`Draft chapter last generated 2024-12-02; P.H. Trinh`

11

> *Author's note*
>
> This chapter remains very much in draft form. In case you are participating as part of the 2024-25 TCC course, you can follow along with the notes in Chapman and Trinh [2019a] (link).

The case of the Schrodinger equation with quadratic potential (the quantum harmonic oscillator) presents an interesting scenario to better understand how the techniques of exponential asymptotics relate to the classical approaches using WKBJ turning-point analysis. Here, the setting consists of a linear eigenvalue problem, studied in the limit the eigenvalue tends to infinity. When reposed as an asymptotic problem as $\epsilon \to 0$, the eigenfunctions and eigenvalues correspond to those WKBJ approximations that satisfy the necessary boundary conditions at infinity, and are carefully matched together at "turning points", where the approximation breaks down.

However, our detour through the Airy equation introduces the idea that, instead of matching directly through turning points, it may be possible to consider analytic continuation in the complex plane—at which point the Stokes phenomena provides the key to the analysis.

11.1 QUANTUM HARMONIC OSCILLATOR

This classic example of a linear eigenvalue problem concerns the time-independent solutions of the Schrödinger equation for the quantum mechanical harmonic oscillator. Consider the differential equation for the wavefunction, $\psi(x)$, given by

$$-\frac{\mathrm{d}^2\psi}{\mathrm{d}x^2} + x^2\psi = E\psi, \tag{11.1}$$

with boundary conditions $\psi \to 0$ as $x \to \pm\infty$ where E are the eigenvalues (the energies). For (11.1), the eigenfunctions can be completely specified in terms of Hermite polynomials[1] and the eigenvalues are given by

$$E = E_n = 2n + 1 \qquad n = 0, 1, 2, , \ldots \tag{11.2}$$

Derivation of the above is an application of regular series solutions for ordinary differential equations, and makes use of the fact that the series representation via Hermite polynomials truncates. For more details, see *e.g.* [Bender and Orszag, 1999, p.332] and [Hannabuss, 1997, p. 21].

[1] We can verify that the eigenfunctions are given by $\psi_n(x) = \mathrm{e}^{-x^2/2}\mathrm{He}_n(\sqrt{2}x)$ with $\mathrm{He}_0(s) = 1$, $\mathrm{He}_1(s) = s$, $\mathrm{He}_2(s) = s^2 - 1$, and so forth.

In cases where the potential function, here $V(x) = x^2$, is not a simple quadratic polynomial, more general approximation techniques are required, and the linear oscillator is forms a classic application of WKBJ techniques. In this case, let us put the differential equation (11.1) in the more typical perturbative form, with $f(z) = y(x)$, where

$$-\epsilon^2 \frac{\mathrm{d}^2 f}{\mathrm{d}z^2} + z^2 f = f, \tag{11.3}$$

achieved by setting $x = E^{1/2} z$ and rewriting $\epsilon = 1/E$. For the discussion to follow, we shall firstly consider z to be a real-valued number, but later it will be useful to consider $z \in \mathbb{C}$.

In the limit $\epsilon \to 0$, we posit the standard WKBJ ansatz, $f(z) \sim A(z)\mathrm{e}^{\mathrm{i}\phi(z)/\epsilon}$ and find that

$$\phi(z) = \pm \int^z \sqrt{1 - t^2}\, \mathrm{d}t, \tag{11.4a}$$

$$A(z) = \frac{\text{const.}}{(1 - z^2)^{1/4}}. \tag{11.4b}$$

As expected, the WKBJ approximation fails at the two turning points, where $z = \pm 1$. We may write down a composite approximation via

$$f(z) \sim a_i A(z)\mathrm{e}^{\mathrm{i}\Phi_i(z)/\epsilon} + b_i A(z)\mathrm{e}^{-\mathrm{i}\Phi_i(z)/\epsilon}, \qquad i = 1, 2, 3 \tag{11.5}$$

where the constant factor in (11.4b) is set to unity. Above, we have defined the exponential arguments as

$$\Phi_{\mathrm{I}}(z) = \int_{-1}^{z} \sqrt{1 - t^2}\, \mathrm{d}t, \quad \Phi_{\mathrm{II}}(z) = \int_{0}^{z} \sqrt{1 - t^2}\, \mathrm{d}t, \tag{11.6}$$

$$\Phi_{\mathrm{III}}(z) = \int_{1}^{z} \sqrt{1 - t^2}\, \mathrm{d}t. \tag{11.7}$$

