Uncommonly accurate energies for the general quartic oscillator

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Recent advances in the asymptotic analysis of energy levels of potentials produce relative errors in
eigenvalue sums of order $10^{-33}$, but few non-trivial potentials have been solved numerically to such
accuracy. We solve the general quartic potential (arbitrary linear combination of $x^4$ and $x^2$) beyond
this level of accuracy using a basis of several hundred oscillator states. We list the lowest 20 eigenvalues
for 9 such potentials. We confirm the known asymptotic expansion for the levels of the pure quartic
oscillator, and extract the next 2 terms in the asymptotic expansion. We give analytic formulas for
expansion in up to 3 even basis states. We confirm the virial theorem for the various energy components
to similar accuracy. The sextic oscillator levels are also given. These benchmark results should be useful
for extreme tests of approximations in several areas of chemical physics and beyond.

1. INTRODUCTION

Since the early days of quantum mechanics, potentials
with analytic solutions have played a crucial role in providing
both insight into more complex problems, and benchmarks
for more general quantum solution methods [1, 2]. The
quartic oscillator is iconic in being a simple potential without
a built-in length scale which does not have a simple analytic
solution [3–7]. The general quartic oscillator (adding both
quadratic and linear terms) is not scale-invariant, and has
been studied in many different contexts in physics [8–10].
In particular, the Mexican hat shape of symmetric double
wells is a paradigm of simple symmetry breaking [8, 11].

In chemical physics, the double well provides important
tests of theories of tunneling in quantum nuclear dynamics
of liquids [8, 11, 12]. In particle physics, it is a prototype of
symmetry breaking, such as occurs in simple field theories
[13, 14]. In mathematical physics, it is a simple case to test
and explore asymptotic approximations [15]. Asymptotic
analysis, especially hyperasymptotics, can yield exquisitely
accurate approximations [16–19]. In the past, many develop-
ments and tests of these methods have been applied to
scale invariant potentials [20–22], but the general quartic
oscillator provides opportunities to look at more complex
cases.

Recent work on one-dimensional potentials [20–22] has
established a deep explicit connection between the gradient
expansion of density functional theory and asymptotic ex-
pansions in powers of $\hbar$ [23]. In one case fractional errors
were below the picoyocto range, i.e., of order $10^{-33}$ [22].
To further develop and test methods in this area, there is
a need for benchmark calculations of this level of accuracy
for non-trivial potentials. This exceeds even quadruple pre-
cision on standard computers, rendering standard numerical
algorithms, even pushed to their convergence limits, difficult to apply. There is also a new area of application:
The breaking of symmetry is a simple prototype of a bond
breaking, in which electrons localize in two separate wells
[24]. Such bond breaking is very difficult to model with standard semi-local density functionals, and their failure has
been traced back to the change in asymptotic expansions in
going from one well to two[21]. In some simple situations,
benchmark electronic structure calculations have been per-
fomed to this level of accuracy (or higher) for systems with
a few electrons [25]. But the purpose of the present study
(and many previous ones) is to explore the underlying princi-
pies behind asymptotic (and other) approximation schemes,
so as to improve the accuracy of less expensive quantum
solvers, such as density functional theory, which can then
be applied to much larger systems. The benchmark data
here provides a quick reference for those exploring basic
questions with analytic one-dimensional models.

![Ground state densities (solid) and potentials (dashed). Legend: $\lambda = 0$ (blue), $\lambda = \lambda_c$ (magenta), $\lambda = 4$
(orange).](image)

FIG. 1. Ground state densities (solid) and potentials
dashed). Legend: $\lambda = 0$ (blue), $\lambda = \lambda_c$ (magenta), $\lambda = 4$
(orange).

