) = (-dS/dx)^{-1/2} \sin(S/\hbar + \pi/4 - \delta). \quad (2)$$

In the classically forbidden Region II ($x_0 < x \leq x_1$) the JWKB wave function has the form

$$\Psi_{\text{II}}(x) = 2b(dQ/dx)^{-1/2} e^{Q/\hbar} + (a + ib)(dQ/dx)^{-1/2} e^{-Q/\hbar}. \quad (3)$$

In Eq. (2), δ is independent of x and is a convenient way to express the trigonometric linear combination (that anticipates the boundary condition at $x = 0$). In Eq. (3), $2b$ and $(a + ib)$ are independent of x and are a convenient way to express the exponential linear combination (that anticipates the connection formula). Both a and b may be complex. As is characteristic of the JWKB method⁶, the “action functions” S and Q are expanded in powers of \hbar^2 :

$$S = S^{(0)} + \hbar^2 S^{(1)} + \hbar^4 S^{(2)} + \dots \quad (4)$$

$$Q = Q^{(0)} + \hbar^2 Q^{(1)} + \hbar^4 Q^{(2)} + \dots \quad (5)$$

For simplicity, we henceforth use units in which $\hbar = 2m = 1$; however, k is to remain explicit and later will be given a numerical value.

We remark that the JWKB $S^{(N)}$ and $Q^{(N)}$ for a linear potential are monomially simple⁷:

$$Q^{(0)} = \zeta_{\text{II}} \quad (6)$$

$$Q^{(1)} = \frac{5}{72} \zeta_{\text{II}}^{-1} \quad (7)$$

$$Q^{(N)} = c^{(N)} \zeta_{\text{II}}^{1-2N} \quad (8)$$

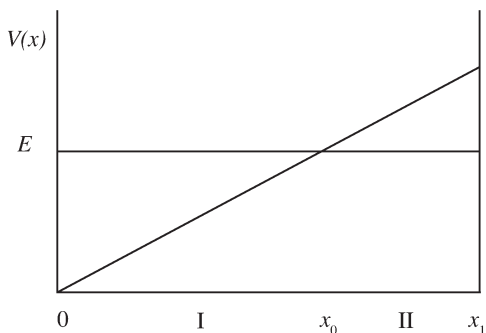


FIG. 1

Particle in a box with a linear potential and a single linear turning point at x_0 . Region I ($0 \leq x \leq x_0$) is classically allowed; Region II ($x_0 \leq x$) is classically forbidden.

$$S^{(0)} = \zeta_1 \quad (9)$$

$$S^{(1)} = -\frac{5}{72} \zeta_1^{-1} \quad (10)$$

$$S^{(N)} = (-1)^N c^{(N)} \zeta_1^{1-2N} \quad (11)$$

where $c^{(N)}$ is a rational constant, and

$$\zeta_I = \zeta_I(x, k, E) = \frac{2}{3k} (E - kx)^{3/2} \quad (12)$$

$$\zeta_{II} = \zeta_{II}(x, k, E) = \frac{2}{3k} (kx - E)^{3/2} . \quad (13)$$

The simplicity of $S^{(N)}$ and $Q^{(N)}$ allows us to take expansions to any particular truncation order $N = N_T$ and permits all attention to be focussed on the connection formulas and the Borel summation method.

III. CONNECTION FORMULA, BOUNDARY CONDITIONS, AND QUANTUM CONDITION

The proper connection formula depends on how x is treated in Region II, where it lies on a Stokes line⁴. It is necessary to “pick sides”. We choose $\text{Im } x = +0$; that is, we consider $(x_0 \leq x \leq x_1)$ to belong to the upper half-plane. (With $\text{Im } x = +0$ and real k , ψ_{II} represents a real function if, and only if, a and b are real. Note that there is a connection problem only if $E < kx_1$; if $E > kx_1$, there is no classical turning point.) The formula that connects ψ_I and ψ_{II} , because of the specification of δ , a , and b in Eqs (2) and (3) and the choice $\text{Im } x = +0$, is^{4,8}

