Large-order Perturbation Theory for a Non-Hermitian $\mathcal{PT}$-symmetric Hamiltonian

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A precise calculation of the ground-state energy of the complex $\mathcal{PT}$-symmetric Hamiltonian $H = p^2 + \frac{1}{4} x^2 + i \lambda x^3$, is performed using high-order Rayleigh-Schrödinger perturbation theory. The energy spectrum of this Hamiltonian has recently been shown to be real using numerical methods. The Rayleigh-Schrödinger perturbation series is Borel summable, and Padé summation provides accurate agreement with the real energy spectrum. Padé analysis provides strong numerical evidence that the once-subtracted ground-state energy considered as a function of $\lambda^2$ is a Stieltjes function. The analyticity properties of this Stieltjes function lead to a dispersion relation that can be used to compute the imaginary part of the energy for the related real but unstable Hamiltonian $H = p^2 + \frac{1}{4} x^2 - \epsilon x^3$.

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It has been conjectured [1] that the spectrum of the complex Hamiltonian

$$H = p^2 + \frac{1}{4} x^2 + i \lambda x^3$$  \hspace{1cm} (1)

is real and positive. Although there is no rigorous proof of this conjecture, it has been argued [2] that the reality and positivity of the spectrum is a consequence of the $\mathcal{PT}$ symmetry of $H$. (Recall that the parity operation acts as $\mathcal{P}: p \rightarrow -p$ and $\mathcal{P}: x \rightarrow -x$ and that the antiunitary time reversal operation acts as $\mathcal{T}: p \rightarrow -p$, $\mathcal{T}: x \rightarrow x$, and $\mathcal{T}: i \rightarrow -i$.) The notion that $\mathcal{PT}$ symmetry can replace the much more restrictive condition of Hermiticity has been studied in the context of quasi-exactly solvable quantum theories [3], new kinds of symmetry breaking in quantum field theory [4,5], and complex periodic potentials [6]. There have been many other instances of non-Hermitian $\mathcal{PT}$-invariant Hamiltonians in physics. Energies of solitons in Toda theories with imaginary coupling have been found to be real [7]. Hamiltonians rendered non-Hermitian by an imaginary external field have been used to study population biology [8] and to study delocalization transitions, such as vortex flux-line depinning in type-II superconductors [9].

In this paper we study the large-order behavior of Rayleigh-Schrödinger perturbation theory for the ground-state energy of the complex $\mathcal{PT}$-symmetric Hamiltonian (1). Note that this Hamiltonian describes a $0 + 1$ dimensional $\phi^3$ field theory, and recall that $\phi^3$ theories were the first quantum field theories in which the divergences of perturbation theory were studied [10]. For the Hamiltonian (1) we find that the perturbation series for the ground-state energy is divergent but Borel summable. Furthermore, by studying the numerical properties of the Padé approximants we infer that the (once-subtracted) ground-state energy considered as a function of $\lambda^2$ is a Stieltjes function. This is a very strong result because it implies analyticity in the cut-$\lambda^2$ plane and other properties. [It is surprising that this Stieltjes condition holds for a complex Hamiltonian such as (1); the proof that the once-subtracted ground-state energy of the conventional $\lambda x^{2N}$ anharmonic oscillator is a Stieltjes function of $\lambda$ makes use of Hermiticity.] We then use these analyticity properties to establish a dispersion relation that yields the precise large-order behavior of the perturbation series.

Let us consider the conventional Rayleigh-Schrödinger perturbation series about the ground state ($E_0 = \frac{1}{2}$) of the harmonic oscillator $H_0 = p^2 + \frac{1}{4} x^2$. The perturbed energy has an asymptotic series representation in powers of $\lambda^2$ because the perturbation $x^3$ is an odd function of $x$:

$$E(\lambda) - \frac{1}{2} \sim \sum_{n=1}^{\infty} b_n \lambda^{2n}.$$  \hspace{1cm} (2)

[We have chosen the form of $H_0$ so that the perturbative expansion coefficients $b_n$ in (2) are integers.]

