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PPPL-5318

Bound State Energies Using Phase Integral Methods

R. B. White

October 2016

Prepared for the U.S. Department of Energy under Contract DE-AC02-09CH11466.

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Bound state energies using Phase integral methods

R.B. White[1]

[1]*Plasma Physics Laboratory, Princeton University,*

P.O. Box 451, Princeton, New Jersey 08543

(Dated: October 18, 2016)

Abstract

The study of asymptotic properties of solutions to differential equations has a long and arduous history, with the most significant advances having been made in the development of quantum mechanics. A very powerful method of analysis is that of Phase Integrals, primarly due to Heading. Key to this analysis are the Stokes constants and the rules for analytic continuation of an asymptotic solution through the complex plane. These constants are easily determined for isolated singular points, by analytically continuing around them and, in the case of analytic functions, requiring the asymptotic solution to be single valued. However, most interesting problems of mathematical physics involve several singular points. By examination of bound state problems involving multiple singular points, we show that the method of Phase Integrals can greatly improve the determination of bound state energy over the simple WKB values.

I. INTRODUCTION

Many differential equations of interest can be put in the form

$$\frac{d^2\psi}{dz^2} + Q(z,E)\psi = 0. \tag{1}$$

For bound state problems the existence of solutions and the energy eigenvalue E can often be determined by Phase Integral methods. Briefly, the WKBJ (and often simply WKB) approximate solutions of Eq. 1, so named after Wentzel, Kramers, Brillouin, and Jeffreys[1], take the form

$$\psi_\pm = Q^{-1/4} e^{\pm i \int^z Q^{1/2} dz}, \tag{2}$$

and provided that $\left|\frac{dQ}{dz} Q^{-3/2}\right| \ll 1$ a general solution of Eq. 1 can be approximated by

$$\psi = a_+\psi_+ + a_-\psi_-. \tag{3}$$

The solutions $\psi_\pm$ are local, not global solutions of Eq. 1. Clearly the inequality is not valid in the vicinity of a zero of $Q(z,E)$, commonly called a turning point. Aside from this, however, $\psi_\pm$ are not approximations of a continuous solution of Eq. 1 in the whole z plane. The method of Phase Integrals, primarily due to Heading[2], consists in relating, for a given solution of Eq. 1, the WKBJ approximation in one region of the z plane to that in another[3, 4].

These regions are separated by the so-called Stokes and anti-Stokes lines associated with $Q(z,\omega)$, and thus the qualitative properties of the solution are determined once these lines are known. The global Stokes (anti-Stokes) lines associated with $Q(z,\omega)$ are paths in the z plane, emanating from zeros or singularities of $Q(z,\omega)$, along which $\int Q^{1/2}(z,\omega)dz$ is imaginary (real). When the zero z_0 is first order, three anti-Stokes lines emanate from z_0. Similarly, one finds that from a double root there issue four anti-Stokes lines, from a simple pole a single line, etc.. In refering to Stokes diagrams, we will refer to both zeros and singularities of Q(z) as singular points, since it is the function $Q^{1/2}$ which is relevant in this diagram.

Along the global anti-Stokes lines the functions $\psi_\pm$ are, within the validity of the WKBJ approximation, of constant amplitude, *i.e.* oscillatory. Along the Stokes lines the WKBJ solutions are exponentially increasing or decreasing with fixed phase. Except at singular

points, the Stokes and anti-Stokes lines are orthogonal. The global anti-Stokes and Stokes lines which are attached to the singular points of the Stokes diagram, along with the Riemann cut lines, determine the global properties of the WKBJ solutions.

In the notation of Heading, including the slow $Q^{-1/4}$ dependence, a WKBJ solution is denoted by

$$(a,z)_s = Q^{-1/4} e^{i\int_a^z Q^{1/2} dz} \tag{4}$$

where the subscript s(d) indicates that the solution is subdominant (dominant); *i.e.* exponentially decreasing (increasing) for increasing $|z-a|$ in a particular region of the z plane, bounded by Stokes and anti-Stokes lines.

