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Should $\mathcal{PT}$ Symmetric Quantum Mechanics Be Interpreted as Nonlinear?

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Abstract

The Feshbach-type reduction of the Hilbert space to the physically most relevant "model" subspace is suggested as a means of a formal unification of the standard quantum mechanics with its recently proposed $\mathcal{PT}$ symmetric modification. The resulting "effective" Hamiltonians $H_{\text{eff}}(E)$ are always Hermitian, and the two alternative forms of their energy-dependence are interpreted as a certain dynamical nonlinearity, responsible for the repulsion and/or attraction of the levels in the Hermitian and/or $\mathcal{PT}$ symmetric cases, respectively. The spontaneous $\mathcal{PT}$ symmetry breaking is then reflected by the loss of the Hermiticity of H_{eff} while the pseudo-unitary evolution law persists in the unreduced Hilbert space.

1 Introduction

Bender and Boettcher [1] tentatively attributed the reality of spectra in non-Hermitian models to the commutativity of the Hamiltonians with the product of the complex conjugation $\mathcal{T}$ (which mimics the time reversal) and the parity $\mathcal{P}$,

$$H = \mathcal{PT}H\mathcal{PT} \equiv H^{\ddagger}. \tag{1.1}$$

An acceptability of this conjecture is supported by the growing empirical experience with the similar models [2] and by the analysis of many examples (1.1) which are partially [3] or completely [4] exactly solvable. In the physics community, a steady growth of acceptance of the $\mathcal{PT}$ symmetric models can be attributed to their phenomenological relevance in solid state physics [5], statistical physics [6], population dynamics [7], in the many-body [8] and supersymmetric [9] context and, last but not least, within the general quantum field theory [10]. A reason why the $\mathcal{PT}$ symmetric models could eventually prove useful in these applications has been sought in the reality of their spectrum.

The latter argument is slightly misleading and has been criticized recently [11] but the debate proves inspiring, involves many separate issues and, apparently, may be expected to continue. In what follows, we intend to join it, emphasizing that the concept of extended, non-Hermitian quantum mechanics with real spectra and $\mathcal{PT}$ symmetric Hamiltonians exhibits multiple parallels with the standard textbook quantum mechanics.

The material is organized as follows. Firstly, Section 2 reviews several features of the symmetry breaking within the standard quantum mechanics. It emphasizes that the commutativity of the Hamiltonian with the parity $\mathcal{P}$ enables us to split the Hilbert space into two subspaces. The loss of this commutativity interrelates these two subspaces but one can still stay within one of them at a cost of the replacement of the Hamiltonian H by its Feshbach's [12] energy-dependent (so called effective) equivalent form $H_{\rm eff}(E)$.

In Section 3 we return to the non-Hermitian models and stress some of their most important specific properties. In particular, the reasons for the introduction of an indeterminate inner product are recollected. We show that in spite of the non-Hermiticity of H, the related pseudo-unitary character of the time evolution represents a good reason for introduction of a certain pseudo-norm.

In Section 4 we formulate the core of our present message and show that the Feshbach's reduction of the $\mathcal{PT}$ symmetric operators $H = H^{\ddagger}$ is Hermitian. As an immediate consequence, at least a part of the spectrum may be real, and its full reality may be expected to occur at least in the case of a certain sufficiently weak non-Hermiticity. Such an idea is also shown to inspire an immediate generalization of the concept of the $\mathcal{PT}$ symmetry. An analogy between Hermiticity and $\mathcal{PT}$ symmetry is established, in spite of the fact that the effective Schrödinger equation must be understood as slightly nonlinear. This nonlinearity is "weak", mediated merely by the energy-dependence of the reduced Hamiltonians $H_{\rm eff}(E)$.

Section 5 contains the discussion of several related questions. We pay some attention to the so called spontaneous $\mathcal{PT}$ symmetry breaking and to the loss of the reality of the energies, not accompanied by any loss of the pseudo-unitarity of the time evolution.

