

ON THE REAL TRACE OF SPECTRUM OF A FAMILY OF \mathcal{PT} -SYMMETRIC HAMILTONIANS

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Abstract

In this paper we give an outline on the real part of energy spectrum of non-Hermitian Hamiltonians $\mathcal{H}_\alpha = p^2 + (-q^4 + i\alpha q)$, where α is a real number. It was showed that when α tends to $-\infty$ some pairs of real branches of the spectrum develop into the range of negative energy levels and coalesce before turning into complex conjugate. This phenomenon for cubic oscillators has been described by Delabaere and Trinh (J.Phys. A: Math. Gen. 33 (2000), 8771-8796), and that motivates our present study.

1. Introduction

Since its first formulation in the late 1990's [2], \mathcal{PT} -symmetric quantum mechanics whose main objects are non-Hermitian Hamiltonians but having \mathcal{PT} -symmetry has attracted much attention of many mathematicians and theoretical physicists. Despite the lack of Hermiticity, many \mathcal{PT} -symmetric Hamiltonians still maintain a number of basic characteristics in common with hermitian Hamiltonians. These characteristics, which are necessary for the formulation of

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traditional quantum mechanics, consist of the reality, discreteness and (lower) boundness of the spectrum [2, 3, 8, 5, 14, 17, 18, 21, 27].

Unfortunately, being \mathcal{PT} -symmetric is not a sufficient condition for Hamiltonians to possess a real spectrum [4, 13, 16, 19]. Naturally, studying of the structure of spectrum of certain \mathcal{PT} -symmetric Hamiltonians is a preliminary step in attempts to construct a conventional physical theory of \mathcal{PT} -symmetric quantum mechanics [9, 7, 22, 23, 32].

Among mentioned references, [16] supplied a rather complete picture about the analysis structure of the spectrum of a family of Hamiltonians $\mathcal{H} = p^2 + i(q^3 + \alpha q)$ associated with (complex) cubic oscillators on the real line. It has been shown (by using the *exact* WKB analysis) that, for $\alpha > 0$ the whole spectrum is real and consists of (infinitely many) determinations of a sole multi-valued analytic function. While these determinations gradually coalesce in pairs before splitting into complex conjugate ones when α tends to minus infinity.

Motivated by this work, our purpose in this article is to explore the real part of spectrum of a similar family of Hamiltonians describing (complex) quartic oscillators. More concretely, we consider a family of non-Hermitian Hamiltonians

$$\mathcal{H}_\alpha = p^2 + (-q^4 + i\alpha q) \quad (1)$$

where $p := -id/dq$ and α is a parameter, which is assumed to be real through the paper.

This assumption furnishes Hamiltonians \mathcal{H}_α with a kind of symmetry, called \mathcal{PT} -symmetry, which is weaker than the Hermiticity, but still keeps spectra of \mathcal{H}_α unchanged under the complex conjugation. In general, a one-dimensional Hamiltonian $\mathcal{H} = p^2 + V(q)$ is said to be \mathcal{PT} -symmetric if it commutes with the composite operator \mathcal{PT} , whose components are defined by the following actions on the complex (p, q) -space

$$\mathcal{P} : \begin{cases} q \mapsto -q \\ p \mapsto -p \end{cases} \quad \text{and} \quad \mathcal{T} : \begin{cases} q \mapsto \bar{q} \\ p \mapsto -\bar{p} \end{cases}$$

As a matter of fact, the requirement for the commutability between H and the combination \mathcal{PT} amounts to forcing $V(q)$ to verify the following equality

$$\overline{V(-\bar{q})} = V(q)$$

Thus, that is the case of \mathcal{H}_α for real α .

For our non-Hermitian Hamiltonian (1), as well as those of general form, the space on which it acts may be no longer a Hilbert space. Instead of $L^2(\mathbb{R})$ as usual, a certain space with an appropriate structure will be involved; for example the space of square-integrable functions $L^2(\gamma)$, where γ is an endless contour in the complex q -plane¹. In particular, our study of the spectrum of

¹For instance, furnishing an appropriate inner product for this kind of space is discussed in [9, 7, 23]

\mathcal{H}_α will concern “bound states”, which are (complex) functions analytic and square-integrable along a contour starting from and ending at infinity at the phases $-\pi/2 \mp \pi/3$.

