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NON-SELF-ADJOINT OPERATORS IN QUANTUM PHYSICS: IDEAS, PEOPLE, AND TRENDS

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1.1 THE CHALLENGE OF NON-HERMITICITY IN QUANTUM PHYSICS

1.1.1 A Few Quantum Physics' Anniversaries, for Introduction

The year of writing this history-oriented chapter on the appeal of non-Hermiticity was also the year of several minor but interesting anniversaries in quantum physics. So let us start by recalling some of these dates.

1.1.1.1 *Hundred Years of the Bohr's Model* In 2013, on occasion of the centenary of the Bohr's model of atom (1) (marking, in a way, the birth of quantum theory), one should appreciate the multitude of results of the first hundred years of our study of quantum world. One of typical characteristics of these developments may be seen in an incessant emergence of dramatic innovations and changes in our perception of what is measurable. The process still remains unfinished. Even the Nobel Prize in Physics for year 2012 was not awarded for the fresh, expensive, and long expected discovery of the Higgs boson in particle physics (which had to wait for one more year) but rather for the invention of "ground-breaking" methods of quantum measurements (2).

One must underline that during the century, the fundamental quantum physics remained a vivid discipline and that its experimental side never ceased to be a

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topical subject. What should be appreciated, in parallel, is the fact that none of these innovations ever disproved any of the apparently counterintuitive basic principles of the theory. One must admire the robust nature of the basic mathematical ideas.

In particular, it was not necessary to change the theory after Herman Feshbach (3) succeeded in describing the usual processes of quantum scattering and reactions in atomic nuclei (*including* the elastic ones) by means of a *complex* effective potential. On this occasion, the “exotic” non-self-adjoint (*alias*, in the physicist’s language, non-Hermitian) operators seem to have entered the scene.

1.1.1.2 Fifty-five Years of the Feshbach’s Non-self-adjoint Hamiltonians For stable quantum systems, the evolution in time is usually assumed generated by a physical Hamiltonian $H = H^{(P)}$ which is defined as acting in a suitable representation $\mathcal{H}^{(P)}$ of the physical Hilbert space of states. It is very important that the popular principle of correspondence, albeit vaguely defined, often enables us to choose, in realistic models, constructively tractable versions of spaces $\mathcal{H}^{(P)}$ and Hamiltonians $H^{(P)}$.

The practical feasibility of calculations quickly decreases during transition to more complicated systems. One may recall multiple examples, say, in nuclear physics where the computer-assisted numerical determination of the bound-state energies hardly remains sufficiently routine even in the lightest nuclei. For the heavier nuclei, the growth of complexity of calculations may be perceived as one of the fundamental methodical challenges in nuclear physics.

As we already mentioned, one of the productive tools of an amendment of the algorithms has been proposed by Feshbach (3). In his considerations, he admits that even if one knows Hamiltonians $H = H^{(P)}$, many time-independent Schrödinger equations $H|\psi\rangle = E|\psi\rangle$ describing bound states (with $E = \text{real}$) or resonant states (with $E = \text{complex}$) prove prohibitively difficult to solve in practice. He recalled that in the majority of applications just the knowledge of the low-lying spectrum of energies is asked for. This led him to the conclusion that a judicious restriction of physical space $\mathcal{H}^{(P)}$ to a suitable subspace $\mathcal{H}^{(R)}$ should be performed in such a way that the reduction of Hamiltonian $H^{(P)} \rightarrow H^{(R)}$ remains compatible with the requirement of an at least partial isospectrality of the two operators.

Ambitious as the project might have seemed, its analysis resulted into a recipe which proved enormously popular and successful in practice (4). In fact, its basic idea is fairly elementary. One simply partitions the “big” Hilbert space $\mathcal{H}^{(P)}$ into two subspaces via projectors Q (on an “irrelevant” part of the bigger Hilbert space $\mathcal{H}^{(P)}$) and $R = I - Q$ (in our present notation, the projector on *the* model space $\mathcal{H}^{(R)}$). This yields the partitioned Schrödinger equation

$$(R + Q)H(R + Q)|\psi\rangle = E(R + Q)|\psi\rangle$$

and formula

$$Q|\psi\rangle = Q[EI - QHQ]^{-1}QH|\phi\rangle, \quad |\phi\rangle = R|\psi\rangle$$



for the Q -projection of the exact wave function, which is, by assumption, less relevant. Its elimination provides the ultimate compactified, nonlinear, “effective” Schrödinger eigenvalue problem

$$H_{\text{eff}}(E) |\phi\rangle = E |\phi\rangle \quad (1.1.1)$$

defined inside the subspace $\mathcal{H}^{(R)}$. The action of the effective Hamiltonian

$$H_{\text{eff}}(E) = RHR + RHQ [EI - QHQ]^{-1} QHR$$

is energy dependent but it remains restricted just to the relevant, R -projected subspace $\mathcal{H}^{(R)}$.

One must emphasize that the required strict isospectrality between H and $H_{\text{eff}}(E)$ is guaranteed. Unfortunately, owing to the manifest energy dependence of $H_{\text{eff}}(E)$, the costs grew high. They became even higher in the original nuclear-reaction context in which the physical values of energies lied in the essential part of the spectrum. One must then generalize the definition of the operator pencil $H_{\text{eff}}(z)$ and start working with the complex values of the variable parameter $z \in \mathbb{C}$.

In the energy range of interest, the spectral shift caused by the presence of z or E in denominators is often being ignored as not too relevant in practice. Still, it must be reemphasized that the simplified effective-Hamiltonian operator $H_{\text{eff}}(z)$ is *manifestly non-self-adjoint* in general.

With such an observation, the projection-operator studies of quantum systems rarely remain restricted to the mere stable dynamical regime with real spectra and unitary evolution in time. The loss of the self-adjoint nature of the effective Hamiltonians is usually interpreted as implying a *necessary* loss of the reality of the energies. Strictly speaking, such a deduction is not always correct. As a counterexample, one may recall, for example, the so-called \mathcal{PT} -symmetric systems and Hamiltonians.

1.1.1.3 Fifteen Years of \mathcal{PT} -symmetry alias Pseudo-Hermiticity In the broader context of preceding paragraph, the abstract formalism of quantum theory encountered an unexpected challenge circa 15 years ago, after several parallel innovative proposals of inclusion, in the mainstream formalism, of certain manifestly non-self-adjoint Hamiltonian-like operators $H \neq H^\dagger$ possessing *strictly real*, bound-state-like spectra. Fortunately, during the subsequent years, the acceptance of such a class of models proved fully compatible with the first principles of quantum theory. Moreover, an intensified study of mathematics of manifestly non-self-adjoint candidates for observables became an inseparable part of quantum theory.

An “official” start of studies of the possibility of having non-self-adjoint operators in a unitary theory may be dated back to 1998 when Bender and Boettcher published their letter (5). Its title “Real spectra in non-Hermitian Hamiltonians having \mathcal{PT} -symmetry” sounded truly provocative at that time because, according to conventional wisdom, the spectra of non-Hermitian operators can hardly be purely real. The explicit construction of a non-Hermitian quantum Hamiltonian $H \neq H^\dagger$



with real spectrum sounded, therefore, like a joke or paradox rather than like a serious scientific proposal¹.

Later on, the situation and attitudes have changed. A sample of the progress is to be reported in this book. As long as the main emphasis will be laid, in the forthcoming chapters, upon the mathematical aspects of the theory, the collected material will be preceded and, in some sense, interconnected by this chapter offering a compact outline of the field, with particular emphasis upon historical and phenomenological context.

