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Level crossings in complex two-dimensional potentials

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Abstract. Two-dimensional $\mathcal{PT}$-symmetric quantum-mechanical systems with the complex cubic potential $V_{12} = x^2 + y^2 + igxy^2$ and the complex Hénon–Heiles potential $V_{\rm HH} = x^2 + y^2 + ig(xy^2 - x^3/3)$ are investigated. Using numerical and perturbative methods, energy spectra are obtained to high levels. Although both potentials respect the $\mathcal{PT}$ symmetry, the complex energy eigenvalues appear when level crossing happens between same parity eigenstates.

Keywords. Non-Hermitian; $\mathcal{PT}$ symmetry; two-dimensional potentials.

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1. Introduction

In 1998, Bender and Boettcher introduced the non-Hermitian $\mathcal{PT}$-symmetric quantum systems [1]. This letter ignited a very active field. Hundreds of papers have been published on various aspects of this new quantum mechanics (for review, please see ref. [2] and references therein).

Most of the studies have been focused on one-dimensional systems, very few have touched two or higher dimensions. In 2001, Bender *et al* studied the complex cubic potential $V_{12} = x^2+y^2+igxy^2$ and $V_{111} = x^2+y^2+z^2+igxyz$. Using perturbation theory, they found real eigenvalues for the three lowest levels. They used the WKB method to confirm the reality of the ground state energy. Their approach also applied to the complex Hénon–Heiles potential $V_{\rm HH} = x^2 + y^2 + ig\left(xy^2 - x^3/3\right)$ [3]. In 2002, Nanayakkara and Abayaratne revisited the $igxy^2$ interaction with a non-degenerated set-up. They computed energy eigenvalues up to $n = 4$. With their choice of parameters, all eigenvalues appear to be real [4]. Later in the same year, Nanayakkara obtained the analytic results for $igxy$ interaction and numerical results in $igxy^3$ and $igxyz^2$ interactions. For all three systems, the author found real spectrum for small enough coupling constant and complex one for large coupling. The interaction of igx^2y^2 is also studied [5]. In 2005, Nanayakkara observed avoided level crossings in both the real cubic interaction gxy^2 and the complex cubic interaction $igxy^2$ [6]. The results have been challenged in a comment by Bíla *et al* in ref. [7]. They pointed out that the quantum system with the real cubic potential is ill-defined and the complex cubic potential has no avoided level crossings.

In this paper, we compute the eigenvalues of two-dimensional systems to high levels with high precision. We study the Hamiltonians associated with the complex cubic potential V_{12}

$$H_{12} = p_x^2 + p_y^2 + x^2 + y^2 + igxy^2 \tag{1}$$

and with the complex Hénon–Heiles potential $V_{\rm HH}$

$$H_{\rm HH} = p_x^2 + p_y^2 + x^2 + y^2 + ig\left(xy^2 - \frac{1}{3}x^3\right). \tag{2}$$

Both Hamiltonians are not Hermitian. Rather, they respect the $\mathcal{PT}$ symmetry and the y parity:

$$[H, \mathcal{PT}] = 0, \quad [H, \mathcal{P}_y] = 0, \tag{3}$$

where the total parity $\mathcal{P}$, the time reversal $\mathcal{T}$, and the y parity $\mathcal{P}_y$ are defined as

$$\begin{aligned}
&\mathcal{P}: i \to i; \quad x \to -x; \quad y \to -y,\\
&\mathcal{T}: i \to -i; \quad x \to x; \quad y \to y,\\
&\mathcal{P}_y: i \to i; \quad x \to x; \quad y \to -y.
\end{aligned} \tag{4}$$

Although the Hamiltonians are complex, the secular equations are real due to the $\mathcal{PT}$ symmetry. They can only depend on g^2. Therefore, both systems are invariant under $g \to -g$.

Since the y parity is an unbroken symmetry, we can diagonalize H and $\mathcal{P}_y$ simultaneously. All the eigenfunctions of H are also eigenfunctions of $\mathcal{P}_y$ with eigenvalues ± 1.