In order to generate such benchmarks and as a simple
example, we consider the generalized quartic oscillator po-
tential:

$$v_\lambda(x) = \frac{x^4}{4} - \lambda \frac{x^2}{2}, \quad (1)$$

where $\lambda$ is a real number, either positive or negative. For
$\lambda = 0$, this is a pure quartic oscillator, which has been
the subject of many investigations. In this paper we will
present the pure quartic oscillator energies for more states
and to more digits than previously computed in Refs. [3–
5]. We also numerically examine the WKB series for the
quartic oscillator closely following Bender & Orszag’s book
[3]. Previous investigations of the WKB approximation of
the quartic oscillator can be found in Refs. [9, 26–29]. We examine the variation of the energy with \( \lambda \) and the effect of a linear term as in Ref. [9]. Our exact energies can be used as inputs to test the semiclassical analysis of Ref. [30]. Other methods of estimating quartic oscillator energies are described in Refs. [3, 4, 29, 31–33]. The exact solution of the quartic oscillator was studied in Refs. [6, 7]. For \( \lambda < 0 \), the minimum is always at \( x = 0 \), with vibrational frequency \( \sqrt{\lambda} \). For \( \lambda > 0 \), the most interesting case, two distinct wells appear, with minima at \( \pm \sqrt{\lambda} \), and frequency \( \sqrt{2\lambda} \). Fig. 1 illustrates some results, showing the density of the ground state and the well for three values of \( \lambda \): 0, \( \lambda_c \), (the critical value of \( \lambda \) at which the ground state energy is zero), and 4. The first is similar in shape to a harmonic oscillator, but with steeper walls, and the density decays more rapidly. The second is particularly flat, as the energy is exactly zero. The third is a typical double-well structure, with two well-localized densities on each side, and a small ‘overlap’ at \( x = 0 \). Thus there is a transition from one well to two, and simple symmetry breaking. Following the behavior of asymptotic expansions with the variation of \( \lambda \) is a toy problem relevant to many fields [15].

In this paper, we show how to calculate extremely accurate results for these potentials using a symbolic manipulation code, such as Mathematica, where manipulations can be performed with an arbitrary number of digits. We summarize results in the main text, and provide some analysis of various regimes. In the supplementary information, we give many tables of results to many digits of accuracy.

2. MOTIVATION

How can energy calculations to 40 decimal places possibly be of practical use? Modern density functional calculations use approximations that have errors larger than 1 kcal/mol, which is of order \( 10^{-5} \) of the total energy of a Ne atom, say. So even 1000 heavy atoms need only 9 digits of accuracy. However, the fundamental approximation behind almost all modern density functional approximations is the gradient expansion. Recent work [20–22] has shown a direct explicit connection between that expansion and summations of the WK expansion, order-by-order. The simplest identification of such asymptotic expansions is to find many terms explicitly, including the asymptotic behavior of the coefficients, and test their accuracy order-by-order with exact results. Because of the extreme accuracy of modern asymptotic methods, these comparisons have involved 33 decimal places in similar cases (linear half-well).

To date, only simple analytic forms have been studied: the harmonic oscillator, particle in a box, the Poschl-Teller well, and the linear half-well [20], all of which have special properties due to their analytic forms. There are many special cases where quasi-analytic solutions are known, such as Ref. [34], but one needs to be able to smoothly approach the semiclassical limit, in which the number of levels diverges. Moreover, we seek techniques that ultimately will be applied to arbitrary (possibly numerically defined) potentials, so those with analytic solutions might always be special cases. The quartic oscillator model studied here contains simple single- and double-well structures that provide numerous examples of parabolic minima (the most generic case) that have no analytic solutions, making them ideal for application of these new methods, but only if extremely accurate results are easily available.

While it may appear that the results in this paper could be easily generated using Mathematica with a single desktop in a short time, the usefulness of this work is in the careful benchmarking of the results, the combined analysis of many different aspects, and the inclusion of asymptotic results, which are unfamiliar to many computational scientists. But the greatest value is likely to be the ability of the many disparate theorists in many fields to extract highly accurate results instantly, without having to reperform the calculations [31].