$$\tan \delta = -b/a . \quad (14)$$

Energy eigenvalues result from the boundary conditions

$$\psi(0) = 0 = \sin(S(0) + \pi/4 - \delta) \quad (15)$$

$$\psi(x_1) = 0 = (dQ/dx)^{-1/2} e^{-Q(x_1)} (2be^{2Q(x_1)} + ib + a) \quad (16)$$

or, equivalently (we start n with 1, because $S(0) \approx \frac{2}{3k} E^{3/2} > 0$),

$$S(0) + \pi/4 - \delta = m\pi \quad (n = 1, 2, \dots) \quad (17)$$

$$b/a = -(2e^{2Q(x_1)} + i)^{-1} \quad (18)$$

which imply

$$\delta = \arctan [(2e^{2Q(x_1)} + i)^{-1}] \quad (19)$$

and what might be called the “quantum condition”

$$S(0) + \pi/4 - \arctan [(2e^{2Q(x_1)} + i)^{-1}] = m\pi \quad (n = 1, 2, \dots) . \quad (20)$$

The energy eigenvalues E_n for which $E_n < kx_1$ are the roots of Eq. (20). For example, if x_1 is large enough that $(2e^{2Q(x_1)} + i)^{-1} \approx 0$, and if we keep just the first term $S(0) \approx S^{(0)}(0) = \zeta_1(0, k, E)$, then

$$E \approx k^{2/3} \left[\frac{3}{2} \left(n - \frac{1}{4} \right) \pi \right]^{2/3} \quad (21)$$

which is a good estimate of the n -th zero of the Airy function, $\text{Ai}(-k^{-2/3}E)$ (cf. ref.⁹).

A. Approximate Quantum Condition; Traditional JWKB

Asymptotically, $|2e^{2Q(x_1)}| \gg |i|$, so that $(2e^{2Q(x_1)} + i) \approx 2e^{2Q(x_1)}$, and one obtains the approximate quantum condition,

$$S(0) + \pi/4 - \arctan \left(\frac{1}{2} e^{-2Q(x_1)} \right) \approx m\pi \quad (n = 1, 2, \dots) . \quad (22)$$

The reader might recognize Eq. (22) as the traditional JWKB result – traditional in the sense that only formally real expansions are used to represent real functions. The equation is in general only approximate: the Borel sum of $Q(x_1)$ is complex, so that Eq. (22) cannot lead to exact, real eigenvalues, whereas Eq. (20) does (vide infra). However, if $Q(x_1)$ is approximated by a

partial sum (all the terms of which are positive), then (i) $2e^{2Q(x_1)}$ is generally greater than 1, and (ii) $2e^{2Q(x_1)}$ is forced by the approximation (of partial sum instead of Borel sum) to be real. For the latter reason the i in $(2e^{2Q(x_1)} + i)$ should be dropped when using partial sums, while the former reason assures us there is otherwise no numerical constraint. What is relevant here is that the first approximation (partial summation), which forces $2e^{2Q(x_1)}$ to be real, induces the second (to drop the i). Thus, Eq. (22) is the “correct” approximate form of the quantum condition when using partial summation. For a discussion of the numerical behavior of partial sums of asymptotic series near a Stokes line, the reader is referred to a paper by Olver¹⁰.

IV. BOREL-SUM APPROXIMANTS

To obtain accurate numerical results with a divergent expansion, it is necessary to use an appropriate numerical technique: in this case, “Borel-sum approximants”. To calculate “Borel-sum approximants”, we adapt the method of Álvarez, Martín-Mayor, and Ruiz-Lorenzo¹¹, viz., the Laplace transform of the partial-fraction resolution of a Padé approximant of the Borel transform. The detailed steps here are: (i) truncate the JWKB series at order $2N_T$ in \hbar ; (ii) divide each \hbar^{2M} -term by $(2M)!$ to form the truncated Borel transform (remember that the terms with odd powers of \hbar in the JWKB series vanish); (iii) form a Padé approximant, which we more or less arbitrarily choose to have numerator and denominator degrees both equal N_T if N_T is even, or respectively $N_T - 1$ and $N_T + 1$ if N_T is odd (since both numerator and denominator have to be polynomials in \hbar^2); (iv) resolve the Padé approximant into partial fractions, which is a sum over (what turns out in the present case to be simple) poles; (v) replace \hbar by $\hbar t$, multiply by e^{-t} , and integrate, making use of the incomplete gamma function or equivalently the exponential integral,