The six constants, a_i and b_i in (11.5) determine the solution in the three regions of $z \in (-\infty, -1) \cup (-1, 1) \cup (1, \infty)$ indexed by $i = 1, 2, 3$, respectively. This yields a composite solution with six unknown constants. The boundedness at infinity is equivalent to two boundary conditions, the continuity of f and f' at $z = \pm 1$ equivalent to four more. Finally there is a free normalisation condition, and hence this is a total of seven boundary conditions. The problem is overdetermined; once the six constants are solved, we can verify that this imposes an additional constraint on the eigenvalue of

$$\epsilon_n = \frac{1}{2n + 1}, \qquad n = 0, 1, 2, \ldots \tag{11.8}$$

A graph of the three WKBJ solutions is shown in fig. 11.1 compared to the exact solution for $\epsilon = 1/11$.

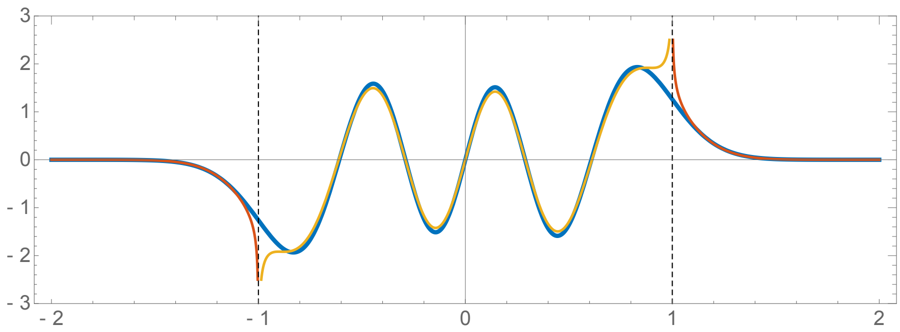

Figure 11.1: WKB solutions in the three regions. Here $\epsilon = 1/11$. The axes correspond to z versus $f(z)$. The blue curve is the exact solution.

11.3 APPROACH USING EXPONENTIAL ASYMPTOTICS

This is treated using the exponential asymptotics methodology in Chapman and Trinh [2019b]. The basic idea is that instead of matching the WKB expansions about the turning points, $z = \pm 1$, we may consider analytic continuation of the solution in the complex plane, thus avoiding the singularities completely. Let us return to the WKBJ approximation in (11.4) and consider the specific choice of

$$f(z) \sim A(z) \exp\left[-\frac{1}{\epsilon}\int_{-1}^{z} \sqrt{t^2-1}\, \mathrm{d}t\right]. \qquad (11.9)$$

We select the branch structure[2] for the square root in the integrand such that $\sqrt{t^2-1} \sim t$ as $t \to \infty$ and $\sqrt{t^2-1} \sim -t$ as $t \to \infty$. Consequently, $f(z)$ is a well-defined WKBJ approximation that satisfies $f \to 0$ as $z \to \pm\infty$ and this suggests a valid approximation for all values of ϵ. Indeed, this leaves the standard mystery of the indeterminacy of ϵ despite the asymptotic approximation satisfying the boundary conditions (to all orders).

However, it is verified that as $f(z)$ in (11.9) is analytically continued from $z = -\infty$ to $z = \infty$ in the lower half-plane, it encountered a Stoke line from $z = -1$ and another from $z = 1$. This is shown in fig. 11.2. Once passed, we have the total leading-order contribution of

$$f(z) \sim A(z)\mathrm{e}^{-\phi_{\mathrm{I}}(z)/\epsilon}\left[1 + \mathrm{i}\mathrm{e}^{2\mathrm{i}\phi(-1)/\epsilon} + \mathrm{i}\mathrm{e}^{2\mathrm{i}\phi(1)/\epsilon}\right]. \qquad (11.10)$$

In order to satisfy the decay condition, we then require

$$\mathrm{i}\mathrm{e}^{2\mathrm{i}\phi(-1)/\epsilon} + \mathrm{i}\mathrm{e}^{2\mathrm{i}\phi(1)/\epsilon} = 0. \qquad (11.11)$$

Simplification then yields those permissible values of $\epsilon = \epsilon_n$ at

$$\frac{2(\phi(1) - \phi(-1)}{\epsilon_n} = (2n+1)\pi, \qquad n = 0, 1, 2, \ldots \qquad (11.12)$$

which is the desired result after use $\phi(1) - \phi(-1) = \pi/2$.