3. METHOD

Our Schrödinger equation is (in units where \( \hbar = m = 1 \))

\[
-\frac{1}{2} \frac{d^2 \psi}{dx^2} + v(x) \psi(x) = \epsilon \psi(x),
\]

so all energies are in Hartrees, all distances in Bohr radii. We expand the eigenfunctions in a basis of harmonic oscillator states, where \( \omega \) can be freely chosen. The Hamiltonian is pentadiagonal, with only a few non-zero matrix elements no more than 2 double-steps off the diagonal. The nonzero matrix elements of the Hamiltonian in the harmonic basis are \( H_{n,n+2k} = h_k \sqrt{n+2k} / 16 \omega^2 \) where \( h_2 = 1 \) and

\[
\begin{align*}
\hat{h}_0 &= 4 \omega(\omega^2 - \lambda)(2n + 1) + 3(2n^2 + 2n + 1), \\
\hat{h}_1 &= 2[2n + 3 - 2\omega(\lambda + \omega^2)],
\end{align*}
\]

and we use the shorthand

\[
\alpha_p = \prod_{m=1}^{p} (\alpha + m), \quad \alpha_0 = 1.
\]

We closely follow Ref. 5 and use the Eigensystem function in Mathematica to diagonalize this matrix for various values of \( \lambda \) and choices of \( \omega \) [35]. We denote by \( N_B \) the number of basis functions included in the calculation (both odd and even, since we did not take advantage of parity). Our default choice of \( |\omega|/N_B \) is \([2/200]\) but we use \([2/400]\) as a baseline for ‘exact’ energies, and report errors relative to those values.

A special case is \( \epsilon = 0 \) for the ground state (magenta in Fig. 1). This happens at \( \lambda = \lambda_c \) which we found using a golden section search to be 1.398258545529855302585947187218312604396, at which the ground state energy is \(-3.955 \times 10^{-41}\). For a different way of finding energies of oscillators of order \( x^{2M} \) using exact quantization conditions see Refs. [32, 33], for an approach using lower bounds see Ref. [31].
4. RESULTS

In this section, we report many different results that may be of interest to different communities under different circumstances. In each case, we also provide a minimal analysis.

4.1. Energetics for different potentials

Here, we simply survey the behavior of the energies and eigenfunctions for various values of $\lambda$. Our focus is primarily on positive values of $\lambda$, which produce the Mexican hat double-well potential.

<table>
<thead>
<tr>
<th>$m$</th>
<th>$\lambda = -1$</th>
<th>$\lambda = 0$</th>
<th>$\lambda = 2$</th>
<th>$\lambda = 4$</th>
</tr>
</thead>
<tbody>
<tr>
<td>0</td>
<td>0.62092703</td>
<td>0.42080497</td>
<td>-0.29952137</td>
<td>-2.66144807</td>
</tr>
<tr>
<td>1</td>
<td>2.02596616</td>
<td>1.50790124</td>
<td>0.04637108</td>
<td>-2.65173172</td>
</tr>
<tr>
<td>2</td>
<td>3.69845032</td>
<td>2.95879569</td>
<td>1.22797281</td>
<td>-0.51029304</td>
</tr>
<tr>
<td>3</td>
<td>5.55777114</td>
<td>4.62122032</td>
<td>2.45984143</td>
<td>0.04637108</td>
</tr>
<tr>
<td>4</td>
<td>7.56842287</td>
<td>6.45350993</td>
<td>3.69845032</td>
<td>0.54300452</td>
</tr>
<tr>
<td>5</td>
<td>9.70914788</td>
<td>8.42845388</td>
<td>5.55777114</td>
<td>0.54300452</td>
</tr>
<tr>
<td>6</td>
<td>11.96454362</td>
<td>10.52783077</td>
<td>7.36888889</td>
<td>0.54300452</td>
</tr>
<tr>
<td>7</td>
<td>14.3236520</td>
<td>12.73833694</td>
<td>9.28322263</td>
<td>0.54300452</td>
</tr>
<tr>
<td>8</td>
<td>16.77645279</td>
<td>15.04975393</td>
<td>11.31134968</td>
<td>0.54300452</td>
</tr>
<tr>
<td>9</td>
<td>19.31695430</td>
<td>17.45393416</td>
<td>13.44312537</td>
<td>0.54300452</td>
</tr>
</tbody>
</table>

TABLE I. The energies at various values of $\lambda$. See Table S1 for more values of $\lambda$, more states, and more digits.