Finally, Section 6 summarizes all our results and emphasizes that the $\mathcal{PT}$ symmetric quantum mechanics with real spectra might admit the standard probabilistic physical interpretation of the wave function on a suitably reduced Hilbert space.

2 A short detour to the standard quantum mechanics

2.1 A parity-preserving oscillator example

The quadratic plus quartic one-dimensional Hamiltonian

$$H(g) = p^2 + x^2 + g\,x^4 \tag{2.1}$$

is extremely popular in perturbation theory where its mathematical study admits the complex couplings g and, therefore, an explicit breakdown of Hermiticity. This qualifies this model as a guide which appears in the standard quantum mechanics [13] as well as in its $\mathcal{PT}$ symmetric alternative [14].

In the former, purely Hermitian case, all the coupling constants in eq. (2.1) are real and the spectral representation of our anharmonic oscillator Hamiltonian (which commutes with the parity $\mathcal{P}$) may be split in the even- and odd-parity eigenstates $|\,n^{(\pm)}(g)\rangle$,

$$H(g) = \sum_{n=0}^{\infty} |\,n^{(+)}(g)\rangle\; \varepsilon_n^{(+)}(g)\,\langle n^{(+)}(g)| + \sum_{m=0}^{\infty} |\,m^{(-)}(g)\rangle\; \varepsilon_m^{(-)}(g)\,\langle m^{(-)}(g)|, \quad g \ge 0.$$

The parity conservation annihilates some matrix elements between the $g = 0$ basis states denoted by the symbols $|\, s_n\rangle = |\, n^{(+)}(0)\rangle$ and $|\, t_n\rangle = |\, n^{(-)}(0)\rangle$,

$$\langle s_m|\, H(g)\, |\, t_n\rangle = \langle t_m|\, H(g)\, |\, s_n\rangle = 0, \qquad m, n = 0, 1, \ldots . \tag{2.2}$$

This induces the so called super-selection $\langle s_m|\, \psi^{(-)}\rangle = \langle t_m|\, \psi^{(+)}\rangle = 0$ and splits the variational Schrödinger equation in the two separate infinite-dimensional matrix sub-problems with a definite parity,

$$\sum_{k=0}^{\infty} \mathcal{F}_{mk}\ \langle s_k|\, \psi^{(+)}\rangle = E\ \langle s_m|\, \psi^{(+)}\rangle, \quad m = 0, 1, \ldots, \qquad \mathcal{F}_{mk} = \langle s_m|\, H(g)\, |\, s_k\rangle,$$
$$\sum_{k=0}^{\infty} \mathcal{G}_{mk}\ \langle t_k|\, \psi^{(-)}\rangle = E\ \langle t_m|\, \psi^{(-)}\rangle, \quad m = 0, 1, \ldots, \qquad \mathcal{G}_{mk} = \langle t_m|\, H(g)\, |\, t_k\rangle.$$

This means that the matrix form of $H(g)$ is the direct sum of the two different matrices $\mathcal{F}$ and $\mathcal{G}$, precisely in the spirit of the Schur's lemma [15].

2.2 Parity-breaking terms and the effective Hamiltonians

For a more general anharmonic oscillator

$$H(f, g) = p^2 + x^2 + f\, x^3 + g\, x^{2N}$$

the parity $\mathcal{P}$ ceases to be a useful symmetry due to the presence of the spatially asymmetric cubic term whose non-vanishing elements form a matrix $\Omega_{mj} = \langle t_m|\, f\, x^3\, |\, s_j\rangle$. Each wave function in $L_2(\mathbb{R})$ must be expanded in the full basis,

$$|\psi\rangle = \sum_{n=0}^{\infty} |s_n\rangle\ h_n^{(+)} + \sum_{m=0}^{\infty} |t_m\rangle\ h_m^{(-)}. \tag{2.3}$$

