A quantum-mechanical anharmonic oscillator

with a most interesting spectrum

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Abstract

We revisit the problem posed by an anharmonic oscillator with a potential given by a polynomial function of the coordinate of degree six that depends on a parameter $\lambda$. The ground state can be obtained exactly and its energy $E_0 = 1$ is independent of $\lambda$. This solution is valid only for $\lambda > 0$ because the eigenfunction is not square integrable otherwise. Here we show that the perturbation series for the expectation values are Padé and Borel-Padé summable for $\lambda > 0$. When $\lambda < 0$ the spectrum exhibits an infinite number of avoided crossings at each of which the eigenfunctions undergo dramatic changes in their spatial distribution that we analyze by means of the expectation values $\langle x^2 \rangle$.

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1 Introduction

Some time ago Herbst and Simon [1] discussed some interesting and baffling features of two one-dimensional Hamiltonians. In one of them, \( H^{(2)}(g) = p^2 + x^2 - 1 + g^4 x^6 + 2g^2 x^4 - 3g^2 x^2 \), the exact ground-state energy is \( E^{(2)}(g) = 0 \) and the coefficients of the perturbation series \( \sum a_n^{(2)} g^{2n} \) vanish for all \( n > 0 \). However, the perturbation series for the eigenvector \( \Omega^{(2)}(g) \) is divergent at least in the norm sense. The related oscillator \( H^{(3)}(g) = H^{(2)}(ig) \) is most interesting because \( 0 < E^{(3)}(g) < D' \exp(-c/g^2) \). Its potential has three wells and there is a kind of asymptotic degeneracy of expected states.

Those models are particular cases of the so-called quasi-exactly solvable Schrödinger equations [2] (and references therein). In fact, Turbiner [2] chose the closely related potential \( V_0(x; a, b) = a^2 x^6 + 2abx^4 + (b^2 - 3a) x^2 - b \) for the discussion of the most interesting problem of phase transition.

The purpose of this paper is the analysis of the spectra of \( H^{(2)} \) and \( H^{(3)} \) because they exhibit several interesting features that may not emerge so clearly from the remarkable theoretical analysis carried out by Herbst and Simon [1] and Turbiner [2]. Present results are shown in section 2 and conclusions in section 3.

2 The model

For simplicity, here we rewrite the Hamiltonian proposed by Herbst and Simon [1] as

\[
H(\lambda) = H^{(2)}(2\sqrt{\lambda}) + 1 = p^2 + x^2 - 12\lambda x^2 + 8\lambda x^4 + 16\lambda^2 x^6. \tag{1}
\]

It exhibits an exact ground-state eigenfunction

\[
\varphi(x) = \exp \left( -x^2/2 - \lambda x^4 \right), \tag{2}
\]

with eigenvalue \( E_0 = 1 \). This solution is only valid for \( \lambda \geq 0 \) because it is not square integrable for negative values of \( \lambda \).
In principle, one expects the eigenfunctions and eigenvalues of $H(\lambda)$ to have perturbation expansions about $\lambda = 0$ of the form
\[
\psi_n(x) = \sum_{p=0}^{\infty} \psi_n^{(p)}(x) \lambda^p,
\]
\[
E_n = \sum_{p=0}^{\infty} E_n^{(p)} \lambda^p.
\] (3)

For the normalized ground-state eigenfunction we have
\[
\psi_0(x) = \frac{\phi(x)}{\sqrt{\langle \phi | \phi \rangle}} = 1 \sqrt{\frac{1}{2 \pi} \frac{1}{4} e^{-x^2/2} [1 + \frac{1}{4} (3 - 4x^4) \lambda + \frac{1}{32} (16x^8 - 24x^4 - 183) \lambda^2 + \ldots]},
\] (4)

but all the perturbation corrections of the corresponding eigenvalue vanish ($E_0^{(j)} = 0, j > 0$) as mentioned above. Therefore, perturbation theory fails to provide suitable values of $E_0(\lambda)$ when $\lambda < 0$. The reason is that this eigenvalue behaves asymptotically as
\[
E_0(\lambda) - 1 \approx A|\lambda|^B e^{-C/|\lambda|}, \lambda < 0.
\] (5)

Figure 1 shows that $E_0(\lambda) - 1$ already behaves in this way. A straightforward least-squares fitting for sufficiently small values of $|\lambda|$ suggests that $A \approx 0.891, B = 0$ (as argued by Herbst and Simon [1]) and $C = 1/8$.

