Observations on the JWKB treatment of the quadratic barrier

Hujun Shen[1] and Harris J. Silverstone[2]

[1] Department of Chemistry, The Johns Hopkins University, 3400 N. Charles St., Baltimore, MD 21218, USA
[2] Department of Chemistry, The Johns Hopkins University, 3400 N. Charles St., Baltimore, MD 21218, USA
hjsilverstone@jhu.edu

Summary. Historically, the "lowest-order" JWKB "parabolic" connection formula between the left and right classically allowed regions for tunneling through a parabolic barrier involved a rather non-JWKB-like square-root $\sqrt{1+\mathrm{e}^{-2\pi(-E)/\hbar}}$ and a non-JWKB phase factor that had been extracted from the asymptotic expansion of the parabolic cylinder function. Generalization to higher order was not obvious. We show how the usual JWKB connection formulas at the linear turning points, combined with matching in a common Stokes region when $\hbar$ is complex, lead to the historical formula and its generalization. The limit of real $\hbar$ is tricky, because Stokes lines coalesce, and the common Stokes region that joins the two turning points disappears. Certain Stokes lines are thus "doubled," but which ones depend on the sign of $\arg\hbar \to \pm 0$. The square root and phase arise from the Borel sum of the "normalization factors" $\mathrm{e}^{\pm\mathrm{i}\sum_{n=1}^{\infty} S_R^{(n)}(\infty)\hbar^{2n-1}}$, which as conjectured by Sato are summed by a gamma function. Real $\hbar$ is a Stokes line for these factors, causing the Borel sums of a single JWKB wave function even in the classically allowed region to be different for $\arg\hbar \to \pm 0$. A proof of Sato's conjecture is given in an Addendum.

Key words: JWKB; connection formula; Borel sum; asymptotic expansion; semiclassical; tunneling

1 Introduction

Miller and Good [1], Ford, Hill, Wakano, and Wheeler [2], Child [3], and Connor [4] established the lowest-order Jeffreys-Wentzel-Kramers-Brillouin (JWKB) connection formula for transmission from $x < -x_0$ to $x > x_0$ through a parabolic barrier $V = -\frac{1}{2}kx^2$, with energy $E < 0$:

$$\mathrm{i}\left(-p^{-1/2}\mathrm{e}^{\frac{\mathrm{i}\pi}{4}+\frac{\mathrm{i}}{\hbar}\int_x^{-x_0} p\,dx} + \mathrm{e}^{\mathrm{i}\phi}\sqrt{1+\mathrm{e}^{-2\pi(-E)/\hbar}}\; p^{-1/2}\mathrm{e}^{-\frac{\mathrm{i}\pi}{4}-\frac{\mathrm{i}}{\hbar}\int_x^{-x_0} p\,dx}\right) \longleftrightarrow \mathrm{e}^{-\frac{\pi(-E)}{\hbar}} p^{-1/2}\mathrm{e}^{\frac{\mathrm{i}\pi}{4}+\frac{\mathrm{i}}{\hbar}\int_{x_0}^{x} p\,dx}, \quad (1)$$

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where $\pm x_0 = \pm\sqrt{-2E}$ are the classical turning points, $p = +\sqrt{x^2 - (-2E)}$, $m = k = 1$, and ϕ is a phase obtained from the large-x asymptotic expansion of the parabolic cylinder function, and which, according to Child [3], "cannot be [determined] by purely phase integral methods."

In the mathematics literature, the two-turning-point problem has been dealt with in some detail by Fedoryuk [5] and in theoretical generality from the point of view of Borel summability by Voros [6], by Aoki, Kawai, and Takei [7],[9], by Kawai and Takei [8], and by Delabaere, Dillinger, and Pham [10],[11]. Complexification with respect to $\hbar$ disentangles coalesced Stokes lines, and the JWKB wave functions are proven to be Borel summable, and therefore exact.

This paper aims to make the mathematical developments more accessible to practitioners via a concrete example, the complete JWKB expansion for the quadratic barrier potential. The JWKB wave function can be found term-by-term in simple closed form to high order; the exact solution is the known parabolic cylinder function. From the application point of view, Eq. (1) raises two immediate questions: (i) Where does the square root in $\sqrt{1 + \mathrm{e}^{-2\pi(-E)/\hbar}}$ come from in the JWKB context? (ii) Is ϕ implicit in the JWKB expansion? More puzzling in the context of physical applications is (iii) the conceptual dilemma inside the barrier ($-x_0 < x < +x_0$): if the JWKB wave function that is exponentially decreasing from $-x_0$ smoothly joins the exponentially increasing wave function from $+x_0$, what happens to the Stokes line of the increasing function that is irrelevant to the decreasing function? Our aim is to look in detail at an example simple enough to be solvable but rich enough to illustrate some of the subtle twists and turns of the exact JWKB method.

The answers, most of which can be found in the paper of Kawai and Takei [8], come from complexification with respect to $\hbar$, Borel summation, the Stokes lines of Stirling's formula for the gamma function, and the disappearance of a domain and coalescence of Stokes lines in the limit of real $\hbar$. The gamma-function Stokes lines are crucial to evaluating the series that converts between "normalization at a turning point" and "normalization at infinity."

In addition, we give in an Addendum an elementary proof of Sato's conjecture about the normalization constant.

2 JWKB wave function for the quadratic barrier

The JWKB solution of the Schrödinger equation for a particle scattered by an inverted parabolic potential (Fig. 1)

$$\left(-\frac{\hbar^2}{2}\frac{d^2}{dx^2} - \frac{1}{2}x^2 - E\right)\psi(x) = 0 \tag{2}$$

has the form

$$\psi_{\mathrm{JWKB}\pm} \sim \dot{S}^{-1/2}\mathrm{e}^{\pm\mathrm{i}(S/\hbar+\pi/4)}\ , \tag{3}$$

$$S(x,\hbar) = \sum_{n=0}^{\infty} S^{(n)}(x)\hbar^{2n}, \qquad \dot{S} \equiv dS/dx\ . \tag{4}$$

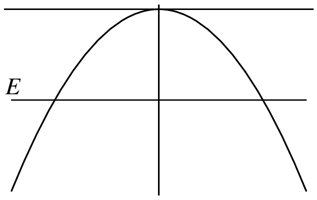

Fig. 1. Inverted-parabola potential

We explicitly take $E < 0$, but there is no difficulty to treat $E > 0$. For notational clarity, the dependence of $S^{(n)}(x)$ on E is suppressed.