Schrödinger equation acquires the partitioned matrix form

$$\begin{pmatrix} \mathcal{F} - E\, I & \Omega^T \\ \Omega & \mathcal{G} - E\, I \end{pmatrix} \begin{pmatrix} \vec{h}^{(+)} \\ \vec{h}^{(-)} \end{pmatrix} = 0,$$

where we may eliminate the Feshbach's [12] "out-of-the-model-space" components

$$\vec{h}^{(-)} = -\frac{1}{\mathcal{G} - E\, I}\, \Omega\, \vec{h}^{(+)}$$

and get the reduced Schrödinger equation containing the effective Hamiltonian which is (presumably, not too manifestly) energy dependent,

$$H_{\text{eff}}(E)\, \vec{h}^{(+)} = E\, \vec{h}^{(+)}, \qquad H_{\text{eff}}(E) = \left(\mathcal{F} - \Omega^T\, \frac{1}{\mathcal{G} - E\, I}\, \Omega \right). \tag{2.4}$$

The energy-dependence of $H_{\text{eff}}(E)$ causes rarely a problem. In numerical context one fixes a trial energy ϱ in $H_{\text{eff}}(\varrho)$ and solves the linearized Schrödinger equation giving a one-parametric family of auxiliary spectra $\{\hat{E}_n(\varrho)\}$. A return to the exact and nonlinear eigenvalue problem (2.4) is then mediated by the selfconsistent determination of the best parameter,

$$\varrho = \hat{E}_n(\varrho). \tag{2.5}$$

Sufficient precision is mostly achieved via the linear approximation

$$H_{\text{eff}}(\varrho)\,\vec{h}^{(+)} = E\,\vec{h}^{(+)}, \tag{2.6}$$

with a single value of ϱ adapted to the practical evaluation of a set of several neighboring energy levels E.

3 $\mathcal{PT}$ symmetric formalism

An interest in the commutativity (1.1) of H with $\mathcal{PT}$ (let us repeat that $\mathcal{P}$ means parity and $\mathcal{T}$ denotes time reversal) grew from several sources. The oldest root of its appeal is the Rayleigh–Schrödinger perturbation theory. Within its framework, Caliceti et al [16] have discovered that a low-lying part of the spectrum in the cubic anharmonic potential $V = x^2 + g\,x^3$ for some *purely imaginary* couplings g is *real*. This establishes an analogy between the Hermitian and some non-Hermitian oscillators, extending the family of the eligible phenomenological potentials.

A non-perturbative direction of analysis has been initiated by Buslaev and Grecchi [17] who were motivated by the physical relevance of non-Hermitian models in field theory. They employed parallels between Hermiticity and $\mathcal{PT}$ symmetry during their solution of an old puzzle of spectral equivalence between apparently non-equivalent quartic interaction models. Bender and Milton [18] underlined in similar context that an ambiguity in boundary conditions exists and is essential for the clarification and consequent explanation of the famous Dyson's paradox in [18]. These studies opened new mathematical as well as interpretation problems. Some of them will be discussed here.

3.1 Modified inner product

In $\mathcal{PT}$ symmetric quantum mechanics the Hamiltonians are non-Hermitian and one often discovers (or, at worst, assumes) that their spectrum is real, discrete and non-degenerate. Even under this assumption, their left eigenvectors (let us denote them by the symbol $\langle\langle\psi|$) need not necessarily coincide with the Hermitian conjugates $\langle\psi|$ of their right eigenvector partners. The Hermitian conjugation must be replaced by its modification,

$$\langle\psi| \to \langle\langle\psi| = \langle\psi|\,\mathcal{P}.$$

Originally, such a replacement has been made and used in the non-degenerate perturbation theory [19] where the Rayleigh–Schrödinger formalism leads to the recursive definition of the products $E^{(k)} \cdot \langle\psi^{(0)}|\,\mathcal{P}|\,\psi^{(0)}\rangle$. They contain the energy correction $E^{(k)}$ multiplied by the unperturbed pseudo-norm which vanishes precisely at the boundary of the applicability of the non-degenerate perturbation formalism. At this boundary a *real* Bender–Wu singularity is crossed [20] so that $\langle\psi^{(0)}|\,\mathcal{P}|\,\psi^{(0)}\rangle \to 0$ and a pair of the energy levels merges [21, 22, 23].