Our first results are the energetics of the first several eigenstates of the generalized quartic oscillator. These values are given to 8 digits in Table I for four values of $\lambda$. In Table S1 in the supplementary information, we give 40 digits for 9 values of $\lambda$ for the first 20 eigenvalues. Here $\lambda = 0$ corresponds to the pure quartic oscillator. As $\lambda$ grows, the eigenvalues inside the double well come in pairs, with ever smaller splitting.

![FIG. 2. First three eigenfunctions (orange, red, magenta) with potentials (blue) at various values of $\lambda$.](image)

We also show the first three stationary states and potentials at various values of $\lambda$ in Fig. 2. As $\lambda$ grows, the ground-state wavefunction develops a minimum at the origin, and the first excited state almost matches it in the bulk of the minimum. By $\lambda = 8$, the wavefunctions are almost indistinguishable, except for their sign.

![FIG. 3. Behavior of the coefficients of the ground-state wave function for the pure quartic oscillator (blue) and double-well potential (red, $\lambda = 8$) in the basis $[2/200]$. In the lower panel stars and open circles denote $c_{2m}$ of opposite signs. See Table S2 for more digits.](image)

In Fig. 3 we show the overlap $c_m$ of the ground-state wave function with even oscillator states in a basis of $[2/200]$ for two values of $\lambda$. The pure quartic oscillator is dominated by the ground-state of the harmonic oscillator, with overlap close to 1, but the magnitude of the double-well coefficients grows before ultimately decaying. In the lower panel, we show that the overlaps decay exponentially, but with varying signs. The broken symmetry well has overlaps that decay significantly more slowly (about 5 orders of magnitude larger).

Lastly, we plot the error in the ground-state density calculated with the first 20 coefficients of $[2/200]$ in Fig. 4 for the double well potential ($\lambda = 8$). This is not the error of the basis set, but simply the error caused by truncation after 20 levels. The error is very small, oscillates in space, and is localized in the two different wells.

4.2. Satisfaction of virial theorem

The virial theorem [36] is a useful check on the accuracy of eigenstates in a basis. It is particularly simple here, as...
4.2 Satisfaction of virial theorem

only accurate energies for the general quartic oscillator

The potential is a sum of two powers of \( x \). For \( v_\lambda(x) \), the virial theorem requires, for any eigensolution

\[
\langle p^2 \rangle + \lambda \langle x^2 \rangle = \langle x^4 \rangle,
\]

with nonzero matrix elements

\[
\begin{align*}
\bar{x}_0^2 &= \bar{p}_0^2 = 2n + 1, \quad \bar{x}_1^2 = -\bar{p}_1^2 = \sqrt{m_2}, \\
\bar{x}_4^2 &= 3(2n^2 + 2n + 1), \quad \bar{x}_3^2 = 2\sqrt{m_2(2n + 3)}, \quad \bar{x}_2^2 = \sqrt{m_4},
\end{align*}
\]

where \( \bar{x}_k = x_{n+k} \sqrt{2\omega} \) and \( \bar{p}_k = p_{n+k} \sqrt{2\omega} \). In particular, at \( \lambda_c \), we find the simple formula:

\[
\frac{\langle p^2 \rangle}{\langle x^2 \rangle} = \frac{\lambda_c}{3}.
\]

In Table II we show how closely our solutions satisfy Eq. 5. This confirms that with [2/200] we have a very good approximation to the exact ground states. Eq. 7 is satisfied to 39 decimal places.

