Spiked potentials and quantum toboggans

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Abstract

Even if the motion of a quantum (quasi-)particle proceeds along a left–right-symmetric (PT-symmetric) curved path $C \neq \mathbb{R}$ in complex plane $\mathbb{C}$, the spectrum of bound states may remain physical (i.e., real and bounded below). A generalization is outlined. First, we show how the topologically less trivial (tobogganic) contours $C$ may be allowed to live on several sheets of a Riemann surface. Second, the specification of a scattering regime is formulated for such a class of models.

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1. Introduction

Let us be interested in the analytic power-law potentials

$$V(x) = \sum_{\beta} g(\beta) x^\beta, \quad \beta \in \mathbb{R}, \quad (1)$$

useful as a schematic phenomenological model as well as a laboratory for testing numerical methods. Among the most popular versions of this choice one finds the polynomially perturbed harmonic oscillator (with even integers $\beta_j = 2j, j = 1, 2, \ldots, j_{\text{max}}$ and with a comparatively easy perturbative tractability [1]) as well as its ‘spiked’ versions (admitting negative integer exponents $\beta_k = -k, k = 1, 2, \ldots, k_{\text{max}}$ – cf [2, 3]). From this background one may derive many mathematically equivalent descendants (1) with rational exponents $\beta \in \mathbb{Q}$ by an elementary change of variables $x$ and $\psi(x)$ in the associated Schrödinger equation [4].

The existence of the latter equivalence transformations (which, in essence, has been revealed by Liouville [5]) will simplify some purely technical aspects of our forthcoming considerations. In particular, it will enable us to restrict our attention just to the most common asymptotically harmonic spiked oscillators

$$V(x) = \frac{g_{(-2)}}{x^2} + \sum_{\beta > -2} g(\beta) x^\beta + x^2, \quad g_{(-2)} = \ell(\ell + 1) > 0. \quad (2)$$
This sum will be assumed finite and containing just subdominant anharmonic terms with rational exponents \( \beta \in (-2, 2) \).

Our specific choice of the quadratic spike in (2) is inspired by its key role in the above-mentioned Liouvillean changes of variables (cf also section 3.1 below) and, first of all, in their implementation by Buslaev and Grecchi [6]. In the latter paper a set of `manifestly non-Hermitian' Hamiltonians with real spectra has been considered, with interactions of the form (1). Surprisingly enough, the presence of the spike proved crucial in the rigorous demonstration of the reality of the spectrum (cf [6] for more details). Another argument supporting the inclusion of a nontrivial centrifugal-like spike may be found in the more recent papers by Dorey, Dunning and Tateo [7, 8] who found a rigorous proof of the reality of the spectrum which has been extended to potentials (2) with \( g(-2) \neq 0 \) in very natural manner.

In a marginal remark Buslaev and Grecchi noticed that their Hamiltonians are \( \mathcal{PT} \)-symmetric,

\[
H_{(\mathcal{PT})} = p^2 + V_{(\mathcal{PT})}(x) \neq H_{(\mathcal{PT})}^{\dagger} \equiv \mathcal{P} H_{(\mathcal{PT})} \mathcal{P}^{-1},
\]

with \( \mathcal{P} \) being parity and \( \mathcal{T} \) complex conjugation (which mimics time reversal). In a historical perspective it is a paradox, therefore, that the present enormous growth of popularity of \( \mathcal{PT} \)-symmetric potentials \( V_{(\mathcal{PT})}(x) \) has not been initiated by the paper [6] but, a few years later, by the doubts-breaking letter of Bender and Boettcher [9] who emphasized that the analyticity of \( V_{(\mathcal{PT})}(x) \) may represent one of hidden reasons for the surprising reality of the spectrum [10].

During the subsequent quick development of the field it became clear that one is allowed to define and integrate the Schrödinger equation with an analytic potential along the whole of the curve \( \xi(t) \equiv \xi(t \equiv \pm \infty) \) during the limits of the \( \mathcal{PT} \)-symmetric potentials \( V_{(\mathcal{PT})}(x) \). What has to be emphasized in parallel is that even for the above elementary \( \epsilon \)-dependent power-law asymptotics of potentials the requirement of the left–right symmetry still leaves the shape of the curve \( \xi(t) \) quite ambiguous. Thus, one considers just the classes of curves \( \xi(t) \) which remain compatible with the same asymptotic boundary conditions on a single Riemann sheet,

\[
\arg x = \arg \xi(t) \in \left\{ \left. \begin{array}{ll}
\frac{\pi}{4} + \frac{\epsilon \pi}{8 + 2 \pi} - \frac{\pi}{4} + \frac{\epsilon \pi}{8 + 2 \pi} - \pi, & t < -1, \\
\frac{\pi}{4} - \frac{\epsilon \pi}{8 + 2 \pi} + \frac{\pi}{4} - \frac{\epsilon \pi}{8 + 2 \pi} - \pi, & t > 1
\end{array} \right\},
\]

for the large arguments \(|t|\) and coordinates \(|\xi(t)|\) and for not too large \( \epsilon \) at least.