Using recursion formulas, we can easily generate as many terms as desired in this expansion. The coefficients $b_n$ alternate in sign, and their magnitude grows rapidly with $n$. The first 20 values are listed in Table 1. We have computed enough of the coefficients $b_n$ so that we can fit the leading large-$n$ behavior as

$$b_n \sim (-1)^{n+1} \frac{60^{n+1/2}}{(2\pi)^{3/2}} \Gamma \left(n + \frac{1}{2} \right) \left[1 - O \left(\frac{1}{n} \right) \right].$$  \hspace{1cm} (3)
Therefore, although divergent, the series in (2) is Borel summable \([11,12]\). Observe that if the factor of \(i\) were absent from the Hamiltonian (1), then the perturbation coefficients \(b_n\) would not alternate in sign and the perturbation series would not be Borel summable.

We have performed a Padé analysis \([11,12]\) on the divergent series for the once-subtracted ground-state energy \([E(\lambda) - \frac{1}{\lambda^2}]/\lambda^2\). Using the first 46 perturbation coefficients \(b_n\), we find that for all real positive \(\lambda^2\) the diagonal Padé sequence \(P_N^M(\lambda^2)\) is monotone decreasing with increasing \(N\), and the off-diagonal Padé sequence \(P_M^{M+1}(\lambda^2)\) is monotone increasing with increasing \(M\):

\[
P_1^0 < P_2^1 < P_3^2 < \ldots < P_M^M < \ldots < P_N^N < \ldots < P_2^1 < P_1^0.
\] (4)

The results for \(\lambda = 0.125\) are shown in Table 2. If the inequalities in (4) hold for all \(N\) and \(M\) and for all real positive \(\lambda^2\), then it is rigorously true that \([E(\lambda) - \frac{1}{\lambda^2}]/\lambda^2\) is a Stieltjes function of \(\lambda^2\) \([12]\). This means that \([E(\lambda) - \frac{1}{\lambda^2}]/\lambda^2\) is analytic in the cut-\(\lambda^2\) plane, vanishes as \(|\lambda^2| \to \infty\), and is a Herglotz function of \(\lambda^2\). [A function \(f(z)\) is said to be Herglotz if \(\text{Im} f(z)\) is positive (negative) when \(z\) is in the upper (lower) plane.] The fact that (4) holds for \(0 \leq M, N \leq 23\) provide strong numerical evidence that \([E(\lambda) - \frac{1}{\lambda^2}]/\lambda^2\) is a Stieltjes function. We stress that this is a much stronger result than merely saying that the divergent series (2) is Borel summable.

Furthermore, in addition to the inequality in (4), the limits of the two Padé sequences appear to be identical. Therefore, we can extract values for the Padé summed energy from the two Padé sequences. The best estimate for the ground-state energy is obtained by averaging the last diagonal and off-diagonal Padé approximants. (To obtain an estimate of the ground-state energy from this average we multiply the average by \(\lambda^2\) and add \(\frac{1}{2}\).) The results are shown in Table 3 for various values of the coupling \(\lambda\). Previous numerical calculations of the ground-state energy were obtained by direct numerical integration of the Schrödinger equation (see Ref. \([1]\)); this technique gave a typical accuracy of about five decimal places. The agreement between the method of numerical integration and the Padé summation is excellent. Moreover, for \(\lambda < \frac{1}{10}\) the Padé technique provides an accuracy of more than ten decimal places. The agreement is better for smaller values of \(\lambda\), as is expected, because of a faster convergence rate of the Padé sequence.

**TABLE I.** The first 20 perturbation coefficients \(b_n\) in the expansion (3) of the ground-state energy for the complex \(\mathcal{PT}\)-symmetric Hamiltonian (1).

| \(n\) | \(b_n\)  |
|------|---------|
| 1    | 11      |
| 2    | -930    |
| 3    | 158836  |
| 4    | -38501610 |
| 5    | 11777967516 |
| 6    | -430048271460 |
| 7    | 181521503378344 |
| 8    | -86827798698581530 |
| 9    | 46402559816523189260 |
| 10   | -27414557425826905074540 |
| 11   | 17754941941607942489064216 |
| 12   | -125174233155326252929874890500 |
| 13   | 9549063685766293430130201941400 |
| 14   | -7841074899699127067193961172389320 |
| 15   | 68982408758305101330092396215438198608 |
| 16   | -6475070010245490659885414541150140103290 |
| 17   | 6460622456476863139999679663986778514033420 |
| 18   | -682918711491699980988331035123263426636150571009020 |
| 19   | 762447929143920959585654339928573065514292039909968 |
| 20   | -89660576791390730762095201994590409692301843683859820 |
TABLE II. The diagonal and off-diagonal Padé sequences $P_N^N(\lambda^2)$ and $P_{N+1}^N(\lambda^2)$ evaluated at $\lambda = 0.125$. Observe the rapid convergence and note that the inequalities in (\textcolor{red}{[1]}\textcolor{red}{[1]}) are satisfied.