[2] This can be argued as follows. We write $\sqrt{t^2-1} = (r_1 r_2)^{1/2}\mathrm{e}^{\mathrm{i}\theta_1/2}\mathrm{e}^{\mathrm{i}\theta_2/2}$ for $t+1 = r_1\mathrm{e}^{\mathrm{i}\theta_1}$ and $t-1 = r_2\mathrm{e}^{\mathrm{i}\theta_2}$. The branch cut from $t = -1$ is taken along $\theta_1 = 2\pi$ while the branch cut from $t = 1$ is taken along $\theta_2 = -pi$. The reader can then verify that $\theta_1 \to -\pi$ and $\theta_2 \to -\pi$ yields the desired sign for $t \to -\infty$ while $\theta_1 \to 2\pi$ and $\theta_2 \to 0$ yields the desired sign for $t \to \infty$.

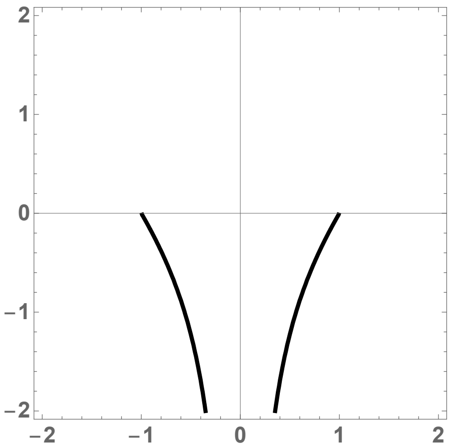

Figure 11.2: Stokes lines for the harmonic oscillator. There is one Stokes line from $z = -1$ and one from $z = 1$.

11.4 OPTICAL TUNNELLING

This should really be removed or truncated.

The original physical derivation from Maxwell's equations is shown by Kath and Kriegsmann [1988], but the (two-dimensional) WKB analysis is quite heuristic. Later, toy models from second-order linear eigenvalue problems were studied, firstly by Paris and Wood [1989], and extended by colleagues to more general one-dimensional models.

Consider

$$-y''(x) - \epsilon x^n y(x) = \lambda y(x), \qquad x \in (0, \infty), n \in \mathbb{Z}^+, \tag{11.13a}$$

$$y'(0) + hy(0) = 0, \qquad h > 0, \tag{11.13b}$$

$$y \text{ behaves as } \mathrm{e}^{\mathrm{i}p(x)} \text{ as } x \to \infty \qquad p(x) > 0. \tag{11.13c}$$

Here, y represents amplitude of an eletromagnetic wave travelling along the centreline of an optic waveguide, with x directed orthogonally to the centreline. The potential function, $-\epsilon x^n$ is connected with the refractive indices of the inner core and outer cladding of the fibre, as well as its curvature.

A regular perturbative scheme indicates that the eigenvalues are given by

$$\lambda = -h^2 + \sum_{n=1}^{\infty} \epsilon^n \lambda_n. \tag{11.14}$$

However, it turns out the eigenvalue expansion in ϵ diverges. The spectrum is real for all algebraic powers of ϵ but in fact there is an exponentially small remainder with non-zero imaginary part.

11.4.1 Exponential asymptotics

It is an interesting property of this problem that the divergent asymptotic expansion of the eigenvalues does not need to be taken into account during a large part of the derivation. The key property of the toy model involves the the turning point(s) located at

$$x^n = -\lambda/\epsilon.$$

Since the eigenvalues satisfy $\lambda \sim -h^2$ as $\epsilon \to 0$, the solution must travel through (or near) this turning point at large x. We re-scale the problem about this turning point:

$$\begin{gathered} w = \delta(x - x_0), \\ \delta = \epsilon^{1/n} \quad \text{and} \quad x_0 = (-\lambda/\epsilon)^{1/n}. \end{gathered} \tag{11.15}$$