In this context our present main message may be formulated as a generalization of the usual definition of the non-intersecting \( \mathcal{PT} \)-symmetric paths \( \Gamma = \odot \) which are reflection symmetric with respect to the imaginary axis. Our generalization will be based on the observation that even in the simplest examples of the type \( V(x) \sim x^{2\epsilon} \) the `standard' branch point in infinity becomes complemented by another branch point in the origin (at all irrational or non-integer \( \epsilon > 0 \)). As a consequence, also the wavefunction \( \psi(x) \equiv \psi[\xi(t)] \) acquires a
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branch point at \( x = 0 \). Even if \( \epsilon \) remains integer this branch point becomes generated by the spike in \( V(x) \) with \( g_{( -2)} \neq 0 \).

In the similar situations people usually use an additional requirement that the whole curve \( \zeta(t) \text{ does not cross the cut} \) (chosen, usually, from \( x = 0 \) upwards). In our recent letter [14] we noticed that one could easily remove the latter restriction and work with the reflection symmetric paths \( C^{(N)} \) with \( N > 0 \) (apparent) self-intersections whenever the wavefunction \( \psi(x) \) possesses a branch point \( x_0(\text{BP}) \) at \( x = 0 \) and ‘lives’ on several Riemann sheets. In such a case (cf the illustrative sample of \( C^{(2)} \) in our present figure 1) the emergence of a nontrivial geometric phase in \( \psi(x) \) after rotation \( x \rightarrow x \cdot e^{2\pi i} \) gives rise to a new, topological source of the possible modification of the energy spectrum.

In our present paper, the latter possibility is further being developed. Although our illustrative examples still remain comparatively simple, we shall, in general, admit the existence of \( x_0(\text{BP}) \) at \( x = 0 \) as well as of some other \( 2M \) non-zero branch points forming the left–right symmetric pairs \( x_{\pm m}^{(\text{BP})} \) with \( m = 1, 2, \ldots M \). Their presence will be again interpreted as reflecting the presence of singularities of the \( PT \)-symmetric potentials \( V(x) \) in complex plane.

In the two brief introductory paragraphs 2.1 and 2.2 of section 2 we shall assume that \( \max(\beta) = \beta_{\max} < 2 \) and \( \min(\beta) = \beta_{\min} > -2 \) in equation (2). Such a requirement (closely related, by the way, to the perturbation-series convergence [15]) will help us to minimize inessential technicalities. As we already noticed, such an assumption of the relative boundedness of the whole anharmonic perturbation in (2) is artificial and can be relaxed via a change of variables. Nevertheless, its use will help us to define \( PT \)-symmetry of \( \psi(x) \) even in the presence of branch points.

In section 3, first of all, the emerging ambiguity of the very concepts of parity \( P \) and of complex conjugation \( T \) will be discussed and the method of its elimination will be clarified. In section 3.1 details will be added for the first nontrivial case with \( M = 0 \). The emergence of difficulties at the higher \( M > 0 \) will then be pointed out in section 3.2.

In the subsequent section 4 we shall discuss the possibilities of the existence of a nontrivial, \( PT \)-symmetric version of the analytic \( S \)-matrix (cf section 4.1). Using a solvable example in section 4.2 we shall finally show that and how this could lead to a new understanding of the \( PT \)-symmetric systems along directions where the first steps have already been made by Ahmed \textit{et al} [16] and by Cannata \textit{et al} [17, 18].

In section 5 we shall summarize the appeal and compactness of the picture allowing the use of trajectories living on several Riemann sheets. The persistence of many technical as well as physical open questions will be emphasized.
2. Potentials possessing a single singularity

The presence of the centrifugal term in \( V(x) \sim x^{2+\epsilon} \) forms a very natural starting point for the use of transfer matrices connecting independent-solution pairs over different asymptotic ‘Stokes sectors’ [7] or ‘wedges’ [9] defined by formulae of type (4). In this perspective one may interconnect the techniques of (exact) WKB approximants [19] and of the Bethe ansatz [8] with the language of monodromy group [20] or of the so-called Stokes geometry [21, 22] as well as with the analyses of solvable models in quantum field theory [23].

The first steps are to be made here in the direction where the eligible Stokes sectors lie on several Riemann sheets pertaining to the analytic solutions \( \psi(x) \) of the differential Schrödinger equations possessing \( 2M+1 \) or \( 2M \) branch points \( x_{\pm m}^{(BP)} = PT x_{\pm m}^{(BP)} \in \mathbb{C} \) with \( m \leq M \) and \( m \geq 0 \) or \( m \geq 1 \), respectively.

2.1. Solvable example: tobogganic harmonic oscillator

The three-dimensional harmonic-oscillator Schrödinger equation with its ordinary differential radial re-scaled form

\[
\left( -\frac{d^2}{dx^2} + \frac{\ell(\ell + 1)}{x^2} + x^2 \right) \psi(x) = E \psi(x)
\]

is one of the most popular illustrations of the formalism of the textbook quantum mechanics (TQM, [24]). Traditionally, its bound states are sought in the usual Hilbert space \( L^2(\mathbb{R}^3) \) and one may make use of the proportionality of the wavefunctions to the Laguerre polynomials,

\[
\psi(x) = \psi_{n,\ell}^{(TQM)}(x) = N_{n,\ell} x^{\ell+1/2} e^{-x^2/2} L_n^{(\ell+1/2)}(x^2),
\]

\[
E = E_{n,\ell}^{(TQM)} = 4n + 2\ell + 3, \quad n, \ell = 0, 1, \ldots
\]