We use different methods to compute the eigenvalues of each system. We found complex conjugate pairs when the levels cross between same y-parity states. At higher level, the level crossing happens at smaller coupling constant. This indicates that no matter how small the coupling constant is, there are always complex eigenvalues at high enough levels. It shows the rich structure in the two-dimensional $\mathcal{PT}$-symmetric quantum systems. One must be very careful when generalizing the results in one-dimensional non-Hermitian quantum mechanics to higher dimensions.

The paper is organized as follows: the methods we used are briefly reviewed in §2, the results of different systems are presented in §3 and §4 and we conclude in §5.

2. Methodology

We use three different methods to study the spectra of Hamiltonians in (1) and (2).

- The first method is the perturbation theory. Because the energy levels of unperturbed Hamiltonian,

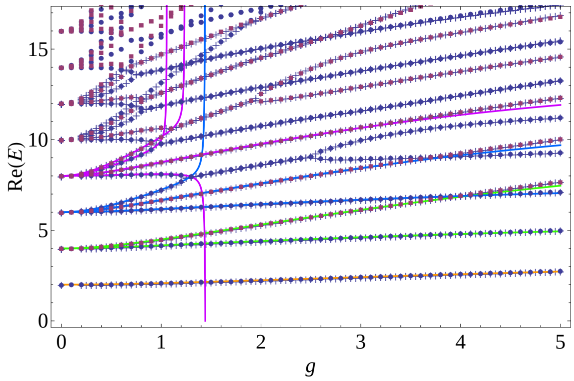

Figure 1. Real parts of the eigenvalues as functions of the coupling constant g with the complex cubic potential. Lines are from perturbative expansion using $(20, 20)$ Padé. Crosses are the results using FEM. Dots are results using the method based on two-dimensional HO basis expansions. Blue disks have even y-parity and purple squares have odd y-parity. The system is symmetric under $g \to -g$ and only the part with positive g is shown.

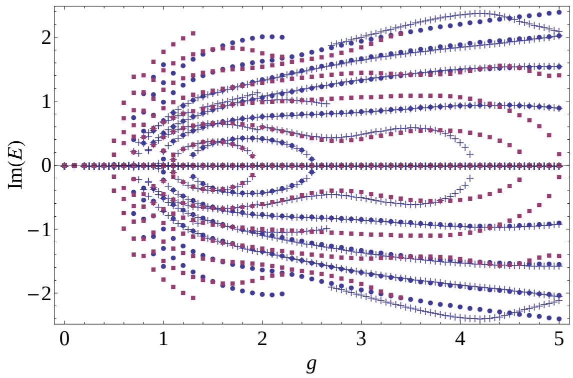

Figure 2. Imaginary parts of the eigenvalues as functions of the coupling constant g with the complex cubic potential. Crosses are the results using FEM. Dots are the results using the method based on two-dimensional HO basis expansions. Blue disks have even y-parity and purple squares have odd y-parity. The system is symmetric under $g \to -g$, only the part with positive g is shown.

$$H_0 = p_x^2 + p_y^2 + x^2 + y^2,$$

has degeneracy, we must apply the degenerate perturbation theory. After getting the eigenvalues as power series of the coupling constant g, we use Padé expansions to extract the information from the divergent series. The results for the two systems are shown as lines in figures 1 and 3, respectively.

- The second method is numerical computation by the finite-element method (FEM). The FEM results for eigenvalues with V_{12} potential are shown as crosses in figures 1 and 2.

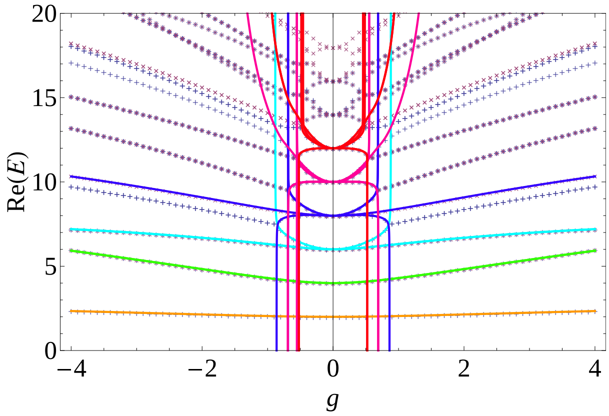

Figure 3. Real parts of the eigenvalues as functions of the coupling constant g with the complex Hénon–Heiles potential. Lines are from perturbative expansion using $(20, 20)$ Padé. Crosses are from HO expansions. Even y-parity states are using $+$ and odd y-parity states are using $\times$.