Our considerations will reflect the selection of topics to be covered by the more mathematically oriented rest of the book. In a sketchy and incomplete, selective outline of key ideas, we intend to restrict our attention to a few moments at which a cross-fertilizing interaction between the phenomenological and formal aspects of the use of non-self-adjoint operators in physics proved particularly motivating and intensive.

1.1.2 Dozen Years of Conferences Dedicated to Pseudo-Hermiticity

Letter (5) inspired a lot of research activities. In the literature, a number of emerging paradoxes was spotted, exposed to a thorough scrutiny—and shown to disappear. At present, one can say that from the point of view of the recent history of quantum physics, the date of publication of this remarkable letter may be perceived as one of the most important turning points. Not only within the theory itself (in which, later, the concepts of stability and evolution were thoroughly revisited and clarified under its influence) but also in experiments.

At present, the progress and publications of the related results in prestigious physics Journals may be followed online, via dedicated bookkeeping webpage as maintained by Daniel Hook (8). Through this page, one can trace the recent history of the field. One can download a lot of papers that caused the change (or rather a complete reversal) of attitude of the international scientific community toward the real spectra in non-Hermitian Hamiltonians.

The change of the paradigm was due to the work by multiple active authors, so the results cannot be summarized easily (cf. review papers (9–11) for many details and references). Among these results, one should recollect, first of all, the introduction of the influential concepts of \mathcal{PT} -symmetry of a quantum Hamiltonian H (i.e., of the rule $H\mathcal{PT} = \mathcal{PT}H$ where symbols \mathcal{P} and \mathcal{T} denote parity and time reversal, respectively) or, after a slight generalization, of the η -pseudo-Hermiticity (or, briefly, pseudo-Hermiticity) of an observable Λ (i.e., of the rule $\Lambda^\dagger \eta = \eta \Lambda$ written in terms of a suitable generalization η of the parity operator).

Although the notion of \mathcal{PT} -symmetry may be already found in 1993 paper (12), it only played a marginal role there. Probably, the concept was in current use even earlier (13). Anyhow, its heuristic relevance and productivity remained practically unknown before 1998.

¹*Pars pro toto*, the imminent voices of criticism may be sampled by the R. F. Streater's comments, propagated via his webpage (6) and book (7).



Several years after 1998, symbol \mathcal{P} entering the \mathcal{PT} -symmetry relation was mostly perceived as the mere parity in one-dimensional bound-state Schrödinger equations

$$\left(-\frac{d^2}{dx^2} + V(x)\right) \psi_n(x) = E_n \psi_n(x), \quad \psi_n(x) \in L_2(-\infty, \infty) \quad (1.1.2)$$

while symbol \mathcal{T} was strictly identified with an antilinear operator of time reversal. Even under these constraints, the appeal of the innovative notion grew quickly. Its use led to conjectures of multiple toy models (1.1.2) with quantum Hamiltonians of the “usual” form $H = p^2 + V(x)$ (and real spectra) but with an “unusual” non-self-adjointness property $H \neq H^\dagger$ in the underlying “friendly” Hilbert space $\mathcal{H}^{(F)}$.

In the contemporary context of quantum model-building practice, the majority of innovations sounded strangely. One of their presentations to a larger audience during an international scientific conference took place in Paris in 2002. On this occasion, the invited speaker (naturally, Carl Bender) plus four other authors (cf. the written form of the talks in proceedings (14)) discussed the response and concluded that the subject might deserve a separate series of dedicated conferences.

Supported by several other enthusiasts, the dedicated series really started, a year later, by the meeting of 27 participants from as many as 13 different countries in Prague (cf. (15)). The next, similarly compact international workshop followed within a year. Subsequently, the number of participants jumped up (i.e., close to one hundred) in 2005, after the transfer of the meeting from Villa Lanna in Prague to the Universities in Istanbul (Turkey, June 2005) and Stellenbosch (South Africa, November 2005), etc².

The proceedings of the PHHQ series of conferences were mostly published in the form of a dedicated and refereed special issue (cf. (17–19), etc.). These materials may be recalled as offering a compact (i.e., introductory, history-oriented, and time-ordered) sample of a few characteristic results, mainly in the field of quantum physics.

Even such a restricted inspection of the history of acceptance of non-self-adjoint operators in quantum physics reveals a sequence of “ups” (i.e., of the periods of a more or less uninterrupted growth), which were followed by “downs,” characterized by a sudden emergence of serious obstacles and crises.

1.2 A PERIODIZATION OF THE RECENT HISTORY OF STUDY OF NON-SELF-ADJOINT OPERATORS IN QUANTUM PHYSICS

1.2.1 The Years of Crises

In retrospective, one of the least expected observations resulting from the recollection of history of \mathcal{PT} -symmetry and pseudo-Hermiticity shows an amazing regularity in the occurrence of crises. Several less regular precursors of these crises may even

²Interested readers may click for more details on the global webpage (16) of the series Pseudo-Hermitian Hamiltonians in Quantum Physics (PHHQ).



be dated before the above-mentioned year 1998. One may recollect, for example, that on the basis of multiple numerical experiments with the *purely imaginary* cubic interaction

$$V(x) = V^{(BZI)}(x) = ix^3, \quad x \in \mathbb{R} \quad (1.2.1)$$

Daniel Bessis with Zinn-Justin already believed, in 1992 at the latest (20), in the strict reality of the bound-state spectrum. Anyhow (was it a crisis?), up to the present author's knowledge, they never published anything on their observations before the years when Carl Bender did.

1.2.1.1 The Year 2001: the First, Spectral-reality-proof Crisis The first “regular” crisis came after circa 3 years of intensified studies of various \mathcal{PT} -symmetric potentials and, in particular, of the Bender's and Milton's (21) (or, if you wish, of the Bender's and Boettcher's (5)) extremely popular model

$$V(x) = V^{(BM)}(x, \delta) = x^2 (ix)^\delta, \quad \delta \geq 0. \quad (1.2.2)$$

In this potential, the choice of the general power-law x -dependence appeared to support an extension of the above-mentioned $\delta = 1$ hypothesis of the reality of the spectrum. During the years 2000 and 2001, nevertheless, people started feeling more and more aware of the lasting absence of a reliable, rigorous proof.

The first proof applicable to the important family of \mathcal{PT} -symmetric models (1.2.2) already appeared in 2001 (22). Just in time. What followed was a quick acceptance of the promising perspective of a noncontradictory existence of the real bound-state energies even when obtained from non-Hermitian Hamiltonians.

The much-required clarification of this point encouraged the community to make the next step and to return, *i.a.*, to the Streater's criticism (6, 7) and to the related doubts about the possible physics behind the new and highly nonstandard models as exemplified by eqs (1.2.1) or (1.2.2). During the first years after the first crisis, the decisive suppression of these doubts has been achieved, basically, via a discovery (or rather rediscovery) of the possibility of using an *ad hoc* inner product and of defining a *different* Hilbert space of states in which a correct probabilistic interpretation of the models can be provided. In this text, we denote such a “second” or “standard” Hilbert space by dedicated symbol $\mathcal{H}^{(S)}$.

1.2.1.2 The Year 2004: the Metric-ambiguity Crisis In the amended Dirac's notation of Ref. (23), the generalized inner products may be defined as overlaps $\langle \phi_1 | \Theta | \psi_2 \rangle$ where operator $\Theta \neq I$ may be called “Hilbert-space metric.” During a year or two, the discovery has been slightly reformulated and found equivalent to a resuscitation of the three-Hilbert-space (THS) quantum-system representation as known and used, in nuclear physics, as early as in 1992 (24)³. In this manner, an overall, sketchy formulation of the theory was more or less completed.