$$\int_0^\infty e^{-t} \frac{1}{t-r} dt = e^{-r} \Gamma(0, -r), \quad \arg r \neq 0 \quad (23)$$

$$= e^{-r} [-\text{Ei}(r) \pm \pi i], \quad 0 < \pm \arg r < \pi. \quad (24)$$

In this way the JWKB series for $S(0)$ and $Q(x_1)$, truncated at order \hbar^{2N_T} , have “Borel-sum approximants” that are a sum of N_T or $N_T + 1$ incomplete gamma functions plus a constant.

Equation (24) explicitly displays the discontinuity of the incomplete gamma function when r falls on the positive real axis, which is implicit in Eq. (23). The “Borel-sum approximants” for $S(0)$ should be real. The “Borel-sum approximants” for $Q(x_1)$ should be complex; in fact,

$$\lim_{N_T \rightarrow \infty} \text{Im } 2e^{\text{Borel-sum approximant } (N_T) \text{ of } 2Q(x_1)} = -i. \quad (25)$$

Thus, some of the roots r in step (iv) for $Q(x_1)$ should fall on the positive t axis, with imaginary part = -0 , corresponding to the lower sign in Eq. (24).

V. NUMERICAL RESULTS

This procedure to calculate “Borel-sum approximants” for both $S(0)$ and $Q(x_1)$ can be implemented¹¹ via ref.¹² which has built-in functions (or packages) for Padé approximant, $\Gamma(n, x)$, and $\text{Ei}(x)$. With both $S(0)$ and $Q(x_1)$ calculated, Mathematica’s FindRoot command can then solve for the roots of Eq. (20).

A. Semi-Infinite Interval

The results of this procedure are displayed in Table I for the first three energy eigenvalues with $k = 300$ and $x_1 = \infty$. This case has $\delta = 0$ (in Eq. (17)) and is an excellent example of a “noncontroversial” use of the connection formula: the JWKB wave function in the classically forbidden Region II is strictly exponentially decreasing.

One should note that to the extent the limit in Eq. (25) is not reached, the calculated energy eigenvalues will have artifactual imaginary parts; they are generally the same order of magnitude or less than the error in the real parts of the calculated energies. Since the limits of the imaginary parts are 0, we drop them at the end. For the partial-sum based calculations in Table I (and later in Table III), we use the approximate quantum condition Eq. (22), as discussed in Section IIIA. The approximate solutions of this equation yield real approximate energy eigenvalues.

One sees in Table I that (i) in all three cases the energies calculated via “Borel-sum approximants” steadily increase in accuracy as N_T increases and numerically converge towards the exact eigenvalues. However, the maximum accuracy of the partial-sum determination of the first three eigenvalues is limited to 2×10^{-2} , 2×10^{-5} , and 3×10^{-8} , respectively, by the asymptotic nature of the JWKB series. For this $x_1 = \infty$ case there is no con-

TABLE I

The errors in the first three energy eigenvalues for $x_1 = \infty$ and $k = 300$, when the eigenvalues are obtained by solving the implicit equation $S(0) = (n - 1/4)\pi$, ($n = 1, 2, 3$), where $S(0)$ is first calculated as a partial sum (Eq. (4)) to order $2N_T$ in h , and where $S(0)$ is second calculated as a "Borel-sum approximant" from the same terms

