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Nonlinearity of perturbations in \mathcal{PT} -symmetric quantum mechanics

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Abstract. In the so called crypto-Hermitian formulation of quantum theory (incorporating, in particular, the \mathcal{PT} -symmetric quantum mechanics as its special case) the unitary evolution of a system is known to be described via an apparently redundant representation of the states in a triplet of Hilbert spaces. Two of them are unitarily equivalent while the auxiliary, zeroth one is unphysical but exceptionally user-friendly. The dynamical evolution equations are, naturally, solved in the friendliest space $\mathcal{H}^{(0)}$. The evaluation of experimental predictions then requires a Hermitization of the observables. This yields, as its byproduct, the correct physical Hilbert space $\mathcal{H}^{(1)}$. The formalism offers the conventional probabilistic interpretation due to the Dyson-proposed unitary equivalence between $\mathcal{H}^{(1)}$ and a certain conventional but prohibitively complicated textbook space $\mathcal{H}^{(2)}$. The key merit of the innovation lies in its enhanced flexibility opening new ways towards nonlocal or complex-interaction unitary models. The price to pay is that the *ad hoc* inner product in the relevant physical Hilbert space $\mathcal{H}^{(1)}$ is, by construction, Hamiltonian-dependent. We show that this implies that the Rayleigh-Schrödinger perturbation theory must be used with due care. The warning is supported by an elementary sample of quantum system near its exceptional-point phase transition. In contrast to a naive expectation, the model proves stable with respect to the *admissible*, self-consistently specified (i.e., physical) small perturbations.

1. Introduction.

In the light of reviews [1, 2, 3, 4, 5] one of the key mathematical characteristics of a quasi-Hermitian (and, in particular, \mathcal{PT} -symmetric) parameter-dependent quantum Hamiltonian $H(\lambda)$ is that the related *physical* Hilbert space proves manifestly λ -dependent in general, $\mathcal{H} = \mathcal{H}^{(1)}(\lambda)$. In practice, fortunately, the experimental predictions are usually made at a fixed λ , via a simplifying *ad hoc* representation of $\mathcal{H}^{(1)}(\lambda)$ in an unphysical, Hamiltonian-independent auxiliary Hilbert space $\mathcal{L} = \mathcal{H}^{(0)}$.

In our present paper we intend to point out that whenever λ is allowed to vary, the conventional linear stability/instability analysis (in which we merely check the influence of the perturbations $H(\lambda) - H(0)$ which are small in \mathcal{L}) must be replaced by a non-linear procedure. Via an elementary example we will show, moreover, that and why the size of the perturbation which appears small in \mathcal{L} may be very large when defined, properly and self-consistently, in the relevant physical Hilbert space $\mathcal{H}^{(1)}(\lambda)$.



2. Formalism: \mathcal{PT} -symmetric quantum mechanics *in nuce*.

The recent growth of popularity of quantum Schrödinger equations containing non-Hermitian Hamiltonian $H \neq H^\dagger$, i.e.,

$$i \frac{d}{dt} |\psi\rangle = H |\psi\rangle \quad (1)$$

has several independent reasons (cf., e.g., the compact outlines of the recent history in [5, 6]).

2.1. The pioneering unbounded-operator toy model of Bender and Boettcher.

One of the most influential motivations of the latter developments lies in the observation made, in 1998, by Bender with Boettcher [7]. They considered the toy-model Hamiltonian

$$H = H(\delta) = -\frac{d^2}{dx^2} + (ix)^\delta x^2, \quad \delta \geq 0 \quad (2)$$

defined on a Hilbert space \mathcal{L} of square-integrable functions living on a suitable complex contour. They revealed (purely empirically, i.e., using certain sophisticated semiclassical as well as purely numerical approximation techniques) that the whole spectrum of energies might be strictly real. This observation was interpreted as a hint that the related evolution law (1) need not necessarily be non-unitary.

An apparent conflict of such a hypothesis with the famous Stone theorem [8] was explained, during the subsequent developments of the idea, as purely terminological. It has been conjectured that the Hamiltonians sampled by Eq. (2) should be perceived as certain unusual generators of unitary quantum evolution [2].