Although the perturbation series for the lowest eigenvalue converges for all $\lambda$ that for its eigenfunction is divergent [1]. As an illustrative example consider the expectation value
\[
\langle x^2 \rangle = \frac{1}{2} - 3 \lambda + 48 \lambda^2 - 1188 \lambda^3 + 39168 \lambda^4 - 1604448 \lambda^5 + \ldots.
\] (6)

for the ground state. In what follows we resort to the notation $X_n = \langle x^{2n} \rangle$ and $X_n^{(j)}$ for the perturbation correction of order $j$. We can easily calculate the perturbation corrections of $E_n^{(j)}$ and $X_n^{(j)}$ analytically to any desired order by means of the hypervirial perturbation method [3]. A least-squares fitting of
the first 1000 perturbation coefficients enables us to estimate the asymptotic expansion

\[ X^{(j)}_1 = (-1)^j 8^j j! \left[ f_0 + \frac{f_1}{j+1} + \frac{f_2}{(j+1)^2} + \ldots \right], \quad j \gg 1, \]  

(7)

where

\[
\begin{align*}
f_0 &= 0.450158158079, \quad f_1 = -0.168809309279, \quad f_2 = -0.30596873069, \\
f_3 &= -0.869104178243, \quad f_4 = -3.78728795807, \quad f_5 = -22.6102214156.
\end{align*}
\]

On keeping just the leading term \( X^{(j)}_1 \approx f_0 (-1)^j 8^j j! \) the Borel sum yields

\[
S(\lambda) = f_0 \sum_{j=0}^{\infty} (-1)^j (8\lambda)^j j! = f_0 \int_0^{\infty} e^{-t} \sum_{j=0}^{\infty} (-1)^j (8\lambda t)^j dt
\]

\[
S_B(\lambda) = f_0 \int_0^{\infty} e^{-t} \frac{e^{\frac{1}{8\lambda} t}}{1 + 8\lambda t} dt = f_0 \frac{e^{\frac{1}{8\lambda}}}{8\lambda} \left[ \text{Shi} \left( \frac{1}{8\lambda} \right) - \text{Chi} \left( \frac{1}{8\lambda} \right) \right],
\]

(8)

where

\[
\text{Shi}(x) = \int_0^x \frac{\sinh t}{t} dt, \quad \text{Chi}(x) = \int_0^x \frac{\cosh t}{t} dt.
\]

(9)

The Borel sum \( S_B(\lambda) \) is complex for \( \lambda < 0 \) and

\[
\Im S_B(\lambda) \sim 0.176715 |\lambda|^{-1} e^{-\frac{1}{4\pi^2}}, \quad \lambda \to 0^-.
\]

(10)

Figure 2 shows that the real part of \( S_B(\lambda) \) exhibits a maximum for \( \lambda < 0 \) like the actual value of \( \langle x^2 \rangle \).

The perturbation series originated in the expansion of a potential about one of its minima can be shown to be non-Borel summable when the potential has degenerate minima [4]. It has been argued that in such a case the imaginary part of the Borel sum is cancelled by the imaginary part of a logarithmic term [4]. In the present case the perturbation series are Padé and Borel-Padé summable for \( \lambda > 0 \) as shown in Figure 3 for \( \langle x^2 \rangle \) (ground state). This figure shows that the Borel summation improves the accuracy of the Padé approximant \([6/6](\lambda)\). However, both summation methods fail for \( \lambda < 0 \).

The perturbation series for the excited states

\[
E_1(\lambda) = 3 + 12\lambda - 144\lambda^2 + 4176\lambda^3 - 172800\lambda^4 + 8892288\lambda^5 + \ldots
\]

\[
E_2(\lambda) = 5 + 48\lambda - 864\lambda^2 + 36864\lambda^3 - 2194560\lambda^4 + 158810112\lambda^5 + .
\]

(11)
are divergent; for example

\[ E_1^{(j)} \sim (-1)^{j+1} \sqrt{j8^j j!}, \]  

was also obtained by numerical least-squares fitting of the analytical perturbation corrections calculated by means of the hypervirial perturbation method [3].

