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Identification of observables in quantum toboggans

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Abstract

Schrödinger equations for 'quantum toboggans' with real energies are given the generalized eigenvalue-problem form $H\psi=EW\psi$, where $H\neq H^\dagger$ and $W\neq W^\dagger\neq I$. The consistent probabilistic interpretation of these models is provided. The new double-series formula for the necessary ad hoc metric $\Theta=\Theta(H,W)$ is derived which defines the acceptable inner products in the physical Hilbert space of states. The formula degenerates to the usual single series in the non-tobogganic trivial-weight limit $W\to I$.

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1. Introduction

For all the sufficiently elementary quantum models which are based on a Hamiltonian H which is self-adjoint, say, in one of the most common Hilbert spaces $\mathbb{L}^2(\mathbb{R}^d)$ of complex integrable functions of d real variables (=coordinates) the identification of all the other eligible candidates for the operators of physical observables is trivial. From the formal point of view, any self-adjoint operator $\mathcal{O} = \mathcal{O}^{\dagger}$ is acceptable [1].

Fifteen years ago Scholtz *et al* [2] emphasized that the same principle applies also in all the less elementary models in quantum theory. They paid attention to the interacting boson model in nuclear physics where the complicated structure of the explicit representation $\mathcal{H}^{(physical)}$ of the Hilbert space of states of a nucleus makes this space unsuitable for explicit calculations. The necessary simplification of some (typically, variational) calculations has been achieved, in this context, via Dyson's mapping $\Omega^{(Dyson)}$ which interrelates the fermionic Hilbert space $\mathcal{H}^{(physical)}$ and a perceivably simpler and much more 'user-friendly' auxiliary bosonic Hilbert space $\mathcal{H}^{(auxiliary)}$ (cf also a few further, more technical remarks relocated to appendix A).

Beyond the framework of nuclear physics the concept of the models which appear to be non-Hermitian 'in a wrong space' occurs also, from time to time, in the framework of field theory [3]. In the late 1990s, the really dramatic development of the models of this type was inspired by the publication of a few papers by Bender $et\ al\ [4,5]$. These authors analyzed several non-Hermitian operators H with real spectra and conjectured that these models could

be perfectly acceptable in physics, for phenomenological purposes at least (for more details, cf the recent review [6]).

In what follows we intend to re-analyze the question of the identification of the operators of observables in the latter non-Hermitian context. In the introductory section 2 we review briefly the class of models of our present interest ('quantum toboggans') and we offer there also a brief review of their mathematical origin (cf section 2.1). This will be complemented by a simple illustrative example (section 2.2) and by a few more technical remarks on the differences between some related Hilbert spaces (appendix A), on the meaning of complex coordinates (appendix B) and on the facilitating mathematical role of the so-called \mathcal{PT} symmetry of the Hamiltonians (cf appendix C).

The presentation of our new results will be separated into two parts. In the first part (section 3) we shall start from an illustrative tobogganic Schrödinger equation. We shall emphasize that the related complex and topologically nontrivial tobogganic paths of coordinates $z^{(N)}(x) \in \mathbb{C}$ are characterized by a winding number N and parametrized by a real $x \in \mathbb{R}$. The rectification transformation is then recommended which maps the original tobogganic, multisheeted curves of the coordinates in the interior of a single complex plane with a cut. We emphasize that in the language of functional analysis, the new form of our tobogganic Schrödinger equation reads $H\psi = EW\psi$ and that it is well defined merely in an auxiliary, unphysical Hilbert space $\mathcal{H}^{(\text{auxiliary})}$. In sections 3.1 and 3.2 we draw some consequences from the fact that $W \neq I$.

The second and main part of our message is formulated in section 4. We emphasize there that whenever $W \neq I$, Schrödinger's generalized eigenvalue problem $H\psi = EW\psi$ requires a new approach when its physical interpretation is concerned. The mathematical core of our innovative proposed strategy is explained in section 4.1 which, in essence, updates the W = I formalism as summarized in appendix A. In a complete parallel we introduce certain sets of appropriate Fourier-like but non-unitary Ω -transformations. Some of the main consequences are clarified in section 4.2. This makes us prepared to address, finally, the principal question of the explicit construction of the physical metric $\Theta = \Theta(H, W)$ in terms of the solutions of our Schrödinger equations (cf section 4.3).

A concise summary of our results will be presented in section 5 where we review, once more, the basic philosophy of the whole approach and where we emphasize that the underlying mathematics is based on a non-unitary generalization of the usual switch between the x and p representations in quantum mechanics. We stress that our recipe coincides with its simpler W = I version in the limit $W \to I$.

2. Tobogganic phenomenological models

2.1. Spiked oscillators

Bender's and Boettcher's \mathcal{PT} symmetric oscillator $V^{(BB)}(x) = x^2 + ix$ (cf appendix C) is easily perceived as a model where the coordinate is complex,

$$r = r(x) = x - i\varepsilon, \qquad x \in (-\infty, \infty).$$
 (1)

Thus, one can write $V^{(\mathrm{BB})}(x) = r^2(x) + \mathrm{const}$ at a suitable $\varepsilon > 0$. Of course, the model is exactly solvable. Still, several less-trivial models have been considered in the recent literature (cf its review in [6]). Many of them were characterized by the presence of the centrifugal term in the potential (cf appendix B). For illustrative purposes let us choose here, therefore, one of the most popular one-dimensional anharmonic-oscillator Schrödinger equations which is

defined along the *complex* straight line (1),

$$\left[-\frac{\mathrm{d}^2}{\mathrm{d}x^2} + \frac{\ell(\ell+1)}{r^2} + \omega^2 r^2 + \mathrm{i}r^3 \right] \varphi_n(r) = E_n(\omega)\varphi_n(r), \qquad r = r(x). \tag{2}$$

In spite of being manifestly non-Hermitian, the latter model still predicts a measurable, strictly real and discrete spectrum of energies which is bounded from below [7].