Begin with a particular solution in one region of the z plane, choosing that combination of subdominant and dominant solutions which gives the desired boundary conditions in this region. The global solution is obtained by continuing this solution through the whole z plane effecting the following changes:

1. Given a solution $\psi = a_d(z_0,z)_d + a_s(z,z_0)_s$, upon crossing a Stokes line emanating from z_0 in a counterclockwise sense a_s must be replaced by $a_s + Sa_d$ where S is the Stokes constant associated with z_0.

2. Upon crossing a cut in a counterclockwise sense, the cut originating from a first order zero of Q at the point z_0, we have

$$\begin{aligned}(z_0,z) &\rightarrow -i(z,z_0)\\ (z,z_0) &\rightarrow -i(z_0,z).\end{aligned} \tag{5}$$

Properties of dominancy or subdominancy are preserved in this process.

3. Upon crossing an anti-Stokes line emanating from z_0, subdominant solutions attached to z_0 become dominant and vice versa.

4. Reconnect from singularity a to singularity b using $(z,a) = (z,b)[b,a]$ with $[b,a] = e^{i\int_b^a Q^{1/2} dz}$.

Using these rules we can pass from region to region across the cuts, Stokes and anti-Stokes lines emanating from a turning point. Beginning with any combination of dominant and subdominant solutions in one region, this process leads to a globally defined approximate solution of Eq. 1.

For an isolated singular point with Q analytic, the Stokes constant can be determined by a continuation around the complex plane, requiring that the WKB approximation be single valued. This gives for $Q = z^n$, the value $S = 2icos(\pi/(n+2))$.

Any function given on the real axis can be analytically continued into the complex plane, resulting in a collection of zeros and singularities associated with the functional form on the axis. Every bound state problem consists of two turning points, with the potential positive outside them, and negative inside. The simplest bound state problem, the harmonic oscillator, given by the Weber equation with $Q = E - z^2$, is unique in that there are no additional zeros or singularities in the complex plane, the function is completely described by the zeros on the real axis. For this case the energy of the bound state as well as the single valuedness of the solution turn out to be independent of the value of the Stokes constant.

In section II we review this case. In sections III and IV we consider Hermitian anharmonic oscillator Hamiltonians with additional zeros above and below the axis, and in section V we consider a non-Hermitian Hamiltonian with three singular points. The shape of these potentials is shown is section VI. Finally in section VII are the conclusions.

II. THE WEBER FUNCTION

The simplest bound state problem is given by the harmonic oscillator potential, with $Q(z) = E - z^2$, real on the real axis with two first order zeros at points $\pm\sqrt{E}$. The Stokes diagram is shown in Fig. 1. The solid lines are Anti Stokes lines, dashed lines are Stokes lines, and cuts are designated with a wavy line. Denoting the Stokes constant as S, we will find that the boundary conditions immediately give the Bohr–Sommerfeld condition, which determines the energy of the bound state, independent of the value of the Stokes constant.

Begin with a subdominant solution at large positive x and continue, assuming Stokes constants the same at each vertex, with $a = \sqrt{E}$:

(1) $(a, z)_s$

(2) $(a, z)_d$

(3) $(a, z)_d + S(z, a)_s$

(3) $[a, -a]_u(-a, z)_d + S(z, -a)_s[-a, a]_u$

But $[-a, a] = e^{-iW}$, $W = \int_{-a}^{a} \sqrt{a^2 - x^2}dx$. Note that the phase of $\sqrt{Q}$ is defined by requiring that $(a, z)_s$ be subdomanant in domain 1, so $i\sqrt{Q} = -real$. The cut locations define the

