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Complex square well—a new exactly solvable quantum mechanical model

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Abstract. Recently, a class of \mathcal{PT} -invariant quantum mechanical models described by the non-Hermitian Hamiltonian $H = p^2 + x^2(ix)^\epsilon$ was studied. It was found that the energy levels for this theory are real for all $\epsilon \geq 0$. Here, the limit as $\epsilon \rightarrow \infty$ is examined. It is shown that in this limit, the theory becomes exactly solvable. A generalization of this Hamiltonian, $H = p^2 + x^{2M}(ix)^\epsilon$ ($M = 1, 2, 3, \dots$) is also studied, and this \mathcal{PT} -symmetric Hamiltonian becomes exactly solvable in the large- ϵ limit as well. In effect, what is obtained in each case is a complex analogue of the Hamiltonian for the square-well potential. Expansions about the large- ϵ limit are obtained.

1. Introduction

The infinite square-well potential,

$$V_{\text{SW}}(x) = \begin{cases} 0 & (|x| < 1) \\ 1 & (|x| = 1) \\ \infty & (|x| > 1) \end{cases} \quad (1.1)$$

is the simplest of all quantum potentials. It is studied at the beginning of any introductory class in quantum mechanics. This model is a useful teaching tool because the eigenvalues and eigenfunctions for this potential can all be found in closed form.

The infinite square-well potential can be regarded as the limiting case of a class of potentials of the form

$$V_M(x) = x^{2M} \quad (M = 1, 2, 3, 4, \dots). \quad (1.2)$$

Here, as $M \rightarrow \infty$, $V_M(x) \rightarrow V_{\text{SW}}(x)$.

The eigenvalues of the Hamiltonian for V_M ,

$$H = p^2 + x^{2M} \quad (1.3)$$

can only be found in closed form for the special case of the harmonic oscillator $M = 1$. For all other positive integer values of M there is no exact solution to these anharmonic oscillators. Thus, the only two exactly solvable cases known are the extreme lower and upper limits $M = 1$ and $M \rightarrow \infty$. The asymptotic behaviour of the eigenvalues of H in equation (1.3) for large M was studied in [1].

In a recent letter [2] the spectra of the class of non-Hermitian \mathcal{PT} -symmetric Hamiltonians of the form

$$H = p^2 + x^2(ix)^\epsilon \quad (\epsilon \geq 0) \quad (1.4)$$

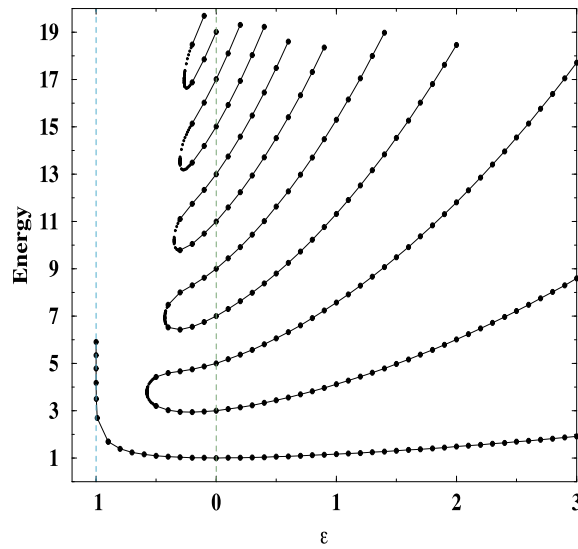


Figure 1. Energy levels of the Hamiltonian $H = p^2 + x^2(ix)^\epsilon$ as functions of the parameter ϵ . There are three regions: when $\epsilon \geq 0$ the spectrum is entirely real and positive. All eigenvalues rise monotonically with increasing ϵ . The lower bound of this region, $\epsilon = 0$, corresponds to the harmonic oscillator, whose energy levels are $E_k = 2k + 1$. When $-1 < \epsilon < 0$, there are a finite number of real positive eigenvalues and an infinite number of complex conjugate pairs of eigenvalues. As ϵ decreases from 0 to -1 , the number of real eigenvalues decreases. As ϵ approaches -1^+ , the ground-state energy diverges. For $\epsilon \leq -1$ there are no real eigenvalues.

were shown to be real and positive. It is believed that the reality and positivity of the spectra are a consequence of \mathcal{PT} symmetry. Here, the case $\epsilon = 0$ is again the harmonic oscillator. For finite values of ϵ larger than zero there is no exact analytical solution for the eigenvalues. However, solutions can be found by numerical integration; the eigenvalues of H in equation (1.4) as functions of ϵ are displayed in figure 1.