Fig 4 shows the energy spectrum for small negative values of \( \lambda \). In order to understand its structure we should pay attention to the form of the potential-energy function. When \( 0 < \lambda < 1/12 \) the potential is a single well and becomes a double well when \( \lambda > 1/12 \), but these cases are not relevant for present discussion. We just mention them for completeness. When \( \lambda < -1/36 \) the potential is a single well; when \(-1/36 < \lambda < 0\) it exhibits three wells, one of them \( V(0) = 0 \) at the origin and the other two at \( \pm x_m \), where

\[ x_m^2 = -\frac{\sqrt{36\lambda + 1} + 2}{12\lambda} = -\frac{1}{4\lambda} - \frac{3}{2} + \frac{27\lambda}{2} - 243\lambda^2 + \ldots \]  

These side wells are separated from the central one by two barriers located at \( \pm x_M \) where

\[ x_M^2 = \frac{\sqrt{36\lambda + 1} - 2}{12\lambda} = -\frac{1}{12\lambda} + \frac{3}{2} - \frac{27\lambda}{2} + 243\lambda^2 + \ldots \]  

Clearly the side wells move away from the origin as \( \lambda \to 0^- \). The values of the potential at these stationary points are \( V(0) = 0 \),

\[ V(x_m) = \left( \frac{\sqrt{36\lambda + 1} + 2}{54\lambda} \right) \left( \frac{\sqrt{36\lambda + 1} + 36\lambda - 1}{54\lambda} \right) = 3 + 9\lambda - 54\lambda^2 + \ldots, \]

\[ V(x_M) = \left( \frac{\sqrt{36\lambda + 1} - 2}{54\lambda} \right) \left( \frac{\sqrt{36\lambda + 1} - 36\lambda + 1}{54\lambda} \right) = -\frac{1}{27\lambda} + 1 - 9\lambda + \ldots. \]

Note that the minima are bounded from below while the maxima increase unboundedly. In the limit \( \lambda \to 0^\circ \) we are left with a harmonic oscillator. The curvatures of the minima and maxima tend to constant values as \( \lambda \to 0^- \)

\[ V''(0) = 2(1 - 12\lambda) \]

\[ V''(x_m) = \frac{8(36\lambda + 1 + 2\sqrt{36\lambda + 1})}{3} = 8 + 192\lambda - 864\lambda^2 + 15552\lambda^3 + \ldots \]

\[ V''(x_M) = \frac{8(36\lambda + 1 - 2\sqrt{36\lambda + 1})}{3} = -\frac{8}{3} + 864\lambda^2 - 15552\lambda^3 + \ldots \]
Figure 4 shows that \( E_0 \) and \( E_1 \) remain isolated and become eigenvalues of the harmonic oscillator when \( \lambda \to 0^- \). The reason is that they are below the minima of the side potentials. The eigenvalues \( E_2, E_3 \) and \( E_4 \) approach each other and become quasi degenerate for intermediate values of \( \lambda \). As \( \lambda \to 0^- \) \( E_2 \) tends to a harmonic-oscillator eigenvalue while the pair \( (E_3, E_4) \) remains quasi degenerate and moves upwards. When \( E_3 \) meets \( E_5 \) there is an avoided crossing after which \( E_3 \) approaches a harmonic oscillator eigenvalue while \( E_5 \) deviates upwards. The same situation takes place between \( E_4 \) and \( E_6 \), the former becomes a harmonic oscillator eigenvalue and the latter moves upwards. All the higher eigenvalues follow the same pattern; for example, \( E_{4k+1}, k = 1,2,\ldots \), remain isolated till they are pushed upwards by a lower odd-parity eigenvalue. The eigenvalues \( (E_{4k+2}, E_{4k+3}, E_{4k+4}) \), \( k = 0,1,\ldots \), become quasi degenerate at intermediate values of \( \lambda \) before the pair \( (E_{4k+3}, E_{4k+4}) \) separates and moves upwards. It seems that every eigenvalue \( E_n \) with \( n > 1 \) undergoes an avoided crossing with a higher eigenvalue of the same symmetry before becoming a harmonic-oscillator eigenvalue. If \( n > 3 \) the eigenvalue \( E_n \) undergoes avoided crossings with \( E_{n-2} \) and \( E_{n+2} \) as illustrated in the more detailed figures 5 and 6. The eigenvalues approach so closely that the avoided crossings appear actual crossings.