The derivatives $\dot{S}^{(n)}(x)$ can be found recursively:

$$\dot{S}^{(0)}(x) = \pm\sqrt{x^2 - (-2E)}\ , \tag{5}$$

$$\dot{S}^{(n)}(x) = \frac{1}{2\dot{S}^{(0)}}\left[\left(\frac{3}{4}\frac{\ddot{S}^2}{\dot{S}^2} - \frac{1}{2}\frac{\dddot{S}}{\dot{S}}\right)^{\text{“}(n-1)\text{”}} - \sum_{k=1}^{n-1}\dot{S}^{(k)}\dot{S}^{(n-k)}\right]\ , \tag{6}$$

$$= \pm(-1)^{n-1}16^{-n}[x^2 - (-2E)]^{-2n+1/2}P_n\left(\frac{1}{x^2/(-2E) - 1}\right)\ . \tag{7}$$

Equation (7) corresponds to the first equation of Lemma A.4 of [8]. The superscript "(n)", as in $\dot{S}^{(n)}$, denotes the coefficient of $\hbar^{2n}$ in the expansion of $\dot{S}$ in powers of $\hbar^2$. As calculated with *Mathematica* [12] to order $n = 50$, the polynomials $P_n(y)$ have positive, integer coefficients. The first three are

$$P_1(y) = 6 + 10y\ , \tag{8}$$

$$P_2(y) = 594 + 2652y + 2210y^2\ , \tag{9}$$

$$P_3(y) = 200556 + 1545948y + 2981700y^2 + 1656500y^3\ . \tag{10}$$

When integrating $\dot{S}^{(n)}(x)$ to get $S^{(n)}(x)$, we choose the "integration constant" to preserve the square-root branch point at the classical turning point, and we choose the sign of the square root that makes $S^{(0)}(x)$ positive where x is classically allowed. Thus $S^{(n)}(x)$ is tied to a particular turning point. For the classically allowed region to the right of the right-hand turning point (labeled by the subscript "R") one finds

$$S_R^{(0)}(x) = +\frac{1}{2}x\sqrt{x^2 - (-2E)} + \frac{-E}{2}\log\left(\frac{x - \sqrt{x^2 - (-2E)}}{x + \sqrt{x^2 - (-2E)}}\right)\ , \tag{11}$$

$$S_R^{(n)}(x) = +x\frac{16^{-n}(-2E)^{-2n+1}}{\sqrt{x^2 - 2(-E)}}T_{3n-2}\left(\frac{1}{x^2/(-2E) - 1}\right)\ , \tag{12}$$

where $T_{3n-2}(y)$ is a polynomial of degree $3n - 2$. The first three are

$$T_1(y) = \frac{2}{3} - \frac{10}{3}y\ , \tag{13}$$

$$T_4(y) = \frac{112}{45} - \frac{56}{45}y + \frac{14}{15}y^2 + \frac{884}{9}y^3 + \frac{2210}{9}y^4 , \quad (14)$$

$$T_7(y) = \frac{15872}{315} - \frac{7936y}{315} + \frac{1984y^2}{105} - \frac{992y^3}{63} + \frac{124y^4}{9} - 20068y^5 - \frac{331300y^6}{3} - \frac{331300y^7}{3} . \quad (15)$$

One can straightforwardly obtain $S_R^{(n)}(x)$ to high order n.

We note that what is called Darwin's expansion [13],[14] for the parabolic cylinder function is essentially the JWKB expansion.

3 Stokes regions; doubled-Stokes lines

At Stokes curves the Borel sum of the dominant JWKB wave function changes discontinuously. If $\arg \hbar = \pm\epsilon \neq 0$, the Stokes curves – on which $\mathrm{i}S^{(0)}(x)$ is real – divide the x plane into five regions; one is shared by both turning points [6],[8],[10],[11]. We number the local regions around the two turning points sequentially. The shared region flips with the sign of $\arg \hbar$, as illustrated in Fig. 2, and disappears when $\hbar$ is real; the region that disappears depends on the sign of $\arg \hbar$. Figure 2 is the "inner part" of Figs. 2.1 and 2.2 of [8], which deals with the more complicated four-turning-point double-well oscillator. One

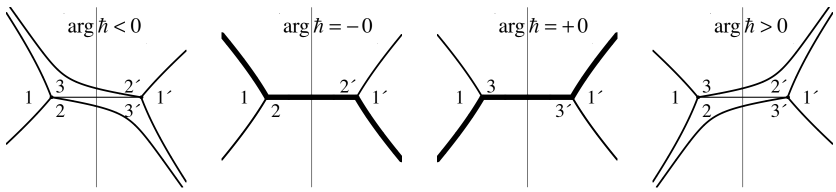

Fig. 2. Stokes lines when $\arg \hbar < 0$, $\arg \hbar = \mp 0$, and $\arg \hbar > 0$, and the specification of Regions 1–3, 1′–3′. The thick, coalesced Stokes lines in the $\arg \hbar = \mp 0$ graphs behave as *doubled-Stokes* lines.

glance is enough to see that the JWKB descriptions of the wave function should be formally different for $|\pm \arg \hbar| > 0$, mirror images, distinct even in the limit of real $\hbar$ [10],[11].

- The overall left-right, 1–1′ connection formula will depend on the sign of $\arg \hbar$, because different Stokes lines are crossed.
- The Borel sum of a JWKB wave function in Region 1′, may depend discontinuously on the sign of $\arg \hbar$, because Region 1′ lies on different sides of the Stokes line emanating from the left turning point towards the right.
- In the limit that $\hbar$ is real, for each turning point the long-range influence of the other turning point squeezes out one of its local Stokes sectors. As

a consequence, moving from the classically allowed sector in the direction of the collapsed sector requires crossing two Stokes lines. We regard the coalesced, thick Stokes lines in the $\arg\hbar = \mp 0$ portions of Fig. 2 as *doubled-Stokes* lines.

- The puzzle of how an exponentially decreasing, Stokes-line-continuous solution can smoothly join an exponentially increasing, Stokes-line-discontinuous solution from the other turning point is explained by Fig. 2: the match is made on only one side of the increasing solution's Stokes line; the limit of real $\hbar$ obliterates the common region from the decreasing solution and forces it to cross an additional (nonlocal) Stokes line.