³One could even trace the idea back to the Dyson's 1956 paper (25) on models of ferromagnetism. Thus, the Dyson's forthcoming 90th birthday (*viz.*, on December 15, 2013) would also be eligible as an item for inclusion in the list of relevant anniversaries.



The ultimate moment of acceptance of \mathcal{PT} -symmetric Hamiltonians by physicists may be identified with the year 2004 of publication of erratum (26). During this year, *any* nontrivial metric $\Theta \neq I$ (known, in the conventional physical terminology, as “non-Dirac” metric) became perceived as a fundamental ingredient in the description of quantum system, in principle at least.

The nontrivial-metric-dependent THS background of the theory was accepted, redirecting attention to the next open problem, namely, to the immanent ambiguity of the THS recipe. People imagined that the assignment of the desirable Hilbert-space metric Θ to a preselected (and, say, \mathcal{PT} -symmetric) Hamiltonian $H \neq H^\dagger$ is far from unique. Deep crisis number two followed almost immediately.

At a comparable speed, the crisis was suppressed, mainly due to an overall acceptance of an additional postulate of observability of a new quantity C called quasi-parity (27) or charge (28). It has been clarified that the requirement of the observability of charge C makes the metric unique. A new wave of optimism followed.

1.2.1.3 The Year 2007: the Nonlocality Crisis The third crisis emerged 3 years later, in 2007, when Jones noticed several counterintuitive features and obstructions to realization of a quantum-scattering-type experiment in \mathcal{PT} -symmetrized quantum mechanics arrangement (29). This discovery forced people to reanalyze the concepts of \mathcal{PT} -symmetry and of the $C\mathcal{PT}$ -symmetry, with the latter name being, for physicists, just the most common alias to the above-mentioned compatibility of the THS representation of quantum systems (using a special metric $\Theta_0 = \mathcal{P}C$) with the standard textbooks on quantum theory where only too often, just for the sake of simplicity, the metric is being set equal to the identity operator.

The simplest way out of the Jones’ trap was proposed by Jones himself. He conjectured that the local complex potentials $V(x)$ should be perceived as “effective,” say, in the Feshbach’s subspace projection sense. In such an approach, the key scattering-unitarity assumption is declared redundant. Although this implies that, say, the flow of mass need not be conserved, that is, certain *deus ex machina* of sinks and sources of particles is admitted, one simply accepts an overdefensive argument that the evolution processes and, in particular, the scattering in a given quantum system is in fact just partially controlled and described by our effective local potentials $V(x)$. In other words, one admits that our information about the quantum dynamics is incomplete.

During the subsequent growth of theoretical efforts, one of the most consequent resolutions of the Jones’ apparent paradoxes was offered in Ref. (30). The main source of misunderstanding has been identified as lying in an inconsistency of our assumptions. In the context of a conventional *unitary* quantum scattering theory, one simply asks for too much when demanding that the scattering potential may be chosen complex *and* local. In a way based on the construction of several explicit models, a transition to nonlocal \mathcal{PT} -symmetric complex forces V was recommended (see more details in the following sections).

1.2.1.4 The Year 2010: the Construction-difficulty Crisis The fourth crisis may be localized, roughly, to the year 2010 when it became clear that the emergent necessity of working with nonlocal potentials might lead to an enormous increase



in technical difficulties during the applications of the unitary THS recipe. The same danger of encountering obstacles was found connected with the need of working with very complicated metrics $\Theta \neq I$ even for originally not too complicated Hamiltonians.

A better profit has been found provided by a “transfer of technologies” beyond quantum physics. Around the year 2010, the active research in the area of quantum theory dropped perceptibly down, therefore. This tendency was clearly reflected by a drastic decrease in the number of foreign participants in the meeting PHHQP IX in 2010 in China (31).

During the crisis, it became clear that the transfer of the concept of \mathcal{PT} -symmetry out of quantum theory may in fact prove not only necessary but also unexpectedly rewarding. A real boom followed, for example, in experimenting with simulations of \mathcal{PT} -symmetry in various gain-or-loss media in nonquantum settings (*pars pro toto*, let us mention here just the quick growth of popularity of \mathcal{PT} -symmetry in nonquantum optics (32)).

Within quantum physics, the boom was paralleled by a reenforcement of interest in the traditional studies of open quantum systems and also of unstable complex systems, with the dynamics controlled by the presence of resonances. Symptomatically, Nimrod Moiseyev’s monograph “Non-Hermitian Quantum Mechanics” (33) dealing with these topics appeared published in 2011.

During the same, first-after-the-crisis year, the place of the jubilee tenth meeting PHHQP (34) (viz., MPI in Dresden) was packed by participants up to the roof again. The conference lasted much longer than usual (viz., full two weeks) and marked the onset of a new period of growth. The meeting was truly successful in putting emphasis on the closeness of connections between the quantum and nonquantum worlds. In addition, the not-entirely-expected influx of a lot of specialists from open-system quantum phenomenology contributed, by feedback, to the subsequent new growth of activities in all of the neighboring fields.

For mathematical physicists, attention has been redirected to the formal aspects of energy-dependent (i.e., nonlinear, effective, and subspace projected) non-self-adjoint Hamiltonians. Last but not least one should mention that as many as two separate special issues of Journals were needed to play the role of proceedings of the remarkable, direction-changing jubilee conference in 2011.

1.2.1.5 At Present: the Ill-defined-metrics Mathematical Crisis Toward the end of 2013, we already know that we are just in the middle of another, fifth serious crisis. Its roots may be traced back to several, not always noticed critical comments on the THS representation formalism as made, in the recent past, by mathematicians (35). The essence of the problem is connected with several failures of the physicists to check the validity of certain necessary mathematical assumptions in their models.

The problem is serious—even for the most popular examples, unexpected “no-go” theorems were proved in the second half of the year 2012 (36). Several parallel attempts at circumventing the obstacles followed (37, 38). Still, the essence of the conflict remains unresolved at present. A final outcome of the last crisis is not yet



known. We only have to stay optimistic, recollecting that up to now, all of the previous crises were overcome. What followed the crisis was always a new phase of the growth of the research activities.

1.2.2 The Periods of Growth

In our present compact review of history of “ \mathcal{PT} -symmetry and all that,” we may take the above-listed crises as separators between the five independent triennials of incorporation of non-self-adjoint operators in standard quantum theory, accompanied by an increasing sophistication of underlying mathematics.

1.2.2.1 The First Period: Between 1998 and 2001 The years between 1998 and 2001 were the years of heuristic innovation of quantum theory which was partially lacking mathematical grounds. The research of this period was all guided by the surprisingly efficient recipes of tentative replacement of the current self-adjointness of Hamiltonians $H = H^\dagger$ by \mathcal{PT} -symmetry or \mathcal{P} -pseudo-Hermiticity. As long as the self-adjointness is usually recalled as implying the reality of the spectrum of bound states, it was rather surprising to reveal, purely empirically, that the same desirable features of stability appeared exhibited by many non-Hermitian Hamiltonians.

The update of the theoretical perspective proved particularly useful for a deeper understanding of field theories with ϕ^3 interactions (14). In quantum mechanics of one-dimensional systems, people studied the possibility of letting the coordinate x in eq. (1.1.2) complex. This led to a perceivable extension of the class of exactly solvable models (cf. (39, 40)).