By virtue of classical results on asymptotic analysis of ordinary differential equations, this problem can be reduced to the complex Sturm-Liouville problem for the (Schrödinger) equation

$$-\phi''(q) + (-q^4 + i\alpha q)\phi(q) = E\phi(q) \tag{2}$$

with boundary conditions

$$\lim_{q \rightarrow \infty, e^{-i5\pi/6}} \phi(q) = 0 \quad \text{and} \quad \lim_{q \rightarrow \infty, e^{-i\pi/6}} \phi(q) = 0 \tag{3}$$

This kind of singular boundary value problem is studied intensively in [28] by virtue of Stokes multipliers.

Starting from a slightly different approach to this problem, our goal is to describe the behavior of the (real) eigenvalues $E_n(\alpha)$ of the problem (2)(3) for various $\alpha \in \mathbb{R}$. The method of investigation is based on the apparatus of “exact WKB analysis” developed by Voros [31] and others [12, 15].

This paper is organized as follows: In section 2 we first give a brief summary of recent results on eigenvalues of problem (2)(3). After recalling some necessary ingredients for WKB calculus, we will state the main result for the case of $\alpha > 0$. The asymptotic behavior of $E_n(\alpha)$ for sufficiently negative α will be the content of Section 3. Surprisingly, we found that the real part of spectrum exhibits a crossing phenomenon similar to the cubic Hamiltonian. The picture of spectrum is sketched out.

2. Asymptotic behavior of the spectrum at $+\infty$

The boundary value problem associated with a second-order linear differential equation with polynomial coefficients has been studied intensively in a pioneer work of Sibuya [28]. By virtue of asymptotic estimates of solutions, solving this kind of eigenvalue problems immediately amounts to exploring zeros of an entire function, the so-called Stokes multiplier.

For our special case, we can transform Eq. (2) into the following

$$-\Phi''(X) + (X^4 - \alpha X + E)\Phi(X) = 0, \tag{4}$$

by using a simple change of variable

$$X := iq; \quad \Phi(X) := \psi(q). \tag{5}$$

The boundary condition now reads

$$\Phi(X) \longrightarrow 0, \quad \text{when} \quad \begin{cases} |X| \longrightarrow +\infty \\ X \in S_{\pm 1} \end{cases} \tag{6}$$

where

$$S_{\pm 1} := \left\{ \left| \arg(X) - \frac{\pm\pi}{3} \right| < \frac{\pi}{6} \right\}.$$

Obviously, the eigenvalues of the problem (4)(6) are exactly those of the problem (2)(3).

Before going further, we now recall some of known facts on eigenvalues of the problem (4)(6) by summarizing recent contributions on the subject [17, 27, 30].

Theorem 1. *For any fixed $\alpha \geq 0$, the boundary value problem for (4) with boundary condition (6) has infinitely many eigenvalues $E_n(\alpha)$. All of them are simple, positive real and*

$$E_n(\alpha) = \left(\frac{(2n-1)\pi}{2K} \right)^{4/3} [1 + \nu_n], \quad \text{for } n \rightarrow +\infty \quad (7)$$

where $K := \int_0^{+\infty} (\sqrt{1+t^4} - t^2) dt > 0$ and $\nu_n \rightarrow 0$.

REMARK 2. The fact that eigenvalues $E_n = E_n(\alpha)$ are nothing but zeros of the entire function $C(\alpha, E)$ implies that each $E_n(\alpha)$ is continuous on $[0, +\infty)$ as functions of α . Therefore, the reality and positivity of the eigenvalues, as well as the simpleness by its very formulation [30], are “open” properties. The statements in Theorem 1 are then still valid for some $\alpha \lesssim 0$. More precisely, it could be extended at least to the bound $\alpha \geq -2$. In particular, for $\alpha = -2$, the lowest eigenvalue is exactly zero, to which the corresponding eigenfunction is $e^{\frac{x^3}{3}}$ (see [6, 27]).