N_T	$E_1 = 104.78005647$ $E_1(N_T) - E_1$		$E_2 = 183.1975604261425$ $E_2(N_T) - E_2$		$E_3 = 247.3986301728020777$ $E_3(N_T) - E_3$	
	partial sum	Borel sum	partial sum	Borel sum	partial sum	Borel sum
0	-80×10^{-2}		-27513×10^{-5}		-15218650×10^{-8}	
1	5×10^{-2}	139739×10^{-8}	430×10^{-5}	$5990007973 \times 10^{-13}$	100702×10^{-8}	$1659066201261 \times 10^{-16}$
2	-2×10^{-2}	-889337×10^{-8}	-40×10^{-5}	$-2119000074 \times 10^{-13}$	-3990×10^{-8}	$-225421385392 \times 10^{-16}$
3	2×10^{-2}	-383925×10^{-8}	9×10^{-5}	$-436742994 \times 10^{-13}$	382×10^{-8}	$-25622869945 \times 10^{-16}$
4	-4×10^{-2}	-45057×10^{-8}	-3×10^{-5}	$-16017376 \times 10^{-13}$	-67×10^{-8}	$-439083533 \times 10^{-16}$
5	10×10^{-2}	91076×10^{-8}	2×10^{-5}	7247534×10^{-13}	18×10^{-8}	89174345×10^{-16}
6	-50×10^{-2}	-4141×10^{-8}	-2×10^{-5}	-327440×10^{-13}	-7×10^{-8}	-2899755×10^{-16}
7		4487×10^{-8}	3×10^{-5}	117604×10^{-13}	4×10^{-8}	563336×10^{-16}
8		-534×10^{-8}	-4×10^{-5}	-11874×10^{-13}	-3×10^{-8}	-39823×10^{-16}
9		464×10^{-8}	9×10^{-5}	4340×10^{-13}	3×10^{-8}	8598×10^{-16}
10		-84×10^{-8}	-26×10^{-5}	-616×10^{-13}	-3×10^{-8}	-878×10^{-16}
11		69×10^{-8}	84×10^{-5}	239×10^{-13}	4×10^{-8}	214×10^{-16}
12		-16×10^{-8}	-334×10^{-5}	-42×10^{-13}	-7×10^{-8}	-28×10^{-16}
13		12×10^{-8}		17×10^{-13}	14×10^{-8}	7×10^{-16}
14		-3×10^{-8}		-4×10^{-13}	-32×10^{-8}	-1×10^{-16}

attention about the connection formula: what is demonstrated is that the “Borel-sum approximants” of the truncated JWKB series yield numerically convergent eigenvalues many orders of magnitude more accurate than by partial summation.

B. Finite Interval

The case $x_1 = 1$ has $\delta \neq 0$ and is an example where the directionality might be questioned: to satisfy the boundary condition in the classically forbidden region at $x_1 = 1$, the JWKB wave function is necessarily a linear combination of the exponentially decreasing and increasing components.

There are two relevant JWKB series, $S(0)$ and $Q(1)$, with independent rates of asymptotic divergence that depend on the numerical values of $\zeta_I(0, k, E)$ and $\zeta_{II}(1, k, E)$ (Eqs (12) and (13)). To visualize the behavior of the series, Fig. 2 presents a semilogarithmic picture of the magnitudes of the terms

