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CONSERVATION OF PSEUDO-NORM IN $\mathcal{PT}$ SYMMETRIC QUANTUM MECHANICS

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ABSTRACT. We show that the evolution of the wave functions in the $\mathcal{PT}$ symmetric quantum mechanics is pseudo-unitary. Their pseudo-norm $\langle\psi|\mathcal{P}|\psi\rangle$ remains time-independent. This persists even if the $\mathcal{PT}$ symmetry itself becomes spontaneously broken.

1. INTRODUCTION

Evolution in quantum mechanics [1]

$$|\psi(t)\rangle = e^{-iHt}\,|\psi(0)\rangle$$

conserves the norm of a state. The assumption $H = H^\dagger$ of the Hermiticity of the Hamiltonian leads to the time-independence of the probability density,

$$\langle\psi(t)|\psi(t)\rangle = \langle\psi(0)|e^{iH^\dagger t}\,e^{-iHt}|\psi(0)\rangle = \langle\psi(0)|\psi(0)\rangle\,. \tag{1}$$

Vice versa, in the light of the Stone's theorem, the unitarity of the evolution implies the Hermiticity of the Hamiltonian.

Apparently, there is no space left for the non-Hermitian Hamiltonians which were recently studied by Bender et al [2]-[22]. The latter formalism may prove inspiring in field theory [3] but, as an extended quantum mechanics, it contradicts the Stone's theorem. In what follows, we intend to clarify this point.

Section 2 reviews a few basic features of the extended formalism which replaces the Hermiticity $H = H^\dagger$ by its weakening $H = H^\ddagger$. The latter property (called $\mathcal{PT}$ symmetry) is explained and several parallels between the symmetries $H = H^\dagger$ and $H = H^\ddagger$ are mentioned. Explicit $\mathcal{PT}$ symmetric square well solutions [4] are recalled as an illustration of the whole idea.

The introductory part of section 3 recollects the regularized spiked harmonic oscillator bound states of ref. [5] as a solvable example of a $\mathcal{PT}$ symmetric system which is defined on the whole real line. With its orthogonality and completeness properties

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kept in mind, we arrive at the first climax of our paper and formulate the appropriate modification of the conservation law (1) in the case of a general non-Hermitian system with the unbroken $\mathcal{PT}$ symmetry.

At the beginning of section 4 the construction of the harmonic bound states is extended to the domain of couplings where the $\mathcal{PT}$ symmetry of the wave functions becomes spontaneously broken. We show how all the Hilbert-space-like concepts of orthogonality and completeness of the states may be generalized accordingly. In particular, the $\mathcal{PT}$ symmetric norm (or rather pseudo-norm) proves so robust that the new conservation law of the type (1) remains valid even in the spontaneously broken regime where the energies cease to be real.

2. $\mathcal{PT}$ SYMMETRIC QUANTUM MECHANICS

The concept of the extended, non-Hermitian quantum mechanics with the requirement of $\mathcal{PT}$ symmetry of its Hamiltonians grew from several sources. The oldest root of its appeal is the Rayleigh-Schrödinger perturbation theory. Within its framework, Caliceti et al [6] have discovered that a low-lying part of the spectrum of the cubic anharmonic oscillator $H = p^2 + x^2 + g\,x^3$ is *real* for the *purely imaginary* couplings g. This establishes many formal analogies with quartic oscillator [7, 8].

A different direction of analysis has been accepted by Buslaev and Grecchi [9] who emphasized and employed some parallels between the Hermiticity and $\mathcal{PT}$ symmetry during their solution of an old puzzle of perturbative equivalence between apparently non-equivalent quartic anharmonic oscillators [23].

A mathematical background of the non-unique choice of the phenomenological Hamiltonians with real spectra has been pointed out, in non-Hermitian setting, by several authors [10]. Bender and Milton [11] emphasized the relevance of the unique analytic continuation of boundary conditions for the clarification and consequent explanation of the famous Dyson's paradox in QED [24].

In the cubic anharmonic models $H = p^2 + x^2 + i\,g\,x^3$ the reality of the energies at the sufficiently small g [6, 12] resembles the quartic case. Bender and Boettcher [13] attributed this connection to the commutativity of the Hamiltonian with the product of the complex conjugation $\mathcal{T}$ (which mimics the time reversal) and the parity $\mathcal{P}$, $H = \mathcal{PT}H\mathcal{PT} = H^\dagger$. An acceptability of this conjecture has been supported by a few partially [14] as well as completely [15] exactly solvable models.