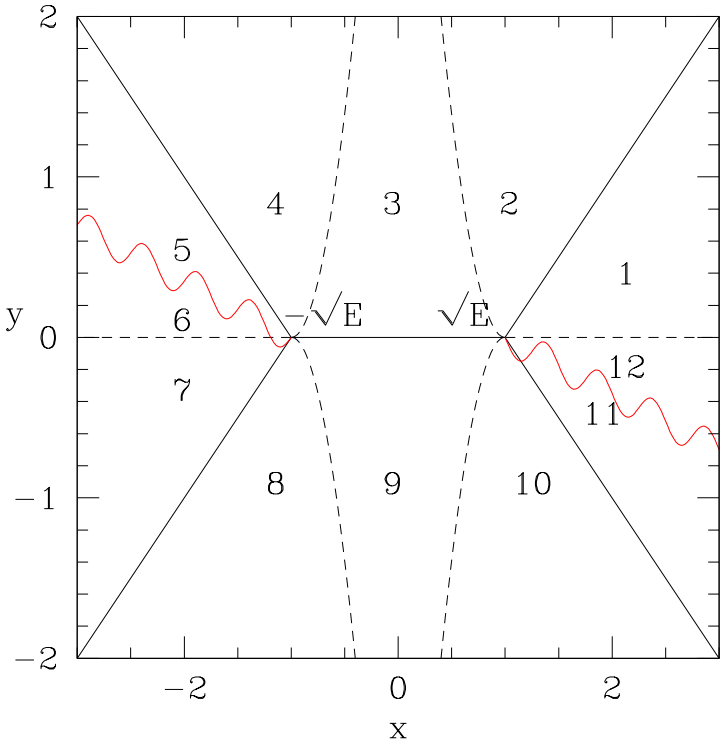

FIG. 1: Stokes plot for the bound state problem $Q = E - z^2$.

phase in other domains.

(4) $e^{iW}(-a,z)_d + S(z,-a)_s(e^{-iW} + e^{iW})$

(5) $e^{iW}(-a,z)_s + S(z,-a)_d 2cosW$

(6) $-ie^{iW}(z,-a)_s - iS(-a,z)_d 2cosW$

Now set the dominant term to zero giving $W = (n+1/2)\pi$, the Bohr Sommerfeld condition, independent of the value of the Stokes constant. Note that $-ie^{iW} = (-1)^n$, the coefficient correctly reflects even and odd symmetry of the solution. Continuing around to domain (12)

(7) $-ie^{iW}(z,-a)_s$

(8) $-ie^{iW}(z,-a)_d$

(9) $-ie^{iW}[(z,-a)_d + S(-a,z)_s]$

(9) $-ie^{iW}[(z,a)_d[a,-a] + S[-a,a](a,z)_s]$

(9) $-ie^{2iW}(z,a)_d - iS(a,z)_s$

(10) $i(z,a)_d$

(11) $i(z,a)_s$

(12) $(a,z)_s$,

we find again a subdominant solution with coefficient equal to one, so the solution is single valued, independent of the value of S provided that the Bohr-Sommerfeld condition on the energy is satisfied. Of course S has a definite value, which can be revealed by constructing an integral representation of the solution, allowing analytic continuation into domain 3 and giving the value of S[5]. In particular one discovers that the Stokes constants do not asymptote to $S = i$, the value for an isolated first order zero, and do not even have magnitude one, they retain information concerning the phase of the solution.

It is important to note that the results of any calcuation are independent of the location of the Riemann cuts, so they can be placed to be convenient for a given calculation.

