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Spectra of $\mathcal{PT}$-symmetric Hamiltonians on tobogganic contours

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Abstract. A non-standard generalization of the Bender potentials $x^2(ix^\varepsilon)$ is suggested. The spectra are obtained numerically and some of their particular properties are discussed.

Keywords. Quantum toboggans; $\mathcal{PT}$ symmetry; complex integration contours.

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1. Introduction

The term $\mathcal{PT}$-symmetric quantum mechanics, although defined to be of a much broader use, was coined in tight connection with C. Bender's analysis of one-dimensional Schrödinger Hamiltonians with potentials

$$V(x) = x^2(ix)^\varepsilon, \tag{1}$$

(see [1]) (we will call them Bender Hamiltonians in the following). This class of operators – characterized by one real parameter ε – contained probably the most exploited Hamiltonian in the history of physics: the $\varepsilon = 0$ harmonic oscillator; but on the other hand, the other members of the family were strange Hamiltonians with imaginary potentials which do not appear physical at all. The aim of the suggested $\mathcal{PT}$-symmetric treatment was to give them an acceptable interpretation and it became a rather standardized procedure since then. One of the key facts which allowed for the physical interpretation was that the spectra of these operators were real at least for some non-zero values of ε, a fact which stems from observation that first, for $\mathcal{PT}$-symmetric operators the complex eigenvalues appear in mutually conjugated pairs, and second, that the spectrum depends continuously on ε. Thus the boundary between real-energy and complex-energy domains can lie only at an exceptional point, i.e. a point where at least two eigenvalues merge. Consequently, one has to depart at least some finite distance on the ε-axis from the non-degenerate harmonic oscillator to see any selected eigenvalue becoming complex. What actually happens in the discussed case is visible at the classical figure (figure 1): the spectrum is real for all positive ε, while at negative ε the lower the energy is, the longer it remains real.

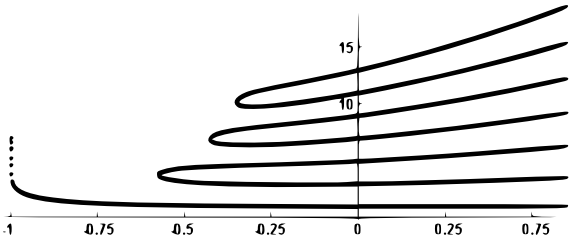

Figure 1. Well-known dependence of the eigenvalues of the Bender Hamiltonian on ε, non-tobogganic case. Complex energies are not shown. Based on numerical calculation it is expected that the value ε_n at which the nth energy becomes complex, tends to zero as $n \to \infty$.

However, the validity of the continuous energy dependence assumption is not obvious. An immediate question of the reader could be: What happens when $\varepsilon = 2$, which yields an obviously unphysical $-x^4$ potential with unbounded continuous spectrum? It is well-known now, that the correct response has to deal with boundary condition in the complex plane. The Hamiltonian which is the proper continuation of the harmonic oscillator in the parameter ε is defined on space of functions which are square-integrable not on the real line, but on some asymptotically straight contour in the complex plane which lies in the correct Stokes sector of the Schrödinger equation. Here, correct means that the sectors are itself a continuation of those sectors which contain the real line in the $\varepsilon = 0$ case. These sectors (also called 'wedges') are turning down in the complex plane as ε increases and for $\varepsilon \geq 2$ they no more contain the real line. Therefore, the conventional $-x^4$ Hamiltonian on $L_2(\mathbb{R})$ is not the only Hamiltonian which deserves this name; in some sense its analogue defined by the same differential equation but with complex boundary conditions is more natural.

For the sake of clarity let us recall that for potentials we are dealing with, the exact choice of the integration contour is irrelevant as long as it lies inside the Stokes sector asymptotically. It became customary to stop mentioning the contour altogether, speaking only about boundary conditions imposed inside a particular sector. On the other hand, the contour is a convenient means for defining the scalar product and, practically, some concrete choice of the contour is necessary for numerical computation. Thus we will speak about integration contours rather than wedge-defined boundary conditions in the rest of the paper, keeping in mind that due to the potential's analyticity, distinct contours with same-wedge asymptotics are equivalent [1a]. It may also be noted that in the special case $\varepsilon = 2$ it is enough to pose the boundary conditions on the shifted real line, i.e. $x = t - ic$ with arbitrary positive constant c (t is a real parameter). For higher ε one has to use bent contours to remain inside the Stokes wedge.