A number of basic questions remained open. First of all, the theory with $H \neq H^\dagger$ remained challenged by the Stone’s theorem and by the apparent loss of the manifest unitarity of the evolution in time. Secondly, the possible physical interpretation of the models having complex coordinates remained temporarily unclear. The first answers to both of these questions only started appearing during the year 2001.

1.2.2.2 The Second Period: Between 2001 and 2004 In a way discussed, reviewed and partially summarized by the participants of the first PHHQP workshop in 2003, the compatibility of the \mathcal{PT} -symmetric quantum models with the Stone’s theorem was achieved via an upgrade and completion of the theory. Although the general pattern was already published and used, in nuclear physics, for more than 10 years (24), the key idea of introduction of a nontrivial Hilbert-space metric Θ and its factorization $\Theta = \Omega^\dagger \Omega$ (i.e., of its reinterpretation as a superposition of mappings Ω and Ω^\dagger) was rediscovered.

The factorization was readapted to the needs of the schematic one-dimensional \mathcal{PT} -symmetric quantum models and to their prospective applications, first of all, in quantum field theory (41). Along several parallel lines of research people then developed multiple new models using, typically, the piecewise constant or point interactions in order to simplify technicalities (42).

The new wave of interest in Hilbert spaces with nontrivial metrics followed. It opened a path toward the innovative studies of many-body systems as well as toward



the first genuine physical applications of the theory in cosmology (43). A clarification has been achieved of the full internal consistency of quantum physics (say, of pion atoms), which is based on the zero-spin relativistic Klein–Gordon version of Schrödinger equation (44).

1.2.2.3 The Third Period: Between 2004 and 2007 One of the important news announced during the 2004 crisis was that the physicist’s definition of \mathcal{PT} -symmetry more or less coincides with the common mathematical concept of Krein-space Hermiticity. This discovery had far-reaching consequences and it accelerated the research. People found motivation for turning attention to the nonunitary formulations of scattering theory (45). The successful implementations of the use of the concept of \mathcal{PT} -symmetry were extended to classical physics, ranging from mechanics (46) up to magnetohydrodynamics (MHD, (47)). The first elementary experiments were proposed in classical optics (48). Within classical electrodynamics, the first microwave simulations of certain characteristic consequences of the transition to \mathcal{PT} -symmetric quantum Hamiltonians $H \neq H^\dagger$ were performed (49).

1.2.2.4 The Fourth Period: Between 2007 and 2010 One of the key challenges encountered during the year 2007 was the apparently incurable loss of the unitarity property in the \mathcal{PT} -symmetry-controlled systems “at large distances,” that is, typically, in the most common quantum-scattering experiments (29). During the subsequent 3 years, one of the solutions was found in the transition from local to nonlocal, “smeared” interaction potentials (50).

In parallel, during these three years of analogies, experiments and simulations people kept paying enhanced attention to classical physics. Thus, experimentalists revealed the practical appeal of certain models of propagation without unitarity, say, within classical electrodynamics. The emergence of spectral singularities has been found relevant and related to the theory of lasers (51). In an even broader context of nonlinear integrable field equations, a transition to \mathcal{PT} -symmetric deformations proved inspiring (52).

The numerical and computer-assisted analyses were found productive (53). After a return to quantum world, it has been revealed, inter alia, that even the explicit construction of a horizon of observability of a pseudo-Hermitian quantum system need not always remain prohibitively difficult (54).

A methodical help started to be sought in an ample use of finite-matrix models. New physical meaning has been assigned to the traditional mathematics of the Jordan-block canonical structures. The related confluence of eigenvalues and their subsequent complexification were connected directly with the physics of the loss of observability of a quantum system in question. Last but not least, the “brachistochrone” paradox has been resolved (55) and multiple “ghost problems” were clarified. On the level of pure theory, the time-dependent version of the THS formalism has finally been formulated (23).

The era between 2007 and 2010 could have been called the era of return to the concept of the Kato’s exceptional points (56). The enhancement of knowledge of the older and new exceptional-point-related phenomena was summarized during



dedicated conference “The Physics of Exceptional Points” as organized by Dieter Heiss in November 2010 in Stellenbosch (57).

1.2.2.5 The Fifth Period: Between 2010 and 2013 During many years of study of quantum models possessing elementary metrics Θ , it became clear that whenever a given, manifestly non-Hermitian observable (say, a Hamiltonian such that $H \neq H^\dagger$ in the “first” Hilbert space $\mathcal{H}^{(F)}$) is considered, and once it is assigned a “Hermitizing” Hilbert-space metric Θ , we may say that

- the original Hilbert space $\mathcal{H}^{(F)}$ (endowed, by definition, with the natural Dirac’s trivial metric $\Theta^{(F)} = I$) must be declared “false”;
- the role of the physical Hilbert space is transferred to the “second” Hilbert space $\mathcal{H}^{(S)}$, which is, by definition, endowed with the nontrivial Hermitizing metric $\Theta = \Theta^{(S)}(H) \neq I$;
- strictly speaking, our observables cannot be called non-self-adjoint as they should be all perceived as living in “sophisticated” $\mathcal{H}^{(S)}$ rather than in “friendly but false” Hilbert space $\mathcal{H}^{(F)}$.

We believe that in place of calling the observable H non-Hermitian (plus, if applicable, \mathcal{PT} -symmetric or pseudo-Hermitian), it makes much better sense to call it “Hermitian in $\mathcal{H}^{(S)}$ ” or, shortly, in a way promoted by Smilga (58), “crypto-Hermitian”.

In this context, mathematicians revealed that the metrics may be often found ill-defined (59). They concluded that our community had to turn attention to the specific features of unbounded operators in infinite-dimensional Hilbert spaces. The decisive relevance of mathematically rigorous definitions and proofs was underlined. The concept of the Riesz basis has been shown to play the particularly important role in the analysis.

All of these considerations are characteristic for the fifth stage of development of the THS theory which lasts up to now. In the context of physics, this phase became strongly interdisciplinary. Behind the above-mentioned return to the study of open quantum systems, one encounters numerous surprises: for example, nonlinear phenomena are studied, typically, in connection with the phenomena of Bose–Einstein condensation (60). New and new theoretical consequences of the presence of exceptional points are being revealed, the traditional WKB analyses acquire various more advanced forms, and so on. Systems with multiple, degenerate exceptional points are considered as forming quantum parallels to the classical instabilities as classified by the Thom’s theory of catastrophes (61, 62).

In experimental physics, anything but a sketchy review (see the following text) is beyond the scope of this text. At present, one is witnessing intensive laser-beam (and other) simulations of non-Hermiticity-related phenomena and the development of multiple other nonquantum systems such as (perhaps, chaotic) billiards, innovative forms of the classical electromagnetic waveguides as well as their formally simplified versions living on the thin wires and forming the so-called quantum graphs (63), and so on.



In theoretical physics, in parallel, the formal problems with metrics (which may not exist) were addressed in a way closely related to the pragmatic analyses of instabilities. A turn of attention to pseudospectra and/or to certain new forms of our understanding of instabilities may be noticed to emerge: *Pars pro toto*, Trefethen's and Embree's book (53) may be recommended as a rich source of information on these subjects.

Before we delve in the literature for more details let us emphasize that now, in the middle of the last crisis, the time seems ripe for a unification of forces of mathematicians and physicists. The point is that the running crisis might prove more serious than ever. From this perspective, the material presented in the subsequent chapters of this book may be perceived as truly topical, indeed.