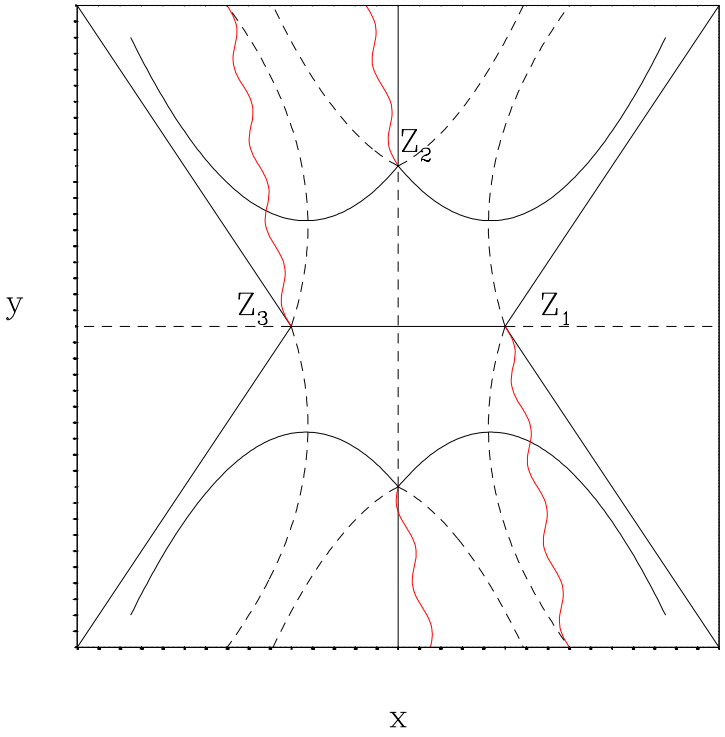

FIG. 2: Stokes plot for the bound state problem $Q = E - z^4$.

III. A FOURTH ORDER POTENTIAL

Now consider a more complicated potential, that of an anharmonic oscillator, with more turning points in the complex plane. As an example we take $Q(z) = E - z^4$. The Stokes structure is shown schematically in Fig. 2. The cuts have been chosen to give symmetry in the continuation between the upper and lower half planes. We assume the Stokes constants to be the same at all singular points.

In order to do the connections, we need the expressions $[k, l] = e^{\int_{z_k}^{z_l} i\sqrt{Q}dz}$. Note that the sheet of $i\sqrt{Q}(z)$ is defined by the cut locations, with the initial sheet determined by the fact that (z_1, z) is subdominant for $x \to +\infty$, meaning that $i\sqrt{Q}(z) = -real$ in this domain.

Carrying out the integrals then gives

$$[1,2] = e^{W/2}e^{iW/2}, \quad [1,3] = e^{iW}, \quad [2,3] = e^{-W/2}e^{iW/2} \tag{6}$$

where $W = E^{3/4}\int_{-1}^{1}\sqrt{1-u^4}du$, and $\int_{-1}^{1}\sqrt{1-u^4}du = 1.74804$.

Begin with a subdominant solution $\psi(z) = (Z_1, z)_s$ at large positive x and continue through the upper half plane above the singularity at $iE^{1/4}$ to large negative x. Choosing

the solution to be real for $x \to \infty$ and using the symmetry of the potential we have

$$Se^{-W} + Se^{iW} = -(-1)^n. \tag{7}$$

Also we find a condition for the vanishing of the dominant solution

$$e^W[1 + S^2] + 2S^2 cos(W) + e^{-W}S^2 = 0. \tag{8}$$

For large turning point separation W is large and we have a solution given by the isolated turning point values, $S = i$ and $W_n = (n + 1/2)\pi$, the usual approximate WKB solution. There is a natural perturbation expansion parameter given by the existence of the exponential term e^{-W}, present because of the additional singular points not on the real axis. Even for the lowest bound state as given by the WKB approximation $e^{-W_0} \simeq 0.2$, and for the next level $e^{-W_1} \simeq 0.009$.

Perturbing about the WKB value $W_n = (n + 1/2)\pi$ gives the solution

$$S = i\left[1 - cos(W_n)e^{-W_n} - \frac{e^{-2W_n}}{2}\right], \qquad cos(W) = -e^{-W_n}. \tag{9}$$

Thus $S = i(1 + e^{-2W}/2)$ and $sin(W) = (-1)^n\sqrt{1 - cos^2(W)} \simeq (-1)^n(1 - e^{-2W}/2)$.

Values of the exact energy levels, the WKB approximation, and the Phase Integral evaluation are shown in table I. For the ground state E_{PI} has a 4 percent error, E_{WKB} has a 20 percent error.