The existence of aforementioned continuation is interesting from different points of view. For example, it is relevant to the Dyson argument about convergence of the perturbative series, which is roughly stated as follows: having a potential $x^2 + gx^4$ (or its field-theoretical counterpart, the argument was originally formulated for quantum electrodynamics [2]) one may use perturbative expansion in g, but since for

any negative g the spectrum collapses to $(-\infty, \infty)$ and the perturbative calculation cannot produce this, the convergence radius of the series ought to be zero and the series is at best asymptotic. The existence of a negative-g Hamiltonian with discrete real and below bounded spectrum invalidates the argument's core assumption: it is now entirely possible that the series converges and gives the spectrum of the complex-plane $-x^4$ potential when evaluated at negative g [3].

2. Quantum toboggans

The observation which we want to point out now is that to force the integration contour to be asymptotically straight and inside the correct Stokes wedges is insufficient to uniquely define the spectra of Hamiltonians with (1). One has to take into account that for non-integer ε the potential lives on multiple Riemann sheets and it matters how the integration contour is distributed upon the sheets. In our presently discussed class of Hamiltonians, the only singularity lies at $x = 0$, which allows us to use only one winding number λ to fully characterize the contour. Hence instead of one $\mathcal{PT}$-symmetric continuation of the harmonic oscillator we obtain an infinite series numbered by distinct integer values of λ. The $\lambda = 0$ trajectory represents only the usually considered case. The higher-λ contours define distinct Hamiltonians which are sometimes referred to as quantum toboggans, and the reason for such denomination is clear when one imagines the Riemann sheets forming a helicoid [3a].

A technical note: To take advantage of the fact that real eigenvalues have to merge before becoming complex, one must take care about the $\mathcal{PT}$ symmetry. In particular, it dictates the position of the branch cut. It has to be chosen to lead upwards along the positive imaginary axis. On the other hand, the potential has to be $\mathcal{PT}$-symmetric on the contour, which, for $\lambda = 0$, forces the contour to pass below the singularity. If one wanted to have the contour bypassing zero from above, which is an equally reasonable option for the harmonic oscillator where no singularity is present, one has to change the potential accordingly to preserve the $\mathcal{PT}$ symmetry of the potential on the contour. Without much surprise this yields

$$V = x^2(-ix)^\varepsilon. \tag{2}$$

Such change of potential together with the change of the contour would obviously be nothing more than the reparametrization $x \to x^*$; as such it leaves the spectrum intact. We can similarly disregard the differences within analogous mutually conjugated pairs of trajectories and potentials even in more complicated settings. Therefore, without loss of generality, we will stick to the definition (1) and keep in mind that the contour must also conform to the $\mathcal{PT}$ symmetry.

The integration contours are schematically drawn in figures 2 and 3. It turns out that the choice of the $\lambda = 1$ contour in figure 2 is inconsistent with $\mathcal{PT}$ symmetry. Instead one has to use the up-down inverted curve, as depicted in figure 3. A general rule is that the centre point of the contour lies below zero (for concreteness say at $x = -i$) on the principal sheet, which is the one where $V(-i)$ is real.

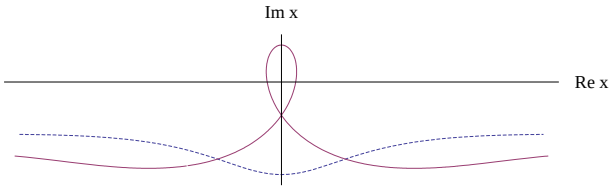

Figure 2. Considered integration contours: a straight one (winding number $\lambda = 0$) is drawn in the dashed line, while its most elementary tobogganic counterpart ($\lambda = 1$) is depicted in solid line. The latter contour is consistent with $\mathcal{PT}$ symmetry only if the branch cut aims downwards. Therefore we need to use an inverted one with potential (1).