| $N$ | $P_N^N$ | $P_{N+1}^N$ |
|-----|---------|-------------|
| 0   | 11.000000000 | 4.739290085 |
| 1   | 7.039037109  | 5.696806799 |
| 2   | 6.347866015  | 5.947606655 |
| 3   | 6.168265727  | 6.026389922 |
| 4   | 6.110857028  | 6.054574069 |
| 5   | 6.089906566  | 6.065678176 |
| 6   | 6.081499968  | 6.070392205 |
| 7   | 6.077873385  | 6.072516805 |
| 8   | 6.076216002  | 6.073522627 |
| 9   | 6.075421823  | 6.074018882 |
| 10  | 6.075028166  | 6.074272525 |
| 11  | 6.074821510  | 6.074406195 |
| 12  | 6.074712942  | 6.074478558 |
| 13  | 6.074653729  | 6.074518675 |
| 14  | 6.074620680  | 6.074541394 |
| 15  | 6.074601848  | 6.074554510 |
| 16  | 6.074590917  | 6.074562214 |
| 17  | 6.074584462  | 6.074566813 |
| 18  | 6.074580592  | 6.074569597 |
| 19  | 6.074578237  | 6.074571306 |
| 20  | 6.074576787  | 6.074572368 |
| 21  | 6.074575882  | 6.074573036 |
| 22  | 6.074575311  | 6.074573460 |

TABLE III. The ground-state energy for the Hamiltonian (\textcolor{red}{[1]}\textcolor{red}{[1]}) for various values of the coupling $\lambda$; the ground-state energy was computed by Padé summation and by direct numerical integration. The Padé sequences were computed for the once subtracted energy $[E(\lambda) - \frac{1}{2}] / \lambda^2$. The diagonal Padé energy refers to the energy extracted from the diagonal Padé sequence $P_N^N(\lambda^2)$, and the off-diagonal Padé energy refers to the energy extracted from the off-diagonal Padé sequence $P_{N+1}^N(\lambda^2)$. The best estimate for Padé energy is the average of the diagonal and off-diagonal values.

| $\lambda$ | Diagonal Padé energy | Off-diagonal Padé energy | Padé energy | Numerical energy |
|-----------|----------------------|--------------------------|-------------|-----------------|
| 0.015625  | 0.50263              | 0.50263                  | 0.50263     | 0.50263         |
| 0.03125   | 0.50998              | 0.50998                  | 0.50998     | 0.50998         |
| 0.0625    | 0.53393              | 0.53393                  | 0.53393     | 0.53393         |
| 0.125     | 0.59492              | 0.59492                  | 0.59492     | 0.59492         |
| 0.25      | 0.71305              | 0.71284                  | 0.71295     | 0.71294         |
| 0.5       | 0.91445              | 0.89035                  | 0.90240     | 0.90026         |
| 1.0       | 1.40007              | 1.05817                  | 1.22912     | 1.16746         |
| 2.0       | 3.16075              | 1.14032                  | 2.15053     | 1.53078         |
The above Padé analysis provides strong evidence that the once-subtracted ground-state energy is analytic in the cut-$\lambda^2$ plane. Thus, we can derive a dispersion relation in the expansion parameter $\lambda^2$ to deduce the leading behavior of the imaginary part of the energy for negative $\lambda^2$. Physically, this means that we can compute the imaginary part of the energy (and hence the decay width) of the unstable ground state of the real Hamiltonian

$$H = p^2 + \frac{1}{4}x^2 - \epsilon x^3. \quad (5)$$

Note that the ambiguity in the choice of the sign of the coupling $\epsilon$ corresponds to choosing the sign of $i$ in (1). This has no effect on the decay width; the sign simply distinguishes the direction (left or right) in which the potential in (5) is unstable.