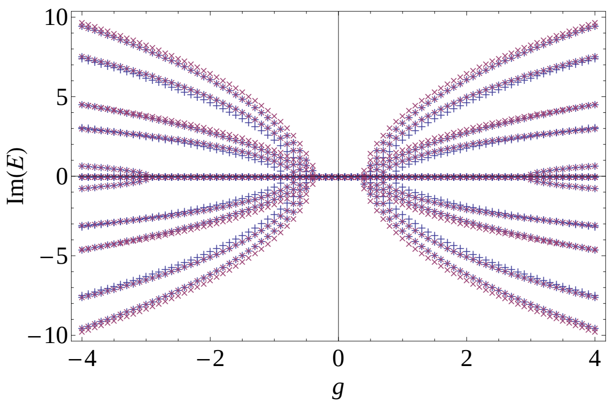

Figure 4. Imaginary parts of the eigenvalues as functions of the coupling constant g with the complex Hénon–Heiles potential. Only the results from HO expansions are shown. Even y-parity states are using $+$ and odd y-parity states are using $\times$.

- The third method is based on the expansion in two-dimensional harmonic oscillator (HO) basis [8]. We first analytically compute the non-vanishing matrix elements of the full Hamiltonian on the two-dimensional HO eigenfunctions basis. Depending on the precision requirement, we truncate the sparse matrix to a finite size, and the eigenvalues of the full Hamiltonian can be obtained by numerically diagonalizing this finite matrix. This method is a mixture of analytic and numerical techniques. It turns out that this is the best way to compute the eigenvalues of the two-dimensional complex Hamiltonians. The results are shown as dots in figures 1 and 2 and crosses in figures 3 and 4.

From figure 1 we can clearly see that all three methods provide consistent information about the real part of the eigenvalues; and figure 2 shows that the two numerical methods are consistent on the imaginary part of the eigenvalues.

3. Eigenvalues with the complex cubic potential

Using perturbation theory, we calculate the eigenvalues as power series of the coupling constant g. Here are the first few terms for the first 10 eigenvalues:

$$
\begin{aligned}
E_{00} &= 2+\frac{5}{48}g^2-\frac{223}{6912}g^4+\frac{114407}{4976640}g^6-\frac{346266143}{14332723200}g^8+\cdots\\
E_{10} &= 4+\frac{11}{16}g^2-\frac{869}{2304}g^4+\frac{737419}{1658880}g^6-\frac{3486539861}{4777574400}g^8+\cdots\\
E_{11} &= 4+\frac{13}{48}g^2-\frac{1519}{6912}g^4+\frac{1535767}{4976640}g^6-\frac{7858558079}{14332723200}g^8+\cdots\\
E_{20} &= 6+\left(\frac{17}{16}+\frac{\sqrt{41}}{8}\right)g^2-\left(\frac{329}{384}+\frac{3407}{768\sqrt{41}}\right)g^4\\
&\quad+\left(\frac{417793}{276480}+\frac{63502133}{7557120\sqrt{41}}\right)g^6\\
&\quad-\left(\frac{952249153}{265420800}+\frac{18548037835009}{892344729600\sqrt{41}}\right)g^8+\cdots\\
E_{21} &= 6+\frac{19}{16}g^2-\frac{1063}{768}g^4+\frac{1606697}{552960}g^6-\frac{4024837709}{530841600}g^8+\cdots\\
E_{22} &= 6+\left(\frac{17}{16}-\frac{\sqrt{41}}{8}\right)g^2-\left(\frac{329}{384}-\frac{3407}{768\sqrt{41}}\right)g^4\\
&\quad+\left(\frac{417793}{276480}-\frac{63502133}{7557120\sqrt{41}}\right)g^6\\
&\quad-\left(\frac{952249153}{265420800}-\frac{18548037835009}{892344729600\sqrt{41}}\right)g^8+\cdots\\
E_{30} &= 8+\left(\frac{115}{48}+\frac{\sqrt{721}}{24}\right)g^2-\left(\frac{9205}{3456}+\frac{260275}{6912\sqrt{721}}\right)g^4\\
&\quad+\left(\frac{3128263}{497664}+\frac{77128555369}{717631488\sqrt{721}}\right)g^6\\
&\quad-\left(\frac{28693057087}{1433272320}+\frac{576524526420731587}{1490147432202240\sqrt{721}}\right)g^8+\cdots\\
E_{31} &= 8+\frac{137}{48}g^2-\frac{888811}{214272}g^4+\frac{1766794711427}{148259082240}g^6\\
&\quad-\frac{16887386781611073971}{410333696734003200}g^8+\cdots
\end{aligned}
$$