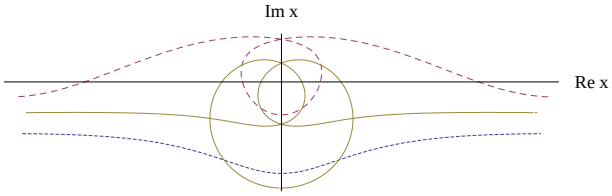

Figure 3. $\mathcal{PT}$-symmetric contours for $\lambda = 1, 2, 3$ of the potential $x^2(ix)^\varepsilon$. In contrast with figure 2, the $\lambda = 1$ contour is chosen inverted with respect to the real axis, confirming the $\mathcal{PT}$ symmetry assumption.

3. Numerical analysis

Unfortunately, the considered potentials are not exactly solvable. Therefore, we have to rely solely on numerical treatment. We use a relatively straightforward method for computation of eigenvalues; we are interested whether real eigenvalues are present – the existence of complex part of the spectrum can be partially deduced from the distribution of the exceptional points – this allows us to significanly simplify the calculation. First of all, a starting energy is chosen. Then we calculate two independent solutions of the differential equation with the chosen energy; let us denote them ψ_1 and ψ_2. The equation has been solved on the contour parametrized as

$$x = t - i \quad \text{for } \lambda = 0, \tag{3a}$$

$$x = i\mathrm{e}^{it}\Theta(\pi - |t|) + (t - \pi - i)\Theta(|t| - \pi) \quad \text{for } \lambda = 1, \tag{3b}$$

$$x = -i\mathrm{e}^{it}\Theta(2\pi - |t|) + (t - 2\pi - i)\Theta(|t| - 2\pi) \quad \text{for } \lambda = 2, \tag{3c}$$

and so on; i.e. the contour consists of a circle of unit radius λ-times encircling the singularity in $x = 0$ and a straight line parallel to the real axis [3b] matched to the circle at $x = -i$. For concreteness the initial conditions for $\psi_{1,2}$ are set in the centre of the contour (i.e. $t = 0$) to satisfy

$$\psi_1(0) = 0, \quad \psi_1'(0) = 1, \tag{4a}$$

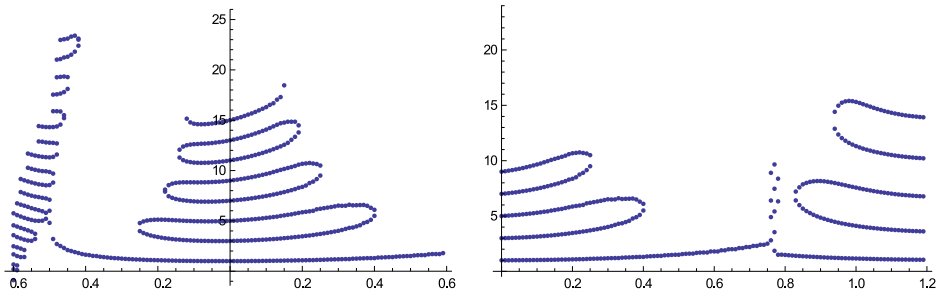

Figure 4. Spectra of Bender Hamiltonian contour with $\lambda = 1$. The graph on the right-hand side illustrates the behaviour around $\varepsilon = 1$ where real eigenvalues emerge again. The algorithm was requested to find only the lowest six real eigenvalues (five on the right graph). Hence the lines corresponding to higher eigenvalues are discontinued where the lower eigenvalue pair emerges. The chaotically distributed points in the upper part of the graph result from the error in the algorithm's implementation which occurs when the demanded number of real eigenvalues is not found. On both graphs, the vertical axis represents the energy while ε is drawn horizontally.

$$\psi_2(0) = 1, \quad \psi_2'(0) = 0. \tag{4b}$$

The number E is an eigenvalue if there exists a linear combination of ψ_1 and ψ_2 which is integrable. Because the asymptotics of the solution is exponential, this is equivalent to the existence of a linear combination tending to zero. In our calculations it is satisfactory to look at the function values at $x_\pm \approx \pm 10$, at least for the lowest eigenstates. The $\mathcal{PT}$ symmetry of the potential plays now a key role. Since we are interested only in the real part of the spectrum we can assume the $\mathcal{PT}$ symmetry of the wave function. The equation for the eigenvalues, which originally reads [3c]

