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New quasi-exactly solvable sextic polynomial potentials

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Abstract

A Hamiltonian is said to be *quasi-exactly solvable* (QES) if some of the energy levels and the corresponding eigenfunctions can be calculated exactly and in a closed form. An entirely new class of QES Hamiltonians having sextic polynomial potentials is constructed. These new Hamiltonians are different from the sextic QES Hamiltonians in the literature because their eigenfunctions obey $\mathcal{PT}$ symmetry rather than Hermitian boundary conditions. These new Hamiltonians present a novel problem that is not encountered when the Hamiltonian is Hermitian: it is necessary to distinguish between the parametric region of unbroken $\mathcal{PT}$ symmetry, in which all of the eigenvalues are real, and the region of broken $\mathcal{PT}$ symmetry, in which some of the eigenvalues are complex. The precise location of the boundary between these two regions is determined numerically using the extrapolation techniques and analytically using the WKB analysis.

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1. Sextic QES Hamiltonians

The purpose of this paper is to introduce a new class of quasi-exactly solvable (QES) Hamiltonians having sextic polynomial potentials. While these new kinds of QES Hamiltonians have positive, real eigenvalues, they have not yet been discussed in the literature because they are not Hermitian. Instead, they are $\mathcal{PT}$ symmetric.

The term *quasi-exactly solvable* (QES) is used to describe a quantum-mechanical Hamiltonian when a finite portion of its energy spectrum and associated eigenfunctions can be found exactly and in a closed form [1]. Typically, QES potentials depend on a parameter J, and for positive integer values of J one can find exactly the first J eigenvalues and eigenfunctions, usually of a given parity. It has been shown that QES systems can be classified by using an algebraic approach in which the Hamiltonian is expressed in terms of the generators of a Lie algebra [2–5].

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Perhaps the simplest example of a QES Hamiltonian having a sextic potential is [6, 7]

$$H = p^2 + x^6 - (4J - 1)x^2, \tag{1}$$

where J is a positive integer. For each positive integer value of J, the time-independent Schrödinger equation for this Hamiltonian,

$$-\psi''(x) + [x^6 - (4J - 1)x^2]\psi(x) = E\psi(x), \tag{2}$$

has J even-parity eigenfunctions in the form of an exponential times a polynomial:

$$\psi(x) = \mathrm{e}^{-x^4/4} \sum_{k=0}^{J-1} c_k x^{2k}. \tag{3}$$

The polynomial coefficients c_k $(0 \leqslant k \leqslant J - 1)$ satisfy the recursion relation

$$4(J - k)c_{k-1} + Ec_k + 2(k + 1)(2k + 1)c_{k+1} = 0, \tag{4}$$

where we define $c_{-1} = c_J = 0$. The simultaneous linear equations (4) have a nontrivial solution for $c_0, c_1, \ldots, c_{J-1}$ if the determinant of the coefficients vanishes. This determinant is a polynomial of degree J in the variable E. The roots of this polynomial are all real and are the J quasi-exact energy eigenvalues of the Hamiltonian (1). Note that all of the QES eigenfunctions (3) of H in (1) have the form of a decaying exponential $\exp\left(-\frac{1}{4}x^4\right)$ multiplying a polynomial. This is the standard form in the literature for the eigenfunctions of any QES Hamiltonian whose potential is a polynomial.

The QES Hamiltonians associated with Hermitian Hamiltonians have been examined in depth and classified exhaustively [1]. However, in 1998 new kinds of Hamiltonians that have positive real energy levels were discovered [8, 9]. These new kinds of Hamiltonians are not Hermitian ($H \neq H^\dagger$) in the usual Dirac sense, where the Dirac adjoint symbol † represents combined transpose and complex conjugation. Instead, these Hamiltonians possess $\mathcal{PT}$ symmetry $H = H^{\mathcal{PT}}$; that is, they remain invariant under combined space and time reflection. This new class of non-Hermitian Hamiltonians has been studied heavily[2] [10, 11] and it has been shown that when the $\mathcal{PT}$ symmetry is not broken, such Hamiltonians define unitary theories of quantum mechanics [13]

The key difference between Hermitian Hamiltonians and complex, non-Hermitian, $\mathcal{PT}$-symmetric Hamiltonians is that with $\mathcal{PT}$-symmetric Hamiltonians the boundary conditions on the eigenfunctions (the solutions to the time-independent Schrödinger equation) are imposed in wedges in the complex plane. Sometimes these wedges do not include the real axis. (A detailed discussion of the complex asymptotic behaviour of solutions to eigenvalue problems may be found in [14].)