REMARK 3. It might be interesting to remark that the leading term of the asymptotic behaviour of large eigenvalues given by (7) does not depend on α .

Our aim in this section is to describe asymptotic behavior of eigenvalues $E_n(\alpha)$ when α tends to $+\infty$ for each fixed n . This kind of problem for a cubic model has been investigated intensively by using the exact WKB analysis [16]. This reference furnishes the global analysis structure of the spectrum not only for real α , but also for any phrase of α in the complex plane. However, in this paper, we limit our considerations only to the case of real α , which guarantees the \mathcal{PT} -symmetry property of Hamiltonian (1). We thus have

Theorem 4. *For $\alpha > 0$, we have*

$$E_n(\alpha) > \frac{3}{4\sqrt[3]{4}} \alpha^{4/3}, \quad \text{for all } n \in \mathbb{N} \quad (8)$$

and for each fixed $n \in \mathbb{N}$, we get

$$E_n(\alpha) \asymp \frac{3}{4\sqrt[3]{4}} \alpha^{4/3} + \alpha^{1/3} \sum_{k=0}^{\infty} \frac{E_{n,k}}{\alpha^k}, \quad \text{when } \alpha \rightarrow +\infty \quad (9)$$

where all $E_{n,k}$ are real number and can be computed by the same algorithm in [12]:

$$\begin{aligned} E_{n,0} &= 1/2 (1 + 2n) \sqrt{6} \sqrt[3]{2}, \\ E_{n,1} &= 1/36 (13 + 42n + 42n^2) \sqrt[3]{2}, \\ E_{n,2} &= -\frac{1}{1296} (-1 + 89n + 273n^2 + 182n^3) \sqrt{6} \sqrt[3]{2}, \\ E_{n,3} &= -\frac{1}{69984} (24517 + 84105n + 115080n^2 + 61950n^3 + 30975n^4) \sqrt[3]{2}, \dots \end{aligned}$$

Further more, the series on the right-hand side of (9) is Borel resumable with respect to α^{-1} and yields exactly the value of $E_n(\alpha)$ via Borel resummation.

The formulation of this statement is essentially originated in the results in our earlier paper [16], while the idea for the proof is radically based on Pham’s work [26]. In the latter reference, Pham has showed the universality of polynomial models and derived a hierarchy, under which one can “see” a model in a higher one. Roughly speaking, our quartic model will be reduced to quadratic or cubic one.

Before proving the theorem, we recall some basic notions of the exact WKB analysis. For a time-independent one-dimensional Schrödinger equation

$$-\hbar^2 \frac{d^2 \varphi}{dq^2} + (V(q) - E)\varphi(q) = 0, \tag{10}$$

the WKB method consists of finding formal solutions of the form

$$\varphi(q) = \left(\sum_{n=0}^{\infty} \varphi_n(q) \hbar^n \right) e^{\frac{i}{\hbar} S(q)}, \tag{11}$$

where $S(q)$ is a solution of the equation

$$(S'(q))^2 = E - V(q) =: p(q)^2$$

To avoid ambiguity caused by the multivalence of $S(q)$, we will define objects locally on the Riemann surface of $p(q)$, which is a 2-fold covering of the complex q -plane eliminated *turning points* (i.e. zeros of $V(q) - E$). For the case $V(q) - E$ is a polynomial, formal solutions of the form (11) are in general resurgent functions, analytically depending on the coefficients of $V(q) - E$ if they are “well normalized” by multiplying an appropriate factor in $\mathbb{C}[[\hbar]]$. This enables us to treat these formal objects as true functions via the Borel-resummation. For more details on these topics we refer the reader to [10, 11, 12, 15, 31].