Table I. Energy Levels $\mathbf{Q = E - z^4}$

n	E_{exact}	E_{wkb}	$cos(W)$	E_{PI}
0	1.0604	0.8671	-0.207879	1.0246
1	3.7964	3.7519	-8.9833×10^{-3}	3.7424
2	7.45567	7.4139	-3.8820×10^{-4}	7.4144
3	11.6374	11.6114	-1.6776×10^{-5}	11.6114
4	16.2618	16.2335	-7.2495×10^{-7}	16.2335

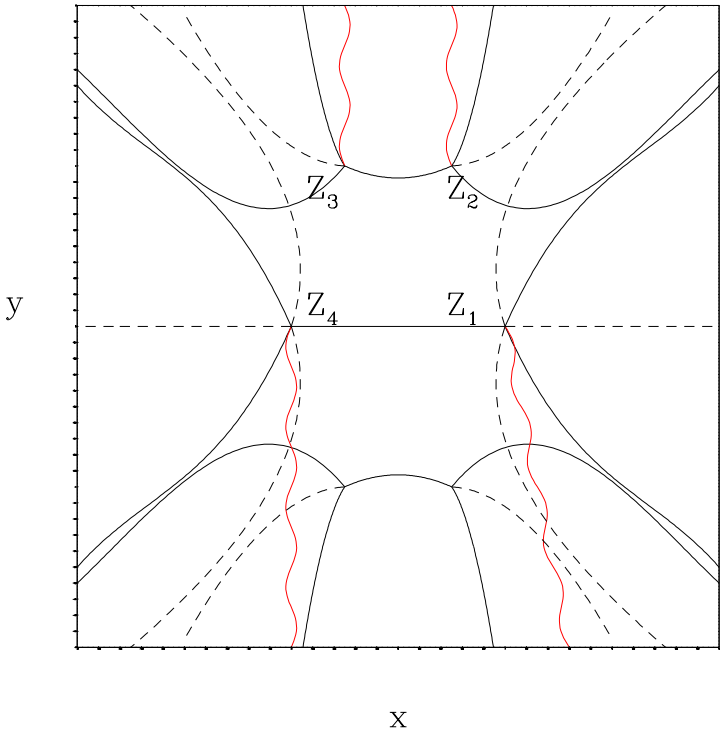

FIG. 3: Stokes plot for the bound state problem $Q = E - z^6$.

IV. A SIXTH ORDER POTENTIAL

Now consider an anharmonic oscillator, with more turning points in the complex plane, $Q(z) = E - z^6$. The Stokes structure is shown in Fig. 3 with first order zeros located at $Z_k = E^{1/6} e^{i(k-1)\pi/3}$ with $k = 1, 2, 3, 4, 5, 6$. We assume the Stokes constants to be the same at all singular points.

In order to do the connections, we need the expressions $[k, l] = e^{\int_{z_k}^{z_l} i\sqrt{Q} z dz}$. Note that the sheet of $i\sqrt{Q}(z)$ is defined by the cut locations, with the initial sheet determined by the fact that (z_1, z) is subdominant for $x \to +\infty$, meaning that $i\sqrt{Q}(z) = -real$ in this domain. Carrying out the integrals then gives

$$[1, 2] = e^{\sqrt{3}W/4} e^{iW/4}, \quad [3, 2] = e^{-iW/2}, \quad [3, 4] = e^{-\sqrt{3}W/4} e^{iW/4}, \tag{10}$$

where $W = E^{2/3} \int_{-1}^{1} \sqrt{1 - u^6} du$, and $\int_{-1}^{1} \sqrt{1 - u^6} du = 1.821488$.