From our present point of view it is remarkable that whenever one uses the complexified coordinates (1) in equation (2), the role of the singularity at r=0 becomes virtually irrelevant. The solvable spiked-harmonic-oscillator illustration of this observation has been described in our letter [8], where the term $\ell(\ell+1)/r^2$ has been noticed bounded at any nonzero shift $\varepsilon>0$. Still, to our great surprise, the spectrum of energies of such a spiked harmonic oscillator, albeit non-equidistant, proved given by a compact formula and remained real and discrete.

A step beyond the scope of equation (2) has been made by Sinha and Roy [9]. These authors were able to complement the elementary harmonic-oscillator example $V(r) = r^2 + \text{const}/r^2$ of [8] with the single centrifugal-like 'spike' at r = 0 by a series of its exactly solvable supersymmetric partners containing a pair of the two left-right symmetric spikes,

$$V(r) \sim \frac{g}{(r-c)^2} + \frac{g}{(r+c)^2} + \text{less singular terms}$$

or a left-right symmetric triplet of the spikes,

$$V(r) \sim \frac{g'}{(r-c')^2} + \frac{h}{r^2} + \frac{g'}{(r+c')^2} +$$
less singular terms

etc. All of these models were defined along the same complex straight lines of equation (1).

2.2. The birth of quantum toboggans: wavefunctions defined over several Riemann sheets

Dorey et al [7] found it entirely natural to replace the regular model (2) with $\ell = \omega = 0$ by its general singular version where ℓ is real and does not vanish. In this perspective the interaction term $\ell(\ell+1)/r^2$ ceased to be related to the angular momenta, of course (cf also [10] in this respect). In [11] we were inspired by this generalization and returned to the study of the role of the parameter ℓ . Our analysis started from the observation that the wavefunctions are analytic so that they must have the following general form near the origin,

$$\psi(r) \sim c_1 r^{\ell+1} + c_2 r^{-\ell}, \qquad |r| \ll 1.$$
 (3)

At a generic real ℓ , the *natural* domain of definition of wavefunctions *must be* the whole logarithmic Riemann surface \mathcal{R} [12] rather than just one of its sheets.

The core of the message of [11] was a mere formulation of a few consequences of the latter facts. We emphasized that immediately after one allows a complexification of the coordinates in Schrödinger equations, there remains no tenable reason for the limitation of our attention to the integration paths of the straight-line form (cf equation (1)) or of the form where a smooth x dependence of $\varepsilon(x) = \varepsilon(-x) > 0$ is admitted,

$$r = r(x) = x - i\varepsilon(x), \qquad x \in (-\infty, \infty)$$
 (4)

(cf, e.g., [13] for illustrative examples).

At this moment, what remained for us to do was an extension of the oversimplified recipe (4). We started from the equivalent formula

$$r[x(\gamma)] = -\mathrm{i}\varrho(\gamma)\,\mathrm{e}^{\mathrm{i}\gamma}, \qquad \varrho(\gamma) = \frac{\varepsilon[x(\gamma)]}{\cos\gamma},$$
 (5)

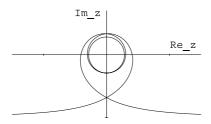


Figure 1. Sample tobogganic curve which three times encircles the origin.

where $r \in \mathbb{C}$ denotes the usual complex coordinate (i.e., an element of a cut complex plane) and where we merely reparametrized our original real parameter $x = x(\gamma) = \varepsilon \tan \gamma$ using an angular variable $\gamma \in (-\pi/2, \pi/2)$.

In the next (and final) step we allowed the angle to run to neighboring Riemann sheets. This was achieved by the mere removal of the restriction on the range of the angle. Alternatively, we may keep the range of $\gamma \in (-\pi/2, \pi/2)$ and modify just slightly the definition of the complex, tobogganic curve of the multisheeted coordinates, yielding, at an arbitrary winding number N,

$$z^{[N]}[x(\gamma)] = -i\varrho^{2N+1}(\gamma) e^{i(2N+1)\gamma}.$$
 (6)

This is the formula we need. It specifies a spiral-shaped curve which may be interpreted as lying on a given logarithmic Riemann surface \mathcal{R} which pertains to a given analytic eigenfunction $\psi(z)$ of our tobogganic Hamiltonian with the single singularity in the origin (for illustration, we choose N=3 in our illustrative figure 1).

Let us agree that we shall reserve the symbol z for the elements of \mathcal{R} . Then, in the vicinity of the origin all our wavefunctions will have the same generic form (3) and only the angle in equation (6) will mark the distinction between the separate Riemann sheets. Hence, we can read the pictures of curves (6) (cf figure 1) as encircling the essential singularity in the origin at a generic ℓ . In effect, these curves extend over an (N+1) plets of the neighboring Riemann sheets of \mathcal{R} . In the same sense, we may also write the tobogganic Schrödinger equations in the form

$$\left[-\frac{\mathrm{d}^2}{\mathrm{d}z^2} + \frac{\ell(\ell+1)}{z^2} + \omega^2 z^2 + \mathrm{i}z^3 \right] \varphi_n^{[N]}(z) = E_n^{[N]}(\omega) \varphi_n^{[N]}(z) \tag{7}$$

which is formally defined on the Hilbert space $\mathbb{L}_2(z^{[N]}[x(-\pi/2, \pi/2)])$ of functions which are quadratically integrable along the spirals $z^{[N]}(x) \in \mathcal{R}$ which, by assumption, N times encircle the origin.