Incidentally, the same differential equation (5) may play the role of an illustrative example in the various consistent formulations of the contemporary \( PT \)-symmetric quantum mechanics [25]. In equation (5) one only has to replace the standard textbook real domain \( D^{(TQM)} = (0, \infty) \equiv \mathbb{R}^+ \) of \( x \), say, by Buslaev’s and Grecchi’s [6] straight contour

\[
C^{(0)} = D^{(PTSQM)} = \{ x \mid t = i\varepsilon, t \in \mathbb{R}, \varepsilon > 0 \}
\]

which is complex, left–right symmetric and ‘twice as long’. As a consequence, there emerge ‘twice as many’ bound-state levels with a not too dissimilar structure. At an arbitrary real \( \alpha(\ell) \equiv \ell + 1/2 \) and discrete \( n = 0, 1, \ldots \) the new solutions retain the closed and compact form

\[
\psi(x) = \psi_{n,\ell,\pm}^{(PTSQM)}(x) = N_{n,\ell,\pm} \sqrt{1+2\alpha(\ell)} x^{\ell+1/2} e^{-x^2/2} L_n^{(\ell+1/2)}(x^2),
\]

\[
E = E_{n,\ell,\pm}^{(PTSQM)} = 4n + 2 \pm 2\alpha(\ell)
\]

and contain now a new discrete quantum number \( q = \pm \) of quasi-parity [26].

2.2. Perturbed tobogganic harmonic oscillators

In [14] we followed the inspiration by [6] and admitted a ‘realistic’ perturbation \( \lambda W(ix) \) of the potential in (5),

\[
\left[ -\frac{d^2}{dx^2} + \frac{\ell(\ell + 1)}{x^2} + x^2 + \lambda W(ix) \right] \psi(x) = E \psi(x).
\]

For technical reasons we constrained our attention to a few particular \( W(ix) \sim \sum_\beta g_\beta(ix)^\beta \).

On this background we imagined that after the perturbation the same differential equation (9) may generate different spectra on different contours.
Basically, what we did was that from the presence of the centrifugal-like singularity in the potential we deduced the topological nontriviality of the Riemann surface on which our wavefunction $\psi(x)$ was defined by the differential equation (9). In what follows we intend to deduce a few further consequences of that observation.

A priori, one might link this type of analysis to monodromy properties (of geometric phase type) of solutions at the branch point. This appealing possibility (mentioned also by the anonymous referee of this paper) is already under an active consideration in the project [27]. In the simpler approach the idea will be pursued here via a replacement of Buslaev’s and Grecchi’s straight contour (7) (and/or of all its admissible analytic-continuation deformations $C^{(BG)}$) by the much broader family of the topologically nontrivial (we called them ‘tobogganic’) contours $C^{(N)}$ which N-times encircle the strong singularity of our Schrödinger equation in the origin.

In an illustrative presentation of a topologically nontrivial trajectory $C^{(N)}$ let us first recollect that in our example (9), the Schrödinger differential equation will still be assumed asymptotically harmonic, with its asymptotically subdominant perturbation $W(i\xi)$ dominated by the term $g_{\beta_{\text{max}}}(i\xi)^{\beta_{\text{max}}}$ with a maximal power $\beta_{\text{max}} < 2$. This means that equation (9) will still possess the two independent asymptotically Gaussian, harmonic-like solutions,

$$
\psi(x) \approx \psi(\pm)(x) = e^{\pm x^2/2}, \quad |x| \gg 1.
$$

\hspace{1cm} (10)

As long as we may expect a generic, irrational value of $\ell$ we may treat these solutions of equation (9) as multi-valued analytic functions defined on a multi-sheeted Riemann surface with a branch point at $x = 0$. This means that along any ray $x_\theta = \varrho e^{i\theta}$ with the large $\varrho \gg 1$ and at almost any angle $\theta$ we may re-label solutions (10) as ‘physical’ (i.e., asymptotically vanishing $\psi(\text{phys})(x)$) and ‘unphysical’ (i.e., asymptotically ‘exploding’ $\psi(\text{unphys})(x)$). It is easy to verify that we have, explicitly,

$$
\psi^{-1}(x) = \begin{cases} 
\psi^{(\text{phys})}(x), & k\pi + \theta \in \left(-\frac{\pi}{4}, \frac{\pi}{4}\right), \\
\psi^{(\text{unphys})}(x), & k\pi + \theta \in \left(\frac{\pi}{4}, \frac{3\pi}{4}\right), 
\end{cases} \quad k \in \mathbb{Z}. \hspace{1cm} (11)
$$

and, vice versa,

$$
\psi^{+1}(x) = \begin{cases} 
\psi^{(\text{unphys})}(x), & k\pi + \theta \in \left(-\frac{\pi}{4}, \frac{\pi}{4}\right), \\
\psi^{(\text{phys})}(x), & k\pi + \theta \in \left(\frac{\pi}{4}, \frac{3\pi}{4}\right), 
\end{cases} \quad k \in \mathbb{Z}. \hspace{1cm} (12)
$$