In the physics community, a steady growth of acceptance of the $\mathcal{PT}$ symmetric models can be attributed to their possible phenomenological relevance. The cubic $H = p^2 + i\,x^3$ has been found relevant in statistical physics [16] and its non-linear perturbations $H = p^2 + (i\,x^3)^{1+\delta}$ were studied in field theory [17]. In all these models, a key argument that they can prove useful in some applications has been based on the reality of their spectrum. This argument is slightly misleading as we shall see in what follows.

2.1. **Solvable illustration: Square well.** The possibility of a spontaneous breakdown of the reality of the energies has been recently studied via a $\mathcal{PT}$–symmetric quartic oscillator $H = p^2 + i\,g\,x + x^4$ [18]. In this model, one spots the sequence of "critical" couplings g_n such that, step by step, the lowest real pair of the bound state energies E_{2n} and E_{2n+1} becomes converted into a complex conjugate doublet

beyond $g = g_n$. Such a pattern may prove characteristic for a fairly broad class of non-Hermitian interactions. For the sake of simplicity of the whole discussion, let us pick up the Schrödinger bound state problem on a finite interval,

$$\left[-\frac{d^2}{dx^2} + V(x)\right] \psi_n(x) = E_n \psi_n(x), \qquad \psi_n(-1) = \psi_n(1) = 0, \tag{2}$$

equipped with one of the most elementary $\mathcal{PT}$ symmetric forces $V(x) = -iT^2 \operatorname{sign} x$. Then, the ansatz

$$\psi_n(x) = \begin{cases} \sin \lambda(x+1), & x < 0, \\ C \sin \kappa(x-1), & x > 0 \end{cases}$$

with $E = k^2$ defines the solutions via the matching condition at $x = 0$. Using an abbreviation $\lambda = p - iq$ and rules

$$\lambda^2 = k^2 - iT^2, \qquad \kappa^2 = k^2 + iT^2 = (\lambda^*)^2$$

we get the elementary matching condition

$$\frac{\tan \lambda}{\lambda} = \text{purely imaginary}$$

which is equivalent to the elementary rule

$$q \sinh 2q = -p \sin 2p.$$

Its numerical solution has been discussed elsewhere [4]. Still, without any detailed numerical computations one can fairly easily see that in the two-dimensional $p - q$ plane, the left-hand-side function forms a valley with zero minimum along the line $q = 0$. The right-hand-side periodically oscillates with an increasing amplitude. One can conclude that the positive solutions $p(q) > 0$ of the latter equation form an infinite family of ovals which are symmetric with respect to the p–axis. The $n - th$ oval is confined between the zeros of the sine function, i.e., between the two lines $p = (2n+1)\pi/2$ and $p = (2n+2)\pi/2$. With the growth of $n = 0, 1, \ldots$, the ovals are longer as their ends move farther and farther from the p–axis. In the $n \gg 1$ asymptotic region, we get the estimate $p_{\text{end}} \approx (n + 3/4)\pi$ and $q_{\text{end}} \approx \ln n$.

As long as the definition of p and q implies that $p = T^2/(2q)$ we get the second curve which is a plain hyperbola in $p - q$ plane. The final solutions (i.e, intersections of this hyperbola with all the ovals) move close to the standard square well solutions in the quasi-Hermitian limit where $n \gg T^2$.

At the opposite extreme, the two lowest real energies determined by the lowest oval cease to exist for the sufficiently strong imaginary part of the force, i.e., for $T^2 > T^2_{\text{crit}} \approx 2 p_{\text{end}} q_{\text{end}}$. In the light of the previous estimates, the values of these critical points will grow with the number n of the oval in question. At $n = 0$ one has $T^2_{\text{crit}} \approx 4.48$ [4].

3. Models with unbroken $\mathcal{PT}$ symmetry

We can summarize that the elementary and exactly solvable $\mathcal{PT}$–symmetric square well model has a spectrum E_n which remains real in a certain non-empty interval of couplings $T \in (0, T_0)$. At the boundary $T = T_0$ with certain exceptional features [25], the lowest energy doublet E_0 and E_1 merges into a single state. The most

immediate fructification of this experience lies in the possibility of its transfer to the $\mathcal{PT}$ symmetric potentials on a "more realistic" infinite interval of coordinates.