Whenever we choose a potential V(z) which is analytic at $z \neq 0$ it is not difficult to realize that the existence of the bound-state solutions $\varphi_n^{[N]}(z)$ of equation (7) will be guaranteed by the following asymptotic boundary conditions,

$$\varphi_n^{[N]}\{z^{[N]}[x(\pm \pi/2)]\} = 0. \tag{8}$$

These two constraints must be considered as lying on the different Riemann sheets. Figure 1 with N=3 may be consulted for illustrative purposes again.

A purely numerical solution of differential equation (7) can be constructed by the standard shooting methods. Indeed, one would have to start at $\gamma \approx -\pi/2$, i.e., on the left asymptotic branch of the curve of figure 1 in our illustration. One has to integrate and move along the curve $z^{[3]}(x)$ toward the origin. The integration path has to change, three times, the Riemann

sheet before completing the full triple rotation around the origin and before reaching, finally, the right asymptotic branch of the integration path at $\gamma \approx +\pi/2$.

In the following section, a non-numerical reinterpretation of such a naive recipe will be proposed and advocated.

3. Rectified tobogganic Schrödinger equations in $\mathcal{H}^{(auxiliary)}$

One of the most efficient methods of the numerical solution of the tobogganic Schrödinger equation (7) may be based on an auxiliary change of the coordinates complemented by the parallel modification of the operators and wavefunctions [11].

In this spirit we are allowed to change the variables from $z \in \mathcal{R}$ to $r \in \mathbb{C}$ and vice versa. For the sake of definiteness let us base this change on the conformal mapping

$$ir = (iz)^{\alpha}, \qquad \alpha = \frac{1}{2N+1}, \qquad N = (0, 1, 2, ...$$
 (9)

and let us assume that the 'rectified' coordinate r lies simply on the line of equation (1). The related toboggan-shaped spirals coincide with $z=z^{[N]}(x)$ at a constant $\varepsilon \neq \varepsilon(x)$. Still, the tobogganic paths resemble the straight lines at the large real parameters,

$$z^{[N]}(x) = -\mathrm{i}\{\mathrm{i} r^{[0]}(x)\}^{2N+1} = (-1)^N x^{2N} \left[x - (2N+1)\mathrm{i}\varepsilon + \mathcal{O}\left(\frac{1}{x}\right) \right]. \tag{10}$$

The latter curves can be interpreted as integration paths of new type. The resulting quantum system generated by the usual Hamiltonian but *redefined* along the new, topologically nontrivial paths carries the name of quantum toboggan.

Let us now return to our tobogganic model (7) with the cubic interaction and with the first nontrivial choice of the winding number N = 1. Via the change of variables (9) this model becomes equivalent to its straight-line rectified rearrangement

$$\left[-\frac{\mathrm{d}^2}{\mathrm{d}x^2} + \frac{L(L+1)}{r^2(x)} + 9\omega^2 r^{10}(x) + 9\mathrm{i}r^{13}(x) \right] \psi_n[r(x)] = 9E_n^{[N]}(\omega)r^4(x)\psi_n[r(x)]$$
(11)

where $r(x) = x - i\varepsilon$ and where

$$\psi_n(r) = z^{-N/(2N+1)} \varphi_n^{[N]}(z), \qquad L = (2N+1) \left(\ell + \frac{1}{2}\right) - \frac{1}{2}.$$

The real one-dimensional variable $x \in (-\infty, \infty)$ can be perceived as a new coordinate. In this way, we managed to return our tobogganic toy model from its fairly exotic representation (7) using wavefunctions $\varphi_n^{[N]}(z)$ defined on complex spirals $z = z^{[N]}(x)$ to its less exotic though still non-self-adjoint differential-equation representation (11) with wavefunctions $\psi_n[r(x)]$ which lie in the entirely standard Hilbert space $\mathbb{L}_2(\mathbb{R}) \equiv \mathcal{H}^{(\text{auxiliary})}$.

The tobogganic generalization of the integration paths (1) is unexpectedly nontrivial. Firstly, its consequences may prove fairly counterintuitive. For example, one encounters bound states called quantum knots [14] even when the potential itself vanishes. Secondly, its mathematical essence immediately inspires various further generalizations. For example, one can introduce tobogganic systems containing more than one branch point [15] and/or describing certain less usual forms of the scattering [16].

3.1. Left and right eigenstates in $\mathcal{H}^{(auxiliary)}$

Our Schrödinger equation (11) is to be solved in the auxiliary, unphysical but 'user-friendly' Hilbert space $\mathcal{H}^{(auxiliary)}$. This illustrates the generic situation in which, in general, the

energy term is absent (i.e., where the 'new energy' is strictly zero). This is one of the most important immediate consequences of the rectification transformation (9) applied to the original tobogganic differential equation (i.e., to equation (7) in our illustrative example).

In the language of functional analysis, our sample Schrödinger equation (11) still has the form of the ordinary differential equation,

$$H|n\rangle = E_n W|n\rangle \tag{12}$$

where the function $W[r(x)] = 9r^4(x) \equiv 9(x - i\varepsilon)^4$ represents an example of the so-called weight operator in the so-called generalized eigenvalue problem (12).

One of the most striking formal features of our tobogganic Schrödinger equation (11) in its version (12) obtained by the change of variables can be seen in its manifest non-Hermiticity in the usual Dirac's sense. More explicitly, in our Hilbert space $\mathcal{H}^{(\text{auxiliary})}$ where the Hermitian conjugation is defined as the usual transposition plus complex conjugation we have $H \neq H^{\dagger}$ and $W \neq W^{\dagger}$ of course.

This means that whenever we return to the standard Dirac's conventions we must be much more careful when using the ket-symbols $|\cdot\rangle$ (denoting the elements of $\mathbb{L}_2(\mathbb{R}) \equiv \mathcal{H}^{(auxiliary)}$) and the bra-symbols $\langle\cdot|$ denoting the corresponding linear functionals of the same Hilbert space which is, of course, self-dual.