The discovery of $\mathcal{PT}$-symmetric Hamiltonians was followed immediately by the discovery of a new class of QES models. Until 1998 it was thought that if the potential associated with a QES Hamiltonian was a polynomial, then this polynomial had to be at least sextic; its degree could not be less than six. This property is in fact true for Hamiltonians that are Hermitian. However, in 1998 it was discovered that it is possible to have a QES *non-Hermitian* complex Hamiltonian whose potential is *quartic* [15]:

$$H = p^2 - x^4 + 2\mathrm{i}ax^3 + (a^2 - 2b)x^2 + 2\mathrm{i}(ab - J)x. \tag{5}$$

Here, a and b are real parameters and J is a positive integer. In [16] the Hamiltonian (5) is generalized to include a centrifugal term of the form $\mathrm{i}d/x + L(L + 1)/x^2$. For a large region of the parameters a and b, the energy levels of this family of quartic Hamiltonians are real,

[2] An excellent summary of the current status and the background of non-Hermitian and $\mathcal{PT}$-symmetric Hamiltonians may be found in [12].

discrete, and bounded below, and the quasi-exact portion of the spectra consists of the lowest J eigenvalues. Like the eigenvalues of the Hamiltonian (1), the lowest J eigenvalues of these potentials are the roots of a Jth-degree polynomial.[3]

The reality of the eigenvalues of H in (5) is ensured by the boundary conditions that its eigenfunctions are required to satisfy. The eigenfunctions are required to vanish as $|x| \to \infty$ in the complex-x plane inside two wedges called *Stokes wedges*. The right wedge is bounded above and below by lines at 0° and -60° and the left wedge is bounded above and below by lines at -180° and -120°. The leading asymptotic behaviour of the wavefunction inside these wedges is given by

$$\psi(x) \sim \mathrm{e}^{-\mathrm{i}x^3/3} \quad (|x| \to \infty). \tag{6}$$

The new class of QES sextic Hamiltonians reported in this paper has the form

$$H = p^2 + x^6 + 2ax^4 + (4J - 1 + a^2)x^2, \tag{7}$$

where J is a positive integer and a is a real parameter. These Hamiltonians are very similar in structure to those in (1) and to the other QES sextic Hamiltonians discussed in the literature [1], but their distinguishing characteristic is that the asymptotic behaviour of their eigenfunctions in the complex-x plane is different.

Let us examine first the asymptotic behaviour of the eigenfunction solutions to the Schrödinger equation (2). For brevity, we call the eigenfunctions in (3) the *good* solutions to (2) because they satisfy the physical requirement of being quadratically integrable. These good solutions decay exponentially like $\exp\left(-\frac{1}{4}x^4\right)$ as $x \to \pm\infty$, while the corresponding linearly independent *bad* solutions grow exponentially like $\exp\left(\frac{1}{4}x^4\right)$ as $x \to \pm\infty$. In the complex-x plane the good solutions (3) decay exponentially as $|x| \to \infty$ in two Stokes wedges that are centred about the positive and the negative real-x axes. These wedges have an angular opening of 45°. The bad solutions grow exponentially in these wedges. At the upper and lower edges of these wedges the good and bad solutions cease to decay and to grow exponentially and they become purely oscillatory.

As we move downward past the lower edges of these wedges, we enter a new pair of Stokes wedges. These wedges also have a 45° angular opening and are centred about the lines $\arg x = -45^\circ$ and $\arg x = -135^\circ$. In these lower wedges, the good solutions grow exponentially as $|x| \to \infty$ and thus they behave like a bad solution.

In the lower pair of wedges we can find solutions to the new class of Hamiltonians in (7) that behave like good solutions. These new $\mathcal{PT}$-symmetric eigenfunctions have the general form of the exponential $\exp(\frac{1}{4}x^4 + \frac{1}{2}ax^2)$ multiplied by a polynomial:[4]

$$\psi(x) = \mathrm{e}^{x^4/4 + ax^2/2} \sum_{k=0}^{J-1} c_k x^{2k}. \tag{8}$$

Hamiltonians having even sextic polynomial potentials are special because such Hamiltonians can be *either* Hermitian or $\mathcal{PT}$-symmetric depending on whether the eigenfunctions are required to vanish exponentially in the 45° wedges containing the positive and negative real-x axes or in the other pair of 45° wedges contiguous to and lying just below

[3] For a nonpolynomial QES $\mathcal{PT}$-symmetric Hamiltonian see [17].