2.2. A rediscovery of the older, Dyson's non-Hermitian Hamiltonians with real spectra.

The rigorous proof of the reality of the spectrum of at least some of the non-Hermitian but \mathcal{PT} -symmetric toy-model Hamiltonians (2) has been offered by Dorey et al [9]. In parallel, the study of numerous other \mathcal{PT} -symmetric models revealed that one of the most straightforward explanations of the reality of their spectra might be sought in their “hiddenly self-adjoint” nature. In the language of mathematics such an explanation was based on the discovery that one simply deals here with a mere reversal of the so called Dyson’s mappings $\Omega : \mathfrak{h} \rightarrow H$ of the most elementary form

$$H = \Omega^{-1} \mathfrak{h} \Omega, \quad \Omega^{-1} \neq \Omega^\dagger, \quad \mathfrak{h} = \mathfrak{h}^\dagger. \quad (3)$$

In the variational-calculation context these Hermiticity-violating invertible mappings were based on the initial choice of a conventional realistic self-adjoint Hamiltonian \mathfrak{h} and of a judiciously pre-selected non-unitary operator Ω . The trick proved useful, mostly in the many-body quantum physics, as an amazingly successful means of the technical and computational simplification of calculations of the low-lying bound-state spectra in nuclear physics [1] and in condensed matter physics [10].

2.3. The Krein-space explanatory mathematics.

The most surprising mathematical ingredient in the Dyson’s calculation recipe may be seen in a highly counterintuitive replacement (3) of a realistic (albeit technically complicated) operator $\mathfrak{h} = \mathfrak{h}^\dagger$ by its *manifestly non-selfadjoint* isospectral avatar H . Thus, the characteristic words of warning appeared in 1960 [11]. From time to time, these words are continuously being repeated, up to these days, by mathematicians [12, 13] as well as by physicists [14, 15].

The deepest essence of the subtle dangers hidden in the tentative replacements $\mathfrak{h} \rightarrow H$ and/or in their Bender-and-Boettcher-inspired inversions $H \rightarrow \mathfrak{h}$ may be seen in the existence of gaps in the mathematical spectral theory for the non-Hermitian avatar operators $H \neq H^\dagger$ (cf., e.g., [16, 17]).

In such a contradictory setting, a decisive and influential encouragement of the study of reconstructions $H \rightarrow \mathfrak{h}$ has been found, in [7], in the special additional \mathcal{PT} -symmetry property $H\mathcal{P}\mathcal{T} = \mathcal{P}\mathcal{T}H$ of the specific admissible non-Hermitian Hamiltonians. Indeed, after the latter property found its mathematical Krein-space-theory re-interpretation $H^\dagger\mathcal{P} = \mathcal{P}H$ [18, 19], the reality of the energy spectra in multiple concrete models appeared much less surprising [20]. The \mathcal{PT} -symmetric quantum mechanics became one of the innovative reformulations of abstract quantum theory [3, 6].

3. The challenge of unbounded \mathcal{PT} -symmetric Hamiltonians

The Dyson's mapping Ω is specific by being, in general, non-unitary, $\Omega^\dagger\Omega = \Theta \neq I$. Between the years 2006 and 2007, the resulting innovative version of the description of the unitary quantum evolution became widely, and often enthusiastically, accepted by physicists.

3.1. A 2012 crisis in \mathcal{PT} -symmetric quantum mechanics

Not so much by mathematicians. In 2012, for example, Siegl with Krejčířík [14] claimed that the Bender's and Boettcher's choice of the benchmark model (2) was, strictly speaking, unfortunate. Indeed, a deeper analysis revealed that such a Hamiltonian *does not* satisfy several necessary mathematical conditions of the applicability of the abstract Dyson's invertible-mapping ideas.

The critical comment [14] on the benchmark example was later followed by a more technical report [15]. The same authors (together with other two coauthors) tried to build there a bridge between the mathematically unsatisfactory ordinary differential operator illustrative examples and an enormous phenomenological success of the abstract concept of \mathcal{PT} -symmetry (cf., in this respect, also the most recent news in [21]). The authors of Ref. [15] followed, in essence, the older recommendations made by numerical mathematicians [22]. They conjectured that the non-Hermitian quantum Hamiltonians should be characterized by the so called pseudospectrum rather than by the mere spectrum. "Giving," in the author's own words, "the mathematical concept of the pseudospectrum a central role in quantum mechanics with non-Hermitian operators" [15].