1.3 MAIN MESSAGE: NEW CLASSES OF QUANTUM BOUND STATES

1.3.1 Real Energies via Non-Hermitian Hamiltonians

1.3.1.1 Successful Heuristics: \mathcal{PT} -Symmetric Toy Models Nowadays, whenever one returns to the past and whenever one recalls the first years of peaceful coexistence of the unusual reality of spectra with the anomalous, non-self-adjoint Hamiltonians exhibiting \mathcal{PT} -symmetry, one most often recollects the Bender's and Boettcher's letter (5). In this work, the *real* bound-state energies were obtained from *complex* potentials using WKB approximation complemented by a routine, brute-force numerical solution of the standard one-dimensional (i.e., ordinary differential) Schrödinger equations (1.1.2) and (1.2.2). The δ -dependence of the numerically evaluated energies $E_n = E_n(\delta)$ which were numbered by $n = 0, 1, \dots$ was sampled, in Ref. (5), in graphical form. One might suspect that the picture of the δ -dependence of the spectrum became one of the most often cited, recalled, represented, and reprinted figures of all of the recent history of quantum mechanics.

1.3.1.2 Search for Terminology Among the less pleasant features of the new direction of research, people found multiple terminological misunderstandings, often attributable to a sharp contrast between the enthusiasm of physicists and a definite scepticism of mathematicians. With time, the gap broadened. People started feeling a need of return to a deeper analysis of mathematical aspects of the field (26, 28, 64).

Fortunately, the birth of terminological conflict was quickly suppressed. First, Mostafazadeh (65) pointed out that in the majority of papers on \mathcal{PT} -symmetry the mathematical meaning of \mathcal{T} was equivalent to Hermitian conjugation yielding a simpler rule $H^\dagger \mathcal{P} = \mathcal{P}H$ of a pseudo-Hermiticity rather than of a symmetry. Langer and Tretter (66) added that the \mathcal{PT} -symmetry *alias* pseudo-Hermiticity of H may conveniently be reread as the property of H being self-adjoint in Krein space, provided only that one endows the latter space with pseudometric that coincides with operator \mathcal{P} .

Ultimately (cf., e.g., Refs. (67, 68) for further references), all of these developments climaxed in a translation of the physics-oriented concepts into the more



traditional mathematical language. A new field of research seemed to be firmly established. Some of its important roots have subsequently been traced to exist already in the past⁴.

1.3.1.3 Search for Methods: Perturbation Theory The reasons for the choice of the particular Bender's and Milton's *alias* Bender's and Boettcher's potential $V^{(BM)}(x, \delta)$ appear entirely formal, in the retrospective at least. Almost certainly, the decision was based on an exceptional amenability of such a toy model to perturbation expansions in a small parameter δ . The method was called, by the authors, delta expansions (cf. Ref. (21) for older references).

The original paper (21) itself remained firmly rooted in physics and, in particular, in quantum field theory. Only its title "Nonperturbative calculation ..." might seem to be in contradiction with what we just wrote about the method. An explanation of the paradox is fairly easy and purely terminological since by "perturbative calculation" people almost invariably mean an application of the most common and traditional Rayleigh-Schrödinger (RS) perturbation-expansion recipe.

In the latter RS recipe, the numerical quantities of interest (say, the bound-state energies of eq. (1.1.2)) are not interpreted as functions of a dynamics-determining parameter (like the above-mentioned exponent δ) but rather as complex functions of an *auxiliary* complex variable $\lambda \in \mathbb{C}$. This RS variable is defined via a scaling generalization $V \rightarrow \lambda V$ of the interaction potential in eq. (1.1.2). Then, one makes use of the simplification of the problem at $\lambda = 0$. Next, after an explicit construction of a suitable Taylor or asymptotic series, say, for the generalized bound-state energies $E_n = E_n(\lambda)$, one finally sets the auxiliary RS variable λ equal to its original, "physical" value of $\lambda = 1$ (69).

The emphasis put, in Ref. (21), on the distinction between the status of being "perturbative" or "nonperturbative" has historical roots. For many years, the specific RS expansions played a key constructive role in relativistic quantum field theory in $D = 3$ dimensions. Naturally, as long as the simplified case of $D = 1$ coincides with quantum mechanics (70), it is not too surprising that one finds, in the related literature, multiple methodically motivated perturbative RS studies of eq. (1.1.2) with various specific potentials (71).

It is particularly interesting to notice that among the latter references there exist several older, mathematically motivated RS-type studies of individual models which are, by our present understanding, \mathcal{PT} -symmetric. In a way pointed out by Álvarez (72) who studied, in 1995, potentials $V(x) = V^{(BM)}(x, \delta)$ at $\delta = 1$, one should certainly return to the 1980 paper (73) by Caliceti et al. These authors proved, rigorously and long before the boom of \mathcal{PT} -symmetry studies, the reality of a set of bound-state energies generated by the asymptotically imaginary cubic anharmonic oscillator well $V(x) = x^2 + V^{(BM)}(x, \delta)$ with specific $\delta = 1$.

The latter proof was based on an RS resummation trick which was rediscovered in 1997 (cf. paper (21)). By Buslaev and Grecchi (12), another \mathcal{PT} -symmetric model

⁴For more detail, the Krein-space interpretation of \mathcal{PT} -symmetry is explained in Chapter 6.



with $V(x) = x^2 + V^{(BM)}(x, \delta)$ and with a larger exponent $\delta = 2$ was considered and given a correct physical interpretation as early as in 1993. These authors listed several other, more than 10 years older references on the $\delta = 2$ model using the RS-expansion techniques. Even these older papers already reported several numerically supported unexpected discoveries of the reality of the spectrum. Alas, the phenomenon had been considered incidental by these authors.

For the localization of the boundaries of the domains of parameters (or multi-parameters) $\delta \in \mathcal{D}$ yielding real spectra, the choice of the RS-resummations and WKB- or δ -expansions was fortunate. In comparison, the applications of alternative perturbation recipes, for example, of the strong-coupling expansion techniques of Ref. (74) proved by far less suitable for the purpose.

1.3.1.4 Search for the Simplest Models with Real Spectra: Numerical Experiments Owing to the apparent simplicity of quartic potential (1.2.2) with exponent $\delta = 2$, the model attracted attention not only in Ref. (12) from 1993 but also, independently, in 2006 (75). The authors of these papers emphasized that one should study all of the members of the $\delta = 2$ family of potentials $V^{(BM)}(x, 2) + \mathfrak{o}(x^4)$ which behave, asymptotically, like a quartic anharmonic oscillator with wrong sign. This means that all of these counterintuitive, repulsive-looking interactions require, in contrast to their predecessors with $\delta < 2$, a particularly careful interpretation and delicate mathematical treatment.

With the growth of the exponent δ in opposite direction, beyond $\delta = 2$, one notices that many simple-minded recipes including most of the above-listed perturbation methods cease to be applicable. One of the main reasons is that the choice of $\delta = 2$ represents a natural boundary of applicability of Schrödinger equation in its real-axis form (1.1.2). Beyond this boundary, one must start treating Schrödinger differential equation as defined at complex “coordinates” x (cf. (76) for basic information).

At any nonnegative exponent δ , one can calculate the eigenvalues $E_n = E_n^{(BM)}(\delta)$ as certain smooth real functions of exponent in the whole interval of $\delta \in (0, \infty)$. It is merely necessary to define the wave functions $\psi_n(x)$, via Schrödinger differential equation, as square-integrable along an *ad hoc* complex curve of coordinates $x = \xi^{(\delta)}(t) \in \mathbb{C}$, with a real parameter $t \in (-\infty, \infty)$. According to Refs. (75, 77), these complex curves are deformable but, for the sake of simplicity, their preferred shape may be chosen elementary, say, in the form of a left–right symmetric hyperbola with downward-running asymptotics in complex plane.