$$\det \begin{pmatrix} \psi_1(E, x_+) & \psi_1(E, x_-) \\ \psi_2(E, x_+) & \psi_2(E, x_-) \end{pmatrix} = 0 \tag{5}$$

is now, having in mind (4a) and (4b), simplified to

$$\operatorname{Re} \psi_1(E, x_+)^* \psi_2(E, x_+) = 0. \tag{6}$$

Note that the left-hand side of (5) is a complex function of energy, whereas the left-hand side of (6) is real. This is clearly an advantage – the zeros of a real function can be determined by the bisection method. The described procedure works well for the case $\varepsilon = 0$ where comparison with the exact results is feasible; the exact result is recovered up to five- or six-digits precision, the precision can be enhanced with some loss of speed. Comparison of the non-tobogganic case with results obtained in [1] shows no significant differences. When $\varepsilon \to 2$ the computation becomes slower if the precision of computation has to be maintained since the solution's asymptotics become more vulnerable to numerical errors.

The results show that the behaviour of eigenvalues depends on the winding number λ. The results for $\lambda = 1$ (see figure 4) exhibit vast differences from the $\lambda = 0$

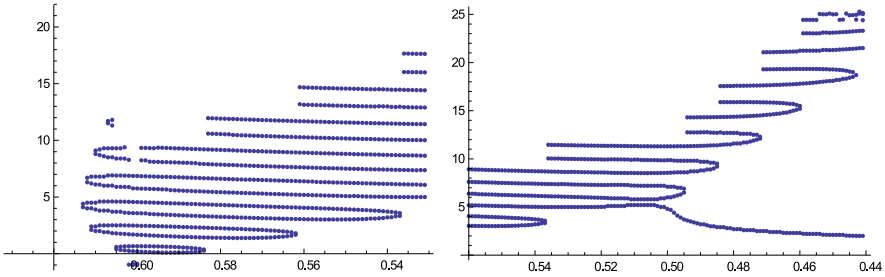

Figure 5. A detail of the critical region between $\varepsilon = -0.45$ and -0.65 for $\lambda = 1$.

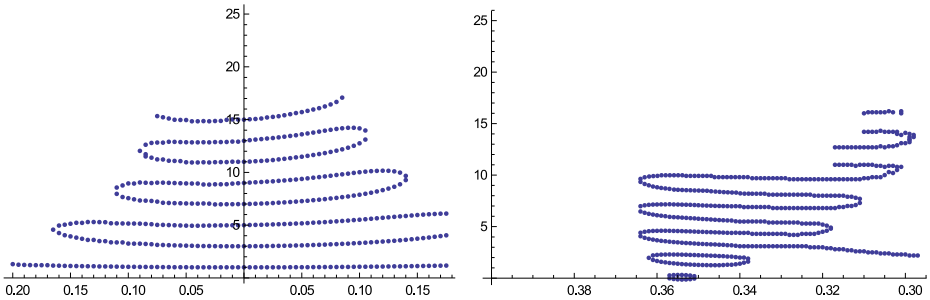

Figure 6. The $\lambda = 2$ case. The region of reality for each eigenvalue is narrower than for $\lambda = 1$. On the right-hand side the critical region is again depicted in a greater detail, its position is moved further to the right with respect to $\lambda = 1$ case.

case. First, except the lowest eigenvalue the spectrum complexifies also at $\varepsilon > 0$. As figure 4 suggests, the region of reality is broader for the low-lying eigenvalues. It is entirely possible that there does not exist either left or right neighbourhood of $\varepsilon = 0$ where the whole spectrum is purely real, in contradistinction to the non-tobogganic contour which yields real spectra for all $\varepsilon > 0$. However, it seems that there is a previously unattested region of real eigenvalues at $\varepsilon < -0.4$, probably not perturbatively accessible since perturbative calculations usually break down in exceptional points. The lowest energy tends to infinity as $\varepsilon \to -1$ in $\lambda = 0$ case; if $\lambda = 1$ it joins the other real eigenvalues in the left region and eventually complexifies in an exceptional point near $\varepsilon = -0.61$ (see figure 5). It is interesting to note that here it does not represent the ground state. The spectrum has to also be real in the vicinity of $\varepsilon \in \mathbb{N}$ since the singularity disappears there and the contours for different λ are equivalent. Consequently the real spectrum of $\lambda = 0$ case must be reproduced (see figure 4).