At the two different real energies $E_1 \neq E_2$ the comparison of the left and right $\mathcal{PT}$ symmetric equations $H|\psi_1\rangle = E_1|\psi_1\rangle$ and $\langle\langle\psi_2|\, H = \langle\langle\psi_2|\, E_2$ leads to the orthogonality $\langle\langle\psi_2|\, \psi_1\rangle = 0$ so that the inner product with metric $\mathcal{P}$ and with the so called quasi-parity $Q_n = \pm 1$ [21, 22] is the natural option. Formally, the disappearance of the self-overlap $\langle\psi|\mathcal{P}|\psi\rangle = 0$ does not imply that the vector $|\psi\rangle$ itself must vanish so that the requirement

$$\langle\psi_n|\mathcal{P}|\psi_m\rangle = Q_n\delta_{mn}, \qquad m, n = 0, 1, \ldots. \tag{3.1}$$

merely "pseudo-normalizes" the solutions (cf. also ref. [24]). A further development of the theory requires the notion of the completeness of the bound states,

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

as well as an innovated spectral representation of a given non-Hermitian $\mathcal{PT}$ symmetric Hamiltonian with real spectrum,

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

It admits various pseudo-Hermitian alternatives and generalizations [25].

3.2 The pseudo-unitarity of the evolution in time

Evolution of bound states in quantum mechanics is mediated (generated) by their Hamiltonian, $|\psi[t]\rangle = \exp(-i\, H\, t)\, |\psi[0]\rangle$. In the models with Hermitian $H = H^\dagger$ the availability of solutions of the time-independent Schrödinger equation simplifies this rule since all the eigenvalues E_n remain real and the time-dependence of the separate eigenstates becomes elementary,

$$|\psi_n[t]\rangle = e^{-i\, E_n\, t}\, |\psi_n[0]\rangle.$$

Although a fully consistent and complete physical interpretation of the general pseudo-Hermitian Hamiltonians is not at our disposal yet, many of their formal features are not entirely new, mimicking the models with indefinite metric in relativistic physics etc. Another significant source of insight are particular examples. In many of them, whenever the real energies E_n are attributed to a non-Hermitian, $\mathcal{PT}$ symmetric Hamiltonian with the property (1.1), we may infer that

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

This formula means that the conservation law concerns the innovated scalar product,

$$\langle\psi[t]|\mathcal{P}|\psi[t]\rangle = \langle\psi[0]|\mathcal{P}|\psi[0]\rangle$$

so that the time evolution of the system is pseudo-unitary.

4 An explanation of the reality of spectra

Any eigenstate of $H = H^\dagger = \mathcal{P}H\mathcal{P}$ (e.g., of $H(g)$ in paragraph 2.1) satisfies the same Schrödinger equation even when it is pre-multiplied by the parity $\mathcal{P}$. Both the old and new eigenstates belong to the same real eigenvalue E which cannot be degenerate due to the Sturm–Liouville oscillation theorems. One of the superpositions $|\psi\rangle \pm \mathcal{P}|\psi\rangle$ must vanish while the other one acquires a definite parity. This is the essence of the mathematical proof of the above-mentioned Schur's lemma. The wave functions are even or odd and the $\mathcal{P}$ symmetry of wave functions cannot be spontaneously broken, $\mathcal{P}|n^{(\pm)}(g)\rangle = \pm|n^{(\pm)}(g)\rangle$.