With the growth of δ , the latter recommended asymptotics must both get closer and closer to the negative imaginary half-axis. In the purely numerical study (77), it has been shown that whenever these “complex-coordinate” asymptotics are *not* turned sufficiently down at a fixed value of δ , a *different* spectrum is obtained.

For each $\delta < 2$, the wave functions $\psi_n(x)$ could have been constructed, from eq. (1.1.2), as solutions which remain square integrable along the real axis of x . For larger exponents $\delta > 2$, on the contrary, each choice of an element $\xi(t)$ of the appropriate class of the deformable nontrivial contours forces us to replace



the original Hilbert space $L_2(-\infty, \infty)$ by another, more suitable Hilbert space of functions over the contour. Then, in order to avoid confusion, it makes sense to change the notation conventions and denote the new Hilbert space by a dedicated symbol, say, $\mathcal{H}^{(F)}$. As mentioned earlier, the superscript $^{(F)}$ may be read as marking “friendly” space.

At any positive $\delta > 0$ in $V^{(BM)}(x, \delta)$, the contour-dependence property of the alternative \mathcal{PT} -symmetric models may be spotted up to the very square-well-shaped limit of $\delta \rightarrow \infty$. In this limit, the bound states of $V^{(BM)}(x, \infty)$ with real energies are simply found living on a thin and down-turned U-shaped complex contour of $x \in \xi^{(\infty)}(t)$ (78). In a slightly more general setting, one could contemplate toboggan-shaped, multilooped generalizations of the contours $\xi(t)$ living, admissibly, on topologically nontrivial, multisheeted Riemann surfaces of x (79).

The contour-dependence phenomenon does not seem to be restricted to the original choice of potentials $V^{(BM)}(x, \delta)$ in eq. (1.1.2). Very similar, numerically supported observations were made in Ref. (80) where we explored an alternative family of the asymptotically exponentially quickly growing trigonometric \mathcal{PT} -symmetric potentials $V^{(FGRZ)}(x, \alpha) = -(i \sinh x)^\alpha$. The main merit of the choice was found in the possibility of return to the standard real line of $x \in (-\infty, \infty)$. Thus, the reality of the coordinate rendered the particle position observable, in principle at least.

1.3.2 Analytic and Algebraic Constructions

Besides the purely numerical nature of the determination of the spectra of bound states in the δ -dependent and \mathcal{PT} -symmetric potentials $V^{(BM)}(x, \delta)$, another shortcoming of the model consisted, for a long time, in the absence of any persuasive nonnumerical demonstration that the whole spectrum is strictly real. The analysis leading to the rigorous proof took several years and the proof itself appeared fairly complicated (22). Let us, therefore, break the tradition and let us recall several simpler parameter-dependent models, which prove solvable in closed form while carrying many of the basic features of a generic \mathcal{PT} -symmetric scenario.

1.3.2.1 Exactly Solvable Example: Harmonic-Oscillator One of the most natural, harmonic-oscillator-resembling candidates for the simplest possible non-Hermitian model with real bound-state spectrum has the following, manifestly \mathcal{PT} -symmetric form as proposed in 1999 (81),

$$V^{(c)}(x, \delta) = (x - ic)^2 + \frac{\delta}{(x - ic)^2}, \quad c > 0, \quad \delta \geq 0, \quad x \in (-\infty, \infty). \quad (1.3.1)$$

The key merit of such a choice lies in the obvious closed-form solvability of the corresponding Schrödinger’s eigenvalue problem (1.1.2). At any positive $c > 0$ and noninteger square root $\alpha = \alpha(\delta) = \sqrt{\delta + 1/4} \notin \mathbb{Z}$, one obtains the complete spectrum of the quantum bound-state energies in c -independent form,

$$E = E_{n,q}^{(\text{HO})}(\delta) = 4n + 2 - 2q \alpha(\delta). \quad (1.3.2)$$



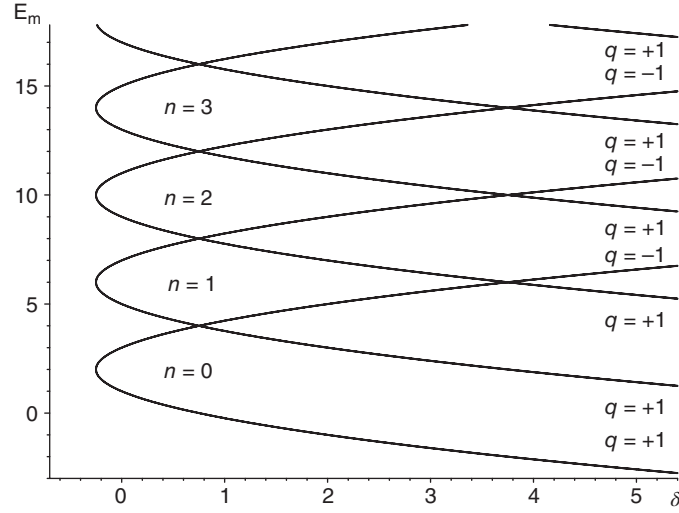


Figure 1.1 The δ -dependence (1.3.2) of the low-lying bound states in the exactly solvable \mathcal{PT} -symmetric potential (1.3.1).

These levels (cf. Fig. 1.1) are numbered by a multiindex $m = \{n, q\}$, which is composed of an integer $n = 0, 1, 2, \dots$ and of the so-called quasi-parity $q = \pm 1$. The related normalizable wave functions are also known in closed form, proportional to Laguerre polynomials (81).

The inspection of the picture reveals that at the exceptional-point (EP) values of $\delta_k^{(\text{EP})} = k^2 - 1/4$ one encounters the unavoided level crossings at $k = 0, 1, \dots$. At these EP coupling strengths, the algebraic and geometric multiplicities of the eigenvalues become different (56). In the language of physics, the EP versions of the model become manifestly unphysical because our generalized harmonic oscillator Hamiltonian $H_\delta^{(\text{GHO})} = -\partial_x^2 + V^{(c)}(x, \delta)$ ceases to be diagonalizable at all of the exceptional couplings $\delta = \delta_k^{(\text{EP})}$.

The mathematical reason lies in the instantaneous EP confluence (i.e., linear dependence, parallelization) of the respective Laguerre-polynomial wave functions of each pair of eigenstates which cross (cf. (81)). In other words, the number of independent eigenstates of each EP Hamiltonian $H_k^{(\text{EP})} = H_{k^2-1/4}^{(\text{GHO})}$ drops to one half. Their set ceases to form a basis in the infinite-dimensional topological vector spaces $\mathcal{H}^{(F)}$ or $\mathcal{H}^{(S)}$. The canonical matrix form of each exceptional $H_k^{(\text{EP})}$ becomes composed of infinitely many two-by-two Jordan blocs. For this reason, one can only speak about *independent* HO models $H_{\delta,k}^{(\text{GHO})}$ which are numbered by $k = 0, 1, \dots$ and which may be parametrized just by a coupling δ out of a finite, k -dependent open interval of $\delta + 1/4 \in (k^2, (k+1)^2)$.

To the left from the leftmost, $k = 0$ EP value of $\delta_0^{(\text{EP})} = -1/4$, *none* of the energies remains real. Owing to eq. (1.3.2), *all* of them suddenly form the complex conjugate pairs with quasi-parities $q = \pm 1$.