4 JWKB connection formulas when $\arg\hbar \neq 0$

To discuss the connection formulas some details are unavoidable: notation for the JWKB wave functions in each region; the basic connection formulas among the regions; the implications of different normalizations; and the differences among the connection formulas that depend on normalization and on the sign of $\arg\hbar$. This section gives these details.

4.1 Notational elaboration

We extend our notation so that the JWKB wave functions are transparently imaginary- or real-exponential of a function positive on the physical axes as in (1), and also in the choice of sign for the square root in (11). To keep the connection formula local, each of the exponentiated functions has a square-root branch point at its associated turning point (a choice of integration constant). Accordingly, we define in addition to S_R, the related Q_R, S_L, and Q_L, which have square-root branch points at either the right or left turning points as labeled, and which in zeroth order are positive in the adjacent classically allowed regions (S) or adjacent classically forbidden regions (Q).

The localized versions of the so-called action functions are defined by

$$\dot{S}_L^{(0)}(x) = -\sqrt{x^2 - (-2E)} = -\dot{S}_R^{(0)}(x) \ , \tag{16}$$

$$S_L^{(0)}(x) = -S_R^{(0)}(x) \ , \tag{17}$$

$$\dot{Q}_L^{(0)}(x) = +\sqrt{(-2E) - x^2} = -\dot{Q}_R^{(0)}(x) \ , \tag{18}$$

$$Q_L^{(0)}(x) = \frac{1}{2} x\sqrt{(-2E) - x^2} - (-E)\arccos\frac{x}{\sqrt{-2E}} + (-E)\pi \ , \tag{19}$$

$$Q_R^{(0)}(x) = (-E)\pi - Q_L^{(0)}(x) \ , \tag{20}$$

$$S_L^{(n)}(x) = -S_R^{(n)}(x) = S_R^{(n)}(-x), \qquad (n \geq 0) \ , \tag{21}$$

$$Q_L^{(n)}(x) = -x\frac{16^{-n}(-2E)^{-2n+1}}{\sqrt{(-2E) - x^2}} T_{3n-2}\left(\frac{1}{x^2/(-2E) - 1}\right) \ , \tag{22}$$

$$Q_R^{(n)}(x) = -Q_L^{(n)}(x) = Q_L^{(n)}(-x), \qquad (n \geq 1) \ . \tag{23}$$

The formal JWKB pairs of wave functions are then

$$\psi_{L,\pm S}(x,\hbar) = (-\dot{S}_L)^{-1/2} \mathrm{e}^{\pm \mathrm{i}(S_L/\hbar + \pi/4)} \ , \tag{24}$$

$$\psi_{L,\pm Q}(x,\hbar) = \dot{Q}_L^{-1/2} \mathrm{e}^{\pm Q_L/\hbar} \ , \tag{25}$$

$$\psi_{R,\pm Q}(x,\hbar) = (-\dot{Q}_R)^{-1/2} \mathrm{e}^{\pm Q_R/\hbar} \ , \tag{26}$$

$$\psi_{R,\pm S}(x,\hbar) = \dot{S}_R^{-1/2} \mathrm{e}^{\pm \mathrm{i}(S_R/\hbar + \pi/4)} \ , \tag{27}$$

Note that

$$\psi_{R,\pm Q}(x,\hbar) = \mathrm{e}^{\pm \frac{(-E)\pi}{\hbar}} \psi_{L,\mp Q}(x,\hbar) \ . \tag{28}$$

4.2 Connection formulas

The connection formulas are obtained by applying the standard JWKB connection formulas [6],[7],[8],[9],[15],[16],[17] at each linear turning point, $x = \pm\sqrt{-2E}$, and by using the identity (28) to match the left and right functions in their common domain: 2 and 2′ for $\arg\hbar > 0$; 3 and 3′ for $\arg\hbar < 0$. We fix a linear combination of the imaginary-exponential solutions on the right in Region 1′, and give the corresponding linear combinations in the other regions in Table 1. The formulas depend on whether $\arg\hbar > 0$ or $\arg\hbar < 0$. The common region in each case has been repeated to list the JWKB wave function in both the left-turning-point and right-turning-point notations.

Table 1. Connection formula when $\arg\hbar \neq 0$

Region	JWKB wave function
1′	$d_+\psi_{R,+S}(x,\hbar) + d_-\psi_{R,-S}(x,\hbar)$
2′	$(d_+ + d_-)\psi_{R,+Q}(x,\hbar) - \mathrm{i}d_-\psi_{R,-Q}(x,\hbar)$
3′	$(d_+ + d_-)\psi_{R,+Q}(x,\hbar) + \mathrm{i}d_+\psi_{R,-Q}(x,\hbar)$
	$\arg\hbar > 0$
2 (= 2′)	$(d_+ + d_-)\mathrm{e}^{\frac{(-E)\pi}{\hbar}}\psi_{L,-Q}(x,\hbar) - \mathrm{i}d_-\mathrm{e}^{-\frac{(-E)\pi}{\hbar}}\psi_{L,+Q}(x,\hbar)$
3	$[d_+ + d_-(1+\mathrm{e}^{-2\frac{(-E)\pi}{\hbar}})]\mathrm{e}^{\frac{(-E)\pi}{\hbar}}\psi_{L,-Q}(x,\hbar) - \mathrm{i}d_-\mathrm{e}^{-\frac{(-E)\pi}{\hbar}}\psi_{L,+Q}(x,\hbar)$
1	$-\mathrm{i}[d_+ + d_-(1+\mathrm{e}^{-2\frac{(-E)\pi}{\hbar}})]\mathrm{e}^{\frac{(-E)\pi}{\hbar}}\psi_{L,+S}(x,\hbar) + \mathrm{i}(d_+ + d_-)\mathrm{e}^{\frac{(-E)\pi}{\hbar}}\psi_{L,-S}(x,\hbar)$
	$\arg\hbar < 0$
3 (= 3′)	$(d_+ + d_-)\mathrm{e}^{\frac{(-E)\pi}{\hbar}}\psi_{L,-Q}(x,\hbar) + \mathrm{i}d_+\mathrm{e}^{-\frac{(-E)\pi}{\hbar}}\psi_{L,+Q}(x,\hbar)$
2	$[d_+(1+\mathrm{e}^{-2\frac{(-E)\pi}{\hbar}}) + d_-]\mathrm{e}^{\frac{(-E)\pi}{\hbar}}\psi_{L,-Q}(x,\hbar) + \mathrm{i}d_+\mathrm{e}^{-\frac{(-E)\pi}{\hbar}}\psi_{L,+Q}(x,\hbar)$
1	$-\mathrm{i}(d_+ + d_-)\mathrm{e}^{\frac{(-E)\pi}{\hbar}}\psi_{L,+S}(x,\hbar) + \mathrm{i}[d_+(1+\mathrm{e}^{-2\frac{(-E)\pi}{\hbar}}) + d_-]\mathrm{e}^{\frac{(-E)\pi}{\hbar}}\psi_{L,-S}(x,\hbar)$

For a quick comparison with (1), set $d_+ = 1, d_- = 0$ in the Region-1 and -1′ rows of Table 1. The exponential ratio $\mathrm{e}^{\frac{(-E)\pi}{\hbar}}$ of the left to right is present, but there is yet no square root. To find the square root, it is necessary to extract the implicit relative normalization factor.