The rigidity of the latter rule is lost during the transition to the $\mathcal{PT}$ symmetric models where any quantity $\exp(i\varphi)$ is an admissible eigenvalue of the operator $\mathcal{PT}$ since its component $\mathcal{T}$ is defined as anti-linear, $\mathcal{T}i = -i$. In more detail, every rule $\mathcal{PT}|\psi\rangle = \exp(i\varphi)\,|\psi\rangle$ implies that we have

$$\mathcal{PTPT}|\psi\rangle = \exp(-i\varphi)\,\mathcal{PT}|\psi\rangle = |\psi\rangle$$

as required. The Schur's lemma ceases to be applicable. In the basis with the properties $\mathcal{PT}|S\rangle = |S\rangle$ and $\mathcal{PT}|L\rangle = -|L\rangle$, the general expansion formula

$$H = \sum_{m,n=0}^{\infty} \left(|S_m\rangle \mathcal{F}_{m,n} \langle S_n| \,+\, |L_m\rangle \mathcal{G}_{m,n} \langle L_n| \,+\, i\,|S_m\rangle \mathcal{C}_{m,n} \langle L_n| \,+\, i\,|L_m\rangle \mathcal{D}_{m,n} \langle S_n|\right)$$

contains four separate complex matrices of coefficients. Once it is subdued to the requirement $H = \mathcal{PT}H\mathcal{PT}$, we get the necessary and sufficient condition demanding that all the above matrix elements of $H = H^\ddagger$ must be real,

$$\mathcal{F}_{m,n} = \mathcal{F}^*_{m,n}, \qquad \mathcal{G}_{m,n} = \mathcal{G}^*_{m,n}, \qquad \mathcal{C}_{m,n} = \mathcal{C}^*_{m,n}, \qquad \mathcal{D}_{m,n} = \mathcal{D}^*_{m,n}. \tag{4.1}$$

As long as the similar trick has led to the superselection rules for the spatially symmetric Hamiltonians, we may conclude that the $\mathcal{PT}$ symmetric analogue of the direct-sum decompositions and superselection rules (2.2) is just the much weaker constraint (4.1).

4.1 Re-emergence of Hermiticity via effective Hamiltonians

Whenever we have a state with the $\mathcal{PT}$-parity equal to $\exp(i\varphi)$, we may try to shift the phase and introduce the new state $|\chi\rangle = \exp(i\beta)|\varphi\rangle$. The action $\mathcal{PT}\,|\varphi\rangle = e^{i\varphi}|\varphi\rangle$ is modified,

$$\mathcal{PT}\,|\chi\rangle = \mathcal{PT}\,e^{i\beta}|\varphi\rangle = e^{-i\beta}\mathcal{PT}\,|\varphi\rangle = e^{i\,(\varphi-2\beta)}\,|\chi\rangle$$

and the $\mathcal{PT}$ parity has changed by -2β. Via the renormalization β we may achieve that the new $\mathcal{PT}$ phase is zero. Such a normalization convention means that

$$|\psi\rangle = \sum_{n=0}^{\infty} |s_n\rangle\; p_n^{(+)} + i \sum_{m=0}^{\infty} |t_m\rangle\; p_m^{(-)},$$

where all the coefficients are real. This revitalizes the analogy with formula (2.3). Our next illustration,

$$H(if,g) = p^2 + x^2 + if\,x^3 + g\,x^4$$

may use the *same* matrix elements $\Omega_{mj} = \langle t_m | \, f \, x^3 \, | \, s_j \rangle$ as above and becomes tractable by the mere replacements $\Omega \to i\,\Omega$, $h_n^{(+)} \to p_n^{(+)}$ and $h_n^{(-)} \to i\,p_n^{(-)}$. This gives very similar, real Schrödinger matrix equation

$$\left(\begin{array}{cc} \mathcal{F} - E\,I & -\Omega^T \\ \Omega & \mathcal{G} - E\,I \end{array} \right) \left(\begin{array}{c} \vec{p}^{\,(+)} \\ \vec{p}^{\,(-)} \end{array} \right) = 0$$