The first example of the possible ambiguity caused by an inappropriate notation emerges when we denote the *n*th eigenstate of *H* by the ket $|n\rangle$ (cf equation (12)). Although the corresponding linear functional is, of course, the bra $\langle n|$, it is *not* proportional to the solution of the Hermitian conjugate version of the equation. Thus, for the elements of $\mathcal{H}^{(\text{auxiliary})}$ which satisfy the latter, 'complementary' Schrödinger equation we *definitely have to* introduce *another* symbol.

In what follows we shall accept the conventions advocated in [17] and specifying the latter eigenvectors (sought as the elements of *the same* auxiliary Hilbert space $\mathcal{H}^{(\text{auxiliary})}$ again) by the mere doubling of the bra or ket symbols. This leads to the following compact form of the 'independent' generalized eigenvalue problem for our 'independent' operators H^{\dagger} and W^{\dagger} ,

$$H^{\dagger}|n\rangle\rangle = E_n^* W^{\dagger}|n\rangle\rangle. \tag{13}$$

Of course, we may rewrite the latter equation in the more natural, conjugate form where the operators would act to the left,

$$\langle \langle n|H = \langle \langle n|WE_n. \rangle \rangle$$
 (14)

In the language of mathematics, the latter version of the second, non-equivalent Schrödinger equation is solved directly in the dual vector space which might be denoted by the symbol $(\mathcal{H}^{(auxiliary)})^{\dagger}$ if necessary.

Let us now emphasize that in general, the rectification mediated by an appropriate change of variables in the corresponding differential Schrödinger equation is an invertible transformation of our original tobogganic eigenvalue problem where the spectrum of the energies $E_n^{[N]}$ has been expected real and where the Hamiltonian and its conjugate operator have been assumed isospectral. These questions have already thoroughly been discussed elsewhere [11]. In the present context this only means that all the key spectral properties of our toboggans will be inherited by the conjugate pair of the *rectified* eigenvalue problems (12) and (13) or (14) in $\mathcal{H}^{(\text{auxiliary})}$ (cf also a few relevant remarks added in appendix C).

A marginal remark may be added concerning the rectified toboggans in a purely pragmatic numerical context where our coefficients $E_n^{[N]}$ need not necessarily be called the energies and where our ket eigenstates can equally well be perceived as the 'alias' zero-energy bound states generated by the Hamiltonian $H^{(\mathrm{alias})} = H - E_n^{[N]}W$. In this sense, for example, our particular

illustrative equation (11) would acquire the standard zero-energy form where one searches for certain particular coupling strengths at the quartic component of the potential.

We may summarize that our task degenerates now to the quantization of the real coefficients $E_n^{[N]}$ at the weight factor W of a well-specified toboggan-oscillator physical origin. We may be sure that the nontriviality of $W \neq I$ cannot become a source of any unexpected mathematical difficulties precisely due to the existence of the possibility of an invertibility of our rectification transformation. Of course, *without* such a pull-back to the original analytic equation for a toboggan the study of our equations containing some more general choices of W would open Pandora's box of many interesting as well as fairly difficult mathematical questions. Here, we need not and will not extend the discussion of these questions beyond our present very specific framework of tobogganic models.

3.2. Biorthogonality and completeness in $\mathcal{H}^{(auxiliary)}$

Let us now re-number the states in $\mathcal{H}^{(auxiliary)}$ directly by their energies, $|n\rangle = |E_n\rangle = |\lambda\rangle$ with the new set of the real indices $\lambda \in \{E_0, E_1, \ldots\}$. In such a reduced notation our two Schrödinger equations (12) and (13) will read

$$H|\lambda\rangle = \lambda W|\lambda\rangle, \qquad \langle\langle \lambda'|H = \langle\langle \lambda'|W\lambda'.$$
 (15)

Under certain general assumptions the left and right generalized eigenstates of our H may be shown to be mutually biorthogonal with respect to the weight operator W,

$$\langle \langle \lambda' | W | \lambda \rangle = \delta_{\lambda, \lambda'} \cdot \sigma_{\lambda}, \qquad \sigma_{\lambda} = \langle \langle \lambda | W | \lambda \rangle. \tag{16}$$

In parallel, the completeness relations in $\mathcal{H}^{(auxiliary)}$ will be assumed in the form

$$I = \sum_{\lambda} |\lambda\rangle \frac{1}{\sigma_{\lambda}} \langle \! \langle \lambda | W. \rangle \!$$
 (17)

Technical details of these formulae have been thoroughly discussed in [17]. Their essence can briefly be summarized as reflecting the fact that *both* the independent Schrödinger equations in (15) are linear and homogeneous. As a consequence, any 'initial', fixed set of these solutions marked by an auxiliary superscript ^[1] can be replaced by another set containing just some *different* multiplication constants and marked by some other superscript.

In what follows, we shall employ the notation convention of [17] where the initial set of eigenvectors $|\lambda\rangle = |\lambda\rangle^{[1]}$ and $\langle\langle\lambda'| = {}^{[1]}\langle\langle\lambda'|$ is allowed to be generalized in accordance with the most elementary rule

$$|\lambda\rangle = |\lambda\rangle^{[\vec{\kappa}]} = |\lambda\rangle^{[1]}/\kappa_{\lambda}, \qquad \langle\langle \lambda'| = {}^{[\vec{\kappa}]}\langle\langle \lambda| = \kappa_{\lambda}{}^{[1]}\langle\langle \lambda| \qquad (18)$$

where $\lambda = E_0, E_1, \ldots$ and any element of the sequence of (complex) constants $\vec{\kappa} = \{\kappa_{\lambda_0}, \kappa_{\lambda_1}, \ldots\}$ is *arbitrarily variable*.