4.3 "Relative normalization factor at ∞"

One can see from (7) that the large-x behavior of $S_R^{(n)}(x)$ is

$$S_R^{(n)}(x) = S_R^{(n)}(\infty) + O(|x|^{-4n+2}), \quad \text{as } |x| \to \infty, \text{ for } n \geq 1 \, . \tag{29}$$

The integration constants $S_R^{(n)}(\infty)$ are determined indirectly by the square-root-branch-point requirement. With the assistance of *Mathematica* [12] to solve (6), (7), (12), and (29), we find that the "squared normalization factor" $e^{+2i\sum_1^\infty S_R^{(n)}(\infty)\hbar^{2n-1}}$ is given "experimentally" through order 50 by

$$N(\hbar)^2 \equiv e^{+2i\sum_1^\infty S_R^{(n)}(\infty)\hbar^{2n-1}} \, , \tag{30}$$

$$= 1 + i\frac{\hbar(-E)^{-1}}{24} - \frac{\hbar^2(-E)^{-2}}{1152} + i\frac{1003\hbar^3(-E)^{-3}}{414720} + \cdots \, . \tag{31}$$

That (31) is the Stirling series associated with $\Gamma(\frac{1}{2} + \frac{i(-E)}{\hbar})$ is a conjecture attributed by Kawai and Takei [8] to Sato, with reference also to Voros [6]. (See also [14]. We give a short "theoretical" proof in the Addendum.) At first glance, $N(\hbar)$ would appear to have magnitude 1. However, $\arg\hbar = 0$ corresponds to a Stokes line [8],[18] of the gamma-function series [with respect to $\frac{1}{2} + i(-E/\hbar)$]. Kawai and Takei (Prop. 2.2 of [8]) further show that

$$N^2 \overset{(B)}{=} \hat{N}^2, (\arg\hbar > 0) \, , \tag{32}$$

$$\overset{(B)}{=} \hat{N}^2 \left(1 + e^{-\frac{\pi(-2E)}{\hbar}}\right), (\arg\hbar < 0) \, , \tag{33}$$

$$\hat{N}^2 \equiv \frac{1}{(2\pi)^{1/2}} \left(\frac{e\hbar}{-E}\right)^{\frac{i(-E)}{\hbar}} e^{\frac{\pi(-E)}{2\hbar}} \Gamma\left(\frac{1}{2} + \frac{i(-E)}{\hbar}\right) \, , \tag{34}$$

where by the symbol $\overset{(B)}{=}$ we mean "equality in the sense of Borel sum," and by $\hat{N}^2$, the right side of (34).

In the limits $\arg\hbar \to \pm 0$, the series for N^2 is evaluated at its Stokes line where it is both discontinuous and not of magnitude 1. The gamma-function reflection formula [13] implies that (for real E),

$$\left|\Gamma(\frac{1}{2} \pm \frac{i(-E)}{\hbar})\right| = e^{-\frac{\pi(-E)}{2\hbar}} \sqrt{\frac{2\pi}{1 + e^{-\frac{\pi(-2E)}{\hbar}}}}, \ (\arg\hbar = 0) \, , \tag{35}$$

from which the magnitudes of N^2, N^{-2}, and $\hat{N}^2$, for $\arg\hbar = \pm 0$, follow:

$$\left|N^2\right| = \left|e^{+2i\sum_{n=1}^\infty S_R^{(n)}(\infty)\hbar^{2n-1}}\right| \overset{(B)}{=} \left(1 + e^{-\frac{\pi(-2E)}{\hbar}}\right)^{\mp 1/2}, (\arg\hbar = \pm 0) \, , \tag{36}$$

$$\left|N^{-2}\right| = \left|e^{-2i\sum_{n=1}^\infty S_R^{(n)}(\infty)\hbar^{2n-1}}\right| \overset{(B)}{=} \left(1 + e^{-\frac{\pi(-2E)}{\hbar}}\right)^{\pm 1/2}, (\arg\hbar = \pm 0) \, , \tag{37}$$

$$\left|\hat{N}^2\right| = \left(1 + e^{-\frac{\pi(-2E)}{\hbar}}\right)^{-1/2}, (\arg\hbar = 0) \, . \tag{38}$$

The JWKB origins of the square-root factor in (1) are thus revealed in (36) – (38). We sharpen this in the next subsection.

4.4 Connection formulas for functions "well-normalized at ∞"

Instead of "square-root" normalization at the turning point, consider instead a normalization by which $S^{(n)}_{R,L}(\infty) = 0$. We attach a superscript $^{[\infty]}$ and define

$$S^{(n)[\infty]}_{L}(x) = S^{(n)}_{L}(x) - S^{(n)}_{L}(-\infty), (n \geq 1) \; , \tag{39}$$

$$S^{(n)[\infty]}_{R}(x) = S^{(n)}_{R}(x) - S^{(n)}_{R}(+\infty), (n \geq 1) \; , \tag{40}$$

$$\psi^{[\infty]}_{R,\pm S}(x,\hbar) = N^{\mp 1}\psi_{R,\pm S}(x,\hbar), \quad \psi^{[\infty]}_{L,\pm S}(x,\hbar) = N^{\mp 1}\psi_{L,\pm S}(x,\hbar) \; . \tag{41}$$

Since $S^{(n)}_{L}(-\infty) = S^{(n)}_{R}(+\infty)$, it is not necessary to distinguish left from right normalization factors N. This is the normalization used by Delabaere, Dillinger and Pham [10],[11] who call such JWKB wave functions "well-normalized at ∞." The connection formulas for the "∞-normalized" JWKB wave functions are given in Table 2. It is particularly significant that when the relative normalization factor N is replaced by its Borel-summed explicit evaluation in terms of $\hat{N}$, there is no $\arg\hbar = 0$ Stokes line in the 1–1′ connection formula. (See the discussion in Sect. 5.)