and the very similar partial solution

$$\vec{p}^{\,(-)} = + \frac{1}{\mathcal{G} - E\,I}\,\Omega\,\vec{p}^{\,(+)}.$$

We have to emphasize that the final, effective Schrödinger equation is Hermitian,

$$H_{\text{eff}}(\varrho)\,\vec{p}^{\,(+)} = E(\varrho)\,\vec{p}^{\,(+)}, \qquad H_{\text{eff}}(\varrho) = \left(\mathcal{F} + \Omega^T\,\frac{1}{\mathcal{G} - \varrho\,I}\,\Omega \right) \tag{4.2}$$

In comparison with the recipe of paragraph 3.2 the only difference is in the sign of the correction term. This makes the connection between the Hermiticity and $\mathcal{PT}$ symmetry particularly tight. Both the Schrödinger equations (2.4) and (4.2) are Hermitian and give the (different) real spectra $E(\varrho)$ at any ϱ. Both these reduced Schrödinger equations prove insensitive to the change of the sign of the coupling matrix Ω but a return to the original Schrödinger equations reveals that the replacement $\Omega \to -\Omega$ is not an equivalence transformation as it changes the wave functions.

4.2 The generalized metric operators $\mathcal{P}$

One has to impose the selfconsistency condition (2.5) but it is clear that this cannot give any complex roots $E(E)$ in the Hermitian case. In contrast, they may freely emerge in the non-Hermitian setting so that the $\mathcal{PT}$ symmetry is less robust than Hermiticity.

All the other parallels between the Hermitian an $\mathcal{PT}$ symmetric models are more straightforward. Once we work just with the effective Hamiltonian (which is always Hermitian), many phenomenologically oriented conclusions concerning the Hermiticity or pseudo-Hermiticity of the full, original Hamiltonian will only depend on the subtle details of an overall energy or rather ϱ-dependence of our model-space Hamiltonian $H_{\text{eff}}(\varrho)$. In this sense, the $\mathcal{PT}$ symmetry may be considered to be just a very special case of the pseudo-Hermiticity.

Let us now return to our original problem once more. Why do the $\mathcal{PT}$ symmetric Hamiltonians have real energies? The above explanation relies on the Hermiticity of $H_{\text{eff}}(\varrho)$, guaranteeing that all the auxiliary $E_n(\varrho)$ are real. The discussion is reduced to the selfconsistency (2.5) and to the reality/complexity of its roots. In this sense the whole parallel between the Hermitian and non-Hermitian coupling of the individual sub-Hamiltonians F and G is based on the mere matrix structure of the Schrödinger equation. Its partitioned form

$$\left(\begin{array}{cc} F - E\,I & \alpha\,A \\ A^\dagger & G - E\,I \end{array} \right) \cdot \left(\begin{array}{c} \vec{u} \\ \vec{w} \end{array} \right) = 0 \tag{4.3}$$

represents simply the Hermitian case at $\alpha = 1$ and the $\mathcal{PT}$ symmetric case at $\alpha = -1$. Thus, the operator $\mathcal{P}$ need not be parity. As long as our previous analysis did not depend on this interpretation, the real energies may be expected to emerge, following the same idea of the effective Hermitization, from the other matrix structures of H.

We may admit, for example, that the block A is not a real matrix at all. One can imagine that the *complex* (and Hermitian or even merely $\mathcal{PT}$ symmetric) sub-Hamiltonians F and G would also lead to the real spectra, at least in the limit of the sufficiently small *complex* coupling matrices A.

Another type of generalization was present in the original Feshbach's proposal [12] where the upper partition F is the most relevant part of the Hilbert space (called "model" space) spanned just by a few most important elements of the basis. The other partition is usually expected to contribute to the observable quantities as a correction. Thus, one might work with the two partitions of different size, $\dim F \neq \dim G$.

Last but not least, one could consider a triple or multiple partitioning which would generalize eq. (4.3). An explicit construction of this type may be found, e.g., in our recent remark [26].