In the past we have always regarded the parameter ϵ as being small; we have defined theories by analytically continuing away from $\epsilon = 0$. However, in this paper we investigate the *large- ϵ* limit of the Hamiltonian in equation (1.4). We will show that in this limit the theory becomes exactly solvable. An exact formula for the k th energy level in the limit of large ϵ is

$$E_k(\epsilon) \sim \frac{1}{4} \left(k + \frac{1}{2}\right)^2 \epsilon^2 \quad (\epsilon \rightarrow \infty). \quad (1.5)$$

More generally, we consider the large- ϵ limit of an *infinite* number of classes of \mathcal{PT} -symmetric Hamiltonians of the form [3]

$$H = p^2 + x^{2M}(ix)^\epsilon \quad (\epsilon \geq 0, M = 1, 2, 3, \dots). \quad (1.6)$$

For each positive integer value of M , these Hamiltonians may be regarded as complex deformations of the Hermitian Hamiltonian $H = p^2 + x^{2M}$ in equation (1.3). In the limit as $\epsilon \rightarrow \infty$ each of these Hamiltonians becomes exactly solvable; the spectrum for large ϵ is given by

$$E_k(M, \epsilon) \sim \frac{1}{4} \left(k + \frac{P}{M+1}\right)^2 \epsilon^2 \quad (\epsilon \rightarrow \infty) \quad (1.7)$$

where $P = 1, 2, 3, \dots, M$.

For the Hamiltonian H in equation (1.6) the Schrödinger differential equation corresponding to the eigenvalue problem $H\psi = E\psi$ is

$$-\psi''(x) + x^{2M}(ix)^\epsilon \psi(x) = E\psi(x). \tag{1.8}$$

To obtain real eigenvalues from this equation it is necessary to define the boundary conditions properly. The regions in the cut complex- x plane in which $\psi(x)$ vanishes exponentially as $|x| \rightarrow \infty$ are wedges. In [2, 3] the wedges for $\epsilon > 0$ were chosen to be the analytic continuations of the wedges for the anharmonic oscillator ($\epsilon = 0$), which are centred about the negative and positive real axes and have angular opening $\pi/(M+1)$. This analytic continuation defines the boundary conditions in the complex- x plane. For arbitrary $\epsilon > 0$ the anti-Stokes' lines at the centres of the left and right wedges lie below the real axis at the angles

$$\begin{aligned} \theta_{\text{left}} &= -\pi + \frac{\epsilon\pi}{4M + 2\epsilon + 4} \\ \theta_{\text{right}} &= -\frac{\epsilon\pi}{4M + 2\epsilon + 4}. \end{aligned} \tag{1.9}$$

The opening angle of each of these wedges is $2\pi/(2M + \epsilon + 2)$. In [2, 3] the time-independent Schrödinger equation was integrated numerically inside the wedges to determine the eigenvalues to high precision. Observe that as ϵ increases from its anharmonic oscillator value ($\epsilon = 0$), the wedges bounding the integration path undergo a continuous deformation as a function of ϵ . As ϵ increases, the opening angles of the wedges become smaller and both wedges rotate downward towards the negative-imaginary axis. Also, note that the angular difference $\theta_{\text{right}} - \theta_{\text{left}} = 2\pi(M + 1)/\epsilon$ approaches zero as ϵ increases.

This paper is organized very simply. In section 2 we consider the special case $M = 1$ in equation (1.4). Then in section 3 we generalize to the case of arbitrary integer M in equation (1.6). Finally, in section 4 we examine expansions about the $\epsilon \rightarrow \infty$ limit of the theory.

2. Special case $M = 1$

The eigenvalues of H in equation (1.4) can be found approximately using WKB theory. The left and right turning points for this calculation lie inside the left and right wedges at

$$\begin{aligned} x_{\text{left}} &= E^{1/(2+\epsilon)} \exp\left(-i\pi + \frac{\epsilon}{2\epsilon + 4}i\pi\right) \\ x_{\text{right}} &= E^{1/(2+\epsilon)} \exp\left(-\frac{\epsilon}{2\epsilon + 4}i\pi\right). \end{aligned} \tag{2.1}$$

As explained in [2], the WKB quantization formula is

$$(k + \frac{1}{2})\pi \sim \int_{x_{\text{left}}}^{x_{\text{right}}} dx \sqrt{E - x^2(ix)^\epsilon} \quad (k \rightarrow \infty) \tag{2.2}$$

where the path of integration is a curve from the left turning point to the right turning point along which the quantity dx times the integrand of equation (2.2) is *real*. This path lies in the lower-half x plane and is symmetric with respect to the imaginary axis. The path resembles an inverted parabola; it emerges from the left turning point and rises monotonically until it crosses the imaginary axis; it then falls monotonically until it reaches the right turning point. As calculated in [2], the WKB quantization formula (2.2) gives

$$E_k \sim \left[\frac{\Gamma\left(\frac{3\epsilon+8}{2\epsilon+4}\right) \sqrt{\pi} \left(k + \frac{1}{2}\right)}{\sin\left(\frac{\pi}{\epsilon+2}\right) \Gamma\left(\frac{\epsilon+3}{\epsilon+2}\right)} \right]^{\frac{2\epsilon+4}{\epsilon+4}} \quad (k \rightarrow \infty). \tag{2.3}$$