Table 2. 1-1′ connection formula for "∞-normalized" JWKB functions

Region	JWKB wave function
1′	$c_+ \mathrm{e}^{-\frac{(-E)\pi}{\hbar}} \psi^{[\infty]}_{R,+S}(x,\hbar) + c_- \mathrm{e}^{-\frac{(-E)\pi}{\hbar}} \psi^{[\infty]}_{R,-S}(x,\hbar)$
	$\arg\hbar > 0$
1	$-\mathrm{i}[c_+ + c_- N^2(1+\mathrm{e}^{-2\frac{(-E)\pi}{\hbar}})]\psi^{[\infty]}_{L,+S}(x,\hbar) + \mathrm{i}(N^{-2}c_+ + c_-)\psi^{[\infty]}_{L,-S}(x,\hbar)$
	$\arg\hbar < 0$
1	$-\mathrm{i}(c_+ + c_- N^2)\psi^{[\infty]}_{L,+S}(x,\hbar) + \mathrm{i}[c_- + c_+ N^{-2}(1+\mathrm{e}^{-2\frac{(-E)\pi}{\hbar}})]\psi^{[\infty]}_{L,-S}(x,\hbar)$
	independent of the sign of $\arg\hbar$
1	$-\mathrm{i}(c_+ + c_- \hat{N}^2)\psi^{[\infty]}_{L,+S}(x,\hbar) + \mathrm{i}(c_- + c_+ \hat{N}^{-2})\psi^{[\infty]}_{L,-S}(x,\hbar)$

4.5 Preliminary comment on the details: generalization of (1)

Formally the connection formulas that connect Region 1′ to 2, 3, and especially 1 are *different*, depending on the sign of $\arg\hbar$. In Table 2, the factor $(1+\mathrm{e}^{-2(-E)\pi/\hbar})$ shifts places; in Table 1 there are even more changes. The differences are a manifestation of the paired-picture view of Fig. 2 and will be discussed in detail in the next section. Here we note that the cleanest generalization of (1) is already contained in Table 2 when $c_+ = 1$ and $c_- = 0$:

$$\mathrm{i}\left(-\psi^{[\infty]}_{L,+S}(x,\hbar) + \hat{N}^{-2}\psi^{[\infty]}_{L,-S}(x,\hbar)\right) \longleftrightarrow \; \mathrm{e}^{-\frac{(-E)\pi}{\hbar}}\psi^{[\infty]}_{R,+S}(x,\hbar) \; . \tag{42}$$

The $\hat{N}^{-2}$ in (42) by virtue of (34) and (38) is exactly the $\mathrm{e}^{\mathrm{i}\phi}\sqrt{1+\mathrm{e}^{-2\pi(-E)/\hbar}}$ of (1) when $\hbar$ is real, but with its JWKB origins clear from (30)–(33). At the same time, the lowest-order JWKB functions in (1) generalize to the the complete "∞-normalized" JWKB functions.

5 Discussion of the connection formula differences and the analytic functions the JWKB functions represent

5.1 Borel sums of $\psi_{R,\pm S}(x,\hbar)$ and of $\psi^{[\infty]}_{R,\pm S}(x,\hbar)$

An advantage of the quadratic barrier is that the exact solutions are the known parabolic cylinder functions, to which the JWKB functions $\psi_{R,\pm S}(x,\hbar) = \dot{S}_R^{-1/2}\mathrm{e}^{\pm\mathrm{i}(S_R/\hbar+\pi/4)}$ are Borel summable (similarly for $\psi_{L,\pm S}$). The proportionality constants can be found by matching asymptotic expansions. Let

$$\eta = \mathrm{e}^{\frac{\mathrm{i}\pi}{8}}\left(\frac{-E}{\mathrm{e}\hbar}\right)^{\frac{\mathrm{i}(-E)}{2\hbar}}, \tag{43}$$

and let $D_\nu(z)$ denote Whittaker's principal parabolic cylinder function (Eq. 19.3.7 of [13]). The ∞-normalized functions have no real-$\hbar$ Stokes line:

$$\psi^{[\infty]}_{R,+S}(x,\hbar) \overset{(B)}{=} \eta\left(\frac{2}{\hbar}\right)^{\frac{1}{4}}\mathrm{e}^{\frac{\pi(-E)}{4\hbar}}D_{-\mathrm{i}(\frac{-E}{\hbar})-\frac{1}{2}}\left(\mathrm{e}^{-\frac{\pi\mathrm{i}}{4}}x\sqrt{\frac{2}{\hbar}}\right), \tag{44}$$

$$\psi^{[\infty]}_{R,-S}(x,\hbar) \overset{(B)}{=} \eta^{-1}\left(\frac{2}{\hbar}\right)^{\frac{1}{4}}\mathrm{e}^{\frac{\pi(-E)}{4\hbar}}D_{+\mathrm{i}(\frac{-E}{\hbar})-\frac{1}{2}}\left(\mathrm{e}^{+\frac{\pi\mathrm{i}}{4}}x\sqrt{\frac{2}{\hbar}}\right). \tag{45}$$

The turning-point-normalized functions do have a real-$\hbar$ Stokes line:

$$\psi_{R,+S}(x,\hbar)$$

$$\overset{(B)}{=} \hat{N}\eta\left(\frac{2}{\hbar}\right)^{\frac{1}{4}}\mathrm{e}^{\frac{\pi(-E)}{4\hbar}}D_{-\mathrm{i}(\frac{-E}{\hbar})-\frac{1}{2}}\left(\mathrm{e}^{-\frac{\pi\mathrm{i}}{4}}x\sqrt{\frac{2}{\hbar}}\right), (\arg\hbar>0), \tag{46}$$

$$\overset{(B)}{=} \hat{N}\eta\left(\frac{2}{\hbar}\right)^{\frac{1}{4}}\mathrm{e}^{\frac{\pi(-E)}{4\hbar}}D_{-\mathrm{i}(\frac{-E}{\hbar})-\frac{1}{2}}\left(\mathrm{e}^{-\frac{\pi\mathrm{i}}{4}}x\sqrt{\frac{2}{\hbar}}\right)\sqrt{1+\mathrm{e}^{-\frac{\pi(-2E)}{\hbar}}}, \quad (\arg\hbar<0), \tag{47}$$