Once we restrict our attention to the more usual scenario (11) we are now prepared to extend the definition (7) of the straight-line version $C^{(0)}$ of the ‘complexified coordinates’ $x \in D^{(PTSQM)}_\varepsilon$ to the Riemann-surface values of the ‘tobogganic trajectories’

$$
D^{(PTSQM,\text{tobogganic})}_{(\varepsilon,N)} = \{x = \varepsilon\varrho(\varphi, N) e^{i\varphi} | \varphi \in (-N+1)\pi, N\pi), \varepsilon > 0 \}
$$

at any positive integer $N > 0$, using a suitable function $\varrho(\varphi, N)$ in the way discussed more thoroughly in [14]. For the sake of definiteness we may parametrize

$$
\varrho(\varphi, N) = \sqrt{1 + \tan^2\frac{\varphi + \pi/2}{2N + 1}}.
$$

This generalizes Buslaev’s and Grecchi’s straight line and Tanaka’s single-sheet curves $\zeta(t)$ ([11], with $N = 0$) to the smooth tobogganic spirals $C^{(N)}$ at all $N > 0$ (in their $N = 2$ sample in figure 1 we choose $\varepsilon = 0.05$).
3. $\mathcal{PT}$-symmetry in the presence of one or more branch points

In the complex plane $\mathcal{K}$ of $x$ equipped with an upwards-oriented cut starting at $x = 0$ the complex-conjugation operation $\mathcal{T} : f(x) \rightarrow f^*(x) \equiv \bar{f}(x^*)$ is easily applied to the potentials $V(x)$ as well as to the related wavefunctions $\psi(x)$. In contrast, the introduction of an appropriately complexified parity operator $\mathcal{P} : x \rightarrow -x$ seems less straightforward as its action upon the line $\mathcal{C}^{(0)}$ proves discontinuous along the negative imaginary half-axis in $\mathcal{K}$.

The doublet of the complex parity-like operators $\mathcal{P}^{(\pm)} : x \rightarrow x \cdot \exp(\pm i\pi)$ might be preferred since both of them remain continuous. This is achieved at the expense of having some $x \in \mathcal{K} = \mathcal{K}_0$ mapped out of the space $\mathcal{K}$, i.e., by definition, into the neighbouring Riemann sheets $\mathcal{K}_{\pm 1}$.

In the language of algebra the less immediate invertibility of the new operators $\mathcal{P}^{(\pm)} \neq (\mathcal{P}^{(\pm)})^{-1}$ makes them even less similar to the standard parity involution. At the same time their action remains independent of our (artificially set) cuts so that its definition and/or visualization becomes facilitated when our (single) cut is suitably rotated by an angle $\beta (\mathcal{K} \rightarrow \mathcal{K}_{\beta})$, cf. a few illustrative pictures in [14]).

After we admit a rotation of the cut, the new problem emerges since also the antilinear action of the operator $\mathcal{T}$ may only be well defined on the whole atlas of the Riemann sheets. One of the two eligible rotation-type innovations $\mathcal{T}^{(\pm)}$ should be considered again, and the same conclusion must finally be applied also to the product of the operators $\mathcal{P}^{(\pm)}\mathcal{T}^{(\pm)}$.

3.1. Toboggans in potentials with a single spike

In the purely technical sense the explicit (say, numerical) construction of bound states $\psi^{(N)}(y)$ in the 'Nth quantum toboggan’ may be made complicated by the changes of the related concepts of the parity and time reversal which become non-involutive, $\mathcal{P}^{(\pm)} \neq (\mathcal{P}^{(\pm)})^{-1}$ and $\mathcal{T}^{(\pm)} \neq (\mathcal{T}^{(\pm)})^{-1}$. In this context, our specific choice of the asymptotically quadratic asymptotics of the potentials of equation (9) and of their manifestly $\mathcal{PT}$-symmetric form $V(x) = x^2 + \lambda W(ix)$ with rational exponents $\beta$ admits a certain clarification mediated by the following $\mathcal{PT}$-symmetry-preserving change of the coordinates [4]:

\[ ix = (iy)^T, \quad \psi(x) = y^{(\tau-1)/2}\psi(y). \quad (14) \]

It may lead to the whole series of the ‘new’, equivalent re-arrangements of our ‘old’ Schrödinger equation (9). Some of them are exceptional as containing solely even powers of the ‘new’ complex coordinate,

\[ -\frac{d^2}{dy^2} + \frac{L(L + 1)}{y^2} + \sum G_k y^k \] \[ \Psi(y) = \varepsilon \Psi(y). \quad (15) \]

Both the Sturm–Liouville bound-state problems (9) and (15) may be tobogganic. They are equivalent by construction. The choice of the constant $\tau$ is dictated by the requirement that for all the rational exponents $\beta$ which appeared in the original, asymptotically subharmonic anharmonicity $W(ix)$ at non-zero couplings $g(\beta)$ we get the even powers in the new polynomial bound-state problem (15),

\[ \beta \cdot \tau = 2m(\beta), \quad m(\beta) = \text{integer for any } \beta. \]