When the parameter ϵ is large, the right-hand side of equation (2.3) simplifies dramatically and we have the result in equation (1.5) with corrections of order $\epsilon \ln \epsilon$. As we will see, this happens to be the exact answer for all energy levels; that is, for *all* values of k . Since the WKB formula in equation (2.3) is only valid for large k with ϵ fixed, it is not at all obvious why the leading-order WKB calculation gives the exact answer.

It is surprising to learn that the energy levels grow as ϵ^2 for large ϵ . Recall that the energy levels of the Hamiltonian in equation (1.3) approach finite limits as $M \rightarrow \infty$. (These limits are the energy levels of the conventional square well V_{SW} in equation (1.1).) To understand why the energy levels for the \mathcal{PT} -symmetric Hamiltonian in equation (1.4) grow as ϵ^2 we use the uncertainty principle. From equation (2.1) we see that the turning points rotate towards each other as $\epsilon \rightarrow \infty$. (They both approach the point $-i$ on the negative imaginary axis.) Indeed, the distance between the turning points is of order $1/\epsilon$. (For the case of the Hamiltonian H in equation (1.3) the turning points stabilize at ± 1 as $M \rightarrow \infty$.) Thus, the quantum particle is trapped in a region whose size Δx is of order $1/\epsilon$. The uncertainty in the momentum Δp of the particle is, therefore, of order ϵ . Finally, since the energy is the square of the momentum, we conclude that the energy levels must be of order ϵ^2 .

Let us rederive this result using the time-energy version of the uncertainty principle. As explained in [2, 3], a *classical* particle described by the Hamiltonian in equation (1.4) exhibits periodic motion. The period T of this complex pendulum is given exactly by the formula

$$T = 4\sqrt{\pi} E^{-\frac{\epsilon}{4+2\epsilon}} \frac{\Gamma\left(\frac{3+\epsilon}{2+\epsilon}\right) \cos\left(\frac{\epsilon\pi}{4+2\epsilon}\right)}{\Gamma\left(\frac{4+\epsilon}{4+2\epsilon}\right)}. \quad (2.4)$$

For large ϵ we have

$$T \sim 4\pi/(\epsilon\sqrt{E}) \quad (\epsilon \rightarrow \infty). \quad (2.5)$$

Multiplying this equation by E gives the product ET on the left-hand side, which, by the uncertainty principle is of order 1. Thus, solving for E , we find again that E is of order ϵ^2 for large ϵ .

This last calculation illustrates an important difference between conventional quantum theories and \mathcal{PT} -symmetric quantum theories. In a conventional Hermitian theory both the classical periodic motion and the WKB path of integration coincide; this *classically allowed* region lies on the real axis between the turning points. For \mathcal{PT} -symmetric theories the WKB contour and the classical path do not coincide. The classical periodic motion follows a path joining the turning points that, like the WKB path, is symmetric about the negative imaginary axis. However, unlike the WKB path, the classical path moves *downward* rather than upward as it approaches the negative-imaginary axis (see, for example, figure 2 of [3]).

Having discussed this problem heuristically, we now give a precise calculation of the spectrum in the limit of large ϵ . We begin by substituting

$$x = \left(-i + \frac{z\pi}{2+\epsilon}\right) E^{\frac{1}{2+\epsilon}} \quad (2.6)$$

into equation (1.8) with $M = 1$. The resulting differential equation[†] for large ϵ is

$$\frac{d^2}{dz^2} \psi(z) + F\pi^2(1 + e^{iz\pi})\psi(z) = 0 \quad (2.7)$$

where

$$F = E/\epsilon^2 \quad (2.8)$$

[†] The Schrödinger equation (2.7) for the complex square well is the analogue of the infinite square well, i.e. the large- M limit in the Schrödinger equation obtained from the Hamiltonian in equation (1.3). But in contrast to the simple trigonometric wavefunctions for the infinite square well, the wavefunctions for the complex square well are given by Bessel functions (see equation (2.13)).

and we have used the identity $\lim_{\epsilon \rightarrow \infty} (1 + x/\epsilon)^\epsilon = e^x$.