<table>
<thead>
<tr>
<th>( \lambda )</th>
<th>( \langle p^2 \rangle )</th>
<th>( \langle x^2 \rangle )</th>
<th>( \langle x^4 \rangle )</th>
<th>( \langle p^2 \rangle + \lambda \langle x^2 \rangle - \langle x^4 \rangle )</th>
</tr>
</thead>
<tbody>
<tr>
<td>-1</td>
<td>0.7096226227</td>
<td>0.3548402512</td>
<td>0.3547823715</td>
<td>-1.0 \times 10^{-69}</td>
</tr>
<tr>
<td>0</td>
<td>0.5610732993</td>
<td>0.4561199557</td>
<td>0.5610732993</td>
<td>-3.8 \times 10^{-68}</td>
</tr>
<tr>
<td>\frac{1}{4}</td>
<td>0.458528308</td>
<td>0.5390764722</td>
<td>0.7559412019</td>
<td>-3.2 \times 10^{-66}</td>
</tr>
<tr>
<td>1</td>
<td>0.4187536838</td>
<td>0.6673186910</td>
<td>1.0860717748</td>
<td>9.6 \times 10^{-67}</td>
</tr>
<tr>
<td>\lambda_c</td>
<td>0.3828873103</td>
<td>0.8214946618</td>
<td>1.5315492412</td>
<td>0.0 \times 10^{-40}</td>
</tr>
<tr>
<td>2</td>
<td>0.405838252</td>
<td>1.2071184727</td>
<td>2.8196207705</td>
<td>1.2 \times 10^{-63}</td>
</tr>
<tr>
<td>4</td>
<td>1.2230281089</td>
<td>3.5787191485</td>
<td>15.5379047030</td>
<td>9.7 \times 10^{-66}</td>
</tr>
<tr>
<td>8</td>
<td>1.9338080508</td>
<td>7.7414002199</td>
<td>63.850008103</td>
<td>-1.6 \times 10^{-51}</td>
</tr>
</tbody>
</table>

In Table II we show the expectation values and their virial sum for different wells with [2/200]. See Table S3 for more digits.

4.3 Tunneling between wells

In this section, we examine both the zero point energy and the tunneling between the symmetric wells that occur for positive \( \lambda \). As mentioned before, the vibrational frequency is \( \sqrt{\lambda} \) for negative \( \lambda \), and \( \sqrt{2\lambda} \) for positive \( \lambda \). Fig. 5 shows the exact zero-point energy and its harmonic approximation, which becomes accurate as \( \sqrt{\lambda} \) grows.

Less trivial is the tunneling between the broken-symmetry wells. A simple WKB analysis[36] yields

\[
\epsilon_\pm = \frac{\omega_0}{2} + \frac{\omega_0 e^{-\phi}}{2\pi},
\]

for the lowest two levels, where \( \omega_0 \) is the vibrational frequency, and \( \phi \) is the decay rate for tunneling, evaluated on the ground-state energy. The splitting is

\[
\Delta \epsilon = \frac{\omega_0}{\pi} e^{-\phi(\lambda)},
\]

and \( \omega_0 = \sqrt{2\lambda} \) in the harmonic approximation. Here \( \phi \) is the integral of the absolute value of the momentum \( p(x) = \)
\[ h_3^{(6)} = 1 \text{ and} \\
\]
\[ h_0^{(6)} = (2n + 1)[10n(n + 1) + 3 (4\omega^4 + 5)], \\
h_1^{(6)} = 3[5n(n + 3) - 4\omega^4 + 15], \\
h_2^{(6)} = 3(2n + 5), \]

i.e., they go one more step away from the diagonal. The energies of the first two sextic oscillator states are given in Table III.

4.5. Analytical results for a few states

It can often be useful to find an approximate solution using just a few basis functions, instead of hundreds. Here we give analytic formulas for the lowest lying even energies as functions of \( \omega \) and \( \lambda \) when only 1, 2, and 3 even oscillator states are used. These expressions can be useful for quick estimates of low-lying eigenvalues. The approximate ground-state energy with one even basis function is

\[ \epsilon_0 = \frac{3}{16\omega^2} + \frac{\omega}{4} - \frac{\lambda}{4\omega}, \quad (N_B = 1). \]