$$\psi_{R,-S}(x,\hbar)$$

$$\overset{(B)}{=} (\hat{N}\eta)^{-1}\left(\frac{2}{\hbar}\right)^{\frac{1}{4}}\mathrm{e}^{\frac{\pi(-E)}{4\hbar}}D_{+\mathrm{i}(\frac{-E}{\hbar})-\frac{1}{2}}\left(\mathrm{e}^{+\frac{\pi\mathrm{i}}{4}}x\sqrt{\frac{2}{\hbar}}\right)\sqrt{1+\mathrm{e}^{-\frac{\pi(-2E)}{\hbar}}}, \quad (\arg\hbar>0), \tag{48}$$

$$\overset{(B)}{=} (\hat{N}\eta)^{-1}\left(\frac{2}{\hbar}\right)^{\frac{1}{4}}\mathrm{e}^{\frac{\pi(-E)}{4\hbar}}D_{+\mathrm{i}(\frac{-E}{\hbar})-\frac{1}{2}}\left(\mathrm{e}^{+\frac{\pi\mathrm{i}}{4}}x\sqrt{\frac{2}{\hbar}}\right), (\arg\hbar<0). \tag{49}$$

The value of $\hat{N}$ is the square root of (34).

5.2 Current densities

Take $\hbar$ to be real and compare (46) and (47):

$$\psi_{R,+S}(x,\hbar-\mathrm{i}0) \overset{(B)}{=} \sqrt{1+\mathrm{e}^{-\frac{\pi(-2E)}{\hbar}}}\,\psi_{R,+S}(x,\hbar+\mathrm{i}0)\ . \tag{50}$$

The implication is that the current density represented by the outgoing-wave JWKB wave function $\psi_{R,+S}$ when $\mathrm{Im}\hbar = -0$ is exactly $(1+\mathrm{e}^{-\frac{\pi(-2E)}{\hbar}})$ times the current density represented by the same formal JWKB wave function when $\mathrm{Im}\hbar = +0$. With (48) and (49), the further implication is that the incoming-wave current density represented by $\psi_{R,-S}$ is $(1+\mathrm{e}^{-\frac{\pi(-2E)}{\hbar}})$ times larger than the outgoing-wave current density represented by $\psi_{R,+S}$ when $\mathrm{Im}\hbar = +0$, but that the reverse is true when $\mathrm{Im}\hbar = -0$. Both these observations are counter-intuitive, in part because the notation for the JWKB wave functions does not indicate that evaluation is taking place on a Stokes line (for $\hbar$) where "real" may Borel-sum to "complex."

In the classically allowed region to the left, the outgoing-wave JWKB function is $\psi_{L,+S}$. By virtue of (21), it has the same current-density "normalization" as $\psi_{R,+S}$, and similarly for $\psi_{L,-S}$ and $\psi_{R,-S}$.

The $\hbar$-Stokes line comes from the implicit normalization factors. The ∞-normalized wave functions do not have a Stokes line with respect to $\hbar$, and the implication from (44) and (45) is that all four of $\psi^{[\infty]}_{L,\pm S}$ and $\psi^{[\infty]}_{R,\pm S}$ share a common current-density normalization.

5.3 Transmission through the barrier

Transmission through the barrier from left to right is specified, in the notations of Tables 1 and 2, by setting $d_- = c_- = 0, d_+ = c_+ = 1$ and taking $\hbar$ real, which yields the following versions of the 1–1′ connection formula:

$$\mathrm{i}\,[-\psi_{L,+S}(x,\hbar+\mathrm{i}0)+\psi_{L,-S}(x,\hbar+\mathrm{i}0)] \longleftrightarrow \mathrm{e}^{-(-E)\pi/\hbar}\psi_{R,+S}(x,\hbar+\mathrm{i}0)\,, \tag{51}$$

$$\mathrm{i}\left[-\psi_{L,+S}(x,\hbar-\mathrm{i}0)+(1+\mathrm{e}^{-2(-E)\pi/\hbar})\psi_{L,-S}(x,\hbar-\mathrm{i}0)\right] \longleftrightarrow \mathrm{e}^{-(-E)\pi/\hbar}\psi_{R,+S}(x,\hbar-\mathrm{i}0)\ , \tag{52}$$

$$\mathrm{i}\left[-\psi^{[\infty]}_{L,+S}(x,\hbar)+\frac{\psi^{[\infty]}_{L,-S}(x,\hbar)}{N(\hbar+\mathrm{i}0)^2}\right] \longleftrightarrow \mathrm{e}^{-\frac{(-E)\pi}{\hbar}}\psi^{[\infty]}_{R,+S}(x,\hbar)\ , \tag{53}$$

$$\mathrm{i}\left[-\psi^{[\infty]}_{L,+S}(x,\hbar)+\frac{(1+\mathrm{e}^{-2(-E)\pi/\hbar})\psi^{[\infty]}_{L,-S}(x,\hbar)}{N(\hbar-\mathrm{i}0)^2}\right] \longleftrightarrow \mathrm{e}^{-\frac{(-E)\pi}{\hbar}}\psi^{[\infty]}_{R,+S}(x,\hbar)\ , \tag{54}$$

$$\mathrm{i}\left[-\psi^{[\infty]}_{L,+S}(x,\hbar)+\mathrm{e}^{\mathrm{i}\phi}\sqrt{1+\mathrm{e}^{-2\pi(-E)/\hbar}}\psi^{[\infty]}_{L,-S}(x,\hbar)\right] \longleftrightarrow \mathrm{e}^{-\frac{(-E)\pi}{\hbar}}\psi^{[\infty]}_{R,+S}(x,\hbar)\,. \tag{55}$$

All five equations, although different, lead by an elementary argument to the same transmission and reflection coefficients: since the outgoing waves are in each case identically normalized, the ratio of the transmission to reflection coefficients is exactly

$$T/R = \mathrm{e}^{-2(-E)\pi/\hbar} \ . \tag{56}$$

From $T + R = 1$, it follows that

$$T = \frac{\mathrm{e}^{-2(-E)\pi/\hbar}}{1 + \mathrm{e}^{-2(-E)\pi/\hbar}} \ , \qquad R = \frac{1}{1 + \mathrm{e}^{-2(-E)\pi/\hbar}} \ . \tag{57}$$

The interesting observation is why the coefficient of the incident wave $\psi_{L,-S}(x,\hbar)$ or $\psi^{[\infty]}_{L,-S}(x,\hbar)$ depends of the sign of $\arg \hbar$. The answer from the preceding subsection is that the relative normalization factor $N(\hbar)$ has a Stokes line for real $\hbar$, and that incoming and outgoing turning-point-normalized JWKB wave functions have different current-density normalizations depending on the sign of $\arg \hbar$. The ∞-normalized functions have a common current-density normalization, but it is still necessary to evaluate (one way or another [19]) the normalization factor $N(\hbar)$.