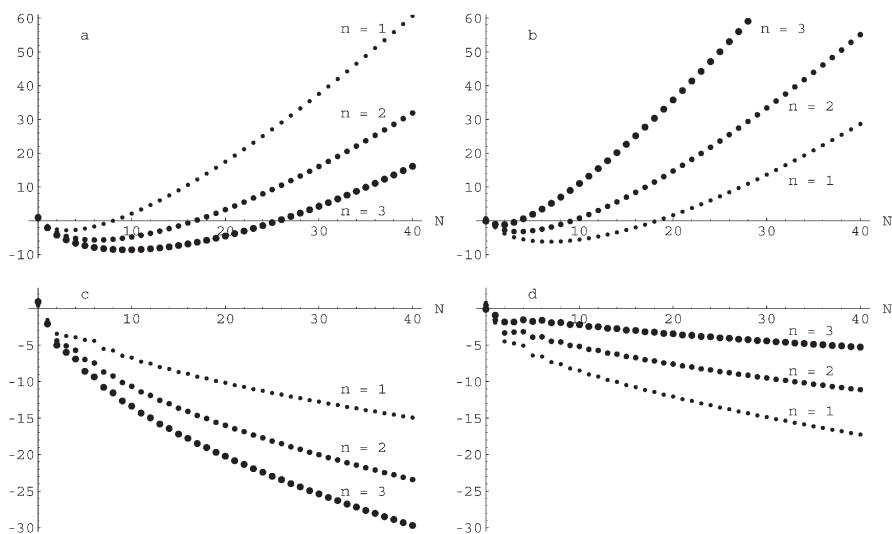


FIG. 2

Study of the divergence of the JWKB expansions for a S and b Q , and the convergence of their “Borel-sum approximants”, c and d. The plots are: a $\log_{10}|S^{(N)}(0)|$; b $\log_{10}|Q^{(N)}(1)|$; c $\log_{10}|(\text{Borel-}\Sigma_{j=0}^N - \text{Borel-}\Sigma_{j=0}^{N-1})S^{(j)}(0)|$; d $\log_{10}|(\text{Borel-}\Sigma_{j=0}^N - \text{Borel-}\Sigma_{j=0}^{N-1})Q^{(j)}(1)|$. The smallest dots are for the first solution, $n = 1$, the medium for $n = 2$, and the largest for $n = 3$. The more negative the logarithm, the smaller the term, the better the convergence. Plots a and b are typical for asymptotic series: the terms first get smaller, then increase without limit. Plots c and d are typical for a geometrically convergent series: the terms get continually smaller, with an approximately linear semilogarithmic plot

both for the JWKB series $\Sigma S^{(N)}(0)$ and $\Sigma Q^{(N)}(1)$, and for the equivalent series obtained by subtracting successive “Borel-sum approximants”. The smaller the magnitudes (i.e., the more negative the logarithms) the more useful the series. The characteristic asymptotic-series behavior shows the terms first decreasing, then increasing without limit (a and b). The characteristic convergent-series behavior is relentless decrease (c and d).

As n increases from 1 to 3, E_n increases, as does ζ_I (Eq. (12)). The smallest $S^{(N)}(0)$ decreases and occurs at higher N (Fig. 2a), and $S(0)$ is easier to calculate (Fig. 2c) – as n increases. At the same time, ζ_{II} (Eq. (13)) decreases, the smallest $Q^{(N)}(1)$ increases and occurs at lower N (Fig. 2b), and $Q(1)$ is harder to calculate (Fig. 2d) – as n increases. With the value $k = 300$, three eigenvalues fall below the maximum of the potential (300), which occurs at $x = x_1 = 1$. For $n = 3$, $\zeta_{II} \approx 0.81$, which is far from asymptotic (∞): the smallest term occurs at $N_T = 2$ with value ca. 0.067 (Fig. 2b); the convergence of the “Borel-sum approximants” to $Q(1)$ is slowest for $n = 3$ (Fig. 2d).

Table II gives the results of energies calculated via “Borel-sum approximants” of $S(0)$ and $Q(1)$, with some indication of which quantity requires the largest number of terms to get the indicated accuracy.

Tables I and II illustrate that the eigenvalues can be obtained to as high an accuracy as computers permit. No limitation on directionality is apparent or appropriate: the formula is bidirectional.

VI. COMMENT ON PARTIAL SUMMATION AND LACK OF DIRECTIONALITY

Eigenvalues calculated by partial summation of the series for $S(0)$ are reported in Table I for the semi-infinite-interval case, and in Table III for both $S(0)$ and $Q(1)$ for the finite-interval case. In the finite-interval case, the approximate, traditional “quantum condition” Eq. (22) can be derived from the traditional connection formula without restriction of directionality. Examination of the results for E_2 and E_3 in Table III, in which representative values for the truncation levels N_S and N_Q are given, show that their minimum truncation errors (2×10^{-5} and 3×10^{-2} , respectively) are 2 to 3 orders of magnitude smaller than the energy shift induced by moving the boundary from ∞ to 1 (0.03845 and 1.61, respectively). The changed boundary condition clearly transmitted the “right” information through the turning point from right to left in the “wrong” direction. That is, the traditional approximate connection formula here is bidirectional.