In a sharp contrast to the Hermitian case where the simple and double-kets coincide, our choice of any numerical factor κ_{λ_j} is now virtually unrestricted. Indeed, the change of any κ_{λ_j} changes *neither* the biorthogonality relations (16) *nor* the completeness relations (17) and neither the values of coefficients σ_{λ} nor the spectral decomposition of our Hamiltonian operator,

$$H = \sum_{\lambda} W|\lambda\rangle \frac{\lambda}{\sigma_{\lambda}} \langle\!\langle \lambda | W. \rangle$$
 (19)

This means that the specific renormalization freedom and the presence and the free variability of the superscript $[\vec{k}]$ should always (at least, tacitly) be kept in mind in what follows.

4. Formula for the metric in $\mathcal{H}^{(physical)}$

4.1. An update of the metric $\Theta_{(Dirac)}^{(auxiliary)} \to \Theta_{(non-Dirac)}^{(physical)}$ at $W \neq I$.

Due to the relations $H \neq H^{\dagger}$ and $W \neq W^{\dagger}$ the space $\mathcal{H}^{(\text{auxiliary})}$ cannot be interpreted and accepted as the Hilbert space of states of our quantum system. Instead, we have to follow and modify the recipe which has been used in the special case where W = I and $H \neq H^{\dagger}$ in $\mathcal{H}^{(\text{auxiliary})}$ [2]. Thus, we shall assume that the correct physical Hilbert space $\mathcal{H}^{(\text{physical})}$ must be introduced via a non-unitary though still invertible mapping of the kets $|\psi\rangle \in \mathcal{H}^{(\text{auxiliary})}$ on their 'spiked-ket' images $|\psi\rangle \in \mathcal{H}^{(\text{physical})}$. In this notation the mapping

$$\Omega: \mathcal{H}^{(auxiliary)} \longrightarrow \mathcal{H}^{(physical)}$$

will be realized by the operators Ω which can be written in the form of the series

$$\Omega = \Omega^{[\vec{\kappa}]} = \sum_{\lambda} |\lambda \rangle \frac{1}{\sigma_{\lambda}} [\vec{\kappa}] \langle \langle \lambda | W \rangle$$
 (20)

containing not yet normalized (i.e., formally, superscript-independent) spiked kets $|\lambda\rangle$. Under this convention, the explicit presence of the superscript in $\Omega^{[\vec{k}]}$ is essential because of the absence of the cancellation between the numerators and denominators,

$$\Omega^{[\vec{\kappa}]} = \sum_{\lambda} |\lambda \rangle \left(\frac{\kappa_{\lambda}}{\sigma_{\lambda}}\right)^{[1]} \langle \! \langle \lambda | W. \rangle$$
 (21)

This indicates that $\Omega^{[\vec{\kappa}]} \neq \Omega^{[\vec{\kappa}']}$ for $\vec{\kappa} \neq \vec{\kappa}'$ and that there exists a 'hidden' ambiguity in the definition

$$|\lambda \rangle = \Omega |\lambda \rangle \in \mathcal{H}^{(physical)}, \qquad \langle \lambda | = \langle \lambda | \Omega^{\dagger} \in (\mathcal{H}^{(physical)})^{\dagger}$$
 (22)

of the same eigenstates (or of their arbitrary linear superpositions) in their two different representations.

In $\mathcal{H}^{(\text{physical})}$ we may now parallel the recipe of [2] and introduce the operator $h = \Omega H \Omega^{-1}$ which represents our original non-Hermitian upper-case Hamiltonian $H \neq H^{\dagger}$ in the new space. The same type of transformation must be used to generate also the physical partner $w = \Omega W \Omega^{-1}$ of our original non-Hermitian weight operator $W \neq W^{\dagger}$. These two lower-case operators are both assumed acting in the physical space so that they must both be self-adjoint in $\mathcal{H}^{(\text{physical})}$.

$$h^{\dagger} = (\Omega^{-1})^{\dagger} H^{\dagger} \Omega^{\dagger} = h, \qquad w^{\dagger} = (\Omega^{-1})^{\dagger} W^{\dagger} \Omega^{\dagger} = w.$$

This implies that in $\mathcal{H}^{(auxiliary)}$ we must have

$$H^{\dagger} = \Theta H \Theta^{-1}, \qquad W^{\dagger} = \Theta W \Theta^{-1} \tag{23}$$

where we abbreviated $\Theta = \Omega^{\dagger}\Omega$. In the special case of W = I this conclusion degenerates to that presented in [2].

Let us now insert expressions (23) in our 'second' Schrödinger equation (13) and compare it with its 'first' form (12). Under the standard non-degeneracy assumption this implies the following elementary proportionality between the eigenkets of H^{\dagger} (=eigen-double-kets) and the metric-premultiplied eigenkets of H (=eigen-single-kets), both being, optionally, superscripted in accordance with equation (18),

$$|\lambda\rangle\rangle^{[\vec{k}]} = \Theta^{[\vec{k}]}|\lambda\rangle^{[\vec{k}]} \cdot q(\lambda). \tag{24}$$

The explicit knowledge of the metric would be needed to extract the values of the proportionality constants $q(\lambda)$ here.

4.2. An update of the eigenstates at $W \neq I$

After the change Ω of the Hilbert space *both* of equations (15) degenerate to the *same* equation which is self-adjoint,

$$h|\lambda\rangle = \lambda w|\lambda\rangle. \tag{25}$$

Under some very general and more or less usual mathematical assumptions its form enables us to deduce the orthogonality relations

$$\langle \lambda | w | \lambda' \rangle = \tilde{\sigma}_{\lambda} \cdot \delta_{\lambda, \lambda'}, \qquad \tilde{\sigma}_{\lambda} = \langle \lambda | w | \lambda \rangle.$$
 (26)

In $\mathcal{H}^{(physical)}$ the completeness relations are also valid,

$$I = I^{\text{(physical)}} = \sum_{\lambda} |\lambda \rangle \frac{1}{\tilde{\sigma}_{\lambda}} \langle \lambda | w$$
 (27)

and the lower-case Hamiltonian h can equally easily be assigned the usual spectral expansion,

$$h = \sum_{\lambda} w |\lambda > \frac{\lambda}{\tilde{\sigma}_{\lambda}} \langle \lambda | w. \tag{28}$$

It is important to add that in the light of our illustrative example (11) the spectrum of the operator w (which is, by construction, isospectral to w) will be assumed non-negative. This will allow us to assume also the positivity of the self-overlaps $\langle \lambda | w | \lambda' \rangle$ in equation (26), etc. Both these assumptions will, of course, significantly simplify our forthcoming considerations.