In order to understand what happens at the avoided crossings we calculated \( \Delta x = \sqrt{\langle x^2 \rangle} \) for some states. This root-mean-square deviation is expected to be larger when the state is localized on the side wells. Figures 7 and 8 show \( \Delta x \) for the states with quantum numbers \( n = 0,2,4,6 \). The states \( n = 0,2 \) do not participate in avoided crossings and the corresponding \( \Delta x \) does not change considerably as \( \lambda \to 0^- \). The state \( n = 4 \) undergoes an avoided crossing and \( \Delta x \) exhibits a jump that suggests that it changes from being localized mainly on the central well to being localized mainly on the side ones. On the other hand, the state \( n = 6 \) appears to be mainly localized on the side wells before the avoided crossing and mainly on the central one after it. In this case the jump is considerably larger indicating that the form of the eigenfunction changes more dramatically.
3 Conclusions

We revisited an old but interesting problem in quantum mechanics and mathematical physics. It has been our purpose to outline some remarkable features of its eigenvalues and eigenfunctions that have not been pointed out before. In particular, the spectrum for $\lambda < 0$ exhibits a rich structure of avoided crossings at which the states that take part undergo dramatic changes in their form. Such changes are clearly revealed by the behaviour of the expectation value $\langle x^2 \rangle (\lambda)$. We also estimated the asymptotic behaviour of the coefficients of the perturbation series and showed that they can be summed by means of Padé approximants and Borel-Padé transformations for $\lambda > 0$. This calculation was greatly facilitated by the hypervirial perturbation method that leads to straightforward recurrence relations for the perturbation corrections to the eigenvalues and expectation values $\langle x^{2n} \rangle$ [3]. At present we do not know if there is any suitable approximation for $\lambda < 0$. In this region we simply resorted to the Rayleigh-Ritz variational method with a basis set of 1000 eigenfunctions of the harmonic oscillator. The reason is that the three widely separated wells pose a quite difficult problem for accurate calculation of the eigenfunctions and eigenvalues. We expect that present investigation may be a suitable complement to previous ones about this problem [1][2].

References

[1] I. W. Herbst and B. Simon, Phys. Lett. B 78 (1978) 304-306. See also erratum Phys. Lett. B 80 (1979) 433.

[2] A. V. Turbiner, Phys. Rep. 642 (2016) 1-71.

[3] F. M. Fernández, Introduction to Perturbation Theory in Quantum Mechanics, (CRC Press, Boca Raton, 2001).

[4] J. Zinn-Justin, Ann. Inst. Fourier, Grenoble 54 (2003) 1259-1285.
Figure 1: $E_0(\lambda) - 1$ calculated by means of the Rayleigh-Ritz variational method (dashed red line) and its least-square fitting using equation (5) (blue points).

Figure 2: Numerical $\langle x^2 \rangle$ (blue, continuous line) and $\Re S_B(\lambda)$ (dashed, red line) for the ground state of the oscillator.
Figure 3: Exact $\langle x^2 \rangle$ (solid line) for the ground state of the oscillator (1) and the [6/6] Padé (circles) and Borel-Padé (squares) sums of the perturbation series.

Figure 4: Part of the spectrum of the anharmonic oscillator (1). Even and odd states are denoted by continuous (blue) and dashed (red) lines, respectively.
Figure 5: Part of the spectrum of even states of the anharmonic oscillator

Figure 6: Part of the spectrum of odd states of the anharmonic oscillator
Figure 7: $\sqrt{\langle x^2 \rangle}$ for the states of the anharmonic oscillator (1) with quantum numbers $n = 0, 2, 4$

Figure 8: $\sqrt{\langle x^2 \rangle}$ for the state of the anharmonic oscillator (1) with quantum number $n = 6$