The case of the lowest eigenvalue E_1 is the most interesting of the three: one sees instantly in Table I that E_1 cannot be calculated via partial summation more accurately than 2×10^{-2} . The difference between E_1 for $x_1 = 1$ and

TABLE II

Numerical convergence of "Borel-sum approximant" method when $x_1 = 1$ and $k = 300$: the errors in the first three energy eigenvalues, with the eigenvalues obtained by solving the equation $S(0) - \arctan [(2e^{2Q(x_1)} + i)^{-1}] = (n - 1/4)\pi$, ($n = 1, 2, 3$), where $S(0)$ is calculated as a "Borel-sum approximant" from terms to order $2N_S$ in \hbar (from Eq. (4)), and where $Q(1)$ is calculated as a "Borel-sum approximant" from terms to order $2N_Q$ in \hbar (from Eq. (5))

$E_1 = 104.78013348$			$E_2 = 183.2360101517839$			$E_3 = 249.01233$		
N_S	N_Q	$E_1(N_S, N_Q) - E_1$	N_S	N_Q	$E_2(N_S, N_Q) - E_2$	N_S	N_Q	$E_3(N_S, N_Q) - E_3$
1	2	139741×10^{-8}	14	25	799×10^{-13}	6	15	95×10^{-5}
2	2	-889339×10^{-8}	14	26	-457×10^{-13}	6	16	-13×10^{-5}
3	2	-383926×10^{-8}	14	27	293×10^{-13}	6	17	113×10^{-5}
4	2	-45056×10^{-8}	14	28	-135×10^{-13}	6	18	-44×10^{-5}
5	2	91076×10^{-8}	14	29	11×10^{-13}	6	19	81×10^{-5}
6	2	-4141×10^{-8}	14	30	10×10^{-13}	6	20	-40×10^{-5}
7	2	4487×10^{-8}	14	31	-53×10^{-13}	6	21	44×10^{-5}
8	2	-534×10^{-8}	14	32	31×10^{-13}	6	22	-25×10^{-5}
9	2	464×10^{-8}	14	33	-37×10^{-13}	6	23	18×10^{-5}
10	2	-84×10^{-8}	14	34	15×10^{-13}	6	24	-12×10^{-5}
11	2	69×10^{-8}	14	35	-14×10^{-13}	6	25	3×10^{-5}
12	2	-15×10^{-8}	14	36	1×10^{-13}	6	26	-4×10^{-5}
13	2	13×10^{-8}	14	37	-3×10^{-13}	6	27	-4×10^{-5}
14	2	-3×10^{-8}				6	28	1×10^{-5}
						6	29	-6×10^{-5}
						6	30	3×10^{-5}
						6	31	-5×10^{-5}
						6	32	3×10^{-5}
						6	33	-4×10^{-5}
						6	34	2×10^{-5}
						6	35	-2×10^{-5}
						6	36	1×10^{-5}

E_1 for $x_1 = \infty$ is 7.7×10^{-5} , more than two orders of magnitude smaller. One might think that to calculate the difference by JWKB partial summation would be hopeless. Quite the contrary is true. If one uses the same truncation level N_S for both cases, the energy difference is accurate to 1 in the fourth significant digit, as seen in Table III.

The traditional connection formula for this problem has no directional limitations, but partial summation does have accuracy limitations.

TABLE III

Asymptotic divergence of partial-sum method when $x_1 = 1$ and $k = 300$: the error in the shift of the first energy eigenvalue, and the errors in the second and third energy eigenvalues; the eigenvalues are obtained by solving the equation $S(0) - \arctan(e^{-2Q(x_1)}/2) = (n - 1/4)\pi$, ($n = 1, 2, 3$), where $S(0)$ is calculated as a partial sum to order $2N_S$ in \hbar (Eq. (4)), and where $Q(1)$ is calculated as a partial sum to order $2N_Q$ in \hbar (Eq. (5)). Although the first eigenvalue can only be calculated to an accuracy of 2×10^{-2} , the difference between the eigenvalue for $x_1 = 1$ and $x_1 = \infty$ can be calculated to better than 1×10^{-8} accuracy, with obvious implications about the bidirectionality of the non-Borel-sum based connection formula