5.4 Conceptualization of the connection formula for real $\hbar$: doubled-Stokes lines

What is the connection formula at the right-hand turning point in the limit that $\arg \hbar = +0$? Region $1'$ to Region $3'$ is normal, but Region $2'$ has disappeared and has been replaced by Region 3 (see Fig. 2). The limit is shown in Table 3. $\psi_{R,+Q}(x,\hbar)$ in Region 3 (new Region $2'$) has an extra term when compared to the old Region $2'$. It would seem descriptive in the light of Fig. 2 to refer to this situation as a doubled-Stokes line. Which Stokes lines are doubled depend on the sign of $\arg \hbar = \pm 0$.

Table 3. Connection formula at the right-hand turning point when $\arg \hbar = +0$ for turning-point-normalized JWKB wave functions

Region	JWKB wave function, ($\arg \hbar = +0$)
$1'$	$d_+ \psi_{R,+S}(x,\hbar) + d_- \psi_{R,-S}(x,\hbar)$
old $2'$ (empty)	$(d_+ + d_-)\psi_{R,+Q}(x,\hbar) - \mathrm{i} d_- \psi_{R,-Q}(x,\hbar)$
3 (new $2'$)	$[d_+ + d_-(1 + \mathrm{e}^{-2(-E)\pi/\hbar})]\psi_{R,+Q}(x,\hbar) - \mathrm{i} d_- \psi_{R,-Q}(x,\hbar)$
$3'$ (normal)	$(d_+ + d_-)\psi_{R,+Q}(x,\hbar) + \mathrm{i} d_+ \psi_{R,-Q}(x,\hbar)$

6 Conclusions

The quadratic barrier provides a solvable illustration of the exact JWKB method. With complexification of $\hbar$, the connection formulas follow directly from the connection formulas at the two linear turning points and the matching of solutions in their common Stokes region, as pictured in Fig. 2. The square root in (1) comes from explicit Borel summation of the implicit normalization factors in the JWKB wave function through the Stirling series to a gamma function. A Stokes line in this $\hbar$-series leads to formulas, including current densities, that depend on the sign of $\arg\hbar = \pm 0$. The understanding of the limiting case of real $\hbar$, and especially the disappearance of the common Stokes region where the left and right functions were matched, is aided by the concept of doubled-Stokes lines.

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Addendum: a straightforward proof of Sato's conjecture

With the stimulation and encouragement of Professors Kawai and Takei, we add this short, straightforward, informal proof of the conjecture by Sato mentioned above.

We adapt the notation of Eq. (1.19) of Kawai and Takei [8] and denote the constant ratios of the Weber and JWKB functions that correspond at large x by c_1 and c_2,

$$c_1 = \frac{D_{-\mathrm{i}(\frac{-E}{\hbar})-\frac{1}{2}}\left(\mathrm{e}^{-\frac{\pi\mathrm{i}}{4}}x\sqrt{\frac{2}{\hbar}}\right)}{\psi_{R,+S}(x,\hbar)} , \tag{58}$$

$$c_2 = \frac{D_{+\mathrm{i}(\frac{-E}{\hbar})-\frac{1}{2}}\left(\mathrm{e}^{+\frac{\pi\mathrm{i}}{4}}x\sqrt{\frac{2}{\hbar}}\right)}{\psi_{R,-S}(x,\hbar)} . \tag{59}$$

The c_2 here differs slightly from C_2 in [8]. Computation of c_1 and c_2 at large x yields [cf. (30), (31), and (43)–(45)]

$$c_1 = (N\eta)^{-1}(\hbar/2)^{1/4}\mathrm{e}^{-\pi(-E)/4\hbar} , \tag{60}$$

$$c_2 = N\eta(\hbar/2)^{1/4}\mathrm{e}^{-\pi(-E)/4\hbar} . \tag{61}$$

The ratio c_2/c_1 is proportional to the square of the relative normalization factor N:

$$\frac{c_2}{c_1} = N^2\eta^2 , \tag{62}$$

$$= \mathrm{e}^{\frac{\pi\mathrm{i}}{4}}\left(\frac{-E}{\mathrm{e}\hbar}\right)^{\frac{\mathrm{i}(-E)}{\hbar}} N^2 . \tag{63}$$

Note that N, $\hbar^{-1/4}c_1$, and $\hbar^{-1/4}c_2$ [(30), (58)–(63)] are all asymptotic expansions in $\hbar/(-E)$ whose Borel sums turn out to have a Stokes discontinuity on $\arg\hbar = 0$. In the present notation, Sato's conjecture takes the form,

$$\frac{c_2}{c_1} = N^2 \mathrm{e}^{\frac{\pi\mathrm{i}}{4}} \left(\frac{-E}{\mathrm{e}\hbar}\right)^{\frac{\mathrm{i}(-E)}{\hbar}} = \frac{\mathrm{e}^{\frac{\pi\mathrm{i}}{4}}\mathrm{e}^{\frac{(-E)\pi}{2\hbar}}}{\sqrt{2\pi}} \Gamma\left(\frac{1}{2} + \frac{\mathrm{i}(-E)}{\hbar}\right) , \quad (\arg\hbar > 0) \ , \quad (64)$$

the important content of which is that the square of the JWKB normalization series (30) is term-by-term exactly the same as the asymptotic power series obtained from the gamma function.

Remark 1 Equation (64) is essential to the connection formulas for the ∞-normalized JWKB wave functions (Table 2) and was obtained from an analysis of the Jost function by Voros [6].

Remark 2 Although N arose here as the relative normalization factor (41) between $\psi_{R,+S}(x,\hbar)$ and $\psi^{[\infty]}_{R,+S}(x,\hbar)$, N *also* carries the ratio of $\psi_{R,+S}(x,\hbar)$ to the Weber function [(58) and (60)]. It is *this fact* that we exploit to evaluate N. Our derivation uses values of the Weber function and its derivative at 0.