The advantage of the differential equation (2.7) is that it is independent of ϵ . (As such, this equation corresponds to the M -independent Schrödinger equation for the square well that is obtained from equation (1.3) in the limit of large M .) In the variable z the turning points at $z = -1$ and 1 are fixed and well separated in the limit of large ϵ . The large- ϵ behaviour of E in equation (1.5) is already evident in equation (2.8). Imposing the appropriate boundary conditions on equation (2.7) gives eigenvalues F that are clearly independent of ϵ . Thus, for large ϵ we see that E grows like ϵ^2 .

Because there is no longer any small parameter in equation (2.7), this equation cannot be solved approximately using a perturbative method such as WKB. It is necessary to solve this equation exactly. Fortunately, we can solve it exactly by making a simple substitution. The change of variable

$$w = 2\sqrt{F}e^{i\pi z/2} \quad (2.9)$$

converts equation (2.7) to a modified Bessel equation [4]:

$$w^2 \frac{d^2}{dw^2} \psi(w) + w \frac{d}{dw} \psi(w) - (w^2 + v^2) \psi(w) = 0 \quad (2.10)$$

where

$$v = 2\sqrt{F}. \quad (2.11)$$

The exact solution to this equation is a linear combination of modified Bessel functions [4]:

$$\psi(w) = C_1 I_v(w) + C_2 K_v(w) \quad (2.12)$$

where C_1 and C_2 are arbitrary constants. Thus, in terms of the z variable we have

$$\psi(z) = C_1 I_v(v e^{i\pi z/2}) + C_2 K_v(v e^{i\pi z/2}). \quad (2.13)$$

We must now impose boundary conditions on $\psi(z)$. Emanating from the turning points at $z = -1$ and 1 are three Stokes' lines (lines along which the solution is purely oscillatory and not growing or falling exponentially) and three anti-Stokes' lines (lines along which the solution is purely exponential and not oscillatory). These Stokes' and anti-Stokes' lines are shown as dashed and solid curves on figure 2. The Stokes' lines emerge from the turning points going up to the left and the right at 30° and also directly down. The anti-Stokes' lines emerge from the turning points going down to the left and the right at 30° and directly up. Note that the Stokes' line going up to the right from the turning point at $z = -1$ joins continuously onto the Stokes' line going up to the left from the turning point at $z = 1$. The anti-Stokes' lines going down to the left from $z = -1$ and down to the right from $z = 1$ eventually become vertical and asymptote to the lines $\text{Re } z = -2$ and $\text{Re } z = 2$. We impose the boundary conditions that $\psi(z) \rightarrow 0$ on these anti-Stokes' lines because these correspond to the centre lines of the wedges in equation (1.9) in the complex- x plane (for $M = 1$).

To summarize, in the large- ϵ limit of the Hamiltonian in equation (1.4), the eigenvalue problem for the scaled eigenvalues F is a two-turning-point problem that lies along an arch-shaped contour. The legs of the arches lie below the real- z axis and approach $\pm 2 - i\infty$. The turning points at $z = \pm 1$ are joined by the Stokes' line lying above the real- z axis as indicated in figure 2. This is the complex version of the infinite square-well problem in elementary quantum mechanics. In the square-well problem there are also two turning points at ± 1 joined by a Stokes' line lying on the real axis. However, there are no anti-Stokes' lines along which the wavefunction dies away exponentially; the wavefunction simply vanishes at the turning points.

The quantized energy levels are determined by imposing the boundary conditions discussed above on the modified Bessel functions in equation (2.13). For simplicity, we

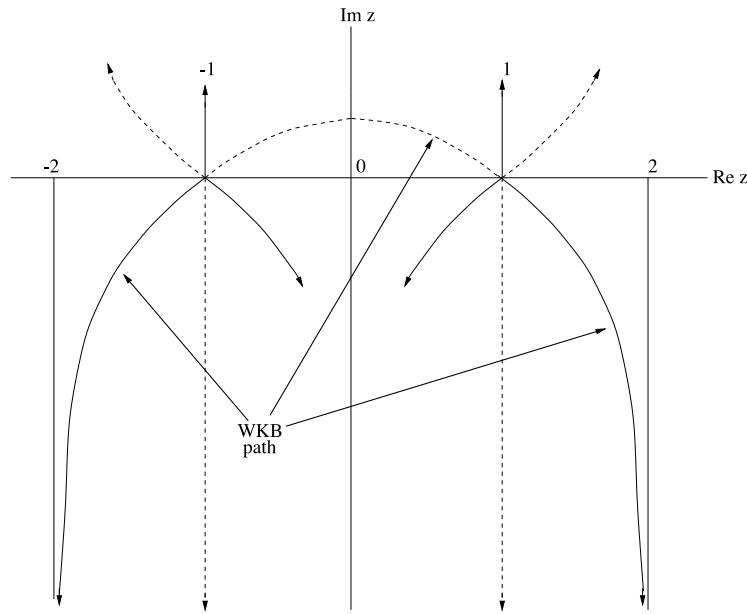


Figure 2. Stokes' lines and anti-Stokes' lines for the differential equation (2.7). Three Stokes' lines (dashed) and three anti-Stokes' lines (solid) emerge from the turning points at $z = \pm 1$. The path of integration for the WKB quantization condition in equation (2.2) corresponds to the arch-shaped dotted curve connecting the turning points.