3.2. A turn of attention towards the bounded-operator Hamiltonians

As long as the unbounded-operator nature of the most popular benchmark model (2) casts the above-mentioned, mathematically well-founded doubts upon the existence of the (for experimentalists, absolutely necessary) Hermitization $H \rightarrow \mathfrak{h}$ of the model, one feels tempted to narrow further the class of the admissible quantum non-Hermitian Hamiltonians with real spectra. The temptation was obeyed, couple of years earlier, by the physics-oriented authors of the older review [1]. Very pragmatically, these authors restricted their attention, exclusively, to the families of the operators of observables which are, in the friendly Hilbert space \mathcal{L} , *bounded*.

The majority of the mathematical obstacles disappeared. Still, the acceptance of the assumption $H \in \mathcal{B}(\mathcal{H})$ by *physicists* seemed surprising. It eliminates, e.g., the Heisenberg algebra from our considerations. At the same time, the pragmatic nature of the reduced scope of the theory remained fully compatible, e.g., with the needs of the so called interacting boson model in nuclear physics [1].

4. Finite-dimensional \mathcal{PT} -symmetric examples

In our present paper we intend to outline the most recent, less dramatic interpretation of the situation (cf., e.g., [23]). We intend to oppose, first of all, the deep scepticism of the disturbing conclusions of Ref. [15] reporting the "unexpected wild properties of operators familiar from \mathcal{PT} -symmetric quantum mechanics".

4.1. The importance of the boundedness of Hamiltonians.

We believe that the latter type of scepticism reflects just a certain conceptual and/or terminological misunderstanding because

- non-Hermitian evolution models found multiple successful applications in *classical* physics [22]. Their “wild properties” can hardly be called “unexpected”: in many models they were studied experimentally, having reflected the existing physical reality, whenever it is characterized by non-Hermiticities;
- many authors interested in the use of the concept of quasi-Hermiticity in *quantum* physics were probably always well aware of the dangers (*pars pro toto*, see a few related comments in [24]).

A part of latter authors resolved the mathematical puzzle, in a very pragmatic manner, either by excluding *all* of the *unbounded* observables from serious considerations, or by giving up the unitarity of the evolution [25]. In both cases, multiple quantum models based on the bounded non-Hermitian Hamiltonians H found their consistent phenomenological applications. In contrast, *none* of the nine illustrative samples of the “specific controversies” as discussed in [14, 15] belongs to the reasonably well understood bounded-operator category.

We may summarize that the high scientific quality of the *mathematical* contents of Refs. [14, 15] should be clearly separated from the added (and, perhaps, involuntarily discouraging) *physical* interpretation of the quasi-Hermitian picture of the *quantum* world. In the latter setting one need not insist on the use of unbounded operators. Even the use of multiple finite-dimensional matrix Hamiltonians proved productive and illuminating, indeed [6].

4.2. The methodical appeal of matrix Hamiltonians.

In our present attempted disentanglement of the puzzle let us cite Ref. [15]: “problems arise if Ω or Ω^{-1} entering the fundamental relation (3) are allowed to be unbounded”. This is true, mainly because the very pragmatic and reasonable postulate of the boundedness of the observables is assumed violated. In the words of *loc. cit.*, the manifestly unbounded operators \mathfrak{h} and H really “cannot be viewed as equivalent representatives of the same physical observable in quantum mechanics” [15]. It makes sense to accept, e.g., the constraint of boundedness.

For the resolution of the paradoxes it is sufficient to recall that even though “there are [still] physical problems where an unbounded similarity transformation could be useful” [15], the study of these models does not seem finished at present [17]. This implies that the acceptance of the assumption of the boundedness of Ω and of Ω^{-1} seems fairly reasonable at present. We recommend that before the clarification of the situation with the unbounded non-Hermitian observables, this constraint should be perceived as a source of reliability of the abstract formalism (cf., e.g., [3]).