The approximate ground- and second-excited states with two even basis functions are:

\[ \epsilon_{\pm} = \frac{3 (\omega^2 - \lambda)}{4\omega} + \frac{21 \pm 2\sqrt{D}}{16\omega^2}, \quad (N_B = 3), \]

\[ D = 8\omega[3\omega (\lambda^2 + \omega^4 + 2\omega) - 2\lambda (\omega^3 + 6)] + 99. \]

With three even basis functions the first three approximate even state energies are (\( n = 0, 2, 4 \)):

\[ \epsilon_n = \frac{1}{48\omega^2} \left[ 15(11 - 4\lambda\omega + 4\omega^3) \\
- (-1)^{n+2} \sqrt{6} D \cos \left( \frac{\phi}{3} + \frac{(n + 1)\pi}{6} \right) \right], \quad (N_B = 5), \]

\[ D = 15[\omega^2 (\lambda^2 + \omega^4 + 4\omega^2) - 7\lambda\omega + 13] - 2\lambda\omega^4, \]

\[ \sin \phi = \frac{9B}{8\sqrt{6}\omega^2}, \]

\[ B = 20\omega^3 (\lambda\omega[51 - 4\omega(\lambda + \omega^2)] + 2[2\omega^6 + 7\omega(3^3 - 15)]) + 4\omega^6 (20\omega^3 - 57) + 5575. \]

At \( \lambda_0 \) (Fig. 7), the least error in the ground state energy is 5.467 \times 10^{-2} at \( \omega = 0.7595 \) with Eq. 14, 4.320 \times 10^{-3} at \( \omega = 1.383 \) with Eq. 15, and 4.563 \times 10^{-4} at \( \omega = 1.854 \) with Eq. 16.

4.6. Error dependence on \( \omega \)

In this paper we have usually set the basis set angular frequency \( \omega \) to 2. Now we analyze what happens to the error of the ground and a highly excited state of the pure

\[ \begin{array}{c|c}
\text{n} & \text{Energy} \\
\hline
0 & 0.43493087878025459238742792925553392774 \\
1 & 1.648311063651709360575374208979389227058 \\
2 & 3.447026714130810318513811929279955987 \\
3 & 5.674137429231210793777941201425803489 \\
4 & 8.24959888596347452014123953299512400416730 \\
5 & 11.1314582800973327594099958109248369395669 \\
6 & 14.28988270823523786346684699297925593899944806 \\
7 & 17.702352219545620799007803069145795820975459 \\
8 & 21.35111718199404164245092730262063053565 \\
9 & 25.22712857036289124841438597544908122878 \\
10 & 29.302053191821526431685743177538338413530 \\
11 & 33.58184072441447465945296478956672311547 \\
12 & 38.052368242715780040920684727674910548 \\
13 & 42.705210613219239798987306117322169371214762 \\
14 & 47.534059451144442611031955694350778521546 \\
15 & 52.53252145069659924991153932257382502470230 \\
16 & 57.695019529286909138098860752008737269497456 \\
17 & 63.0164936069367007526199870383520713 \\
18 & 68.4923253127971812054761641800704809075654 \\
19 & 74.118277288288342368118468014333735452468298 \\
\end{array} \]
4.6 Error dependence on $\omega$

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$M = 1$
$M = 2$
$M = 3$

$\Delta E_0$

FIG. 7. The errors of the analytic expressions for the approximate ground state with 1, 2, and 3 even basis functions and $\lambda = \lambda_c$.

$N_B = 40$
$N_B = 50$
$N_B = 60$

$\Delta E_0 \times 10^{17}$

FIG. 8. The errors of the ground state and 19th excited state (i.e. 10th odd state) as a function of $\omega$. See Table S5 for more digits.

4.7. Quartic potential as perturbation

Consider the case where $\lambda$ is large and negative, and treat the quartic potential as a perturbation. This problem and it’s analytic structure was studied in Refs. [27, 28, 38]. The zeroth, first, and second order contributions to the energies are

$$\epsilon^{(0)}_n = \left(n + \frac{1}{2}\right) \sqrt{|\lambda|},$$

$$\epsilon^{(1)}_n = \frac{3(2n^2 + 2n + 1)}{16|\lambda|},$$

$$\epsilon^{(2)}_n = \frac{-\left(1 + 2n\right)[17n(n + 1) + 21]}{128|\lambda|^{5/2}}. \tag{17}$$

Fig. 9 shows the resulting error in the ground state energy.