Return to our point, we need to know how the altitude of solutions $\varphi(q)$ in (11) changes when q varies in the complex plane. For fixed $\hbar > 0$ and a choice of determination of $p(q)$, this is controlled by the factor $e^{\frac{i}{\hbar} S(q)}$. We call *Stokes*

lines (resp. *anti-Stokes lines*) of Eq. (10) the curves in the q -plane emanating from a turning point, along which $\Im(\frac{i}{\hbar}S(q))$ (resp. $\Re(\frac{i}{\hbar}S(q))$) is constant. Obviously, along a Stokes line that ends at infinity, the solution (11) vanishes or increases fastest, according to the sign of the real part of $\frac{i}{\hbar}S(q)$. A solution $\varphi(q)$ is said to be *recessive* (resp. *dominant*) along an endless Stokes line L if it vanishes (resp. grows) exponentially when q tends to infinity along L . A set of rules that allow to observe the alternation of dominance for solutions (11) can be found in [12].

Proof of Theorem 4: Consider a value of $\alpha > 0$, sufficiently large. By the quasi-homogeneity, Eq. (2) can be reduced to the form of Schrödinger equation

$$-\hbar^2 \frac{d^2 \varphi}{dq^2} + (-q^4 + iq - \widehat{E})\varphi(q) = 0, \tag{12}$$

by introducing a (small) parameter \hbar and changing its variables

$$\hbar := \alpha^{-1} > 0, \quad q \mapsto q\hbar^{-1/3}, \quad E := \widehat{E}\hbar^{-4/3}, \quad \phi(q) \mapsto \varphi(q). \tag{13}$$

The unique *real* critical value of potential $-q^4 + iq$ is $\widehat{E}_{crit} = \frac{3}{4\sqrt[3]{4}}$. Some previous investigations show that we can also get much information about energy levels of (12) by locating \widehat{E} only near the critical value \widehat{E}_{crit} . Some typical Stokes patterns for $\widehat{E} \simeq \widehat{E}_{crit}$ are drawn in Fig. 1.

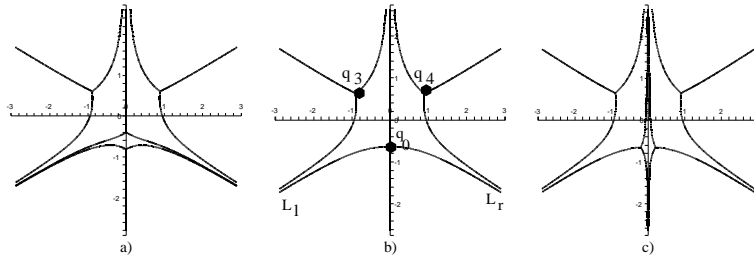


Figure 1: Stokes patterns of Eq. (12) for \widehat{E} near \widehat{E}_{crit} .

The “bound-states” problem for (12) can be solved geometrically as follows. Starting with a (non-null) solution $\varphi(q)$ recessive along Stokes line L_l , which is at the phase $-5\pi/6$ and bounds the domain containing the negative imaginary half-axis, we make all possible analytic continuations of $\varphi(q)$ to a domain containing L_r (the same as L_l but at the phase $-\pi/6$, see Fig. 1), in the manner as in [12]. Next, we eliminate all the obtained solutions which are dominant along L_r . This manipulation usually reduces to a more analytic

problem, which is to solve an equation (the so-called *secular equation*) and known as the *quantization condition*.

In spirit of Pham’s work [26], by ignoring Stokes lines² attached to two turning points q_3 and q_4 on Fig. 1, we can see a Stokes pattern of quadratic model, i.e. that of simple harmonic oscillator.

As a consequence, we infer that the quantization condition cannot occur for $\widehat{E} < \widehat{E}_{crit}$. Indeed, this case involves a pattern of Airy’s type, where L_l and L_r can be considered as two consecutive Stokes lines. This implies the latter estimates of the theorem³.