In the $t = \lambda^2$ plane there is a cut along the negative $t$ axis, and in the standard way [10, 11] the $b_n$ coefficients are related to the discontinuity across the cut by the exact formula

$$b_n = \frac{1}{\pi} \int_0^\infty \frac{dt}{t^n} D(-t), \quad (6)$$

where $D(-t)$ ($t > 0$) is the imaginary part of $E(\lambda) - \frac{1}{2}$, evaluated with $\lambda^2$ negative. From the growth estimate (3) we deduce that

$$D(-t) \sim -\frac{\epsilon^{\frac{1}{3}}}{2\sqrt{2\pi t}} [1 + O(t)] \quad (t \to 0^+). \quad (7)$$

Thus, the leading contribution (for small $\epsilon$) to the imaginary part of the energy for the unstable ground state of the Hamiltonian (5) is

$$\text{Im}[E(\epsilon)] \sim \frac{\exp(-\frac{1}{60\epsilon^2})}{(2\pi)^{3/2} \epsilon} \quad (\epsilon \to 0^+). \quad (8)$$

There are several ways to check this result. First, it agrees with a direct leading-order WKB calculation [11] of the imaginary part of the energy of the unstable ground state of the real Hamiltonian (5). Second, applying the “bounce” method [17] to the real unstable Hamiltonian (5) we find that

$$\text{Im}[E(\epsilon)\text{bounce} \sim \epsilon S_0^{1/2} \exp(-S_0) \quad (\epsilon \to 0^+), \quad (9)$$

where the action $S_0$ of the bounce solution is given by

$$S_0 = 2 \int_0^\frac{1}{\epsilon} dx \sqrt{\frac{1}{4}x^2 - \epsilon x^3} = \frac{1}{60\epsilon^2} \quad (10)$$

Finally, the answer in (8) is in agreement with the variational perturbation theory analysis in Ref. [18]. In fact, Ref. [18] contains a higher-order WKB expression for $\text{Im}[E(\epsilon)]$. Inserting this higher-order WKB result into the dispersion relation (1), we obtain a WKB-based prediction for the corrections to the leading-order growth of the $b_n$ coefficients given in (3):

$$b_n^{\text{WKB}} \sim (-1)^{n+1} \frac{60^{n+1/2}}{(2\pi)^{3/2}} \Gamma\left(n + \frac{1}{2}\right) \left[1 - \frac{169}{120(n - \frac{9}{2})} - \frac{44507}{28800(n - \frac{9}{2})(n - \frac{11}{2})} \right. \left. - \frac{1920000(n - \frac{7}{2})(n - \frac{9}{2})(n - \frac{11}{2})}{42944342679817} - \frac{82944000000(n - \frac{5}{2})(n - \frac{7}{2})(n - \frac{9}{2})(n - \frac{11}{2})}{342541916236654541} \right. \left. - \frac{398131200000000(n - \frac{3}{2})(n - \frac{5}{2})(n - \frac{7}{2})(n - \frac{9}{2})(n - \frac{11}{2})}{933142404651551165943} \right. \left. - \frac{143327232000000000(n - \frac{1}{2})(n - \frac{3}{2})(n - \frac{5}{2})(n - \frac{7}{2})(n - \frac{9}{2})(n - \frac{11}{2})}{189244716209} \right]. \quad (11)$$

With these higher-order corrections, this growth estimate of the $b_n$ coefficients is spectacularly accurate. For example,
\[ \frac{b_{WKB}^{46}}{b_{46}} = 1.0000000807. \] (12)

To conclude we note that the strategy employed here to relate the large-order Rayleigh-Schrödinger perturbation theory coefficients of a stable (and Borel-summable) problem to the imaginary part of the energy of an unstable (and Borel-nonsummable) problem is familiar from the quartic double-well potential \( H = p^2 + \frac{1}{4}x^2 + gx^4 \), which is stable when \( g > 0 \) and unstable when \( g < 0 \) [13]. The novelty in this paper is that we begin with a complex Hamiltonian \( H = p^2 + \frac{1}{4}x^2 + i\lambda x^3 \) which, despite being non-Hermitian, nevertheless appears to be stable in the sense that it has a real and positive (and discrete) energy spectrum and a Borel-summable perturbation expansion for the ground-state energy. We can then relate the large-order perturbation coefficients to the imaginary part of the energy of an unstable state of the real but unstable Hamiltonian \( H = p^2 + \frac{1}{4}x^2 - \epsilon x^3 \). It is interesting to note that the quartic case is relevant to the physics of instantons [20,17] while the cubic case is relevant to ‘bounces’ in scalar field theories [17] and to string perturbation theory [21].

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