4.8. Asymmetric wells

We now examine the effect of breaking the symmetry of $v_\lambda(x)$ by adding a linear term

$$v_{\lambda,\alpha}(x) = \frac{x^4}{4} - \lambda \frac{x^2}{2} + \alpha x. \tag{18}$$

We only examine the case $\lambda = 4$. In Table IV, we show both the energies for the case $\alpha = 0.1$ and their difference from the unperturbed case $\alpha = 0$. As one side of the well is depressed and the other elevated, for the low-lying states,
TABLE IV. The first twenty energies when \( \alpha = 0 \) is reported. All energies are accurate to the 41 digits given.

<table>
<thead>
<tr>
<th>( n )</th>
<th>( B_{2n} )</th>
</tr>
</thead>
<tbody>
<tr>
<td>0</td>
<td>( 1.74805389283297819764 )</td>
</tr>
<tr>
<td>1</td>
<td>( -0.149707253419490259 )</td>
</tr>
<tr>
<td>2</td>
<td>( 0.03855515184539294104 )</td>
</tr>
<tr>
<td>3</td>
<td>( -0.0001929122099439287 )</td>
</tr>
<tr>
<td>4</td>
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<tr>
<td>5</td>
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<tr>
<td>6</td>
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</tr>
<tr>
<td>7</td>
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</tr>
<tr>
<td>8</td>
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</tr>
<tr>
<td>9</td>
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</tr>
<tr>
<td>10</td>
<td>( -0.00000144739478696102 )</td>
</tr>
</tbody>
</table>

TABLE VI. The known WKB coefficients reported to twenty digits.

4.9. Asymptotic solution of pure quartic oscillator

The asymptotic solution of the pure and generalized quartic oscillator has been studied many times before [3, 9, 10, 26]. We analyze only the pure quartic oscillator and closely follow Bender & Orszag [3]. The WKB series for a pure quartic oscillator with potential \( v(x) = x^4 \) yields the implicit formula

\[
\sum_{m=0}^{\infty} A_{2m}(4\epsilon^{3/2})^{1/2-m} = \left( n + \frac{1}{2} \right) \pi, \tag{19}
\]

with the known \( A_{2n} \) reported in Table V and in Refs. [3, 39]. One can invert this implicit expression to an explicit formula for each level:

\[
\epsilon_n = 2^{1/3} \sum_{m=0}^{\infty} B_{2m} \left( n + \frac{1}{2} \right)^{4/3-2m}. \tag{20}
\]

We give the known \( A_{2n} \) and \( B_{2n} \) coefficients numerically in Table VI to twenty decimal places. The analytic forms of the \( B_{2n} \) coefficients are given by

\[
B_{2n} = (-1)^{n/2} \frac{\pi^{2-n} \beta_n}{\Gamma(n/2)^8/3}, \tag{21}
\]

where the \( \beta_n \) are polynomials of order \( n/2 \) in \( \gamma \):

\[
\beta_n = C_n \sum_{k=0}^{n/2} a_{n,k} \gamma^k, \tag{22}
\]

where \( \gamma = \Gamma(1/4)^8/\pi^4 \). This allows the 11 known \( \beta_{2n} \) to be given by the constants in Table VII.