Under the boundedness assumption, virtually all of the misunderstandings disappear. Citing the words of Ref. [15], “if Ω in (3) is bounded and boundedly invertible” and if “the spectrum is discrete,” then “the \mathcal{PT} -symmetry can be understood through an older notion of quasi-Hermiticity [1, 11] and the quantum-mechanical description . . . is consistent: [non-Hermitian] H and [self-adjoint] \mathfrak{h} represent the same physical system” [15]. We can summarize that the authors of [15] confirm that their criticism concerns, exclusively, the ill-chosen illustrations rather than the essence of the quasi-Hermitian theories themselves (cf. also Proposition 3 in [15]).

Unfortunately, the misunderstandings still survive in the literature because only too many papers on the subject did not sufficiently strongly emphasize the absolute necessity of the construction of the positive, bounded and boundedly invertible metric operators $\Theta = \Omega^\dagger \Omega$ [3]. We appreciate also the opportunity of emphasizing that these constructions are feasible, first of all, for the class of the non-Hermitian *matrix* Hamiltonians with real spectra.

5. Perturbation theory.

After the acceptance of the assumption of the boundedness of the observables and Hamiltonians there emerges another, independent question of an enormous importance. Whenever the pseudospectrum remains trivial (i.e., whenever the \mathcal{PT} -symmetric quantum system remains mathematically acceptable), we still need, in applications, a phenomenologically most important reliable information about the *response* of the system to its small perturbations.

Naturally, the latter study of the role of perturbations must be performed in the *physical* Hilbert space $\mathcal{H}^{(1)}$. This makes the constructive analyses unexpectedly difficult. Feasible, perhaps, just in the finite-dimensional models again. Let us mention now some of the related technicalities.

5.1. Parameter-dependent matrix Hamiltonians.

Once we take into consideration our non-Hermitian Schrödinger Eq. (1), and once we assume, along the traditional lines of consideration, that the Hamiltonian can vary with a parameter, we may select, in the simplest possible scenario, the linear functions

$$H(\lambda) = H(0) + \lambda V. \quad (4)$$

For the (presumably, real) energy spectrum $\{E_n(\lambda)\}$ of our Hamiltonian $H(\lambda)$ we may recall the relevant mathematical theory [26] and, under certain very general analyticity assumptions, we may try to search for the energies, at any excitation $n = 0, 1, \dots$, via the constructive Rayleigh-Schrödinger perturbation-series ansatz

$$E_n(\lambda) = E_n(0) + \lambda E_n^{(1)} + \lambda^2 E_n^{(2)} + \dots \quad (5)$$

In this formulation of the problem our present main message is that the only way towards the answers must proceed through the difficult constructive analysis of the physical Hilbert space of states $\mathcal{H}^{(1)}$ which is *not* independent of the Hamiltonian and λ , i.e., we must write $\mathcal{H}^{(1)} = \mathcal{H}^{(1)}(\lambda)$ and *construct* this space at each individual λ

5.2. The challenge of the parameter-dependence of the physical Hilbert space.

Naturally, the task is difficult. The space $\mathcal{H}^{(1)}(\lambda)$ may be expected to be represented in some conventional auxiliary Hilbert space \mathcal{L} (say, in $\mathcal{L} = L^2(\mathbb{R})$). In such a strictly constructive setting every change of parameter may be expected to induce a change of the physical space $\mathcal{H}^{(1)}(\lambda)$. In other words, the change also involves the so called metric operator $\Theta(\lambda)$.

The way out of the dead end may be twofold. In one we give up the requirements of the unitarity, and we reclassify our model as effective. This means that the Hilbert space \mathcal{L} will be declared physical. With the unitarity manifestly broken, and with no tedious construction of the physical Hilbert space $\mathcal{H}^{(1)}(\lambda)$ needed, the system is reinterpreted as an open quantum system.

In our present, more ambitious and unitary-evolution version of the theory it is necessary to construct the nontrivial inner product in $\mathcal{H}^{(1)}(\lambda)$,

$$\langle \psi | \Theta(\lambda) | \psi' \rangle \quad (6)$$

at each separate parameter λ . This implies, in general, the change of the set of the admissible observables, i.e., the change of the whole quantum system in question. The change of the geometry in $\mathcal{H}^{(1)}(\lambda)$ may imply, in parallel, also a possible reclassification of the perturbations which appeared small in the auxiliary user-friendly working Hilbert space \mathcal{L} . Indeed, these operators may prove very large in the relevant Hilbert space $\mathcal{H}^{(1)}(\lambda)$.