All relations (26)–(28) are of a rather academic value since all the mathematical manipulations should preferably be performed in the simpler Hilbert space $\mathcal{H}^{(auxiliary)}$, anyhow. Still, all of them improve our insight in the possible physics behind our models which can solely be discussed inside the physical Hilbert space $\mathcal{H}^{(physical)}$.

The mapping Ω can be read as returning us back from the 'correct' $\mathcal{H}^{(physical)}$ to the 'simpler' Hilbert space $\mathcal{H}^{(auxiliary)}$. In particular, in the light of equation (22) we may complement the proportionality relation (24) by another formula,

$$\langle \lambda | \Theta = \langle \lambda | \Omega$$

which enables us to transfer equations (26) and (27) to $\mathcal{H}^{(\text{auxiliary})}$.

$$\langle \lambda | w | \lambda' \rangle = \langle \lambda | \Theta W | \lambda' \rangle = \langle \lambda | \Theta | W | \lambda' \rangle = \tilde{\sigma}_{\lambda} \cdot \delta_{\lambda, \lambda'}, \tag{29}$$

$$I = I^{\text{(auxiliary)}} = \sum_{\lambda} |\lambda\rangle \frac{1}{\tilde{\sigma}_{\lambda}} \langle \lambda | \Theta W.$$
 (30)

A similar translation applies also to the alternative spectral decomposition

$$H = \sum_{\lambda} W |\lambda\rangle \frac{\lambda}{\tilde{\sigma}_{\lambda}} \langle \lambda | \Theta W \tag{31}$$

of our Hamiltonians in $\mathcal{H}^{(auxiliary)}$. In the light of equation (24), the only difference from the respective equations (16), (17) and (19) degenerates to the following relation between the tilded and untilded overlaps:

$$\tilde{\sigma}_{\lambda} = \langle \lambda | \Theta W | \lambda \rangle = \left[\frac{1}{q(\lambda)} \right]^* \sigma_{\lambda}, \qquad \sigma_{\lambda} = \langle \langle \lambda | W | \lambda \rangle$$
 (32)

which are all, incidentally, \vec{k} independent.

4.3. The ultimate double-series update of Θ at $W \neq I$

Let us return to the simpler Hilbert space $\mathcal{H}^{(\text{auxiliary})}$ and, via a suitable multiplier in the eigen-double-kets $|\lambda\rangle$, let us postulate that $\sigma_{\lambda}=1$. In parallel, in $\mathcal{H}^{(\text{physical})}$, the maximum of simplicity will be achieved by setting $\tilde{\sigma}_{\lambda}=1$ via a premultiplication of our basis vectors $|\lambda\rangle$ by some suitable numerical constants at each energy λ . Thus, we shall have $q(\lambda)=1$ in equation (24) as well as in equation (32), i.e.,

$$\langle \lambda | w | \lambda \rangle = 1.$$
 (33)

Under these updated conventions we shall be allowed to work, without any loss of generality, with the simplified $\sigma_{\lambda} = 1$ versions of equations (16) and (17) and with the similarly simplified representation (19) of the Hamiltonian H.

Even though we have no direct access to the metric Θ and/or to the overlaps and matrix elements defined in terms of the 'inaccessible' and 'prohibitively complicated' vectors $|\lambda \succ \in \mathcal{H}^{(physical)}$ we can still recall the definition of the mappings Ω and write

$$\Theta = \Omega^{\dagger} \Omega = \sum_{\lambda \lambda'} W^{\dagger} |\lambda\rangle\rangle M_{\lambda,\lambda'} \langle\langle \lambda' | W, \qquad M_{\lambda,\lambda'} = \langle \lambda | \lambda' \rangle.$$
 (34)

The not yet known matrix M of coefficients cannot vary with the (tacitly present) superscripts $[\vec{k}]$ so that, in the light of equation (21), there is no cancellation between numerators and denominators and

$$\Theta^{[\vec{\kappa}]} \neq \Theta^{[\vec{\kappa}']}$$
 for $\vec{\kappa} \neq \vec{\kappa}'$.

The change of the superscripts will change the metric only via the eigenvectors of H^{\dagger} (cf equation (18)) so that we can rewrite the superscript dependence of the metric in equation (34) in the following explicit form:

$$\Theta^{[\vec{\kappa}]} = \sum_{\lambda,\lambda'} W^{\dagger} |\lambda\rangle\rangle^{[1]} \kappa_{\lambda}^{*} M_{\lambda,\lambda'} \kappa_{\lambda'}^{[1]} \langle\langle \lambda' | W.$$
(35)

Now we return to the factorization $\Theta = \Omega^{\dagger}\Omega$ of the metric and to identity (33) and definition (20). We insert all of these formulae in equation (29). This gives the relation

$$\langle \lambda | \Theta W | \lambda' \rangle = \sum_{\lambda''} \langle \lambda | \lambda'' \rangle \langle \langle \lambda'' | W^2 | \lambda' \rangle = \delta_{\lambda, \lambda'}. \tag{36}$$

Once we succeed in evaluating all the necessary 'input' matrix elements $\langle \langle \lambda | W^2 | \lambda' \rangle \rangle$, the 'missing' matrix of coefficients $M_{\lambda,\lambda'} = \langle \lambda | \lambda' \rangle$ will be defined as its inverse,

$$M = S^{-1}, \qquad S_{\lambda,\lambda'} = \langle \langle \lambda | W^2 | \lambda' \rangle.$$
 (37)

This result is to be inserted in formula (35) for the metric Θ . Our task is completed.