Changing to differentiation in w, we seek to solve

$$\delta^2 y''(w) = -Q(w;\lambda) y, \tag{11.16a}$$

$$y'(-\delta x_0) + hy(-\delta x_0) = 0, \tag{11.16b}$$

$$y \text{ behaves as } \mathrm{e}^{\mathrm{i}p(w)/\delta} \text{ as } w \to \infty, \tag{11.16c}$$

all primes now denote differentiation in w, and we have defined $Q(w) = Q(w;\lambda)$ via

$$Q(w) = [w + (-\lambda)^{1/n}]^n + \lambda. \tag{11.17}$$

The procedure now follows similar to Chapman and Trinh [2019b]. First, upon substitution of the WKB ansatz,

$$y = A(w)\mathrm{e}^{\mathrm{i}\phi/\delta} \sim \sum_{m=0}^{\infty} \delta^m A_m \mathrm{e}^{\mathrm{i}\phi/\delta},$$

we have

$$\frac{\mathrm{d}\phi}{\mathrm{d}w} = \pm Q(w)^{1/2}. \tag{11.18}$$

We select the positive sign and define ϕ with $\phi = 0$ at the turning point, thus

$$\phi = \int_0^w Q(t)^{1/2} \, \mathrm{d}t. \tag{11.19}$$

We have again the same differential equation for $A(w)$, with

$$\delta A'' + [2\mathrm{i}\phi']A' + [\mathrm{i}\phi'']A = 0. \tag{11.20}$$

With the series expansion for A, the leading-order solution satisfies

$$A_0 = \frac{C}{(-\phi')^{1/2}}, \tag{11.21}$$

so that as $w \to \infty$, the leading-order WKB expansion satisfies

$$y_{\mathrm{III}} \sim \frac{C}{(-\phi')^{1/2}} \mathrm{e}^{\mathrm{i}\phi/\delta}, \tag{11.22}$$

which is consistent with the outgoing radiation condition (11.16c). In consider the values of ϕ, we consider the branch such that for $w < 0$, $\mathrm{e}^{\mathrm{i}\phi/\delta}$ is decaying as $w \to -\infty$. For the solution shown in fig. 11.3, with the branch cut taken along the negative real axis, this corresponds to evaluating the solution just below the branch cut. The key, however,

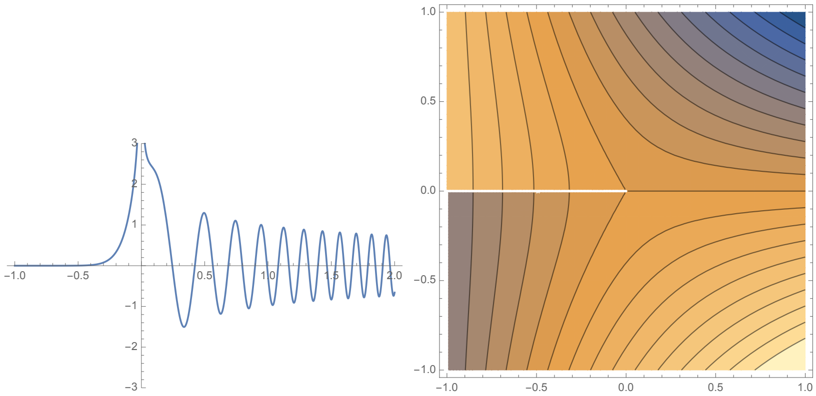

Figure 11.3: $\delta = 0.05$, $h = 1$, $\lambda = -h^2$, $n = 2$ evaluated on $w - 10^{-12}\mathrm{i}$.

is that in order to satisfy the boundary conditions (11.16b), we must consider the switching-on of the secondary exponential $\mathrm{e}^{-\mathrm{i}\phi/\delta}$.

The late-orders analysis proceeds the same as for the previous problems, with

$$A_m(w) \sim \frac{B(w)\Gamma(m+\gamma)}{[\chi(w)]^{m+\gamma}}$$

$$\chi(w) = 2\mathrm{i}\phi(w) \qquad B(w) = \frac{\Lambda}{[\phi'(w)]^{1/2}}$$

Let us examine the Stokes lines. As $w \to 0$, we have that $Q \sim aw$ where $a = n(-\lambda)^{(n-1)/n}$. Consequently,

$$\chi \sim \frac{4\mathrm{i}}{3} a w^{3/2}. \tag{11.23}$$

!!! Think we want LHP

It may be convenient to take the branch cut along the positive w-axis. Consequently, there are there are Stokes lines at $\mathrm{Arg}(w) = \pi/3$ and $5\pi/3$. Let us assume that the analytic continuation is done into the upper half-w-plane.