$\Delta E_1 = E_1 _{x_1=1} - E_1 _{x_1=\infty} = 0.000077012$			$E_2 = 183.2360101517839$			$E_3 = 249.01233$		
N_S	N_Q	$\Delta E_1(N_S, N_Q) - \Delta E_1$	N_S	N_Q	$E_2(N_S, N_Q) - E_2$	N_S	N_Q	$E_3(N_S, N_Q) - E_3$
1	6	219×10^{-9}	0	3	-27578×10^{-5}	3	0	29×10^{-2}
2	6	-47×10^{-9}	1	3	430×10^{-5}	3	1	-3×10^{-2}
3	6	7×10^{-9}	2	3	-40×10^{-5}	3	2	-24×10^{-2}
4	6	59×10^{-9}	3	3	8×10^{-5}	3	3	-85×10^{-2}
5	6	-366×10^{-9}	4	3	-4×10^{-5}	3	4	-161×10^{-2}
6	6	3208×10^{-9}	5	3	2×10^{-5}			
			6	3	-3×10^{-5}			
			7	3	2×10^{-5}			
			8	3	-5×10^{-5}			
			9	3	9×10^{-5}			
			10	3	-26×10^{-5}			
			11	3	83×10^{-5}			
			12	3	-333×10^{-5}			

TABLE IV
Errors in direct "Borel-sum approximants" for the energy eigenvalues as a single power series in $[(n - 1/4)\pi + \delta_n]^{-1}$, Eq. (26)

N_S	$E_1(N_S) - E_1$		$E_2(N_S) - E_2$		$E_3(N_S) - E_3$	
	$x_1 = \infty$	$x_1 = 1$	$x_1 = \infty$	$x_1 = 1$	$x_1 = \infty$	$x_1 = 1$
7	2357×10^{-8}	2357×10^{-8}	80667×10^{-13}	80389×10^{-13}	412300×10^{-16}	365149×10^{-16}
8	-581×10^{-8}	-581×10^{-8}	-12385×10^{-13}	-12340×10^{-13}	-41247×10^{-16}	-36139×10^{-16}
9	334×10^{-8}	334×10^{-8}	3511×10^{-13}	3497×10^{-13}	7227×10^{-16}	6259×10^{-16}
10	-92×10^{-8}	-92×10^{-8}	-642×10^{-13}	-639×10^{-13}	-909×10^{-16}	-780×10^{-16}
11	57×10^{-8}	57×10^{-8}	208×10^{-13}	207×10^{-13}	191×10^{-16}	162×10^{-16}
12	-17×10^{-8}	-17×10^{-8}	-44×10^{-13}	-43×10^{-13}	-29×10^{-16}	-24×10^{-16}
13	11×10^{-8}	11×10^{-8}	16×10^{-13}	16×10^{-13}	7×10^{-16}	6×10^{-16}
14	-4×10^{-8}	-4×10^{-8}	-4×10^{-13}	-4×10^{-13}	-1×10^{-16}	-1×10^{-16}

for $x_1 = \infty$	$\delta_1 = 0$	$\delta_2 = 0$	$\delta_3 = 0$
	$E_1 = 104.78005647$	$E_2 = 183.1975604261425$	$E_3 = 247.3986301728020777$
for $x_1 = 1$	$\delta_1 = 0.0000265456$	$\delta_2 = 0.00173861329621003531$	$\delta_3 = 0.084819831196108922086$
	$E_1 = 104.78013348$	$E_2 = 183.2360101517839$	$E_3 = 249.0123255633977249$

VII. MATHEMATICAL ANALYSIS via THE JWKB EXPANSION

As a bonus, it is interesting and instructive to note that, because of the structure of the $S^{(N)}$ (Eq. (11)), the quantum condition (20) can be solved for E , or more cleanly $\frac{2}{3k} E^{3/2}$, explicitly as a series in $(n - \frac{1}{4})\pi + \delta$, by using Mathematica's InverseSeries command:

$$\frac{2}{3k} E_n^{3/2} = (n - \frac{1}{4})\pi + \delta + \frac{5}{72 [(n - \frac{1}{4})\pi + \delta]} - \frac{1255}{31104 [(n - \frac{1}{4})\pi + \delta]^3} + \dots \quad (26)$$