3.1. **$\mathcal{PT}$ symmetric harmonic oscillators.** A nontrivial example which is solvable on the full real line is the $\mathcal{PT}$ symmetric harmonic oscillator described by the differential Schrödinger equation of ref. [5],

$$\left[-\frac{d^2}{dx^2}+\frac{G}{(x-i\delta)^2}-2i\delta\, x+x^2\right]\psi_n(x)=E_n\,\psi_n(x)\,,\quad \psi_n(x)\in L_2(-\infty,\infty)\,. \tag{3}$$

This equation with $G>-1/4$ can be interpreted as a confluent hypergeometric equation where an elementary change of the coordinate $x=r+i\,\delta$ eliminates all the unusual imaginary terms. At the same time, due to the analyticity of such a transformation, one can simply keep r on the real line with a small complex half-circle circumventing the singularity in the origin ($r=0$). Without any loss of generality we can then work with the complex general solution of our equation. It is available in closed form,

$$\psi(x)=C_{(+)}r^{1/2-\alpha}e^{r^2/2}\;{}_1F_1\left[\frac{1}{4}(2-E-2\alpha),1-\alpha;r^2\right]$$
$$+\,C_{(-)}r^{1/2+\alpha}e^{r^2/2}\;{}_1F_1\left[\frac{1}{4}(2-E+2\alpha),1+\alpha;r^2\right]\,.$$

This facilitates the use of the asymptotic boundary conditions. In the standard way described in any textbook [26] the idea works without alterations since the general solutions grow exponentially unless one of the confluent hypergeometric series terminates to a Laguerre polynomial. This gives the compact wave functions

$$\psi_N(r)=\mathcal{N}\,r^{1/2-Q\,\alpha}\,e^{-r^2/2}\,L_n^{(-Q\,\alpha)}(r^2)$$

with the quasi-parity $Q=\pm1$, main quantum number $n=0,1,\ldots$ and subscripted index $N=2n+(1-Q)/2$. The energies

$$E_N=4n+2-2\,Q\,\alpha\,,\qquad \alpha=\sqrt{G+\frac{1}{4}}\,,\qquad G>-\frac{1}{4} \tag{4}$$

remain real for the positive centrifugal-like parameters $\alpha>0$. These energies decrease/grow with G for the quasi-even/quasi-odd quasi-parity Q of the state, respectively.

If necessary, we can return to the Hermitian case and reproduce the usual radial harmonic oscillator solutions, provided only that we cross out the "unphysical" quasi-even states. These states violate the textbook boundary conditions [1]. The only exception concerns the regular limit (one-dimensional case) with $G=0$ (i.e., $\alpha=1/2$) and two parities $Q=\pm1$. In this sense, the full spectrum (4) of our complexified oscillator represents a comfortable formal link between the seemingly different one- and three-dimensional Hermitian cases [19].

3.2. **Scalar product and orthogonality.** Let us return to a general Hamiltonian $H=H^\dagger$ and assume that its spatial parity $\mathcal{P}$ becomes manifestly broken, $\mathcal{P}H\mathcal{P}=\mathcal{T}H\mathcal{T}\neq H$. We may define the quasi-parity as a constant integer $Q_n=(-1)^n$ in the $n-$th state. This generalizes the above square well and harmonic oscillator constructions and applies also to the quartic oscillator of ref. [18] in a constrained domain of the couplings $g\in(0,g_0)$.

In the first step we introduce the indeterminate scalar product defined by the prescription $\langle\phi|\mathcal{P}|\psi\rangle$ of ref. [20]. It does not possess the property of definiteness and defines merely a pseudo-norm. The disappearance of the self-overlap $\langle\psi|\mathcal{P}|\psi\rangle = 0$ does not imply that the vector $|\psi\rangle$ must vanish by itself.