For the case $\widehat{E} \gtrsim \widehat{E}_{crit}$, the quantization condition can be established easily by using the same reasonings in [12, Section III] (see also [16]). It is found exactly of the (Bohr-Sommerfeld) form

$$s(E_r, \hbar) = n \tag{14}$$

where $s = s(E_r, \hbar)$ is a (formal) power series of \hbar , the so-called *monodromy exponent* of $\varphi(q)$ (for details see [12]) at the double turning point q_0 and E_r is the *rescaled* energy induced by locating \widehat{E} near the critical value

$$\widehat{E} := 3\sqrt[3]{2}/8 + \hbar E_r. \tag{15}$$

Since there is no bounded Stokes line attaching to the double turning point q_0 , it turns out that s is an expansion Borel summable in the direction of $\arg(1/\hbar) = 0$ and resurgent with respect to $1/\hbar^4$. By theorem of implicit (resurgent) functions [24, 15], Eq. (14) can be solved formally for each $n \in \mathbb{N}$ under the form of Rayleigh-Schödinger series

$$E_r^n = \sum_{k=0}^{\infty} E_{n,k} \hbar^k \tag{16}$$

where the coefficients $E_{n,k}$ can be computed by the algorithm described in [12, Section V]. A crucial point here is that series (16) is still Borel summable, so we can “recover” E_r^n by the Borel resummation as the following

$$E_r^n = E_r^n(\hbar) = E_{n,0} + \int_0^{+\infty} b(\xi) e^{-\xi/\hbar} d\xi$$

where

$$b(\xi) := \sum_{k=1}^{\infty} E_{n,k} \frac{\xi^{k-1}}{\Gamma(k)}$$

²These Stokes lines are not intervened in the quantization condition.

³This can be also verified directly by the same way as in [29, Thm. 2].

⁴In fact, s is resummable in a larger range by analytically continuing $1/\hbar$ into the complex plane. The possible obstacles are nothing but periods of action integral $S(q)$ with respect to cycles surrounding q_0 and q_3, q_4 respectively.

is Borel transform of (16). The fact that Borel sum of a series admits that series itself as an asymptotic expansion completes the proof, up to getting back the initial variables.

3. Picture of spectrum for $\alpha < 0$.

We begin this section with a remark that when α varies in the negative half-axis, the eigenvalue problem (4)(6) admits zero as one of its eigenvalues infinitely many times (e.g. see [6]). For $E = 0$, the general solutions of (4) in fact can be written out in terms of Whittaker functions (see [1]). We can see without difficulty that there are infinitely many values of $\alpha < 0$ such that Eq. (4) admits solutions vanishing exponentially when X tends to infinity in both sectors S_{\pm} . For instance, for the sequence $\alpha_k = -6k - 4$ ($k \in \mathbb{N}$) of values of α , the mentioned Whittaker functions can be reduced to Laguerre polynomials so that the eigenfunctions corresponding to the eigenvalue $E = 0$ are exactly of the form of elementary functions

$$\Phi_{eigen}(X)|_{\alpha=-6k-4} = X e^{X^3/3} Q_k(X)$$

where Q_k is a polynomial of X^3 of degree k . From this observation, we can predict the appearance of negative eigenvalues when α takes negative values.

Similarly to the previous section, by rescaling variables

$$\hbar := -\alpha^{-1} > 0, \quad q \mapsto q\hbar^{-1/3}, \quad E := \widehat{E}\hbar^{-4/3}, \quad (17)$$

we can reduce Eq. (2) to the form

$$-\hbar^2 \frac{d^2 \varphi}{dq^2} + (-q^4 - iq - \widehat{E})\varphi(q) = 0. \quad (18)$$

The quantization condition for the bound states problem associated with Eq. (18) is established by the same manner as above. Some typical Stokes patterns in this case are drawn in Fig. 2.

We should notice that, there exists a value \widehat{E}_0 of real \widehat{E} such that the quantization condition for Eq. (18) cannot be occurred for $\widehat{E} < \widehat{E}_0$. Our numerical computation yields $\widehat{E}_0 \simeq -0.79$, corresponding to which the Stokes pattern possesses two bounded Stokes lines (Fig. 2, part b)). As a matter of fact, an Airy's model will be involved for $\widehat{E} < \widehat{E}_0$ and this explains why the quantization condition is impossible (Fig. 2, part c)).