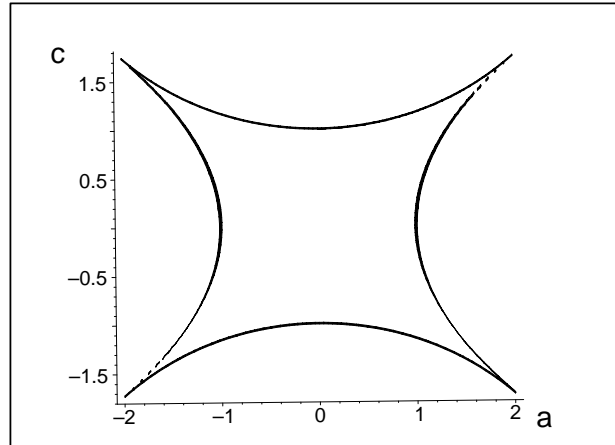


Figure 1. The boundary of domain $\mathcal{D}^{(physical)}$

6. An illustration.

It is necessary to accept the counterintuitive, unexpected and physics-changing sensitivity of the generic metric $\Theta(\lambda)$ to the changes, however small, of the parameter.

6.1. An exactly solvable toy model of Ref. [27].

The most elementary illustration of our above considerations can be offered by the following four-by-four real-matrix toy-model Hamiltonian of Ref. [27],

$$H(a, c) = \begin{pmatrix} -3 & c & 0 & 0 \\ -c & -1 & -a & 0 \\ 0 & a & 1 & c \\ 0 & 0 & -c & 3 \end{pmatrix}. \quad (7)$$

The quadruplet of the related eigenvalues (i.e., of the bound state energies) has an elementary closed form

$$E_{\pm, \pm}(a, c) = \pm \frac{1}{2} \sqrt{20 - 4c^2 - 2a^2 \pm 2\sqrt{64 - 64c^2 + 16a^2 + 4c^2a^2 + a^4}}. \quad (8)$$

All of these four values remain real (i.e., potentially, observable) if and only if a and c lie inside a left-right and up-down symmetric part $\mathcal{D}^{(physical)}$ of the $a - c$ plane, with the shape resembling a deformed square with protruded vertices (cf. Figure 1).

Inside and only inside the latter parametric domain it makes sense to speak about the existence and observability as well as about the stable and unitary time evolution of the quantum system in question. From a parallel, purely mathematical perspective, our physical Hilbert space $\mathcal{H}^{(1)}(\lambda)$ can only be introduced and constructed inside this domain, irrespectively of the choice of the possible perturbative reparametrization of the two free parameters $a = a(\lambda)$ and $c = c(\lambda)$ in Eq. (7).

6.2. Perturbations of the toy model near its quantum-phase-transition exceptional-point dynamical boundary.

The most interesting parts of $\mathcal{D}^{(physical)}$ can be found near the vertices, i.e., in the dynamical regime of maximal non-Hermiticity in the auxiliary and manifestly unphysical Hilbert space \mathcal{L} . Once the distance from the vertex gets parametrized by a positive parameter $\lambda \ll 1$, the

interior of $\mathcal{D}^{(physical)}$ admits (say, in the vicinity of the lower left vertex) the following remarkable re-parametrization $(a, c) \rightarrow (\lambda, \alpha)$,

$$a = a(\lambda) = 2 \left[-1 + \lambda + \alpha \lambda^2 + \mathcal{O}(\lambda^3) \right], \quad c = c(\lambda) = \sqrt{3} \left[-1 + \lambda - \alpha \lambda^2 + \mathcal{O}(\lambda^3) \right].$$

For the sufficiently small values of λ we wish to stay inside $\mathcal{D}^{(physical)}$. This means [27] that the energies remain real if and only if we fix the value of our new free parameter α inside the following interval,

$$-\frac{1}{4} + \mathcal{O}(\lambda) < \alpha < \frac{2}{9} + \mathcal{O}(\lambda). \quad (9)$$

Near the vertex such a spike-shaped “admissible” domain (in which, and only in which, the metric $\Theta(\lambda)$ and the physical Hilbert space $\mathcal{H}^{(1)}(\lambda)$ do exist) is extremely narrow. In this specific, counterintuitive scenario, *all* quantum world (i.e., its states as well as operators) *must* find its representation *inside* $\mathcal{H}^{(1)}(\lambda)$, *not* outside. *Any* move out of this space cannot be given any operational physical meaning and interpretation. At the same time, this phenomenologically prohibited move might have been realized by a perturbation which appears small when measured, incorrectly, inside the unphysical Hilbert space \mathcal{L} .