We can use our highly accurate energies to extract higher order coefficients. We define the deviation from the \( 2m \)-th order WKB approximation as

\[
\Delta \epsilon_n^{(2m)} = \epsilon_n - \epsilon_n^{(2m-2)} \tag{23}
\]

which, according to Eq. 20, has the asymptotic form

\[
\Delta \epsilon_n^{(2m)} = B_{2m} X_n^{m-2} + B_{2m+2} X_n^{m-2+1} + \ldots, \tag{24}
\]

where

\[
X_n = \left( n + \frac{1}{2} \right)^{-2}, \tag{25}
\]
yielding

\[ \Delta_n^{(2m)} X_n^{2/3-m} = B_{2m} + B_{2m+2}X_n + B_{2m+4}X_n^2 + \ldots \]  

(26)

Thus by calculating accurate energies, multiplying them by \( X_n^{2/3-m} \), and fitting to a line, we confirm the WKB coefficients up to twentieth order and find the next two coefficients numerically, as shown in Fig. 11. Our most accurate approximations to \( B_{22} \) and \( B_{24} \) were calculated using \( 3/3000 \) to be \( B_{22} = -1.2052792 \times 10^4 \) and \( B_{24} = 2.98 \times 10^6 \), which are accurate to the number of digits shown. To speed up the calculation we took advantage of parity and calculated the odd and even energies separately using the ParallelTable function in Mathematica [35].

6. FUNDING INFORMATION

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5. CONCLUSIONS

We have used Blinder’s method to extract many quantities from the general quartic oscillator to many digits [5]. We have considered many distinct limits and scenarios where these benchmark results might be useful. We have covered energetics of eigenstates, the virial theorem, tunneling between wells, the sextic oscillator, analytic forms in a few basis functions, error dependence on choice of \( \omega \), perturbation theory in the quadratic term, asymmetric wells, and asymptotic analysis of WKB results for the pure quartic case. In all cases, we have provided preliminary analysis and compared with the exact results. Some of this work should also prove useful for pedagogy. This would include both the use of Mathematica to generate accurate results and the derivations of various results in this context. Users who wish to replicate our results can start with Ref. [5] and modify the Hamiltonian with a quartic potential using the matrix elements in Eq. 6. But the two examples of asymptotic techniques are beyond most standard curricula, and unfamiliar to most theorists. Refs. [3, 20, 22, 40] provide a pedagogical introduction to such methods.
Appendix A: Derivation of asymptotic splitting formula

We now explain how to derive Eq. 11, the asymptotic approximation to $\Delta \epsilon = \epsilon_1 - \epsilon_0$ in the limit $\lambda \to \infty$.
We introduce the shorthand $\eta = (2/\lambda)^{3/4}$ so $\lambda \to \infty \implies \eta \to 0_+$. In terms of $\eta$ Eq. 10 of the main text becomes

$$\phi(\eta) = 4 \eta^2 \int_0^{\sqrt{1-\eta}} dx \sqrt{(1-x^2)^2 - \eta^2}. \quad (A1)$$

In the limit $\eta \to 0_+$,

$$\phi^{(0)}(\eta) = 4 \eta^2 \int_0^1 dx (1 - x^2) = \frac{(2\lambda)^{3/2}}{3}. \quad (A2)$$

We evaluate Eq. A1:

$$\phi(\eta) = \frac{8}{3\eta^2} \sqrt{1 + \eta F(\eta)}, \quad (A3)$$

where $F(\eta) = \mathcal{E}(y) - \eta \mathcal{K}(y)$, $y = (1 - \eta)/(1 + \eta)$ and

$$\mathcal{K}(x) = \int_0^{\pi/2} \frac{d\theta}{f(x, \theta)}, \quad \mathcal{E}(x) = \int_0^{\pi/2} d\theta f(x, \theta), \quad (A4)$$

with $f(x, \theta) = \sqrt{1 - x \sin^2 \theta}$ [41]. The following expansion will prove useful shortly:

$$F(\eta) = 1 - \frac{\eta}{2} + \frac{3}{16} \eta^2 (1 - 6 \ln 2 + 2 \ln \eta) + \mathcal{O}(\eta^3), \quad (A5)$$
as $\eta \to 0_+$ [42]. Inserting Eq. A5 into Eq. A3 and expanding around $\eta = 0$, yields

$$\phi^{(2)}(\lambda) = \frac{(2\lambda)^{3/2}}{3} - \frac{3}{4} \ln \lambda - \frac{1}{4} (2 + 9 \ln 2). \quad (A6)$$

The above equation combined with Eq. 9 leads to the final result, Eq. 11 of the main text.