In the inner region, let us set $w = A\sigma$, so that

$$y_{\sigma\sigma} = \sigma y, \tag{11.24}$$

with

$$A = \left(-\frac{\delta^2}{a}\right)^{1/3} = \mathrm{e}^{\pi\mathrm{i}/3}\frac{\delta^{2/3}}{a^{1/3}}. \tag{11.25}$$

We choose the branch of A so that the matching with the WKB solution is via only the Airy Ai function. In particular, note that for $w \to \infty$ along $w > 0$, $\sigma = \mathrm{e}^{\pi\mathrm{i}/3} a^{1/3} w/\delta^{2/3}$, so since a is approximately real and positive, the matching is done as $|\sigma| \to \infty$ along the ray $\pi/3$. In this region, the Airy Bi function is unbounded, and hence in the inner region,

$$y \sim A_1 \,\mathrm{Ai}(\sigma) \tag{11.26}$$

The matching procedure indicates that

$$\gamma = 0 \qquad \Lambda = \frac{1}{2\pi}. \tag{11.27}$$

11.4.2 Stokes smoothing and eigenvalues

Stokes smoothing yields the fact that, as the regular series in $A(w)$, is analytically continued past Stokes lines, it switches-on a subdominant exponential given by

$$A_{\text{exp}} \sim \pm \frac{2\pi \mathrm{i}}{\delta^\gamma} \frac{\Lambda}{(-\phi')^{1/2}} \mathrm{e}^{-\chi/\delta} = \pm \frac{\mathrm{i}}{(-\phi')^{1/2}} \mathrm{e}^{-\chi/\delta}. \tag{11.28}$$

The $\pm$ signs correspond to crossing the Stokes lines in the counterclockwise or clockwise directions in the w-plane. Consequently, as eq. (11.22) crosses the Stokes line, we have the switching

$$\frac{C}{(-\phi')^{1/2}} \mathrm{e}^{\mathrm{i}\phi/\delta} \mapsto \frac{C}{(-\phi')^{1/2}} \mathrm{e}^{\mathrm{i}\phi/\delta} \pm \mathrm{i} \frac{C}{(-\phi')^{1/2}} \mathrm{e}^{-\mathrm{i}\phi/\delta}. \tag{11.29}$$

However, the negative real axis is also a Stokes line corresponding to the exponential $\mathrm{e}^{-\mathrm{i}\phi/\delta}$. Thus the extra term switched-on in (11.29) switches-on a further multiple of $\mathrm{e}^{\mathrm{i}\phi/\delta}$ and this is an example of the higher-order Stokes Phenomenon. Since the analytic continuation only proceeds to the real axis, then only half of the switching multiple of i is incurred. Thus,

$$\pm \mathrm{i} \frac{C}{(-\phi')^{1/2}} \mathrm{e}^{-\mathrm{i}\phi/\delta} \mapsto \pm \mathrm{i} \frac{C}{(-\phi')^{1/2}} \mathrm{e}^{-\mathrm{i}\phi/\delta} \left(\pm \frac{\mathrm{i}}{2}\right) (\pm \mathrm{i}) \frac{C}{(-\phi')^{1/2}} \mathrm{e}^{\mathrm{i}\phi/\delta}. \tag{11.30}$$

In total then, we have

$$y \sim \begin{cases} \left[\frac{1}{(-\phi')^{1/2}}\right] \mathrm{e}^{\mathrm{i}\phi/\delta} \\ \left[\frac{1}{(-\phi')^{1/2}}\right] \mathrm{e}^{\mathrm{i}\phi/\delta} \pm \left[\frac{\mathrm{i}}{(-\phi')^{1/2}}\right] \mathrm{e}^{-\mathrm{i}\phi/\delta} \\ \left[\frac{1}{2(-\phi')^{1/2}}\right] \mathrm{e}^{\mathrm{i}\phi/\delta} \pm \left[\frac{\mathrm{i}}{(-\phi')^{1/2}}\right] \mathrm{e}^{-\mathrm{i}\phi/\delta} \end{cases} \tag{11.31}$$

We now use the solution, valid along the negative real axis, in the boundary condition of eq. (11.16b),

$$y'(-\delta x_0) + hy(-\delta x_0) = 0. \tag{11.32}$$

First, we have that

$$hy(-\delta x_0) \sim \left[\frac{h\lambda^{-1/4}}{2\mathrm{i}}\right] \mathrm{e}^{\mathrm{i}\phi/\delta} \pm \left[h\lambda^{-1/4}\right] \mathrm{e}^{-\mathrm{i}\phi/\delta} \tag{11.33}$$

$$\delta y'(-\delta x_0) \sim \left[\frac{\lambda^{1/4}}{2} + \mathcal{O}(\delta)\right] \mathrm{e}^{\mathrm{i}\phi/\delta} \mp \left[\mathrm{i}\lambda^{1/4} + \mathcal{O}(\delta)\right] \mathrm{e}^{-\mathrm{i}\phi/\delta}. \tag{11.34}$$