7. Summary

The study of pseudospectra defined in the manifestly unphysical Hilbert space \mathcal{L} (as performed, e.g., in Refs. [15, 22]) may lead to an incorrect prediction of the emergence of quantum instabilities in unitary systems. At the same time, the same predictions of wild anomalies will be correct and realistic in multiple other, non-unitary settings. In these scenarios (which were not considered here) the properties of the pseudospectrum in \mathcal{L} will be relevant, reflecting simply the physical reality of the genuinely non-Hermitian systems.

In other words, whenever we give up the requirements of the unitarity (cf. section 1.7.2 in [6]), or whenever we leave the quantum world and “de-quantize” (returning, say, to the classical optics – cf. section 1.7.3 in [6]) we may observe the wild behavior caused by an effective incorporation of uncontrolled interactions with an environment. Thus, in the open quantum systems the emergence of various sorts of the wild behavior is not too surprising [28].

In the isolated quantum unitary cases, on the contrary, the strongly counterintuitive “extreme narrowness” of the corners of the domain of “admissible” physical parameters as sampled by Figure 1 is not surprising, either. The spike with $a(\lambda)/2 - c(\lambda)/\sqrt{3} = \mathcal{O}(\lambda^2)$ appears truly sharp. Virtually *all* of the $\mathcal{O}(\lambda)$ perturbations must be re-classified, in the relevant geometry of the physical Hilbert space, as too strong, non-quasi-Hermitian and, therefore, inadmissible. Pushing the quantum system in question out of the physical Hilbert space, i.e., out of the theoretically postulated and experimentally realizable dynamical regime.

The inadequacy of the auxiliary-space criteria of the smallness of the perturbations is obvious. Such an observation is generic, independent of illustrative examples. It is necessary to emphasize that the inadequacy gets strengthened whenever the system moves closer to the boundary $\partial\mathcal{D}^{(physical)}$. Naturally, once we decide to observe the basic postulates of quantum theory of closed and stable systems, we are not allowed to leave the admissible parametric domain $\mathcal{D}^{(physical)}$ at all.

In applications, the localization of the latter domain and/or of its boundary may be a difficult task. In such a situation, a significant help and insight in the problem may be provided by a return to the information provided by the analysis of the pseudospectrum. In the wording provided after Proposition 3 in Ref. [15]: “Proposition 3 can be conveniently used in the reverse sense, where the presence of nontrivial pseudospectrum for a given operator H immediately implies that the operator cannot possess a physically relevant (i.e. bounded and boundedly invertible) metric”. In other words, whenever we decide to represent a quantum system in

the (physical) Hilbert space with a *fixed* nontrivial metric $\Theta \neq I$, we can easily accept the nontriviality of the metric operator $\Theta(\lambda) \neq I$ but we *cannot* ignore its impact upon the geometry of the physical space and, first of all, upon the contents of the probabilistic predictions. They simply cannot be made without the knowledge of $\Theta(\lambda)$, trivial or not.

This is the main key to the resolution of the paradoxes. The role of the Hamiltonian-dependence of the geometry on the perturbation is decisive. The issue must be treated with great care, in spite of being strongly counterintuitive. The size of the perturbations (as well as all of the related stability/instability issues) must be analyzed self-consistently, in an iterative, non-linear manner. Indeed, the use of the correct physical norm is obligatory. All of the *feasible* experiments over the system's perturbations can find their unique meaning, realization and interpretation *exclusively* inside the Hamiltonian- and perturbation-dependent Hilbert space $\mathcal{H}^{(1)}(\lambda)$ with a *fixed*, constant $\lambda = \lambda_0$.

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