[4] Note that $\psi(x)$ in (8) is a function of x^2 and thus all of the QES wavefunctions are symmetric under parity reflection $(x \to -x)$. In general, $\mathcal{PT}$-symmetric Hamiltonians, such as $H = p^2 - x^4$, are not symmetric under parity reflection because the parity operator $\mathcal{P}$ changes the complex domain of the Hamiltonian operator. As a consequence, the expectation value of the x operator is nonvanishing (see [18]). Nevertheless, the special QES eigenfunctions in (8) *are* parity-symmetric. We believe that the parity operator may therefore be used to distinguish between the QES and the non-QES portions of the Hilbert space.

these wedges in the complex-x plane. In [19] complex sextic potentials were examined but the wavefunctions exhibited the conventional asymptotic behaviour $\exp\left(-\frac{1}{4}x^4\right)$ rather than the new asymptotic behaviour in (8). We thank M Znojil for pointing this out to us. The solutions for these two different boundary conditions are somewhat related. Specifically, a good solution in one pair of wedges becomes a bad solution in the other pair of wedges. However, a bad solution in one pair of wedges does not become a good solution in the other pair of wedges, as we now explain.

Given a good solution $\psi_{\rm good}(x)$ in one pair of wedges, we use the method of reduction of order [20] to find the bad solution. We seek a bad solution in the form $\psi_{\rm bad}(x) = \psi_{\rm good}(x)u(x)$, where $u(x)$ is an unknown function to be determined. Substituting the bad solution into the Schrödinger equation $-\psi''(x)+V(x)\psi(x) = E\psi(x)$, we get the differential equation satisfied by $u(x)$:

$$\psi_{\rm good}(x)u''(x) + 2\psi'_{\rm good}(x)u'(x) = 0. \tag{9}$$

We solve this equation by multiplying by the integrating factor $\psi_{\rm good}(x)$ and obtain the result

$$\psi_{\rm bad}(x) = \psi_{\rm good}(x)\left(\int^x {\rm d}s[\psi_{\rm good}(s)]^{-2} + C\right), \tag{10}$$

where C is an arbitrary constant.

This bad solution always grows exponentially in the two wedges in which the good solution decays exponentially. How does this bad solution behave in the other pair of wedges in which the good solution grows exponentially? We can always choose the constant C so that the bad solution vanishes as $|x| \to \infty$ in *one* of these two wedges. However, in the other of the two wedges, the bad solution will always grow exponentially. Thus, while the good solution becomes bad as we cross from one pair of wedges to the other, the bad solution does not become good.

2. Determination of the $\mathcal{PT}$ boundary

The difference between the Hermitian Hamiltonians in (1) and the $\mathcal{PT}$-symmetric Hamiltonians in (7) is that the Hermitian Hamiltonians always have real eigenvalues. The $\mathcal{PT}$-symmetric Hamiltonians in (7) have real eigenvalues only if the $\mathcal{PT}$ symmetry is unbroken; if the $\mathcal{PT}$ symmetry is broken, some of the eigenvalues will be complex. Thus, it is crucial to determine whether the $\mathcal{PT}$ symmetry is broken. We will see that there is a range of values of the parameter a in (7) for which the energy levels are real and this is the region of unbroken $\mathcal{PT}$ symmetry. Outside this region some of the eigenvalues appear as complex-conjugate pairs.

Let us illustrate the difference between the regions of broken and unbroken $\mathcal{PT}$ symmetry by examining some special solutions of the Schrödinger equation

$$-\psi''(x) + [x^6 + 2ax^4 + (4J - 1 + a^2)x^2]\psi(x) = E\psi(x), \tag{11}$$

corresponding to H in (7). First, consider the case $J = 1$. The unique eigenfunction solution to (11) of the form in (8) is $\psi(x) = \exp\left(\frac{1}{4}x^4 + \frac{1}{2}ax^2\right)$ and the corresponding eigenfunction is $E = -a$. Note that E is real so long as a is real. Thus, for $J = 1$ there is no region of broken $\mathcal{PT}$ symmetry.