Begin with a subdominant solution $\psi(z) = (Z_1, z)_s$ at large positive x and continue through the upper half plane above all singularities to large negative x. Choosing the solution to be real for $x \to \infty$ and using the symmetry of the potential, but also noting that

with the choice of cuts we have $Q^{1/4} = e^{i\pi/2}$ for large positive x and $Q^{1/4} = e^{-i\pi/2}$ for large negative x we find

$$(-1)^n i = 1 + S^2[1 + cos(W) + isin(W) + 2e^{-\sqrt{3}W/2}cos(W/2)]. \tag{11}$$

Also we find a condition for the vanishing of the dominant solution

$$1 + e^{\sqrt{3}W/2}cos(W/2) + S^2[e^{\sqrt{3}W/2} + 2cos(W/2) + e^{-\sqrt{3}W/2}]cos(W/2) = 0, \tag{12}$$

giving $S^2 = -1 + O(e^{-\sqrt{3}W})$.

For large turning point separation W is large and we have a solution given by the isolated turning point values, $S = i$ and $W_n = (n + 1/2)\pi$, the usual approximate WKB solution. A first order perturbation about the WKB value W_n gives the solution

$$S = i, \qquad cos(W) = -2e^{-\sqrt{3}W_n/2}cos(W_n/2). \tag{13}$$

It is interesting to note that these solutions break down at the second order, meaning that one or more of the Stokes constants has a second order correction not given by Eq. 12. Note that Eq. 12 is real, but expanding $sin(W)$ in Eq. 11 to give $sin(W) \simeq (-1)^n(1-cos(W)^2/2)$ gives an additional second order imaginary term, and there is no second order term to balance it, and we conclude that S^2 must possess an imaginary second order term, not given by Eq. 12.

Values of the exact energy levels, the WKB approximation, and the Phase Integral evaluation are shown in table II. For the ground state E_{PI} has a 4 percent error, E_{WKB} has a 30 percent error.

Table II. Energy Levels $\mathbf{Q = E - z^6}$

n	E_{exact}	E_{wkb}	$cos(W)$	E_{PI}
0	1.1448	0.8008	-0.36206	1.1009
1	4.3332	4.1612	2.3888×10^{-2}	4.1929
2	9.0731	8.9535	1.5727×10^{-3}	8.9508
3	14.9195	14.8316	-1.0354×10^{-4}	14.8314
4	21.7140	21.6224	-6.81617×10^{-6}	21.6224

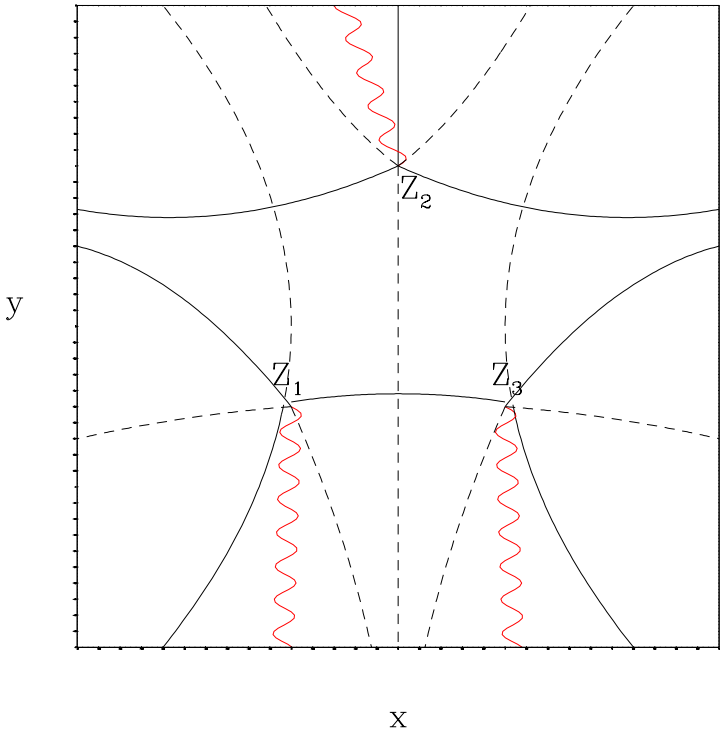

FIG. 4: Stokes plot for the bound state problem, $Q = E + (iz)^3$.