In a historical remark, let us add that the concept of quasi-parity was introduced in Ref. (27). Such a choice of name originated from the coincidence of q with the usual parity of wave functions in the self-adjoint limit of the vanishing coupling $\delta \rightarrow 0$. In the context of quantum physics where one prefers speaking about eigenvalues of operators of observables (24), the value of q may be reinterpreted as an eigenvalue of a charge C for each $H_{\delta,k}^{(\text{GHO})}$ (cf. Ref. (28)).

1.3.2.2 Algebraic Solvability: Truncated Anharmonic Oscillators For the next-to-trivial harmonic-oscillator potential (1.3.1) the above-mentioned exact, closed-form analytic solvability of \mathcal{PT} -symmetric Schrödinger equation (1.1.2) is not too surprising because this differential equation can be given the Gauss hypergeometric form. For phenomenological purposes, the model does not seem too exciting, either. It merely offers two mutually shifted copies of the usual equidistant harmonic-oscillator spectrum.

In applications, one usually asks for more. Typically, an enhanced flexibility of a weakly anharmonic model is often welcome. In a suitable basis, one then deforms the equidistant spectrum using a suitable perturbation,

$$H^{(\text{AHO})}(g) = H^{(\text{AHO})}(0) + \mathcal{O}(g),$$

$$H^{(\text{AHO})}(0) = H^{(\text{HO})} = \begin{bmatrix} 1 & 0 & 0 & \dots \\ 0 & 3 & 0 & \dots \\ 0 & 0 & 5 & \ddots \\ \vdots & \vdots & \ddots & \ddots \end{bmatrix}.$$

One may recall, for example, the real and antisymmetric bidiagonal (i.e., nearest-neighbor) anharmonicity $V(g) = H^{(\text{AHO})}(g) - H^{(\text{AHO})}(0)$ in the form of truncated and \mathcal{PT} -symmetrized N by N matrices as introduced in Ref. (54). Once we omit, for the sake of brevity, the discussion of the cases with odd matrix dimensions $N = 2J + 1$, we arrive at the series of tilded real Hamiltonian matrices with $N - 1 = 2J - 1$ free parameters,

$$\tilde{H}_{(a)}^{(2)} = \begin{bmatrix} 1 & a \\ -a & 3 \end{bmatrix}, \quad \tilde{H}_{(a,b,c)}^{(4)} = \begin{bmatrix} 1 & b & 0 & 0 \\ -b & 3 & a & 0 \\ 0 & -a & 5 & c \\ 0 & 0 & -c & 7 \end{bmatrix}, \dots$$

For illustration purposes, let us further shift the energy scale and impose an additional symmetry upon perturbations. The resulting untilded operators $H^{(2J)}$ will then depend on J real parameters,

$$H^{(2)} = \begin{bmatrix} -1 & a \\ -a & 1 \end{bmatrix}, \quad H^{(4)} = \begin{bmatrix} -3 & b & 0 & 0 \\ -b & -1 & a & 0 \\ 0 & -a & 1 & b \\ 0 & 0 & -b & 3 \end{bmatrix}, \dots \quad (1.3.3)$$



At any positive integer J , the key advantage of the model is that after an ample use of MAPLE-assisted symbolic-manipulation algebra (cf. (82) for technical details), one can qualitatively determine the shape of the boundaries $\partial\mathcal{D}^{(J)}$ of the compact J -dimensional real domains $\mathcal{D}^{(J)}$ of parameters a, b, \dots for which the spectrum of energies remains real and nondegenerate.

This feature makes the model truly exceptional. The computer-assisted form of its solvability makes the model particularly appealing for applications as it enables us to realize multiple alternative scenarios of the loss of the reality of the spectrum (i.e., of an onset of instability) via the whole family of nonnumerical benchmark explicit realizations (cf. (62) for more details and for a more extensive discussion).

1.3.3 Qualitative Innovations of Phenomenological Quantum Models

1.3.3.1 Exceptional Points as Points of a Quantum Horizon One of the most remarkable mathematical aspects of the sequence (1.3.3) of the real-matrix N by N toy-model Hamiltonians may be seen in the feasibility of a partially nonnumerical description of their spectra, especially near their exceptional-point degeneracies (54, 82). In this context, a typical result of symbolic-manipulation analysis is an “optimal,” λ -parametric, and dimension-dependent reparametrization $a \rightarrow A, b \rightarrow B, \dots$ yielding the same sequence of matrices in new form, namely,

$$H_{[A]}^{(2)}(\lambda) = \begin{bmatrix} -1 & \sqrt{1-A\lambda} \\ -\sqrt{1-A\lambda} & 1 \end{bmatrix}, \quad H_{[A,B]}^{(4)}(\lambda) =$$

$$= \begin{bmatrix} -3 & \sqrt{3}\sqrt{\lambda' - B\lambda^2} & 0 & 0 \\ -\sqrt{3}\sqrt{\lambda' - B\lambda^2} & -1 & 2\sqrt{\lambda' - A\lambda^2} & 0 \\ 0 & -2\sqrt{\lambda' - A\lambda^2} & 1 & \sqrt{3}\sqrt{\lambda' - B\lambda^2} \\ 0 & 0 & -\sqrt{3}\sqrt{\lambda' - B\lambda^2} & 3 \end{bmatrix}$$

(where we abbreviated $\lambda' = \lambda'(\lambda) = 1 - \lambda$), etc.

In the weakly non-Hermitian dynamical regime with small off-diagonal elements a, b, \dots , the spectra of eigen-energies remain safely real. In contrast, the spectra of the more strongly non-Hermitian matrices $H_{[A,B,\dots,Z]}^{(2,J)}(\lambda)$ may be expected to complexify at some critical couplings—take just $J = 1$ with energies $E_{\pm} = \pm\sqrt{1-a^2} = \pm\sqrt{A\lambda}$ for illustration.

By analogy, one may expect (and, if asked for, prove (82)) that at any dimension $N = 2J$ the complexifications are always encountered during a decrease in the apparently redundant auxiliary real parameter $\lambda > 0$. In this manner, one can determine the $(J - 1)$ -dimensional exceptional-point boundary $\partial\mathcal{D}^{(2J)}$ of the J -dimensional “physical” domain $\mathcal{D}^{(2J)}$ of parameters A, B, \dots, Z for which the spectrum stays real (i.e., in which the time evolution of the quantum model in question remains unitary).

After one exempts the $J = 1$ model as oversimplified, one may conclude that in order to determine the points of the horizon of quantum stability (i.e., of the



hypersurface $\partial D^{(2J)}$ at arbitrary dimension $N = 2J$ (*mutatis mutandis*, analogous conclusions apply to odd $N = 2J + 1$ (82)), one only has to evaluate the Kato's exceptional points $\lambda^{(\text{EP})} = \lambda^{(\text{EP})}(A, B, \dots, Z)$ as functions of the J new variable couplings A, B, \dots, Z .

The main purpose and benefit of the above-outlined sophisticated though still fully nonnumerical reparametrization of the model is connected with the heavily computer-assisted guarantee (54) that a complete confluence (plus subsequent complexification) of *all* of the $2J$ real eigenvalues E takes place at the vanishing uppercase couplings $A = B = \dots = Z = 0$ *plus* at the vanishing "extreme" exceptional point $\lambda^{(\text{EEP})} = 0$.

In the language of quantum phenomenology, the latter extreme exceptional point may be perceived as representing a quantum catastrophe or collapse, resembling the quantum versions of phenomena such as Big Bang or Big Crunch in quantum gravity (see Ref. (62) for more details). After a return to mathematics and to the questions of geometry of the space of original parameters a, b, \dots, z , one may conclude that at any dimension $N = 2J$, the quantum horizon has the shape of the hypersurface of a hypercube with protruded vertices.