We see that the old asymptotically dominant interaction term $x^2$ is replaced by the new maximal-power term $-\tau^2(iy)^{4\tau-2}$ (i.e., $\tau$ must be integer or half-integer). The original energy term is tractable as an interaction term proportional to a constant $x^0$, i.e., we may set $-E = \lambda g(0)x^0$. In this way the constant $E$ acquires the role of one of the coupling constants after the transformation, $G_{\tau-1} = (-1)^{\frac{1}{2} + \tau}E$. In the opposite direction, one gets the ‘new’
energy term from the old coupling \( g(\beta, \tau) \) (which may be, incidentally, equal to zero) with \( \beta = -2 + 2/\tau \). Similarly, the old and new centrifugal terms must obey the rule
\[
\tau^2 (\ell + \frac{1}{2})^2 = (L + \frac{1}{2})^2.
\]
Due to the conservation of \( \mathcal{P}\mathcal{T}\)-symmetry by the change of variables (14) the ‘new’ spiked polynomial interaction representation (15) of our toboggan (9) (using, for economy reasons, the minimal parameter \( \tau \)) must have real coupling constants and will be called ‘canonical’ in what follows.

Transformation (14) of coordinates induces the replacement of the ‘old’ contour \( [x \in C(N)] \) by its ‘new’ map \( [y \in C'(N')] \) where, by construction, \( N' \leq N \). In this way the transformation may lower the winding number. In principle, one may even employ a ‘very large’ \( \tau \) in (14) (which need not be (half)integer in such a case) and achieve a replacement of any single-branch-point tobogganic operator of equation (9) with \( N > 0 \) by its formally equivalent non-tobogganic representation (15) with \( N' = 0 \).

In an alternative presentation we may select a specific ‘old’ \( \mathcal{P}\mathcal{T}\)-symmetric tobogganic domain \( D_{(\mathcal{PTSQM}, \text{tobogganic})}^{(\epsilon, N)} \) such that the equivalence transformation (14) replaces it by Buslaev’s and Grecchi’s straight line \( C^{(0)} \). In other words, all the subtleties arising in connection with the definition of the \( \mathcal{P}\mathcal{T}\)-symmetry may entirely easily be solved by their pull-back from the non-tobogganic canonical Schrödinger equation (15).

We may summarize that the original left–right-reflection-symmetric interpretation of the \( \mathcal{P}\mathcal{T}\)-symmetry of any \( \psi(x) \) (defined, in \( K_0 \), on the straight line \( C^{(0)} \) with the geometric centre at \( \phi = \pi/2 = 0 \) (in the notation of equation (13)) finds its easy and intuitively appealing generalization in the \( \delta \to -\delta \) geometric symmetry of the spirals of the type \( C^{(N)} \) with respect to their ‘main vertex’ at \( \phi = -\pi/2 \). For our purposes each tobogganic spiral \( C^{(N)} \) may be assigned its conjugate partner by using just the (arbitrarily selected) action of one of the eligible rotations \( T^\pm \),
\[
(c^{(N)})^\dagger = D_{(\mathcal{PTSQM}, \text{tobogganic})}^{(\epsilon', N)} , \quad \epsilon' = \epsilon \cdot e^{i\pi} \quad \text{or} \quad \epsilon' = \epsilon \cdot e^{-i\pi} .
\]

The non-tobogganic, standard complex conjugation is re-obtained at \( N = 0 \).

3.2. Toboggans in potentials with more spikes

In [28] another hidden source of emergence of a centrifugal singularity can be spotted in the reconstruction of a spiked \( V_1(x) \) from its regular supersymmetric partner \( V_0(x) \). This idea has further been pursued by Sinha and Roy [29] who started from a regular \( \mathcal{P}\mathcal{T}\)-symmetric harmonic oscillator \( V_0(x) \) and proposed the construction of the whole series of potentials \( V_k(x) \) with \( k \) different centrifugal-like singularities on the real line. We may briefly summarize their recipe as specifying the two supersymmetric partner potentials
\[
V_\pm(x) = W^2(x) \pm W'(x)
\]
in terms of their shared superpotential \( W(x) \) which is, in its turn, defined by the well-known formula [30]
\[
W(x) = -\frac{\psi'_m(x)}{\psi_m(x)}
\]
in terms of an ‘input’ wavefunction \( \psi_m(x) \). The point is that any wavefunction can be used now, due to the regularization effect of the \( \mathcal{P}\mathcal{T}\)-symmetrization [31]. In this sense, the \( m \)-plet of the (simple) nodal zeros of the \( m \)th excited state \( \psi_m(x) \) converts into the simple poles of \( W(x) \) (the zeros cannot cancel due to the Sturm–Liouville oscillation theorem) and into the
second-order poles of at least one of the potentials in (17) (one should keep in mind that the poles brought by both the terms in (17) can—and often do—cancel).

It is now easy to imagine that the generic Riemann surface pertaining to the generic analytic wavefunction \( \psi(x) \) will have two branch points (say, in \( x = \pm 1 \)) at \( m = 2 \) (etc). Unfortunately, the corresponding potentials (say, \( V(x) = x^2 + \frac{G}{(x-1)^2} + \frac{G^*}{(x+1)^2} \)) etc) do not seem to admit closed-form solutions in any generic case with irrational \( G \). Hence, any future analysis of the related bound states will have to rely upon sophisticated numerical methods \[27\].