V. A NON HERMITIAN HAMILTONIAN

Non-Hermitian Hamiltonians having PT symnmetry have been shown to have real spectra, following a conjecture by D. Bessis that the spectrum of the Hamiltonian $H = p^2 + x^2 + ix^3$ is real and positive. A non-Hermitian Hamiltonian problem studied by Bender and Boettcher[6] is given by the function $Q(z) = E + (iz)^N$. The energy spectrum is positive because of symmetry under the product of parity and time reversal. As an example we take $N = 3$.

The Stokes diagram is shown in Fig. 4, with three singular points located at $E^{1/3}e^{i\pi/2}$, $E^{1/3}e^{-i\pi/6}$, and $E^{1/3}e^{-i5\pi/6}$. Subdominant regions include the positive and negative real axis for $|x| \to \infty$. We carry out the continuation in the upper half complex plane in order to take account of the singular point at Z_2.

In order to do the connections, we need the expressions $[k, l] = e^{\int_{z_k}^{z_l} i\sqrt{Q}zdz}$. Note that the sheet of $i\sqrt{Q}(z)$ is defined by the cut locations, with the initial sheet determined by the fact that (z_3, z) is subdominant for $x \to +\infty$, meaning that $i\sqrt{Q}(z) = -real$ in this domain.

Carrying out the integrals then gives

$$[1,2] = e^{\sqrt{3}W/2}e^{-iW/2}, \quad [1,3] = e^{-iW}, \quad [2,3] = e^{-\sqrt{3}W/2}e^{-iW/2} \tag{14}$$

where $W = E^{5/6}cos(\pi/6)\int_{-1}^{1}\sqrt{1-u^3}du$, and $\int_{-1}^{1}\sqrt{1-u^3}du = 1.68262$.

Begin for positive real x with $\psi(z) = (Z_3, z)_s$, and continue to large negative x, giving a subdominant and a dominant term, which we set to zero, giving

$$0 = e^{\sqrt{3}W}(1+S^2) + 2S^2cos(W) + e^{-\sqrt{3}W}S^2 \tag{15}$$

leaving

$$\psi(z) = -(Z_1, z)_s(Se^{-\sqrt{3}W} + Se^{iW}), \tag{16}$$

very similar to the equations found in section III, since the Stokes structure in the upper half plane is the same. In this case the differential equation is not real, but choosing symmetric integration paths from $x = 0$ asymptotically along the Stokes lines to the right and to the left, and using the symmetry of $Q(z)$ we again conclude that the phases of the solutions for large positive x and large negative x are equal within a sign.

The cut locations give the fact that whereas $Q^{1/4} = e^{i\pi/4}$ for large positive x, $Q^{1/4} = e^{i3\pi/4}$ for large negative x, so in fact choosing the eigenfunction to be real for $x \to +\infty$ and requiring that it be real for large negative x gives from Eq. 16 $cos(W) + e^{-\sqrt{3}W} = 0$. Again in this case the asymptotic value of the Stokes constant is given by $S = i + O(\epsilon^2)$ with $\epsilon = e^{-\sqrt{3}W}$.

The first few energy levels for $N = 3$, with WKB and numerical values given by Bender, and values from this Phase Integral analysis are given in Table III. The WKB ground state energy has an error of 6 percent, and the Phase Integral value an error of 0.6 percent.

Table III. Energy Levels $\mathbf{Q = E - iz^3}$

n	E_{exact}	E_{wkb}	$cos(W)$	E_{PI}
0	1.1562	1.09427	-6.5834×10^{-2}	1.1496
1	4.1092	4.08949	-2.8533×10^{-4}	4.0892
2	7.5621	7.54898	-1.2366×10^{-6}	7.54898
3	11.3143	11.3043	-5.3598×10^{-9}	11.3043
4	15.2916	15.2832	-2.3228×10^{-11}	15.2832