5 Discussion

5.1 What happens after a spontaneous breakdown of $\mathcal{PT}$ symmetry

A puzzle emerges when the non-Hermiticity grows and certain doublets of real energies merge and form, subsequently, complex conjugate pairs. Explicit examples of such a possibility range from the $\mathcal{PT}$ symmetric square well on a finite interval [27] up to many quasi-exactly solvable models [28] and virtually all the shape invariant potentials on the whole real line [29].

Let us recollect the harmonic oscillator example $H = p^2 + r^2 + G/r^2$ of ref. [21] and the two possible forms of its energy spectrum. At $G > -1/4$ one encounters the purely real and discrete levels $E_N = 4n + 2 - 2\,Q\,\gamma$ with $\gamma = \sqrt{-G - 1/4} > 0$ and $n = 0, 1, \ldots$. These levels (distinguished by their quasi-parity $Q = \pm 1$) are to be compared with the complex conjugate pairs $E_N = 4n + 2 - 2\,i\,Q\,\delta$ which replace the above set at the strongly negative coupling $G < -1/4$ in $\delta = \sqrt{-G - 1/4} > 0$. We see that once we remove the constraint $G > -1/4$, the $\mathcal{PT}$ symmetry of the wave functions breaks down *for all the levels at once*, at $G = -1/4$ [29].

In such a context let us now assume that the solution of a given non-Hermitian Schrödinger equation gives at least two energies which are mutual complex conjugates,

$$H|\psi_+\rangle = E\,|\psi_+\rangle, \qquad H|\psi_-\rangle = E^*\,|\psi_-\rangle. \tag{5.1}$$

We may re-write these two Schrödinger equations in their respective Hermitian conjugate form with $H^\dagger = \mathcal{P}\,H\,\mathcal{P}$ acting 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 now recollect the following four,

$$\begin{aligned}
\langle\psi_+|\,\mathcal{P}\,H|\psi_+\rangle &= E^*\,\langle\psi_+|\,\mathcal{P}\,|\psi_+\rangle, \qquad & \langle\psi_+|\,\mathcal{P}\,H\,|\psi_+\rangle &= E\,\langle\psi_+|\,\mathcal{P}\,|\psi_+\rangle,\\
\langle\psi_-|\,\mathcal{P}\,H|\psi_-\rangle &= E^*\,\langle\psi_-|\,\mathcal{P}\,|\psi_-\rangle, \qquad & \langle\psi_-|\,\mathcal{P}\,H\,|\psi_-\rangle &= E\,\langle\psi_-|\,\mathcal{P}\,|\psi_-\rangle.
\end{aligned}$$

Their comparison suggests that for $E \neq E^*$ the self-overlaps must vanish,

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

We must extend the above rule (3.1) and complement it by an off-diagonal pseudo-normalization

$$\langle \psi_+ | \mathcal{P} | \psi_- \rangle = [\, \langle \psi_- | \mathcal{P} | \psi_- \rangle \,]^* = c \tag{5.2}$$

with any suitable $c \in \mathbb{C}$.

5.2 The pseudo-norm and its conservation

For the sake of simplicity let us assume that the $\mathcal{PT}$ symmetry is broken just at the two lowest states (cf. the examples [27, 14]). Besides the above-mentioned modification of the orthogonality relations, one has to change the first two terms in the decomposition of unit,

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

This is a new form of the completeness relations. The parallel spectral decomposition of the Hamiltonian in question contains the similar two new terms,

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

Finally, the pseudo-unitary time dependence of wave functions acquires the following new compact form,

$$|\psi[t]\rangle = e^{-iHt} \, |\psi[0]\rangle = \left(|\psi_+\rangle \frac{1}{c^*} \, e^{-i\,E\,t} \, \langle \psi_- | \mathcal{P} \right) + \left(\; |\psi_-\rangle \, \frac{1}{c} \, e^{-i\,E^*\,t} \, \langle \psi_+ | \mathcal{P} \right)$$
$$+ \sum_{n=2}^{\infty} |\psi_n\rangle \, e^{-i\,E_n\,Q_n\,t} \, \langle \psi_n | \mathcal{P} | \psi[0] \rangle.$$