5. Summary

Many quantum Hamiltonians with real spectra which appeared manifestly non-Hermitian in the current Dirac's sense were recently re-assigned a new, consistent probabilistic interpretation mediated by a new metric Θ in the physical Hilbert space of states. For certain models of this type (exemplified here by 'quantum toboggans'), Mostafazadeh's spectral-expansion formula for Θ [18] ceases to be applicable because their Schrödinger equation acquires the generalized eigenvalue-problem form $H\psi=EW\psi$ containing an invertible though not necessarily positive-definite weight $W\neq I$. For all of these models we derived the necessary generalized spectral-expansion formula for Θ .

We started our considerations from a given non-Hermitian tobogganic Hamiltonian playing the usual role of the generator of the time evolution but acting, very unusually, along a certain topologically nontrivial path $z^{[N]}$ of complex coordinates. Via a suitable change of variables we achieved a rectification of this path and obtained a much more usual non-Hermitian representation H of the Hamiltonian operator in an auxiliary Hilbert space $\mathbb{L}_2(\mathbb{R})$.

For the purely pragmatic reasons we constrained our attention to the mere 'first nontrivial' toboggans with the single branch point. Our formulation of the corresponding bound-state problem has been facilitated by their rectification. Still, as long as the change of the variables induced a nontrivial weight operator W in our Schrödiger equation, the standard recipes of dealing with similar situations proved inapplicable and we were forced to modify them accordingly. Fortunately, via a subsequent non-unitary mapping Ω we were able to replace the non-Hermitian 'upper-case' operators H and W by their respective 'lower-case' avatars h and W defined as Hermitian in another, physical Hilbert space of states $\mathcal{H}^{(physical)}$.

We should emphasize that in similar models, the non-unitary correspondence between two Hilbert spaces is of a key importance. Its main purpose lies in a *decisive simplification* of mathematics (i.e., of the solution of equations) in one of the spaces, combined with a facilitated return to the consistent probabilistic interpretation of the system in the other one. In this sense, our tobogganic models also fit very well the basic methodical premise that the lower-case, 'correct' representation h of the Hamiltonian appears, in the purely technical terms, *too complicated* in comparison with H.

Having paid our main attention to the correct physical interpretation of the elementary though nontrivial tobogganic models we formulated a straightforward $W \neq I$ generalization of the known W = I theory of [2]. We succeeded in a derivation of the explicit formula for the metric operator Θ . We revealed that the coefficients in this formula coincide with an inverse of certain matrix S representing the square of the weight operator W in a certain basis. In this sense, our formula degenerates to the older theories in the limit $W \to I$ where S becomes a diagonal matrix.

Another conclusion resulting from our formula for Θ is that without essential changes, the ambiguity problem in the assignment of Θ to a given set of observables $A_j \neq A_j^{\dagger}$ (containing the Hamiltonian $H = A_0$, etc) survives the transition to the systems with a nontrivial weight operator W. Indeed, when we only take the Hamiltonian $H = A_0$ into consideration, the same infinite sequence of arbitrary complex parameters κ_{λ} enters the formula for the metric (cf equation (35)) in *both* the W = I and $W \neq I$ scenarios.

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Appendix A. Non-unitary maps Ω in quantum models with W = I

The most disturbing feature of all the Dyson-like invertible mappings Ω of spaces as studied in [2] is their non-unitarity, $\Omega^{\dagger} \neq \Omega^{-1}$. Due to it, the 'tractable' Hamiltonians H in the space $\mathcal{H}^{(\text{auxiliary})}$ are manifestly non-Hermitian. This is not too essential of course—for all the physical predictions one can always return to the (in our present notation, lower-case) pull-backs of Hs in $\mathcal{H}^{(\text{physical})}$,

$$h = \Omega H \Omega^{-1}. \tag{A.1}$$

Even if operators (A.1) themselves remain, by assumption, too complicated for computational purposes, they are still observable, i.e., self-adjoint in their own Hilbert space $\mathcal{H}^{(physical)}$,

$$h^{\dagger} = (\Omega^{-1})^{\dagger} H^{\dagger} \Omega^{\dagger} = h.$$

From this relation one deduces that

$$H^{\dagger} = \Theta H \Theta^{-1}, \qquad \Theta = \Omega^{\dagger} \Omega.$$
 (A.2)

We should note that our use of the symbol Θ for the 'metric operator' is not too widespread, being equivalent to T or η_+ or \mathcal{CP} or $e^{\mathcal{Q}}$ of [2] or [18] or [19] or [20], respectively.

The identification of all the other observables A_1, A_2, \ldots in the 'tractable' Hilbert space $\mathcal{H}^{(auxiliary)}$ remains entirely straightforward. Once we return to the derivation of equation (A.2) we immediately see that all of these operators must obey the same intertwining rule as the Hamiltonian,

$$A_j^{\dagger}\Theta = \Theta A_j. \tag{A.3}$$

In order to avoid confusion or lengthy explanations ('in which space?'), the authors of [2] suggested to call all these 'admissible' operators of observables 'quasi-Hermitian'.