Combining with $hy(-\delta x_0)$, we have

$$\left[\frac{\lambda^{1/2}}{2} - \frac{\mathrm{i}h}{2} + \mathcal{O}(\delta)\right] \mathrm{e}^{\mathrm{i}\phi/\delta} \pm \left[-\mathrm{i}\lambda^{1/2} + h + \mathcal{O}(\delta)\right] \mathrm{e}^{-\mathrm{i}\phi/\delta} = 0. \tag{11.35}$$

Let us define

$$\tau \equiv -\frac{\mathrm{i}\phi(-\delta x_0)}{\delta} = -\frac{\mathrm{i}}{\delta} \int_0^{-\delta x_0} [(t + \delta x_0)^n + \lambda]^{1/2} \, \mathrm{d}t. \tag{11.36}$$

So that

$$\mathrm{i}\lambda^{1/2} \sim \frac{h(\pm 1 - (\mathrm{i}/2)\mathrm{e}^{-2\tau} + \mathcal{O}(\delta \mathrm{e}^{-\tau}))}{\pm 1 + (\mathrm{i}/2)\mathrm{e}^{-2\tau} + \mathcal{O}(\delta \mathrm{e}^{-\tau})}, \tag{11.37}$$

or that

$$\lambda \sim -h^2 + \left[\pm 2\mathrm{i}h^2 + \mathcal{O}(\delta)\right]\mathrm{e}^{-2\tau}. \tag{11.38}$$

Next, we can verify that

$$\tau = \frac{(-\lambda)^{\frac{n+2}{2n}}}{\delta} S(n), \qquad S(n) = \int_0^1 (1-u^n)^{1/2}\, \mathrm{d}u = \frac{\sqrt{\pi}\Gamma(1/n+1)}{2\Gamma(1/n+3/2)}. \tag{11.39}$$

In particular, $S(1) = 2/3$ and $S(2) = \pi/4$. Noting that

$$\begin{aligned}\frac{(-\lambda)^{\frac{n+2}{2n}}}{\epsilon^{1/n}} &= \frac{\left(h^2 + \epsilon\lambda_1 + \ldots\right)^{\frac{n+2}{2n}}}{\epsilon^{1/n}} \\ &= \frac{h^{\frac{n+2}{2}}}{\epsilon^{1/n}} + \left(\frac{n+2}{2n}\right)\lambda_1 h^{\frac{n+2}{2}-2}\epsilon^{1-1/n} + \mathcal{O}(\epsilon^{2-1/n}).\end{aligned}$$

Crucially, if $n = 1$, then the correction term, which involves $\lambda_1 = -1/(2h)$ must be used, since it produces a constant pre-factor in $\mathrm{e}^{-2\tau}$. Otherwise, the corrections terms are lower order for $n = 2, 3, \ldots$.

Thus to leading order for $n = 2, 3, \ldots$ the imaginary eigenvalue is given by

$$\lambda_{\text{exp}} \sim \pm 2h^2\mathrm{e}^{-2\tau} \sim \pm 2h^2 \exp\left[-\frac{2S(n)}{\epsilon^{1/n}} h^{(n+2)/n}\right], \tag{11.40}$$

while for $n = 1$,

$$\lambda_{\text{exp}} \sim \pm \frac{2h^2}{\mathrm{e}} \exp\left[-\frac{4}{3\epsilon} h^3\right]. \tag{11.41}$$

Taking the lower sign, this matches [Paris and Wood, 1989, p. 284].

11.4.3 Notes

Firstly, the above derivation seems to show that it is not necessary to examine the divergent series of

$$y \sim \sum_{m=0}^{\infty} \delta^m A_m \mathrm{e}^{\mathrm{i}\phi/\delta}, \tag{11.42}$$

simultaneously to the divergent series of

$$\lambda = \sum_{m=0}^{\infty} \epsilon^m \lambda_m = \sum_{m=0}^{\infty} \delta^{nm} \lambda_m \tag{11.43}$$

as long as the WKB form includes the entire λ form in the definition of ϕ. It would be interesting to develop the exponential asymptotics with the λ expansion and confirm that the theory is the same—that is, the late orders are not affected by the divergence of λ.

Secondly, there seems to be great scope in extending the Paris and Wood [1989] analysis in light of the Chapman and Trinh [2019b] direction – i.e. consideration of non-integral n and different potential functions.