impose these conditions on the vertical lines $z = \pm 2 - iy$, where $y \rightarrow +\infty$. In terms of the variable y the wavefunction ψ in equation (2.13) becomes

$$\psi(y) = C_1 I_\nu(\nu e^{-i\pi} e^{\pi y/2}) + C_2 K_\nu(\nu e^{-i\pi} e^{\pi y/2}) \quad (2.14)$$

at $z = -2 - iy$, and

$$\psi(y) = C_1 I_\nu(\nu e^{i\pi} e^{\pi y/2}) + C_2 K_\nu(\nu e^{i\pi} e^{\pi y/2}) \quad (2.15)$$

at $z = 2 - iy$.

Our objective now is to simplify these equations by making the arguments of the modified Bessel equations entirely real and positive. To do so we use the following functional equations satisfied by I_ν and K_ν [4]:

$$\begin{aligned} I_\nu(e^{m\pi i} z) &= e^{m\nu\pi i} I_\nu(z) \\ K_\nu(e^{m\pi i} z) &= e^{-m\nu\pi i} K_\nu(z) - i\pi \frac{\sin(m\nu\pi)}{\sin(\nu\pi)} I_\nu(z) \end{aligned} \quad (2.16)$$

where m is an integer. According to these relations, equation (2.14) becomes

$$\psi(y) = C_1 e^{-\nu\pi i} I_\nu(\nu e^{\pi y/2}) + C_2 [e^{\nu\pi i} K_\nu(\nu e^{\pi y/2}) + i\pi I_\nu(\nu e^{\pi y/2})] \quad (2.17)$$

and equation (2.15) becomes

$$\psi(y) = C_1 e^{\nu\pi i} I_\nu(\nu e^{\pi y/2}) + C_2 [e^{-\nu\pi i} K_\nu(\nu e^{\pi y/2}) - i\pi I_\nu(\nu e^{\pi y/2})]. \quad (2.18)$$

Next, we use the asymptotic behaviour of the modified Bessel functions for large positive argument. The function $I_\nu(r)$ grows exponentially and the function $K_\nu(r)$ decays exponentially

Table 1. Comparison of the numerical values of $F(\epsilon)$ with that predicted in equation (2.22) for the ground state $k = 0$ of an $x^2(ix)^\epsilon$ theory. The second column gives the exact values of the ground-state energy for various values of ϵ in the first column. The third column gives the values of F obtained from the exact energy in the second column using equation (4.1), which is a more precise version of equation (2.8). Finally, in the fourth and fifth columns the first and second Richardson extrapolants [5] of the numbers in the third column are given. Note that the exact values of $F(\epsilon)$ and their Richardson extrapolants rapidly approach the asymptotic value $\frac{1}{16} = 0.0625$.

ϵ	$E_0(\epsilon)$	$F(\epsilon)$	$R_1(\epsilon)$	$R_2(\epsilon)$
8	5.553 31	0.078 25	—	—
18	20.676 29	0.069 98	0.063 36	—
28	46.943 24	0.067 42	0.062 81	0.062 59
38	84.787 28	0.066 17	0.062 66	0.062 53
48	134.437 52	0.065 42	0.062 60	0.062 51
58	196.034 17	0.064 93	0.062 57	0.062 51

for large positive r [4]:

$$\begin{aligned}
 I_\nu(r) &\sim \frac{1}{\sqrt{2\pi r}} e^r & (r \rightarrow +\infty) \\
 K_\nu(r) &\sim \sqrt{\frac{\pi}{2r}} e^{-r} & (r \rightarrow +\infty).
 \end{aligned}
 \tag{2.19}$$

Eliminating the growing exponentials in equations (2.17) and (2.18) gives a pair of linear equations to be satisfied by the coefficients C_1 and C_2 :

$$\begin{aligned}
 C_1 e^{-\nu\pi i} + C_2 i\pi &= 0 \\
 C_1 e^{\nu\pi i} - C_2 i\pi &= 0.
 \end{aligned}
 \tag{2.20}$$

A nontrivial solution to equation (2.20) exists only if the determinant of the coefficients vanishes:

$$\det \begin{pmatrix} e^{-\nu\pi i} & i\pi \\ e^{\nu\pi i} & -i\pi \end{pmatrix} = -2i\pi \cos(\nu\pi) = 0.
 \tag{2.21}$$

Hence, $\nu = k + \frac{1}{2}$, and from equation (2.11), we have the *exact* result

$$F = \frac{1}{4} (k + \frac{1}{2})^2 \quad (k = 0, 1, 2, 3, \dots).
 \tag{2.22}$$

Finally, we use equation (2.8) to obtain the large- ϵ behaviour of the eigenvalues E given in equation (1.5). We verify this result numerically in table 1.