As a consequence, we can conclude that, for each fixed $\alpha < 0$, all the (negative) real eigenvalues are necessarily lower bounded:

$$E_n(\alpha) > \widehat{E}_0(-\alpha)^{4/3}.$$

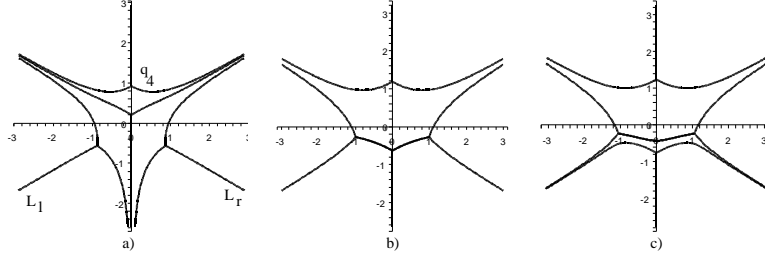


Figure 2: Some Stokes patterns for Eq. (18).

Now we consider a certain generic value $\widehat{E} > \widehat{E}_0$. The corresponding Stokes pattern is given in the part *a*) of Fig. 2. It can be seen homeomorphically, after erasing three Stokes lines attached to q_4 , that the Stokes pattern exhibits a cubic model (Fig. 3, the left part), which is investigated in detail in [16].

By the same arguments as in the former section, the quantization condition for bound states requires cancelling all the solutions which become dominant along L_r after being extended analytically from another that is recessive along Stokes line L_l . With the convenience of using notations in [16], the secular equation simply reads

$$1 - 2e^U \sin(\pi s) = 0, \quad (19)$$

where U and s are resurgent Borel-resummable expansions of \hbar (depending analytically on \widehat{E} , even regularly in the sense of [15]) and defined by

$$\begin{aligned} U = U(\widehat{E}, \hbar) &= \frac{i}{2\hbar} \int_{\gamma^* + \gamma} p(q, \widehat{E}) dq + O(\hbar) \\ s = s(\widehat{E}, \hbar) &= -\frac{1}{2} + \frac{1}{2\hbar\pi} \int_{\gamma^* - \gamma} p(q, \widehat{E}) dq + O(\hbar) \end{aligned} \quad (20)$$

The cycles γ and γ^* in these formulae (Fig. 3) are mutually symmetric under the real conjugation $q \longleftrightarrow -\bar{q}$. This implies the reality of U and s .

Our next step is to solve Eq. (19), then try to translate the results into (E, α) -space by inverting the following consecutive maps

$$(E, \alpha) \mapsto (\widehat{E}, \hbar) \mapsto (U, s). \quad (21)$$

This can be done very easily by repeating the arguments and computations in [16]. We should notice that the solutions U and s in (19) can be simultaneously *real* only for $U \geq -\ln 2$. Therefore, for $\alpha \ll -1$ (i.e. $\hbar \simeq 0$) and $U \gtrsim -\ln 2$,

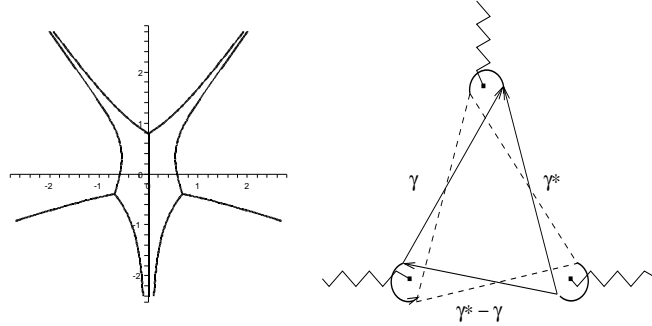


Figure 3: Real trace of spectrum for large $\alpha > 0$ and near crossing points for $\alpha < 0$.

we can deduce from (20) that

$$i \int_{\gamma^* + \gamma} p(q, \widehat{E}) dq \lesssim 0. \tag{22}$$

This requirement gives $\widehat{E} \lesssim 0$. We thus can see that when $\alpha \rightarrow -\infty$, the real eigenvalues $E_n(\alpha)$ in fact locate much higher than the curve $E = \widehat{E}_0(-\alpha)^{4/3}$ in the (E, α) -plane.