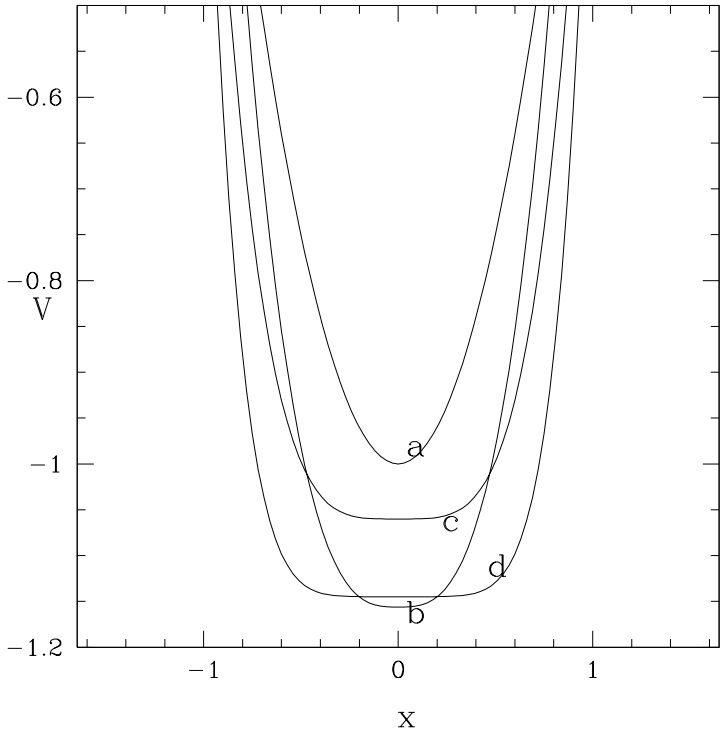

FIG. 5: Potentials for the four cases discussed, the harmonic oscillator associated with the Weber equation, $V = x^2 - E$, (a), the non-Hermitian potential $Q = E + (iz)^3$ (b), and the Hermitian anharmonic oscillators $V = x^4 - E$ (c), and $V = x^6 - E$ (d). The exact ground state energies were used for each plot.

VI. POTENTIALS

The four potentials for these cases are plotted in Fig. 5. The harmonic oscillator potential (a) $V(x) = z^2 - E$ and the two anharmonic oscillator potentials (c) $V(x) = z^4 - E$ and (d) $V(x) = z^6 - E$ are real on the real axis, $z = x$. The potential associated with $Q = E + (iz)^3$ (b) is real and subdominant along the lines $y = -|x|/\sqrt{3}$, giving $V(x) = |x|^3(\sqrt{3} - 1/3) - E$. The energies used in the plot are the ground state values. It is seen that the degree of distortion from the harmonic oscillator potential shape is inceasing larger for the $(iz)^3$ and the z^4 and z^6 cases, associated with the larger number of singularities in $Q(z)$ in addition to the two turning point singularities. We see that the error in the WKB energy levels increases with the deviation from the harmonic oscillator potential shape, along with a corresponding improvement of the Phase Integral evaluation over the WKB value.

VII. CONCLUSION

A proper use of Phase Integral methods can improve the eigenvalue determination for bound states significantly compared to a simple WKB evaluation. This improvement increases along with the increasing deviation of the potential shape from that of a harmonic oscillator. It is remarkable that the asymptotic value of the Stokes constant in each case is $S = i$, the value for an isolated first order zero. Of course the bound state energies do not form an open set, so S is not determined as an analytic function, only the values at the bound eigenstates are fixed. For all potentials possessing zeros or singularities in the complex plane in addition to the principal turning points, a small parameter is defined by $exp\int(i\sqrt{Q})dz$, with the integration taken from them to the principle turning points, allowing a perturbation expansion. No such parameter exists for the Weber equation.

It has not escaped the author's attention that with present day computing the numerically correct eigenvalues are easily obtained, so this result is only of theoretical interest.

Acknowledgement This work was partially supported by the U.S. Department of Energy Grant DE-AC02-09CH11466. The author acknowledges useful exchanges with Cheng Tang and constant encouragement from his grandson Enrico.

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