3. Arbitrary integer M

The calculation of the energy levels for the general class of theories given in equation (1.6) is a straightforward generalization of the calculation for the case $M = 1$ in section 2. The crucial ingredient in the calculation is understanding the array of Stokes' and anti-Stokes' lines along which we impose the boundary conditions. This difference leads to M -dependent wavefunctions, but the condition that determines the eigenvalues is still a simple trigonometric equation.

Just as for the case $M = 1$, we scale the differential equation (1.8) using equation (2.6). In the limit as $\epsilon \rightarrow \infty$ the resulting differential equation is identical to equation (2.7) except that now there is a factor of $(-1)^{M+1}$ multiplying the exponential term. Again, we define F as

in equation (2.8) and change to the variable w as prescribed by equation (2.9). This gives the differential equation

$$w^2 \frac{d^2}{dw^2} \psi(w) + w \frac{d}{dw} \psi(w) - [(-1)^{M+1} w^2 + \nu^2] \psi(w) = 0 \quad (3.1)$$

which is the generalization of equation (2.10). In this equation ν is defined as before by equation (2.11). Note that except for the appearance of the $(-1)^{M+1}$ multiplying the w^2 term this equation is independent of M .

To solve equation (3.1) we consider the two cases of odd M and even M separately. If M is odd this equation is identical to equation (2.10), and the general solution is that given in equation (2.12). If M is even, equation (3.1) is no longer a modified Bessel equation, but instead is just the standard Bessel equation. Hence, in this case the general solution to equation (3.1) is a linear combination of the ordinary Bessel functions J_ν and Y_ν :

$$\psi(w) = C_1 J_\nu(w) + C_2 Y_\nu(w). \quad (3.2)$$

Thus, in terms of the variable z the wavefunction in this case is

$$\psi(z) = C_1 J_\nu(\nu e^{i\pi z/2}) + C_2 Y_\nu(\nu e^{i\pi z/2}). \quad (3.3)$$

Although it appears that this solution is independent of the parameter M , one must recall that the boundary conditions do depend on M . Thus, the wavefunctions and energy eigenvalues do indeed depend on M . To be precise, for a given M the Stokes' lines emanating from $z = \pm M$ are joined by a string of adjacent arches of length 2. The anti-Stokes' lines leave $\pm M$ and asymptote to the lines $\text{Re } z = \pm(M + 1)$.

For odd M we impose the boundary conditions as for the case $M = 1$ except that the wavefunction ψ vanishes along different lines. For even M the wavefunctions in equation (3.3) must first be expressed in terms of modified Bessel functions using the functional equations [4]

$$\begin{aligned} J_\nu(iz) &= e^{v\pi i/2} I_\nu(z) \\ Y_\nu(iz) &= \frac{-2}{\pi} e^{-v\pi i/2} K_\nu(z) + i e^{v\pi i/2} I_\nu(z) \end{aligned} \quad (3.4)$$

and then be treated using the same procedure as for odd M .

Although the matrix elements for the linear equations obtained for odd M and even M are quite different, the eigenvalue conditions are similar. For $M = 2$ the condition is

$$\cos(2\nu\pi) = -\frac{1}{2} \quad (3.5)$$

whose solution is

$$\nu = k + \frac{1}{3} \quad \text{and} \quad \nu = k + \frac{2}{3}. \quad (3.6)$$

Thus, for large ϵ the energy is given by

$$E = \frac{1}{4} \left(k + \frac{P}{3} \right)^2 \epsilon^2 \quad (3.7)$$

where $P = 1, 2$. Note that this result is the $M = 2$ case of equation (1.7). This expression is verified numerically in table 2 for the case of the ground state energy corresponding to $k = 0$ and $P = 1$. For arbitrary M one obtains the result in equation (1.7).