An exhaustive analysis of the possibilities of the construction of the left–right symmetric tobogganic trajectories which would encircle the pair of branch points \( x = \pm 1 \) would be complicated. One of reasons is that both the halves of these trajectories must be permitted to travel freely between the two singularities before they finally escape in infinity.

The problem of classification of all the possible topologically nontrivial toboggan trajectories would become even more interesting in the case of more than two branch points in the bound-state wavefunctions \( \psi(x) \). At the same time, this problem looks still rather academic on our present level of knowledge. For this reason, let us now rather turn our attention to the (as far as we know, equally open) questions connected with the possibilities of a tobogganic generalization(s) of the usual textbook scattering states.

4. Scattering theory for toboggans

4.1. The concept of scattering along curved trajectories

Up to now we kept the \( \mathcal{PT} \)-symmetric version of quantum mechanics of toboggans specified by the bound-state boundary conditions at both the ends of the curves \( C^N \), i.e., in the light and notation of equation (11), by the pairs of the constraints

\[
\psi(\varrho \cdot e^{i\theta}) = 0, \quad \varrho \gg 1 \tag{20}
\]

where

\[
\theta + k_{\text{sub}} \pi \in \left( -\frac{\pi}{4}, \frac{\pi}{4} \right).
\]

Two different subscripts \( \text{sub} = \text{in} \) and \( \text{sub} = \text{out} \) were considered, marking the angle of the ‘initial’ and ‘final’ Stokes-line ray, respectively. This means that we have to select \( k_{\text{out}} = 0 \) and \( k_{\text{in}} = 1 \) at \( N = 0 \), \( k_{\text{out}} = -1 \) and \( k_{\text{in}} = 2 \) at \( N = 1 \), \( k_{\text{out}} = -2 \) and \( k_{\text{in}} = 3 \) at \( N = 2 \), etc.

Now, let us search further inspiration in certain reflectionless (or, if you wish, standing-wave) real-line Hermitian models as studied in letter \[16\]. We will contemplate their generalization to our present \( \mathcal{PT} \)-symmetric tobogganic context. In fact, the generalization is not difficult as it is sufficient to combine our present differential Schrödinger equation

\[
H_{(\mathcal{PT})} \psi(x) = E \psi(x) \tag{21}
\]

with the appropriately generalized scattering boundary conditions. This means that we require that the incoming beam moves along a specific (often called ‘anti-Stokes’) line,

\[
\psi(\varrho \cdot e^{i\theta_{\text{in}}}) = \psi_{(i)}(x) + B \psi_{(f)}(x), \quad \varrho \gg 1, \quad \theta_{\text{in}} = \text{fixed}. \tag{22}
\]

This scattering-like wavefunction is composed of the normalized incident wave \( \psi_{(i)}(x) \approx e^{i\varrho^2/2} \) in superposition with the reflected \( \psi_{(r)}(x) \approx e^{-i\varrho^2/2} \). Similarly we select the outcoming beam

\[
\psi(\varrho \cdot e^{i\theta_{\text{out}}}) = (1 + F) \psi_{(i)}(x), \quad \varrho \gg 1, \quad \theta_{\text{out}} = \text{fixed} \tag{23}
\]
which contains just the transmitted wave \( \psi(t)(x) \approx e^{\text{i} \varphi/2} \). This notation generalizes the standard textbook scattering on the real line and could be also reformulated in the language of the transfer and/or monodromy matrices [20] in an extension to the case where our complex path of coordinates is different from the standard straight real line. Our present notation \( B \) and \( F \) reminds the reader of the coefficients called, respectively, the ‘backward scattering’ and ‘forward scattering’ amplitudes in physics.

For our present, asymptotically \( x^2 \)-dominated potentials (2) with \( \beta_{\text{max}} < 2 \) we can specify the ‘in’ and ‘out’ \( \varphi \to \infty \) asymptotics of the respective lower-edge and upper-edge \( PT \)-symmetric scattering curves \( A_{(L)}^{(N)} \) and \( A_{(U)}^{(N)} \) in closed form,

\[
\begin{align*}
A_{(L)}^{(N)} &\to \varrho e^{i \theta_{\text{in}}}, \quad \theta_{\text{in}} = -(N + 3/4)\pi, \\
A_{(U)}^{(N)} &\to \varrho e^{i \theta_{\text{in}}}, \quad \theta_{\text{in}} = -(N + 5/4)\pi, \\
A_{(L)}^{(U)} &\to \varrho e^{i \theta_{\text{out}}}, \quad \theta_{\text{out}} = (N - 1/4)\pi, \\
A_{(U)}^{(U)} &\to \varrho e^{i \theta_{\text{out}}}, \quad \theta_{\text{out}} = (N + 1/4)\pi.
\end{align*}
\]

These choices preserve the \( PT \)-symmetry of the new anti-Stokes tobogganic scattering contours \( A^{(N)} \) obtained as the edge-of-the-wedge boundaries, i.e., the respective upper or lower limiting extremes \( A_{(L)}^{(N)} \) or \( A_{(U)}^{(N)} \) of the preceding deformable bound-state contours \( C^{(N)} \) at a given \( N \).