The value of the scalar product is conserved in time,

$$\langle \psi[t] | \mathcal{P} | \psi[t] \rangle = \langle \psi[0] | \mathcal{P} | \psi[0] \rangle.$$

A weakened form of the Stone's theorem could be re-established for the pseudo-unitary evolution allowing non-Hermitian Hamiltonians $H = H^{\ddagger}$. We see that this may be done not only in the $\mathcal{PT}$ symmetric systems characterized by the real spectra but also in the domain of couplings where this symmetry is spontaneously broken. A parallel to the unbroken case is established. As long as the vanishing self-overlaps $\langle\langle \psi | \psi \rangle = 0$ cease to carry any information about the phase and scaling of $|\psi\rangle$, the complexified pseudo-norm may be re-introduced via the off-diagonal rule (5.2) if needed. In the light of eqs. (5.1) which indicate that we may choose $|\psi_-\rangle = \mathcal{PT}|\psi_+\rangle$, we may drop the unit operators $\mathcal{P}^2 = 1$ from all the overlaps and conclude that our definition of the inner product should be rewritten in the form

$$\langle\langle \psi | \psi' \rangle = \langle \psi | \vec{\mathcal{T}} | \psi' \rangle, \tag{5.3}$$

where the superscripted arrow indicates that the antilinear operator $\mathcal{T}$ should be understood as acting, conventionally, to the right. This makes this more universal definition a bit clumsy. Fortunately, whenever the $\mathcal{PT}$ symmetry is not broken, this new prescription is equivalent to the old one and can replace it in the orthogonality relations (3.1) etc.

6 Summary

In the current literature we are witnessing an increase of interest in the non-Hermitian Hamiltonians exhibiting $\mathcal{PT}$ symmetry and combining promising features (e.g., a "non-robust" existence of real spectra) with several unanswered questions. We motivated our present considerations, mainly, by the apparent lack of any clear probabilistic interpretation of wave functions.

Mathematically, it is reflected by the non-unitarity of the time evolution and by the concept of quasi-parity $Q = \pm 1$ introduced via a few examples and specified as a certain "analytic continuation" of the ordinary quantum number of parity. On the spiked harmonic oscillator we illustrated its role of a physical criterion which distinguishes between the quasi-odd and quasi-even solutions. In a parallel to the Hermitian picture we eliminated the latter states from the "relevant" Hilbert space using the standard Feshbach projection method.

A formal support for the latter conjectured transition $H \to H_{\text{eff}}$ may be seen in a necessity of suppression of the indeterminate character of the pseudo-norm within physical space. This has been amply rewarded. A deep connection between the Hermitian and $\mathcal{PT}$ symmetric H has been found in the shared Hermiticity of their projected forms H_{eff}. The H_{eff} of the respective Hermitian and $\mathcal{PT}$ symmetric origin differs just by the sign $\alpha = \pm 1$ of the correction term.

We hope that we have answered our original question: The non-Hermitian $\mathcal{PT}$ symmetric quantum mechanics seems to find, in its specific and Hermitian projected form, a fairly natural interpretation. We have reached a new level of understanding of what happens in the non-Hermitian systems. There seems to exist a certain natural boundary of the domain $\mathcal{D}$ of parameters in H. In its interior the energies stay real. In the other words, the "non-obligatory" $\mathcal{PT}$ symmetry of the wave functions themselves becomes (people usually say spontaneously) broken on the boundary of $\mathcal{D}$. The algebraic manifestation of the crossing of this boundary (the pseudo-norm vanishes) is reflected by the disappearing roots in the selfconsistency or graphical rule (2.5).

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