The main merit of such a definition of the scalar product lies in the observation that it leads to the usual orthonormality of the left and right eigenstates of the $\mathcal{PT}$ symmetric Hamiltonians and Schrödinger equations [8],

$$\langle\psi_n|\mathcal{P}|\psi_m\rangle = Q_n\delta_{mn}\,, \qquad m,n = 0,1,\ldots$$

The completeness relations also acquire the form mentioned in ref. [20],

$$\sum_{n=0}^{\infty} |\psi_n\rangle\, Q_n \langle\psi_n|\mathcal{P} = I\,.$$

The related innovated spectral representation of our non-Hermitian $\mathcal{PT}$ symmetric Hamiltonians can be written in a bit unusual but fully transparent manner,

$$H = \sum_{n=0}^{\infty} |\psi_n\rangle\, E_n\, Q_n \langle\psi_n|\mathcal{P}\,.$$

This enables us to infer that the time evolution of the corresponding system is pseudo-unitary,

$$|\psi(t)\rangle = e^{-iHt}\,|\psi(0)\rangle = \sum_{n=0}^{\infty} |\psi_n\rangle\, e^{-i\,E_n\,Q_n\,t}\,\langle\psi_n|\mathcal{P}|\psi(0)\rangle\,,$$

and preserves the value of the scalar product in time,

$$\langle\psi(t)|\mathcal{P}|\psi(t)\rangle = \langle\psi(0)|\mathcal{P}|\psi(0)\rangle\,.$$

We have to stress that the Stone's theorem (which relates the unitary evolution law to the Hermitian underlying Hamiltonians) finds the first interesting extension here.

4. Spontaneously broken $\mathcal{PT}$ symmetry

4.1. **Harmonic oscillator inspiration.** Clear parallels between the Hermitian and non-Hermitian $\mathcal{PT}$ symmetric Hamiltonians remain marred by the possibility that in the latter case the reality of the spectrum could break down at certain couplings. We have seen that "step-by-step", at an increasing sequence of the couplings, the levels can cease to be real even for the most transparent square well and quartic examples. Here, we are going to explain that from a formal point of view, the break-down of the $\mathcal{PT}$ symmetry can still remain quite innocent in its physical consequences.

When we return to the harmonic oscillator example (3), we can mimic the break-down of the $\mathcal{PT}$ symmetry when we remove the constraint $G > -1/4$ which was inherited from the standard Hermitian quantum mechanics where its violation would cause the unavoidable fall of the particles into the attractive strong singularity in the origin [1].

In the present non-Hermitian context, one cannot find any persuasive excuse why the smaller couplings $G < -1/4$ could not be admitted as legitimate. Of course, they give the purely imaginary parameters $\alpha = i\gamma = i\sqrt{-1/4 - G}$ but the rest of the construction in subsection 3.1 would remain perfectly valid. In particular, the termination of the hypergeometric series will definitely determine the normalizable

solutions existing at the complex energies. This is a puzzle which is to be resolved here.

Our illustrative harmonic oscillator energies form the two complex families,

$$E_N = 4n + 2 - 2iQ\gamma, \qquad \gamma = \sqrt{-G - \frac{1}{4}} > 0, \qquad G < -\frac{1}{4}. \tag{5}$$

These energies (as well as their Laguerre-polynomial wave functions) are numbered, as above, by the quasi-parity $Q = \pm 1$ and by the integers $n = 0, 1, \ldots$ in the index $N = 2n + (1 - Q)/2$.

We are going to demonstrate now that the similar families of the complex energies can still be interpreted as admissible solutions. We shall see that, rather counterintuitively, there exists in fact no acceptable reason why the complex spectrum (5) should be forgotten [21].

We have to return to a model-independent argumentation. In the case of the broken symmetry, we shall only assume that the two solutions with $E \neq E^*$ have to be sought simultaneously.

4.2. **The case of the complex conjugate pairs of the energies.** In a way inspired by ref. [22] we may assume that the $\mathcal{PT}$ symmetry of the Hamiltonian becomes broken by a pair of the wave functions. One gets the two respective Schrödinger equations

$$H|\psi_+\rangle = E\,|\psi_+\rangle\,, \qquad H|\psi_-\rangle = E^*\,|\psi_-\rangle\,.$$

As long as we have $H \neq H^\dagger = \mathcal{P}H\mathcal{P}$, we may also re-write our equations in the form of action of the Hamiltonian to the left,

$$\langle\psi_+|\,\mathcal{P}H = E^*\,\langle\psi_+|\,\mathcal{P}, \qquad \langle\psi_-|\,\mathcal{P}H = E\,\langle\psi_-|\,\mathcal{P}\,.$$