Observe that the magnitude of the energy eigenvalues decreases as M increases. At first glance this might seem surprising, but it can be easily understood in terms of the uncertainty principle. As M increases, the anti-Stokes' lines on which we impose the boundary conditions for the differential equation (1.8) move away from the negative imaginary axis, as we can see from equation (1.9). For example, for fixed ϵ the anti-Stokes' lines for $M = 2$ are separated by a greater distance than for $M = 1$; the anti-Stokes' lines for $M = 3$ are separated by a greater

Table 2. Comparison of the numerical values of $F(\epsilon)$ with that predicted in equation (3.7) for the ground state $k = 0, P = 1$ of an $x^4(ix)^\epsilon$ theory. The second column gives the exact values of the ground-state energy for various values of ϵ in the first column. The third column gives the values of F obtained from the energy in the second column using equation (4.1). Finally, in the fourth and fifth columns the first and second Richardson extrapolants [5] of the numbers in the third column are given. Note that the exact values of $F(\epsilon)$ and their Richardson extrapolants rapidly approach the asymptotic value $\frac{1}{36} = 0.0277778$.

ϵ	$E_0(\epsilon)$	$F(\epsilon)$	$R_1(\epsilon)$	$R_2(\epsilon)$
8	2.651 28	0.050 35	—	—
18	9.214 77	0.035 51	0.026 61	—
28	20.705 25	0.032 32	0.027 22	0.027 40
38	37.320 10	0.030 97	0.027 46	0.027 66
48	59.168 65	0.030 23	0.027 56	0.027 72
58	86.317 66	0.029 77	0.027 64	0.027 75

distance than for $M = 2$, and so on. Hence, the uncertainty in the position Δx increases with M . By the uncertainty principle, this increase in the uncertainty of the position corresponds to a decrease in the uncertainty of the momentum, and thus, a decrease in the energy. This argument explains the large- M behaviour of the result in equation (1.7).

4. Higher-order corrections to the $\epsilon \rightarrow \infty$ limit for $M = 1$

In this section we show how to calculate the corrections to the large- ϵ behaviour in equation (1.5). These corrections are of order ϵ and $\epsilon \ln \epsilon$. From these higher-order calculations we obtain an extremely accurate approximation E_k for all k . Our asymptotic analysis begins with the change of variable in equation (2.6), but we use a more precise version of equation (2.8):

$$F(\epsilon) = \frac{E^{\frac{\epsilon+4}{\epsilon+2}}}{(\epsilon + 2)^2}. \tag{4.1}$$

We find that the function $F(\epsilon)$ is a series in inverse powers of ϵ of the form $F = f_0 + f_1\epsilon^{-1} + f_2\epsilon^{-2} + \dots$. The coefficient $f_0 = F(\infty)$ is given in equation (2.22). Our objective here is to calculate f_1 , and from this to calculate the first correction to E .

In addition to $F(\epsilon)$, the wavefunction ψ is also a series in inverse powers of ϵ , $\psi(z) = \psi_0 + \psi_1(z)\epsilon^{-1} + \psi_2(z)\epsilon^{-2} + \dots$. Using this series and collecting like powers of ϵ we obtain the following sequence of differential equations:

$$\begin{aligned} \epsilon^0 : \frac{d^2}{dz^2} \psi_0(z) + f_0\pi^2(1 + e^{iz\pi})\psi_0(z) &= 0 \\ \epsilon^{-1} : \frac{d^2}{dz^2} \psi_1(z) + f_0\pi^2(1 + e^{iz\pi})\psi_1(z) &= - \left[f_0\pi^2 e^{iz\pi} \frac{z^2}{2} + f_1(1 + e^{iz\pi}) \right] \pi^2 \psi_0(z) \\ \epsilon^{-2} : \frac{d^2}{dz^2} \psi_2(z) + f_0\pi^2(1 + e^{iz\pi})\psi_2(z) &= - \left[f_0\pi^2 e^{iz\pi} \frac{z^2}{2} + f_1(1 + e^{iz\pi}) \right] \pi^2 \psi_1(z) \\ &\quad - \left[f_0 e^{iz\pi} \left(z^2 \pi^2 + z^3 \pi^3 i - \frac{z^4 \pi^4}{8} \right) + f_1 e^{iz\pi} \frac{z^2 \pi^2}{2} + f_2(1 + e^{iz\pi}) \right] \pi^2 \psi_0(z). \end{aligned} \tag{4.2}$$

The first equation is exactly equation (2.7). The second equation contains the coefficient f_1 . To solve for f_1 we observe that the solution to the homogeneous part of the equation is just the solution to the first equation. This suggests using the method of reduction of order; to wit, we let $\psi_1(z) = u_1(z)\psi_0(z)$. To solve the resulting equation for f_1 we then multiply by $\psi_0(z)$ and integrate over the WKB path with respect to z . The first equation can be used to

Table 3. Comparison of the numerical value of the coefficient f_1 in equation (4.6) with a fit to the exact values of $F(\epsilon)$ for the case of the ground state $k = 0$ of an $x^2(ix)^\epsilon$ theory. The second column gives the exact values of the ground-state energy for various values of ϵ in the first column. The third column gives the approximation to f_1 obtained from $F(\epsilon)$ by subtracting off the leading large- ϵ behaviour given in equation (2.22). In the fourth and fifth columns the first and second Richardson extrapolants [5] of the numbers in the third column are given. Note that the approximations in the third column and their Richardson extrapolants rapidly approach the asymptotic value of $f_1 = \gamma/4 = 0.144\,304$.