An extension of this construction to the potentials asymptotically dominated by the other powers of the coordinate may be based on the use of formula (14) and is left to the reader.

4.2. Illustration: tobogganic scattering by the harmonic-oscillator well

For illustration let us now omit the perturbation \( W(ix) \) from equation (9) and discuss the solution of the resulting simplified Schrödinger differential equation

\[
\left[ -\frac{d^2}{dx^2} + \frac{\alpha^2 - 1/4}{x^2} + x^2 \right] \psi(x) = E \psi(x), \quad \alpha = \ell + \frac{1}{2},
\]

say, along the path \( A_{(L)}^{(0)} \), i.e., in the first nontrivial scattering regime. In the first step let us notice the \( x \leftrightarrow -x \) and \( \alpha \leftrightarrow -\alpha \) symmetries of equation (25) and recollect that on the asymptotic parts of the selected scattering trajectory \( A_{(L)}^{(0)} \) we may set \( x^2 = -ir \) with the real \( r \ll -1 \) along the asymptotic part of the ‘in’ branch and with \( r \gg +1 \) for the ‘out’ branch, respectively.

In the second step we shall set \( E = 2\mu \) and restrict our attention to the generic case, ignoring, in a way paralleling the bound-state construction [26], the exceptional integer values of \( \alpha \). This allows us to construct the general analytic solution \( \psi(x) \) of our ordinary differential Schrödinger equation (25) of the second order, in the scattering regime, as a superposition of the expression proportional to a confluent hypergeometric function,

\[
\chi_{(\alpha)}(r) = r^{1/2} \left[ \alpha + \frac{1 - \mu}{2} \right] F_1 \left( \frac{\alpha + 1 - \mu}{2}, \alpha + 1; -ir \right)
\]

with its linearly independent partner \( \chi_{(-\alpha)}(r) \).

In the third step we may employ the well-known \( |r| \gg 1 \) estimate for hypergeometric functions [32] and get the compact final asymptotic formula

\[
r^{1/2} \chi_{(\alpha)}(r) \approx e^{ir/2} r^{\mu/2} \exp[-i\pi(\alpha + 1)/4] + e^{-ir/2} r^{-\mu/2} \exp[i\pi(\alpha + 1)/4].
\]

(27)
Its inspection reveals that at the generic $\alpha > 0$ and $\mu = E/2 > 0$ the dominant asymptotic $|x| = |\sqrt{r}| \gg 1$ behaviour of the wavefunctions is ‘rigid’,

$$\psi_{\text{in,out}}(x) \approx r^{-1/4(\alpha + \mu)/2} e^{i\pi/2} \exp[-i\pi(-\alpha + 1)/4] \frac{\Gamma(-\alpha + 1 + \mu)/2}{\Gamma(-\alpha + 1 + \mu)/2} + \text{corrections.} \quad (28)$$

We may conclude that the scattering properties of our model remain trivial unless the energies acquire specific values at which the dominant term (28) would vanish. This observation is not surprising. Indeed, even the ‘scattering’ boundary conditions may lead to the quantization of the spectrum of energies in the way illustrated in [16]. Incidentally, the authors of the latter reference preserved the traditional, non-tobogganic real-line contour $A^{(0)} \equiv \mathbb{R}$ in their model ‘fine-tuned’ to the specific asymptotics of their interaction $V(x) \sim -x^4$. From our present point of view their particular choice of the contour is in fact not unique. Its ambiguity may be interpreted as a generic feature of the analytic models.

In a different perspective our result (28) resembles the standard scattering in the Coulomb field [32] where the phase shift of the oscillations of the scattered wave remained coordinate dependent due to the not sufficiently rapid asymptotic decrease of the potential. In other words, the standard textbook Coulombic scattered waves $\psi_{\text{out}}^{(Coul)}(r)$ are ‘distorted’ by a power-law factor as well,

$$\sin(kr \text{ const}) \to \sin(kr + \text{const} \cdot \log r + \text{const}).$$

In our equations (27) and (28), conceptually the same power-law distortion of the ‘free waves’ $\psi_{\text{in,out}}(r)$ occurs.

For this reason a suitably modified definition of the scattering matrix $S$ (measuring the change of the ratio of two independent solutions due to the scattering) would be needed. Mathematically, the present construction of the scattering states for the nontrivial power-law potentials is clear and almost obvious since our curved contours (24) represent a very natural generalization of the usual real line of $x$. At the same time, a real application/applicability of this construction represents a truly open problem. One must keep in mind that the coordinates $x$ themselves lie on the complex contours (24) and cannot be understood as directly observable, therefore. Presumably, for this reason (and in full analogy with the parallel $\mathcal{PT}$-symmetric bound-state problems), the correct physical interpretation of our unusual scattering states generated by the asymptotically nontrivial power-law potentials would again require the construction and specification of an appropriate non-local operator of the physical metric $\Theta$ [33].