Next, consider the case $J = 2$. Now, there are two eigenfunctions. The two eigenvalues are given by

$$E = -3a \pm 2\sqrt{a^2 - 2}. \tag{12}$$

Table 1. Critical values, $[a_{\rm crit}(J)]^2$, of the parameter a^2 listed as a function of J. When a^2 is greater than this critical value, the eigenvalues of the $\mathcal{PT}$-symmetric Hamiltonian H in (7) are all real. Thus, this is the region of unbroken $\mathcal{PT}$ symmetry. The $\mathcal{PT}$ symmetry is broken when $a^2 < [a_{\rm crit}(J)]^2$. Note that the differences between successive values of $[a_{\rm crit}(J)]^2$ appear to be approaching a limit and this is indeed the case. In fact, the numerical value of this limit is exactly 12. Thus for large J, the critical values have the simple asymptotic behaviour $[a_{\rm crit}(J)]^2 \sim 12J$.

J	$[a_{\rm crit}(J)]^2$	$[a_{\rm crit}(J+1)]^2 - [a_{\rm crit}(J)]^2$
2	2	
3	10.587 470 0363	8.587 470 0363
4	20.551 533 4397	9.964 063 4033
5	31.053 455 2654	10.501 921 8257
6	41.851 956 9727	10.798 501 7073
7	52.840 939 0328	10.988 982 0601
8	63.963 634 8939	11.122 695 8611
9	75.185 875 5649	11.222 240 6710
10	86.485 395 1835	11.299 519 6186
11	97.846 807 2286	11.361 412 0451
12	109.259 033 5351	11.412 226 3065
13	120.713 791 3596	11.454 757 8245
14	132.204 725 9144	11.490 934 5548
15	143.726 846 1067	11.522 120 1923
16	155.276 172 0922	11.549 306 4512
17	166.849 402 0446	11.573 229 9524
18	178.443 911 7241	11.594 509 6795
19	190.057 407 9492	11.613 496 2251
20	201.688 027 3595	11.630 619 3103

Thus, there is now an obvious transition between real eigenvalues (unbroken $\mathcal{PT}$ symmetry) and complex eigenvalues (broken $\mathcal{PT}$ symmetry). Evidently, the eigenvalues are real if $a \geqslant \sqrt{2}$ or if $a \leqslant -\sqrt{2}$.

We find that for any positive integer value of $J > 1$, the eigenvalues E for H in (7) are entirely real if a^2 is greater than some critical value $[a_{\rm crit}(J)]^2$ that depends on J. These critical values up to $J = 20$ are shown in table 1.

Observe from table 1 that the critical values of $[a_{\rm crit}]^2$ grow monotonically with increasing J. We have therefore also calculated the differences between successive critical values of a^2. These differences also grow monotonically with increasing J, but they appear to be levelling off and seem to be approaching a limiting value. To see whether the differences are indeed approaching a limiting value as J increases, we have plotted in figure 1 these differences as a function of $1/J$. This plot suggests that the differences tend to the value 12 as $J \to \infty$.

To determine whether it is true that these differences really do approach limit 12, it is necessary to extrapolate the sequence of differences to its value at $J = \infty$. To do so we have calculated the Richardson extrapolants [20] of the sequence of differences. The *first* Richardson extrapolants, $R_1(J)$, of these differences are listed in table 2. Observe that the sequence $R_1(J)$ rises more slowly and quite convincingly appears to be approaching the value 12. The differences $R_1(J+1) - R_1(J)$ between successive Richardson extrapolants are also shown.

To test further the hypothesis that $R_1(J)$ tends to the limiting value 12 as $J \to \infty$, we have calculated successive Richardson extrapolants of the Richardson extrapolants $R_1(J)$ in table 2. The successive extrapolants are listed in Table 3 and they provide very strong numerical