In the semi-infinite-interval case, $\delta = 0$, and Eq. (26) is an explicit asymptotic expansion for (the two-thirds power of) E_n as a function of n . (It is essentially an asymptotic expansion for the zeros of $\text{Ai}(-z)$ (with $z = k^{-2/3}E$) in powers of $[(n - \frac{1}{4})\pi]^{-1}$.) In both cases, the only information about (i) which eigenvalue, and (ii) the boundary condition at x_1 , comes in through the values of n and δ . If Eq. (26) is evaluated by Borel summation, for any truncation level N_S , the N_S -“Borel-sum approximant” is an explicit function of $(n - \frac{1}{4})\pi + \delta$. Plugging in appropriate values of n and δ leads to explicit values for E_1 , E_2 , and E_3 for the two cases, as exhibited in Table IV.

VIII. CONCLUSION

The convergence of the “Borel-sum approximants” to the exact eigenvalues, as presented in Tables I, II, and IV, could not happen for both of these two companion cases – one in which the wave function decreases exponentially in the barrier region, the other in which the wave function is a linear combination of decreasing and increasing components – if the connection formulas⁴ were incorrect or if they were one-directional. Additionally, partial summation of the divergent series here yields results of accuracy limited not by the connection formula, but only by the asymptotics (in the normal way), as presented in Tables I and III. This implies that the traditional connection formula is also not one-directional here. One sees that the nature of Borel summation is to turn a divergent series into a convergent sequence. The significance of Borel summation is that (i) each series, on either side of the turning point, is in one-to-one correspondence with the same analytic function, and (ii) the values of the analytic function on either side of the turning point determine the values on the other, by analytic continuation. Along any path, analytic continuation is bidirectional.

Finally, we point out as another application of chemical interest, that using the Borel summability of the JWKB wavefunctions and the connection

formulas without directional restriction, Aoki, Kawai and Takei¹³ have recently solved the calculation of non-adiabatic transition probabilities in a Landau-Zener problem with three levels.

REFERENCES AND NOTES

1. Benderskii V. A., Goldanskii V. I., Makarov D. E.: *Phys. Rep.* **1993**, *233*, 195.
2. Dingle R. B.: *Asymptotic Expansions: Their Derivation and Interpretation*, p. 295. Academic Press, New York 1973.
3. Fröman N., Fröman P. O.: *J. Math. Phys.* **1998**, *39*, 4417.
4. Silverstone H. J.: *Phys. Rev. Lett.* **1985**, *55*, 2523.
5. Shen H., Silverstone H. J.: *Int. J. Quantum Chem.* **2004**, *99*, 336.
6. Messiah A.: *Quantum Mechanics*. North-Holland Publ. Co., Amsterdam 1961–62.
7. Silverstone H. J. in: *Modern Electronic Structure Theory* (D. R. Yarkony, Ed.), Chap. 10, Eqs (195)–(207). World Scientific Publishing Co., Singapore 1995.
8. Ref.⁷, Eqs (209) and (211), which pertain explicitly to the case that the classically forbidden region is to the right.
9. Abramowitz M., Stegun I. A. (Eds): *Handbook of Mathematical Functions*, Eqs (10.4.94) and (10.4.105). Dover, New York 1965.
10. Olver F. W. J.: *SIAM Rev.* **1980**, *22*, 188.
11. Álvarez G., Martín-Mayor V., Ruiz-Lorenzo J. J.: *J. Phys. A: Math. Gen.* **2000**, *33*, 841.
12. Wolfram S.: *The Mathematica Book*. Cambridge University Press and Wolfram Media, Champaign 1999.
13. Aoki T., Kawai T., Takei Y.: *J. Phys. A: Math. Gen.* **2002**, *35*, 2401.