5. Summary and outlook

One of the most important innovations brought by the $\mathcal{PT}$-symmetric quantum mechanics is that it decouples its models and observables (say, quantum Hamiltonians $H$) from an immediate correspondence to their classical analogues. In particular, once we allow that the coordinates $x$ become complex (i.e., the ‘position’ of a ‘particle’ ceases to be observable), the experimental observability of these quantities is, naturally, lost. Their role remains formal and purely auxiliary. Suitable functions $f(x)$ of these quantities may still be treated as elements of the Hilbert (or Krein [11]) space in an ‘easily tractable’ representation but the values $x$ of their argument cannot be understood as eigenvalues of an operator of ‘position’ anymore. In physical context this loss of observability for some ‘obvious operators of coordinates’ finds its closest analogue in relativistic quantum mechanics where one encounters a contradictory and unobservable ‘Zitterbewegung’ of the Dirac particles [24], etc.

In the mathematical setting the best-developed rigorous analysis (which may be exemplified by the recent paper by Trinh [21] and references listed therein) exists for
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polynomial potentials. Using an explicit reference to the underlying theory of the corresponding linear differential equations of second order in complex plane [34] one may formulate a number of theorems. Unfortunately, the bulk of the available mathematical theory has not been extended to an appropriate incorporation of singular terms in $V(x)$ nor to the problem of scattering.

In such a setting our present paper studied the formal Hamiltonians of quantum toboggans which do not seem to have any obvious source or inspiration in classical mechanics. In a way characteristic for modern physics, the real use of their formal development may only be expected to come a posteriori. In this spirit our present paper filled the gap since without an explicit construction of scattering states, the concept of quantum toboggans considered just as a bound-state problem along topologically nontrivial complex trajectories seemed incomplete.

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References

[1] Fluegge S 1971 Practical Quantum Mechanics I (Berlin: Springer)
[2] Harrell E M 1977 Ann. Phys., NY 105 379
[3] Hall R L, Saad N and von Keviczky A B 2002 J. Math. Phys. 43 94
[4] Znojil M 1994 J. Phys. A: Math. Gen. 27 4945
[5] Liouville J 1837 J. Math. Pure Appl. 1 16
[6] Buslaev V and Grechín V 1993 J. Phys. A: Math. Gen. 26 5541
[7] Dorey P, Dunning C and Tateo R 2001 J. Phys. A: Math. Gen. 34 5679
[8] Dorey P, Dunning C and Tateo R 2001 J. Phys. A: Math. Gen. 34 L391
[9] Bender C M and Boettcher S 1998 Phys. Rev. Lett. 24 5243
[10] Bender C M, Boettcher S and Meisinger P N 1999 J. Math. Phys. 40 2021
[11] Tanaka T 2005 Preprint hep-th/0605035
[12] Bender C M and Túrberner A V 1993 Phys. Lett. A 173 442
[13] Fernández F M, Guardiola R, Ros J and Znojil M 1999 J. Phys. A: Math. Gen. 32 3105
[14] Znojil M 2005 Phys. Lett. A 342 36
[15] Kato T 1976 Perturbation Theory for Linear Operators (Berlin: Springer)
[16] Ahmed A, Bender C M and Berry M V 2005 J. Phys. A: Math. Gen. 38 L627
[17] Cannata F and Ventura A 2006 Czech. J. Phys. 56 (Preprint quant-ph/0606006)
[18] Cannata F, Dedonder J-P and Ventura A 2006 Scattering in PT-symmetric quantum mechanics Preprint quant-ph/0606129
[19] Voros A 1999 J. Phys. A: Math. Gen. 32 5993
Dorey P, Milicic-Strator A and Tateo R 2004 Beyond the WKB approximation in PT-symmetric quantum mechanics Preprint hep-th/0410013
[20] Arnold V I 1998 Geometrical Methods in the Theory of Ordinary Differential Equations 2nd edn (Berlin: Springer)
Zołdek H 2006 The Monodromy Group (Basel: Birkhauser)
[21] Trinh D T 2005 J. Phys. A: Math. Gen. 38 5665
[22] Takei Y (ed) 2005 Recent Trends in Exponential Asymptotics (Kokyuroku Series vol 1424) (Kyoto: RIMS)
[23] Dorey P, Dunning C and Tateo R 2004 Czech. J. Phys. 54 35
[24] Messiah A 1961 Quantum Mechanics (Amsterdam: North Holland)
Styer D F et al 2002 Am. J. Phys. 70 288
[25] Scholtz F G, Geyer H B and Hahne F J W 1992 Ann. Phys., NY 213 74
[26] Mostafazadeh A 2002 J. Math. Phys. 43 205, 2814, 3944 and 6343
Bender C M, Brody D C and Jones H F 2002 Phys. Rev. Lett. 89 270401
[27] Znojil M 1999 Phys. Lett. A 259 220
[27] Stefani F, Günther U and Znojil M in preparation
[28] Znojil M, Cannata F, Bagchi B and Roychoudhury R 2000 Phys. Lett. B 483 284
[29] Sinha A and Roy P 2004 Czech. J. Phys. 54 129
[30] Cooper F, Khare A and Sukhatme U 1995 Phys. Rep. 251 267
[31] Znojil M 2004 J. Phys. A: Math. Gen. 37 10209
[32] Fluegge S 1971 Practical Quantum Mechanics I (Berlin: Springer) p 292
[33] Znojil M 2005 Czech. J. Phys. 56 (September issue)
[34] Sibuya Y 1975 Global Theory of a Second Order Linear Differential Equation with Polynomial Coefficient (Amsterdam: North Holland)