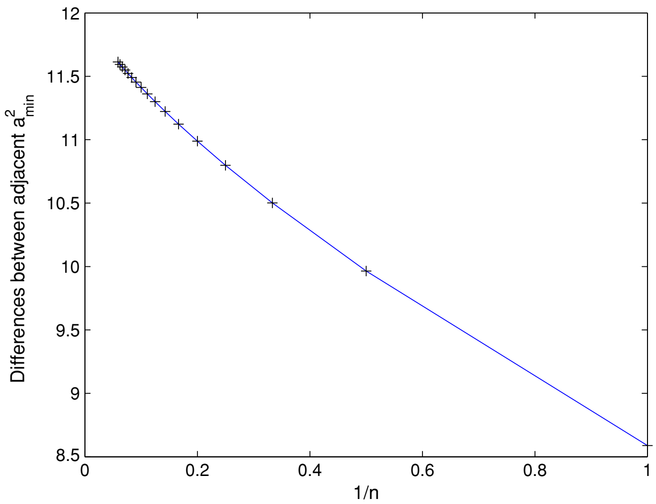

Figure 1. The differences $[a_{\rm crit}(J+1)]^2 - [a_{\rm crit}(J)]^2$ taken from table 1 plotted as a function of $1/J$. Observe that as J increases, these differences tend towards the limiting value 12.

Table 2. First Richardson extrapolants $R_1(J)$ of the sequence of differences $[a_{\rm crit}(J+1)]^2 - [a_{\rm crit}(J)]^2$ taken from table 1. Note that $R_1(J)$ rises slowly and smoothly towards its limiting value 12. The differences between successive Richardson extrapolants are also listed.

J	$R_1(J)$ series	$R_1(J+1) - R_1(J)$
1	11.340 656 7704	
2	11.577 638 6705	0.236 981 90
3	11.688 241 3518	0.110 602 68
4	11.750 903 4718	0.062 662 12
5	11.791 264 8657	0.040 361 40
6	11.819 509 5305	0.028 244 66
7	11.840 472 2516	0.020 962 72
8	11.856 551 4577	0.016 079 21
9	11.869 554 6582	0.013 003 20
10	11.880 073 0055	0.010 518 35
11	11.888 878 5336	0.008 805 52
12	11.896 347 9526	0.007 469 42
13	11.902 771 7144	0.006 423 76
14	11.908 360 9386	0.005 589 23
15	11.913 272 8866	0.004 911 95
16	11.917 627 1918	0.004 354 30

evidence that $\lim_{J\to\infty}\left([a_{\rm crit}(J+1)]^2 - [a_{\rm crit}(J)]^2\right) = 12$. From this we conclude that for large J the asymptotic behaviour of the critical value of a^2 is given by

$$[a_{\rm crit}(J)]^2 \sim 12J \quad (J \to \infty). \tag{13}$$

Our numerical analysis provides convincing evidence that for large J the boundary between the regions of broken and unbroken $\mathcal{PT}$ symmetry is given by the asymptotic behaviour in (13). We will now verify this result analytically by using WKB methods [20]. From our numerical analysis we know that the first eigenvalues to become complex conjugate pairs are always the highest, and this implies that WKB is the appropriate tool for investigating the $\mathcal{PT}$ boundary for large J.

Table 3. Repeated Richardson extrapolants of the sequence of Richardson extrapolants in Table 2. This table provides strong and convincing numerical evidence that Richardson extrapolants $R_1(J)$ tend to the limiting value 12 as $J \to \infty$. This implies that for large J the critical values of a^2 grow linearly with J (see equation (13)).

J	$R_1(J)$	R of $R_1(J)$	R of R of $R_1(J)$	R of R of R of $R_1(J)$
1	11.340 656 7704	11.814 620 5706	12.004 272 8584	11.991 279 2745
2	11.577 638 6705	11.909 446 7145	11.997 776 0665	11.986 964 6719
3	11.688 241 3518	11.938 889 8318	11.994 172 2683	11.988 773 2331
4	11.750 903 4718	11.952 710 4409	11.992 822 5095	11.997 845 9499
5	11.791 264 8657	11.960 732 8547	11.993 827 1976	11.948 363 0075
6	11.819 509 5305	11.966 248 5785	11.986 249 8326	12.116 806 5542
7	11.840 472 2516	11.969 105 9005	12.004 900 7928	11.837 703 1045
8	11.856 551 4577	11.973 580 2620	11.984 001 0818	12.098 246 0411
9	11.869 554 6582	11.974 738 1309	11.996 694 9661	11.972 635 6846
10	11.880 073 0055	11.976 933 8144	11.994 289 0380	11.998 315 6753
11	11.888 878 5336	11.978 511 5620	11.994 655 0959	
12	11.896 347 9526	11.979 856 8565		
13	11.902 771 7144			

For the potential $V(x) = x^6 + 2ax^4 + (a^2 + 4J - 1)x^2$, the leading-order WKB quantization condition, valid for large n, is

$$\left(2n + \tfrac{1}{2}\right)\pi \sim \int_{T_1}^{T_2} \mathrm{d}x \sqrt{E_n - V(x)} \quad (n \to \infty), \tag{14}$$

where $T_{1,2}$ are the turning points. Note that there is a factor of $2n + \frac{1}{2}$, rather than $n + \frac{1}{2}$, on the left side of this asymptotic relation because we are counting *even*-parity eigenfunctions.