The overall picture does not change significantly when $\lambda = 2$. The overall pattern is similar to $\lambda = 1$ (see figure 6). Possibly another region of real spectrum exists near $\varepsilon = -1$, but the computation becomes lengthy and unreliable in those points, since near $\varepsilon = -1$ the solutions do not decrease enough rapidly; we are not confident in results obtained in this region by the above-described method and leave this problem for future investigation.

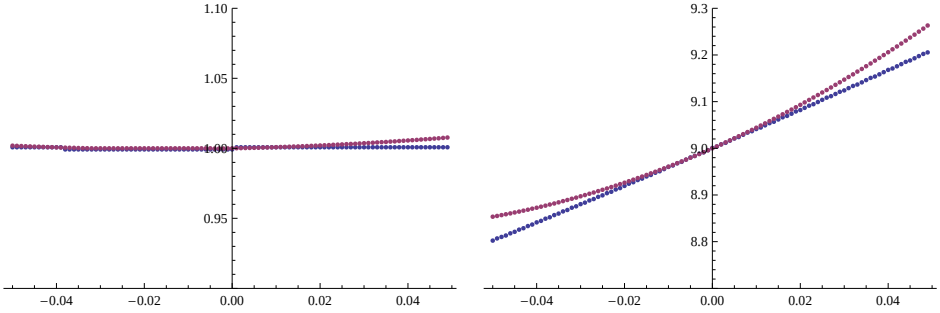

Figure 7. The first (left) and fifth (right) eigenvalues plotted against ε for $\lambda = 0$ and $\lambda = 1$ (the latter is the less straight dependence).

4. Summary

The introduction of tobogganic contours into the Bender potentials produces another version of $\mathcal{PT}$-symmetric Hamiltonian. Though they are closely related to the original non-tobogganic Hamiltonian, they are indeed different and exhibit qualitatively distinct behaviour with exceptional points standing between intervals of reality including the points $\varepsilon = n, n \in \mathbb{N}$. In an alternative approach, one can change the variable to unbend the contour, this leaves e.g. the $\lambda = 1$ Hamiltonian in the form

$$-\frac{\psi''}{9y^4} - \frac{2\psi'}{y} + i^{\varepsilon} y^{6+3\varepsilon} \tag{7}$$

after putting $x = y^3$. Such transformations were discussed in [4]. They are interesting as a method that allows to simply transform the problem to an ordinary differential equation of one real variable. On the other hand, the Schrödinger-like form of the Hamiltonian is lost, which makes the example less physically appealing.

If we are interested only in the transition between the harmonic oscillator and the negative quartic oscillator, the choice of λ is clearly irrelevant. For integer ε there is no singularity and distinctly winded contours must yield identical spectra. Therefore, it can be said that any tobogganic Hamiltonian defines good continuation of the harmonic oscillator, and the $\lambda = 0$ special case is only 'incidentally' privileged due to its real spectrum.

It may also be noted that the dependence on λ is non-perturbative in ε. The equality of the linear approximation coefficients for distinct λ is visible from figure 7. Up to the first order the energy is, independent of the contour selection,

$$E_n = 2n + 1 + \frac{\varepsilon}{2} \digamma\left(\frac{2\lceil n/2 \rceil + 1}{2}\right), \tag{8}$$

$\digamma$ is the di-gamma function [4a].

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[1a] In fact one can even release the asymptotic straightness condition provided that the contour does not oscillate too rapidly in the asymptotic region. The technical details of equivalence between contour integrability and boundary conditions in infinity are beyond the scope of this article
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[3] C M Bender, D C Brody and H F Jones, *Am. J. Phys.* **71**, 1095 (2003)
[3a] Suggested imagination is, of course, consistent only when infinite number of sheets are present
[3b] This choice puts a limit on the applicability of the method to $\varepsilon < 2$
[3c] The energy dependence of the solution is made explicit in the following
[4] M Znojil, *Phys. Lett.* **A342**, 36 (2005)
[4a] $\digamma(x) = (\log\Gamma(x))'$ where Γ is the standard Euler gamma function