$$E_{32} = 8 + \left(\frac{115}{48} - \frac{\sqrt{721}}{24}\right) g^2 - \left(\frac{9205}{3456} - \frac{260275}{6912\sqrt{721}}\right) g^4 + \left(\frac{3128263}{497664} - \frac{77128555369}{717631488\sqrt{721}}\right) g^6 - \left(\frac{28693057087}{1433272320} - \frac{576524526420731587}{1490147432202240\sqrt{721}}\right) g^8 + \cdots$$

$$E_{33} = 8 + \frac{13}{48} g^2 - \frac{85457}{214272} g^4 + \frac{126990201721}{148259082240} g^6 - \frac{998074124043859297}{410333696734003200} g^8 + \cdots. \tag{5}$$

We actually continue this expansion up to the order of g^{40}, then use $(20, 20)$ Padé to extract the information from the divergent series. The results are shown as lines in figure 1. From the figure, we may see that some Padé expansions have poles and cross each other.

In the same figure, we show the real parts of eigenvalues from FEM as crosses and from HO expansions as dots. The two sets of numerical results clearly agree with each other. Surprisingly, up to the crossing points, the Padé expansions fit the numerical results very well.

Although the Hamiltonian H_{12} has $\mathcal{PT}$ symmetry, some energy eigenvalues are complex. The imaginary parts of the eigenvalues by two numerical methods are shown in figure 2.

From figure 1, we observe two types of level crossings. If the crossing is between different y-parity states, the eigenvalues remain real. One example of this type is the crossing between the third and fourth lowest states near $g = 4$. If the crossing is between same y-parity states, then eigenvalues become complex conjugate pairs. For example, the sixth and seventh lowest states cross near $g = 1.4$.

We also observed that the level crossing happens in higher levels at smaller value of coupling constant. This indicates that no matter how small the coupling constant is, there is always complex eigenvalues at high enough levels. There is no critical value, $g_c > 0$, such that for $|g| < g_c$, the entire spectrum is real.

4. Eigenvalues with the complex Hénon–Heiles potential

In the case of the complex Hénon–Heiles potential, a similar patten appears. The energy eigenvalues become complex when $g \neq 0$. There are special features for this interaction.

- First, there are all rational numbers in every term of eigenvalues in the perturbation expansion.
- Second, there is an accident degeneracy between odd and even y-parity. Most of the energy levels are degenerated, but interestingly, not all of them. For example, $E_{10} = E_{11}$, $E_{21} = E_{22}$ and $E_{30} = E_{31}$, but $E_{32} \neq E_{33}$. In fact, E_{32} and E_{33} are the same up to the order of g^2, but for the order of g^4 and higher, they separate. This patten remains the same for higher exciting states:

  - For even $n \geq 2$, $E_{n1} = E_{n2}$, $E_{n3} = E_{n4}$, etc.
  - For odd $n \geq 3$, $E_{n0} = E_{n1}$, $E_{n4} = E_{n5}$, etc.
  - For odd $n \geq 3$, $E_{n2} \neq E_{n3}$ starting from the order of g^4.
- Third, E_{53} appears to be non-alternating in signs in the expansion, and this is a unique case up to $n = 9$.