For large $n = J$ we approximate the integral in (14) by making the asymptotic substitution $a \sim \sqrt{J}b$, where b is a number to be determined. In order to verify the asymptotic behaviour in (13), we must show that $b = \sqrt{12}$. We then make the scaling substitutions

$$x = yJ^{1/4} \qquad \text{and} \qquad E_J \sim FJ^{3/2} \tag{15}$$

because for large J we can then completely eliminate all dependence on J from the integral. We thus obtain the condition

$$2\pi = \int_{y=U_1}^{U_2} \mathrm{d}y \sqrt{F - [y^6 + 2by^4 + (b^2+4)y^2]}, \tag{16}$$

where $U_{1,2} = T_{1,2}J^{-1/4}$ are zeros of the algebraic equation

$$y^6 + 2by^4 + (b^2+4)y^2 - F = 0. \tag{17}$$

Next, following the analysis in [7], we assume that in this large-J limit the polynomial in (17) factors as

$$(y^2 - \alpha)^2(y^2 - \beta) = 0. \tag{18}$$

The correctness of this factorization assumption will be verified in the subsequent analysis. We then expand (18);

$$y^6 - y^4(\beta + 2\alpha) + y^2(\alpha^2 + 2\alpha\beta) - \alpha^2\beta = 0. \tag{19}$$

Comparing coefficients of like powers of y in (17) and (19), we obtain the three equations

$$F = \alpha^2\beta, \tag{20}$$

$$2b = -2\alpha - \beta, \tag{21}$$

$$b^2 + 4 = \alpha^2 + 2\alpha\beta. \tag{22}$$

Subtracting the square of equation (21) from three times (22), we get $\beta-\alpha = \pm\sqrt{b^2 - 12}$, and solving this equation simultaneously with (21), we get expressions for α and β:

$$3\alpha = -2b - \sqrt{b^2 - 12}, \tag{23}$$

$$3\beta = -2b + 2\sqrt{b^2 - 12}. \tag{24}$$

We then substitute (23) and (24) into (20) to obtain

$$F = -\tfrac{2}{27}(b - \sqrt{b^2 - 12})(2b + \sqrt{b^2 - 12})^2. \tag{25}$$

Finally, we calculate the value of the number b. Our procedure is simply to show that the special choice $b^2 = 12$ is consistent with the limiting WKB integral in (16). With this choice we can see from (23) and (24) that $\alpha = \beta = 4/\sqrt{3}$ and that (16) reduces to

$$2\pi = \int_{y=-\alpha}^{\alpha} \mathrm{d}y(\alpha - y^2)^{3/2} = 2\int_{y=0}^{\alpha} \mathrm{d}y(\alpha - y^2)^{3/2}. \tag{26}$$

We simplify this integral by making the substitution $y = \sqrt{u\alpha}$, and obtain

$$\tfrac{3}{8}\pi = \int_{u=0}^{1} \mathrm{d}u\, u^{-1/2}(1 - u)^{3/2}, \tag{27}$$

which is an exact identity. Thus, we may conclude that $b^2 = 12$. This verifies the asymptotic formula in (13) for the location of the $\mathcal{PT}$ boundary.

Furthermore, we can see that $F = \frac{64}{9}\sqrt{3} \approx 12.3$. Thus, we obtain a formula for the large-J asymptotic behaviour of the largest QES eigenvalue at the $\mathcal{PT}$ boundary:

$$E_J \sim \tfrac{64}{9}\sqrt{3}J^{3/2} \quad (J \to \infty). \tag{28}$$

The difference between this WKB calculation and that done in [7] for the Hermitian QES sextic Hamiltonian (1) is that here we have a critical value, $b = \sqrt{12}$, or $a \sim \sqrt{12J}$. This critical value defines the boundary between the regions of broken and unbroken $\mathcal{PT}$ symmetry for the $\mathcal{PT}$-symmetric Hamiltonian in (7). There is no analogue of this boundary for Hermitian Hamiltonians.

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