The left part of Figure 4 illustrates some of eigenvalues $E_n(\alpha)$ near their “crossing” points, where they collapse in pairs before splitting into complex conjugates. These curves are nothing but the reciprocal image of *real* solutions of Eq. (19) via the sequence (21). Numerical computation has been done at the value $\widehat{E} = -0.03$ by the same method as in [16]. It should notice that for $\widehat{E} = 0$, the left hand side in (22) is exactly zero⁵. The analytic structure of $E(\alpha)$ can be investigated similarly as in [16], but it goes further than our considerations in this text. To summarize, we can state the following

Theorem 5. *For α varies decreasingly from 0 to $-\infty$, the eigenvalues $E_n(\alpha)$ gradually develop into the range of $E < 0$ in the (E, α) -plane and collapse in pairs at points $\alpha_{[n/2]} < 0$ (known as their square-root branch points) before splitting into complex conjugates in the complex E -plane.*

REMARK 6. We can also estimate values of $\alpha_{[n/2]}$ by the same method as in [16, Theorem 4.2]. Their distribution is apparently regular at large indexes

$$\alpha_m = -(Cm + D) + O(m^{-1})$$

⁵The corresponding anti-Stokes pattern exhibits bounded anti-Stokes lines [16, Fig.11].

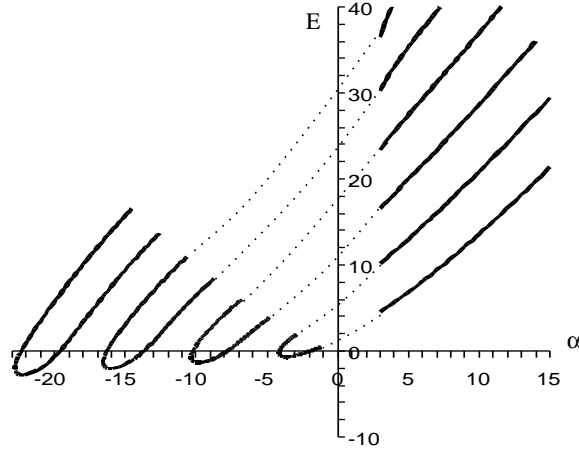


Figure 4: Real trace of spectrum for large $\alpha > 0$ and near crossing points for $\alpha < 0$.

where $C > 0, D$ are computable constants depending only on the range of considered α . The first value in our case is $\alpha_0 = -4.145245086$.

REMARK 7. From the very formulation, our description on the spectrum does not include the part corresponding to small $|\alpha|$. However, we believe that no singular behavior occurs in this gap. Here the dotted lines on Fig. 4 are only for illustration.

4. Conclusion

In this paper, we have explored the shape of the real energy spectrum of \mathcal{PT} -symmetric Hamiltonians \mathcal{H}_α associated with a family of complex quartic oscillators. It turns out that the real trace of the spectrum exhibits many features similar to those in the cubic case. The most interesting common property in both cases is that the real spectrum consists of infinitely many curves of a sole multivalent analytic function of α , growing like a power of $\alpha \gg 0$ and developing into complex conjugates in pairs when α tends to negative infinity. Yet a generalization for higher models was not mentioned and can be investigated by the same methods as in this paper.

Our analysis is essentially to reduce our model to well-known ones according to Pham’s point of view on the hierarchy of model [25, 26]. This reduction,

together with the applicability of the semiclassical asymptotic analysis, may be also useful for the studying of the spectrum of Hamiltonians of the more general type $p^2 - (iq)^m + i\alpha q$. Of course, for this kind of Hamiltonians, the triple (or higher) confluence of turning points does not appear so that the exact WKB methods in [12] are still applicable.

Even though there are some gaps in our understanding of the global structure, our study, together with earlier works [4, 15, 16], once again strengthens the effectiveness of the *exact* WKB analysis in investigating of the asymptotic behavior of the energy spectrum of this kind of Hamiltonians.

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