ϵ	$E_0(\epsilon)$	$R_0(\epsilon)$	$R_1(\epsilon)$	$R_2(\epsilon)$
8	5.553 31	0.125 97	—	—
18	20.676 29	0.134 60	0.141 50	—
28	46.943 24	0.137 67	0.143 21	0.143 89
38	84.787 28	0.139 26	0.143 72	0.144 18
48	134.437 52	0.140 24	0.143 94	0.144 25
58	196.034 17	0.140 90	0.144 06	0.144 28

simplify this equation and the left-hand side becomes the expression $u_1(z)\psi_0^2(z)$ evaluated at the end points. Since $\psi_0(-i\infty) = 0$, the left-hand side equals zero, and we can solve for f_1 in quadrature form. To be explicit,

$$f_1 = -\frac{1}{2} f_0 \pi^2 \frac{\int_{-2-i\infty}^{2-i\infty} dz z^2 \psi_0^2(z) e^{iz\pi}}{\int_{-2-i\infty}^{2-i\infty} dz \psi_0^2(z) (1 + e^{iz\pi})}. \quad (4.3)$$

To prepare for evaluating these integrals we change to the variable w in equation (2.9) with $F = f_0$ and obtain

$$f_1 = \frac{1}{2} \frac{\int_{-\infty+i\delta}^{-\infty-i\delta} dw w \psi_0^2(w) \ln^2\left(\frac{w}{2\sqrt{f_0}}\right)}{\int_{-\infty+i\delta}^{-\infty-i\delta} \frac{dw}{w} \psi_0^2(w) \left(1 + \frac{w^2}{4f_0}\right)} \quad (4.4)$$

where δ is infinitesimal and the contour of integration goes around the origin.

For the case $k = 0$ these integrals are easy to evaluate because $f_0 = \frac{1}{16}$ and $\psi_0(w) = I_{1/2}(w) + K_{1/2}(w)/\pi = e^w/\sqrt{2\pi w}$. Substituting these expressions into equation (4.4) gives

$$f_1 = \frac{1}{2} \frac{\int_{-\infty+i\delta}^{-\infty-i\delta} dw e^{2w} \ln^2(2w)}{\int_{-\infty+i\delta}^{-\infty-i\delta} dw e^{2w} \left(4 + \frac{1}{w^2}\right)}. \quad (4.5)$$

By carefully evaluating the discontinuities across the branch cut and the residues at the singularities of the integrands, we obtain

$$f_1 = \gamma/4 \quad (4.6)$$

where γ is Euler's constant. Combining this result with equation (4.1) and solving for E in the limit of large ϵ yields

$$E = \frac{1}{16}\epsilon^2 - \frac{1}{4}\epsilon \ln \epsilon + \frac{1}{4}(1 + \gamma + 2 \ln 2)\epsilon + O(\ln \epsilon). \quad (4.7)$$

By comparison, if we calculate to next order in WKB, we obtain for the k th energy level:

$$E_k \sim \left[\frac{\Gamma\left(\frac{8+3\epsilon}{4+2\epsilon}\right) \sqrt{\pi} \left(k + \frac{1}{2}\right)}{\sin\left(\frac{\pi}{2+\epsilon}\right) \Gamma\left(\frac{3+\epsilon}{2+\epsilon}\right)} \right]^{\frac{4+2\epsilon}{4+\epsilon}} \left[1 + \frac{(2+\epsilon)(1+\epsilon) \sin\left(\frac{2\pi}{2+\epsilon}\right)}{6\pi \left(k + \frac{1}{2}\right)^2 (4+\epsilon)^2} \right] \quad (k \rightarrow \infty). \quad (4.8)$$

Taking the large- ϵ limit of this expression gives

$$E = \frac{\epsilon^2}{16} - \frac{1}{4}\epsilon \ln \epsilon + \frac{1}{4} \left(\frac{7}{3} + \ln 2 \right) \epsilon + O(\ln \epsilon). \quad (4.9)$$

The appearance of a $\log \epsilon$ term in this behaviour is a consequence of the structure of equation (4.1). Note that the coefficient of the ϵ term for WKB differs from the exact result but WKB is numerically very accurate. WKB gives 0.756 62 compared with 0.740 88 for the exact result.

In table 3 the results of a Richardson extrapolation [5] of the exact values of $F(\epsilon)$ are given. These results verify that the value of f_1 is correct.

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