Here are the first few terms for the first 21 eigenvalues:

$$
\begin{aligned}
E_{00} &= 2 + \frac{1}{18}g^2 - \frac{11}{864}g^4 + \frac{6089}{933120}g^6 - \frac{2221951}{447897600}g^8 + \cdots \\
E_{10} &= E_{11} = 4 + \frac{7}{18}g^2 - \frac{133}{864}g^4 + \frac{30191}{233280}g^6 - \frac{67779467}{447897600}g^8 + \cdots \\
E_{20} &= 6 + \frac{31}{18}g^2 - \frac{145}{288}g^4 + \frac{200923}{186624}g^6 - \frac{40752209}{29859840}g^8 + \cdots \\
E_{21} &= E_{22} = 6 + \frac{5}{9}g^2 - \frac{83}{144}g^4 + \frac{432493}{466560}g^6 - \frac{133188257}{74649600}g^8 + \cdots \\
E_{30} &= E_{31} = 8 + \frac{26}{9}g^2 - \frac{535}{432}g^4 + \frac{180037}{46656}g^6 - \frac{296084959}{44789760}g^8 + \cdots \\
E_{32} &= 8 + \frac{5}{9}g^2 - \frac{1123}{432}g^4 + \frac{1416869}{233280}g^6 - \frac{3963323843}{223948800}g^8 + \cdots \\
E_{33} &= 8 + \frac{5}{9}g^2 - \frac{115}{432}g^4 + \frac{12121}{46656}g^6 - \frac{15676999}{44789760}g^8 + \cdots \\
E_{40} &= 10 + \frac{91}{18}g^2 - \frac{2065}{864}g^4 + \frac{1208431}{186624}g^6 - \frac{1731827209}{89579520}g^8 + \cdots \\
E_{41} &= E_{42} = 10 + \frac{35}{9}g^2 - \frac{1085}{432}g^4 + \frac{1285823}{93312}g^6 \\
&\qquad - \frac{1478364167}{44789760}g^8 + \cdots \\
E_{43} &= E_{44} = 10 + \frac{7}{18}g^2 - \frac{2485}{864}g^4 + \frac{1063615}{186624}g^6 \\
&\qquad - \frac{1819581169}{89579520}g^8 + \cdots \\
E_{50} &= E_{51} = 12 + \frac{127}{18}g^2 - \frac{1205}{288}g^4 + \frac{814129}{46656}g^6 \\
&\qquad - \frac{1958220799}{29859840}g^8 + \cdots \\
E_{52} &= 12 + \frac{85}{18}g^2 - \frac{2633}{288}g^4 + \frac{1370563}{29160}g^6 - \frac{20818356203}{149299200}g^8 + \cdots \\
E_{53} &= 12 + \frac{85}{18}g^2 + \frac{55}{288}g^4 + \frac{70673}{5832}g^6 + \frac{354058961}{29859840}g^8 + \cdots \\
E_{54} &= E_{55} = 12 + \frac{1}{18}g^2 - \frac{1457}{288}g^4 + \frac{329257}{29160}g^6 \\
&\qquad - \frac{9599275547}{149299200}g^8 + \cdots .
\end{aligned} \tag{6}
$$

As in the previous section, we actually continue this expansion up to the order of g^{40}, then use $(20, 20)$ Padé to extract the information from the divergent series. The results are shown as lines in figure 3.

The results from HO expansions are shown as crosses in the same figure. Once again, we found the Padé expansions fit the numerical results up to the crossing points.

The $\mathcal{PT}$ symmetry is also broken in this Hamiltonian. Some eigenvalues cross and form complex conjugate pairs. The imaginary parts of the eigenvalues by HO expansions are shown in figure 4.

5. Concluding remarks

We concluded that both Hamiltonians have complex spectra. The origin of this broken $\mathcal{PT}$ symmetry is unclear. It could be due to the interaction between Hermitian and non-Hermitian potentials as in ref. [9]. It could also be due to the level contraction instead of level repulsion in the non-Hermitian quantum mechanics.

The results indicate that there is no critical value of the coupling constant to have reality in this degenerated set-up. In the analogue with the $igxy$ interaction studied in ref. [5], it is possible that small enough coupling constant exhibits entire real spectrum in the non-degenerated set-up. This would be confirmed by a future study.

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