Remark 3 The calculation is unexpectedly straightforward because of a most fortuitous result: that both $\psi_{R,+S}(0,\hbar)$ and $\mathrm{d}\psi_{R,+S}(x,\hbar)/\mathrm{d}x|_{x=0}$ can be calculated from the single asymptotic power series $\dot{Q}_R(0)$, which in turn can be "Borel-summed" via the equality of the logarithmic derivatives of the JWKB and Weber [13] functions.

Sketch of proof By (60) and (61) it is sufficient to calculate c_1, since

$$c_2 = \sqrt{\hbar/2}\,\mathrm{e}^{-\pi(-E)/2\hbar}/c_1 \ . \quad (65)$$

We specify that $\arg\hbar > 0$, so that there is no Stokes discontinuity in the Borel sum of $\psi_{R,+S}(x,\hbar)$ when x is continued from $x = +\infty$ to $x = 0$ (the point at which the potential is stationary). That is, $\psi_{R,+S}(x,\hbar) \leftrightarrow \psi_{R,+Q}(x,\hbar)$. [Cf. Table 1 and Fig. 2; the relevant regions are $1'$ and $2'$. We do not need $\psi_{R,-S}(x,\hbar) \leftrightarrow \psi_{R,+Q}(x,\hbar) - \mathrm{i}\psi_{R,-Q}(x,\hbar)$.] The essential fortunate fact is that $Q_R(x,\hbar) - (-E)\pi/2$ is an odd function of x (also all even derivatives are odd; all odd derivatives are even—see Secs. 2 and 4.1), which leads to

$$\psi_{R,+Q}(0,\hbar) = [-\dot{Q}_R(0,\hbar)]^{-1/2}\mathrm{e}^{(-E)\pi/2\hbar} \ , \quad (66)$$

$$\dot{\psi}_{R,+Q}(0,\hbar) \equiv \mathrm{d}\psi_{R,+Q}(x,\hbar)/\mathrm{d}x|_{x=0} = -\frac{1}{\hbar}[-\dot{Q}_R(0,\hbar)]^{+1/2}\mathrm{e}^{(-E)\pi/2\hbar} \ , \quad (67)$$

$$\dot{Q}_R(0,\hbar) = \hbar\frac{\dot{\psi}_{R,+Q}(0,\hbar)}{\psi_{R,+Q}(0,\hbar)} \ , \quad (68)$$

$$= \hbar\frac{\frac{\mathrm{d}}{\mathrm{d}x}D_{-\mathrm{i}(\frac{-E}{\hbar})-\frac{1}{2}}\left(\mathrm{e}^{-\frac{\pi\mathrm{i}}{4}}x\sqrt{\frac{2}{\hbar}}\right)_{x=0}}{D_{-\mathrm{i}(\frac{-E}{\hbar})-\frac{1}{2}}(0)} \ , \quad (\arg\hbar > 0) \ , \quad (69)$$

$$= -2\mathrm{e}^{-\pi\mathrm{i}/4}\sqrt{\hbar}\frac{\Gamma\left(\frac{3}{4} + \frac{1}{2}\mathrm{i}\frac{(-E)}{\hbar}\right)}{\Gamma\left(\frac{1}{4} + \frac{1}{2}\mathrm{i}\frac{(-E)}{\hbar}\right)} \ , \quad (\arg\hbar > 0) \ . \quad (70)$$

c_1 follows from evaluation of the wave-function ratio at $x = 0$ and the gamma-function duplication formula [13]:

$$c_1 = \frac{D_{-\mathrm{i}(\frac{-E}{\hbar})-\frac{1}{2}}(0)}{\psi_{R,+S}(0,\hbar)} , \tag{71}$$

$$= \frac{\mathrm{e}^{-\pi \mathrm{i}/8}\pi^{1/4}\hbar^{1/4}\mathrm{e}^{-(-E)\pi/2\hbar}}{\sqrt{\Gamma\left(\frac{1}{2}+\mathrm{i}\frac{(-E)}{\hbar}\right)}} , \quad (\arg\hbar > 0) . \tag{72}$$

Equations (72) and (65) give (64).

References

1. Miller, S.C., Good, R.H.: Phys. Rev., **91**, 174 (1953).
2. K. W. Ford, D. L. Hill, M. Wakano and J. A. Wheeler, Ann. Phys. (NY), **7**, 239 (1959).
3. M. S. Child, *Semiclassical Mechanics with Molecular Applications* (Oxford University Press, Oxford, 1991).
4. J. N. Connor, Molec. Phys., **15**, 37 (1968).
5. M. V. Fedoryuk, *Asymptotic Analysis* (Springer-Verlag, Berlin, 1993).
6. A. Voros, Ann. Inst. Henri Poincaré, **39**, 211 (1983).
7. T. Aoki, T. Kawai and Y. Takei, in *Special Functions,ICM-90 Satellite Conference Proceedings*, edited by M. Kashiwara and T. Miwa (Springer-Verlag, Berlin, 1991), p. 1.
8. T. Kawai and Y. Takei, in *Analyse Algébrique des Perturbations Singulière. I: Méthodes Résurgentes*, edited by L. Boutet de Monvel (Hermann, Paris, 1994), p. 85.
9. T. Aoki, T. Kawai and Y. Takei, Sugaku Expositions, **8**, 217 (1995).
10. E. Delabaere, H. Dillinger and F. Pham, J. Math. Phys., **38**, 6126 (1997).
11. E. Delabaere and F. Pham, Ann. Inst. Henri Poincaré Phys. Théor., **71**, 1 (1999).
12. S. Wolfram, *The Mathematica Book* (Cambridge University Press and Wolfram Media, Champaign, 1999).
13. M. Abramowitz and I. A. Stegun, *Handbook of Mathematical Functions* (National Bureau of Standards, Washington, D.C., 1964).
14. C. G. Darwin, Quart. J. Mech. Appl. Math., **2**, 311 (1949).
15. H. J. Silverstone, Phys. Rev. Lett., **55**, 2523 (1985).
16. H. Shen and H. J. Silverstone, Int. J. Quantum Chem., **99**, 336 (2004).
17. M. V. Berry and K. E. Mount, Rep. Prog. Phys., **35**, 315 (1972).
18. R. B. Paris and A. D. Wood, J. Comp. and Appl. Math., **41**, 135 (1992).
19. G. Álvarez, V. Martín-Mayor and J. J. Ruiz-Lorenzo, J. Phys. A, **33**, 841 (2000).