Appendix B. The birth of models with complex coordinates and W = I

It is well known that in nuclear, atomic and molecular systems many features of the observed bound-state spectra can often be very well understood and explained via an elementary differential Hamiltonian

$$H^{(\text{rad})} = -\frac{d^2}{dr^2} + \frac{\ell^{(\text{rad})}(\ell^{(\text{rad})} + 1)}{r^2} + V^{(\text{rad})}(r)$$
(B.1)

(units $\hbar = 2m = 1$) where the phenomenological requirements are usually reflected by an appropriate adaptation of the real potential $V^{(\text{rad})}(r)$ defined along the real and nonnegative coordinate $r \in (0, \infty)$. For pragmatic reasons this potential is often chosen as confining. Then, the spectrum itself remains always 'acceptable', i.e., real and discrete and bounded below.

It is rather surprising to reveal that the spectrum *can* stay real, discrete and bounded below even for certain *complexified* potentials and/or paths of coordinates. For illustration one might recollect the early works by Caliceti *et al* [21] or by Buslaev and Grecchi [10]. Before all of these apparent 'curiosities' fell into oblivion there appeared, in 1998, the influential letter by Bender and Boettcher [5] which we already cited above. This letter offered a numerically and semi-classically inspired hypothesis that the energies may be expected to stay real and discrete for *many* complex potentials. An unexpectedly intensive growth of interest in the similar models followed (cf [6] or [22] for more references).

In the context of the similar concrete examples it soon appeared to be easy to prove the reality of the energies for a large family of the exactly solvable complex potentials [23]. Subsequently, in 2001, Dorey *et al* [7] rigorously proved also Bender's and Boettcher's hypothesis for the original class of the field-theory-related power-law complex potentials of [5]. They were even able to introduce more parameters (generalizing also the (half-) integer $\ell^{(\text{rad})}$ in equation (B.1) [10] to any real parameter ℓ) and succeeded in an *explicit* specification of the boundaries of the domains $\mathcal D$ of these parameters where the reality of the whole spectrum is guaranteed.

Appendix C. The role of $\mathcal{P}\mathcal{T}$ symmetry at $W \neq I$

An important formal feature of our illustrative tobogganic examples can be seen in the so-called $\mathcal{P}\mathcal{T}$ symmetry (cf [6]) where \mathcal{P} denotes space-reversal (i.e., parity) while \mathcal{T} represents the time reversal (i.e., in effect, Hermitian-conjugation antilinear operator). Such a feature of the toboggan-like models can be interpreted here as the *doublet* of the parity-pseudo-Hermiticity properties

$$H^{\dagger} = \mathcal{P}H\mathcal{P}^{-1}, \qquad W^{\dagger} = \mathcal{P}W\mathcal{P}^{-1}.$$
 (C.1)

The main role of this 'generalized symmetry' lies in possible simplification of the necessary proof that all the energies remain real, $E_n = E_n^*$, i.e., that the states of the underlying quantum system remain observable.

In addition, the generalized \mathcal{PT} symmetry (C.1) will enable us to replace equation (13) by its equivalent representation

$$H\mathcal{P}^{-1}|n\rangle\rangle = E_n W \mathcal{P}^{-1}|n\rangle\rangle. \tag{C.2}$$

From equation (12) and from another simplifying assumption that the spectrum is nondegenerate we immediately deduce that we must have

$$|n\rangle\rangle = \mathcal{P}|n\rangle Q_n \tag{C.3}$$

where the coefficients of proportionality Q_n called quasi-parities [24] are, in principle, arbitrary. Still, one must keep in mind that once we postulate the standard biorthogonality and completeness relations, $\langle (n'|n) \rangle = \delta_{nn'}$, and $I = \sum_n |n\rangle \langle (n|)$, we are forced to define the quasi-parities $Q_n = Q_n(\kappa_n)$, at all the energy levels, in terms of the matrix elements of the parity operator,

$$Q_n(\kappa_n) = \frac{1}{[\kappa_n] \langle n | \mathcal{P} | n \rangle^{[\kappa_n]}}.$$

Thus, knowledge of these matrix elements fixes the values of quasi-parities, while equation (C.3) replaces the second Schrödinger equation (13) as it becomes an *explicit definition* of its solutions. This fact can, of course, shorten the ultimate construction of Θ very significantly.

For illustrative purposes, non-Hermitian anharmonic oscillators are often being chosen in the literature. As we already mentioned, the birth of interest in these models dates back to the letter [5]. In this letter, one of the key ideas of all the subsequent developments of the subject has been presented via the most elementary harmonic oscillator Hamiltonian $H = p^2 + x^2$ defined in the usual Hilbert space $\mathbb{L}_2(\mathbb{R})$. It has been noticed there that this Hamiltonian has a real spectrum $(E_n = 2n + 1)$ and that it is, at the same time, \mathcal{PT} symmetric (for the time being, we can simply understand the latter concept as a left-right invariance of H in the complex plane of H0. In the next step Bender and Boettcher (H0 emphasized that both the latter features remain unchanged when one adds a manifestly non-Hermitian linear interaction term H1. In the third step they re-analyzed this type of correspondence on several other examples and conjectured that there may exist H1 symmetry of the system

An important source of the appeal of using the phenomenological operators of the latter class should be sought in the feasibility of working with them in the 'unphysical' Hilbert space $\mathbb{L}_2(\mathbb{R}) \equiv \mathcal{H}^{(\text{auxiliary})}$ where they remain 'sufficiently elementary' (i.e., typically, ordinary differential) operators. In the context of field theory, this idea of simplicity motivated, *inter alia*, the study of Hamiltonian densities containing the most elementary parity-violating interaction terms, typically of the form $ig\varphi^3(\vec{x},t)$ [4]. In the context of mathematics, many properties of these models found their explanation by means of a return to their most elementary

but already nontrivial quantum-mechanical predecessors. For example, in the late 1980s the one-dimensional non-Hermitian potential

$$V^{(CGM)}(r) = \omega^2 r^2 + ir^3$$
 (C.4)

was chosen for detailed perturbation studies [21, 25].

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