Out of all the possible resulting overlaps, let us compare the following two,

$$\langle\psi_+|\,\mathcal{P}H|\psi_+\rangle = E^*\,\langle\psi_+|\,\mathcal{P}\,|\psi_+\rangle\,, \qquad \langle\psi_+|\,\mathcal{P}H\,|\psi_+\rangle = E\,\langle\psi_+|\,\mathcal{P}\,|\psi_+\rangle$$

and, in parallel,

$$\langle\psi_-|\,\mathcal{P}H|\psi_-\rangle = E^*\,\langle\psi_-|\,\mathcal{P}\,|\psi_-\rangle\,, \qquad \langle\psi_-|\,\mathcal{P}H\,|\psi_-\rangle = E\,\langle\psi_-|\,\mathcal{P}\,|\psi_-\rangle\,.$$

These alternatives imply that for $E \neq E^*$ the self-overlaps must vanish,

$$\langle\psi_+|\,\mathcal{P}\,|\psi_+\rangle = 0\,, \qquad \langle\psi_-|\,\mathcal{P}\,|\psi_-\rangle = 0\,.$$

This leads to several interesting consequences. Firstly, we are free to employ the following less common normalization

$$\langle\psi_+|\,\mathcal{P}\,|\psi_-\rangle = [\ \langle\psi_-|\,\mathcal{P}\,|\psi_+\rangle\ ]^* = c\,,$$

and, wherever needed, re-normalize $c \to \pm 1$. This convention is less common but can be still interpreted as a generalized orthonormality condition in any two-dimensional subspace of the linear pseudo-normalized space of the $\mathcal{PT}$ symmetry breaking states.

4.3. **Evolution under the broken $\mathcal{PT}$ symmetry.** For the sake of simplicity, let us assume that the $\mathcal{PT}$ symmetry is broken just at the two lowest states. The necessary modification of the completeness relations adds then just the two new terms to the sum over the unbroken ψ_n's,

$$I = |\psi_+\rangle \frac{1}{c^*} \langle\psi_-|\mathcal{P} \ + \ |\psi_-\rangle \frac{1}{c} \langle\psi_+|\mathcal{P} \ + \ \sum_{n=2}^{\infty} |\psi_n\rangle \, Q_n \langle\psi_n|\mathcal{P} \, .$$

The forthcoming modification of the spectral decomposition of the Hamiltonian adds the similar two new terms to the sum over the unbroken energies,

$$H = |\psi_+\rangle \frac{E}{c^*} \langle\psi_-|\mathcal{P} \ + \ |\psi_-\rangle \frac{E^*}{c} \langle\psi_+|\mathcal{P} \ + \ \sum_{n=2}^{\infty} |\psi_n\rangle \, E_n Q_n \langle\psi_n|\mathcal{P} \, .$$

Finally, the pseudo-unitary time development acquires the compact form as well,

$$|\psi(t)\rangle = e^{-iHt} \, |\psi(0)\rangle \, ,$$

$$e^{-iHt} = |\psi_+\rangle \frac{1}{c^*} e^{-i\,E\,t} \langle\psi_-|\mathcal{P} \ + \ |\psi_-\rangle \frac{1}{c} e^{-i\,E^*\,t} \langle\psi_+|\mathcal{P} \ + \ \sum_{n=2}^{\infty} |\psi_n\rangle e^{-i\,E_n\,Q_n\,t} \langle\psi_n|\mathcal{P} \, .$$

It is quite amusing to discover that the value of the scalar product is conserved,

$$\langle\psi(t)|\mathcal{P}|\psi(t)\rangle = \langle\psi(0)|\mathcal{P}|\psi(0)\rangle \, .$$

A full parallel to the conventional quantum mechanics is established.

5. Summary

We may summarize that far beyond the boundaries of the ordinary quantum mechanics, the above-mentioned difficulties with the implications of the Stone's theorem in $\mathcal{PT}$ symmetric context were shown related to the "hidden" use of a pseudo-norm. *Vice versa,* after one admits that the vanishing (pseudo-)norm need not imply the vanishing of the state, a modified version of the Stone's theorem is recovered. We have shown that the appropriately defined self-overlaps of the states remain unchanged in time not only in the systems characterized by the preserved $\mathcal{PT}$ symmetry, but also in the domains of couplings where this symmetry is spontaneously broken.

A consistent and complete interpretation of the extended quantum formalism is not at our disposal yet. Still, several new features of it have been revealed here. For example, it seems to mimic some properties of the indefinite metric which is already of quite a common use, say, in relativistic physics.

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