An analysis of the geometry of these hypersurfaces near their full-confluence EEP vertices is feasible nonnumerically. At any dimension $N = 2J$ and at the sufficiently small λ , there exist $\lambda \rightarrow 0$ limits of certain two smooth real functions $\mu_N^2(\lambda)$ and $\nu_N^2(\lambda)$ such that the *complete* reality of the spectrum is guaranteed by the *single* inequality sampled by the following first few relations

$$-\mu_4^2(0) \leq 2A/2 - B \leq +\nu_4^2(0), \quad N = 4,$$

$$-\mu_6^2(0) \leq 6A/2 - 4B + C \leq +\nu_6^2(0), \quad N = 6,$$

$$-\mu_8^2(0) \leq 20A/2 - 15B + 6C - D \leq +\nu_8^2(0), \quad N = 8,$$

and so on, with $\mu_4^2(0) = 1/4$ and $\nu_4^2(0) = 4/9$, and so on (cf. (82) for more details).

1.3.3.2 The Feshbach's Effective Hamiltonians Revisited In one of the areas in which the old and new ideas merged, the applicability of non-self-adjoint operators has been sought and found in an immediate transfer of the concept of evolution in time from the usual physical Hilbert space $\mathcal{H}^{(P)}$ in which the evolution is unitary to its alternative $\mathcal{H}^{(F)}$ in which the unitarity would be violated. It should be pointed out that one of the most natural visualizations of such a transfer is provided by the above-mentioned Feshbach's reduction of $\mathcal{H}^{(P)}$ to a subspace $\mathcal{H}^{(R)}$ playing the role of the false space $\mathcal{H}^{(F)}$.

For one of the most immediate applications of the idea of the loss of Hermiticity of Hamiltonians during space-reduction $\mathcal{H}^{(P)} \rightarrow \mathcal{H}^{(R)}$, we may return to letter (55). Its authors explained the impact of the reduction of spaces on the measurable properties of the so-called quantum brachistochrone, the name of which derives from the Greek "brachistos" (= the shortest) and "chronos" (= time). The core of the explanation lied in the fact that the full Hilbert space $\mathcal{H}^{(P)}$ may be perceived as carrying additional



degrees of freedom, a dynamical coupling to which may be made responsible for the loss of Hermiticity (as well as for its multiple consequences) inside subspace $\mathcal{H}^{(R)}$.

In another, more traditional illustration of the space-reduction scenario, one may speak about the so-called open quantum systems in which, typically, the products of a decay of an unstable system simply move out of the reduced Hilbert space. Naturally, the instability gets immediately removed via a return to the full space.

Whenever one decides to stay inside the reduced, false space $\mathcal{H}^{(F)} = \mathcal{H}^{(R)}$, the reference to the above-cited Feshbach's projector-operator isospectrality may remain just vague and implicit during the concrete approximative calculations. In applications to atomic and molecular systems, the underlying reduction-by-projection simplifications may be found in the background of multiple approximate calculations (cf. their detailed account in (33)). As a conceptual guide to qualitative analyses of resonance and various other phenomena emerging in unstable atomic nuclei, precisely the same idea may also be used (cf., e.g., review paper (83) giving further references).

As already mentioned, the popularity of the latter type of correspondence climaxed in 2011 when, for all of the above-listed reasons, the specialists in the study of open systems and the models with effective Hamiltonians $H = H_{eff}(E)$ happened to form the majority of participants of the tenth non-self-adjoint-operator conference PHHQP 2011 (34) in Dresden. The extension of the phenomenological scope to complex-energy quantum systems proved clearly beneficial because it reattracted the attention of theoreticians to the analysis of the behavior of quantum systems near the horizons of their stability (84).

In the subsequent years, the last crisis emerged but it did not hit the models using effective Hamiltonians $H = H_{eff}(E)$ because their phenomenological interpretation does not require any construction of the metric Θ at all. As a consequence, many people started paying attention to the deeper analysis of the phase transitions connected with the spontaneous breakdown of \mathcal{PT} -symmetry (cf. the following sections in this respect).

For illustration of the possible (although, up to now, not too much explored) survival of the overlap between quantum model-building strategies based on the traditional (i.e., effective, trivial-metric-requiring) and on the \mathcal{PT} -symmetric (i.e., non-self-adjoint, nontrivial-metric-requiring), Hamiltonians H let us now recall Ref. (85). The puzzling energy dependence of the effective Hamiltonian $H_{eff}(E)$ has been reanalyzed there via its possible rearrangement and rigorous transformation to the two alternatives of the effective Hamiltonian denoted as mappings $H_{eff}(E) \leftrightarrow K \neq K^\dagger$ and $H_{eff}(E) \leftrightarrow L \neq L^\dagger$.

The main conclusion was that one can make both of the new isospectral partner Hamiltonians non-self-adjoint but, by construction, energy-independent, $K \neq K(E)$ and $L \neq L(E)$. The nonlinear eigenvalue problem (1.1.1) has been, in this manner, linearized. What is important is that the change did not destroy the immanent, phenomenologically appealing possibility of the loss of the reality of the bound-state energies E at the boundary $\delta \in \mathcal{D}$ of the domain of the stability-supporting variable parameters.

1.3.3.3 Systems Exhibiting Nonlinear Supersymmetry The elementary and exactly solvable non-self-adjoint harmonic oscillator (1.3.1) has been found to play an interesting role in the framework of the so-called supersymmetric (SUSY) quantum mechanics (86). Initially, people found it impossible to parallel, strictly, the existing self-adjoint constructions and to implement any non-self-adjoint operator into the usual SUSY-representation pattern. Nevertheless, a partial success has been achieved after a transition to the algebras of the so-called nonlinear SUSY *alias* second-order SUSY (SSUSY, (87, 88)). In the latter, broadened framework, it appeared feasible to generalize the well-known correspondence between the exact solvability of Schrödinger equation (1.1.2) and a SUSY-related property of shape invariance of the corresponding potential $V(x)$. The results of these efforts may be found summarized, for example, in paper (39).

In such a context, potential (1.3.1) reacquired the status of one of the simplest special cases of the whole shape-invariant and/or SSUSY-algebra-related family of solvable interactions. For this reason, it makes sense to return to this example, in the new SSUSY context, in more detail. Skipping the majority of technicalities and physics interpretations that may be, after all, found explained in Refs (88) and (89), let us merely display the most common SUSY generators formed by Hamiltonian \mathcal{G} and by the two usual SUSY charges,

$$\mathcal{G} = \begin{bmatrix} H_{(\text{Left})} & 0 \\ 0 & H_{(\text{Right})} \end{bmatrix}, \quad \mathcal{Q} = \begin{bmatrix} 0 & 0 \\ A & 0 \end{bmatrix}, \quad \tilde{\mathcal{Q}} = \begin{bmatrix} 0 & B \\ 0 & 0 \end{bmatrix} \quad (1.3.4)$$

(cf., e.g., eqs Nr. (15)–(17) in Ref. (86), respectively). Once we further postulate that $H_{(\text{Left})} = B \cdot A$ and $H_{(\text{Right})} = A \cdot B$, the triplet of operators (1.3.4) will generate, by construction, a representation of SUSY algebra $\mathfrak{sl}(1/1)$ based on the following linear anticommutator and commutator relations,

$$\{\mathcal{Q}, \tilde{\mathcal{Q}}\} = \mathcal{H}, \quad \{\mathcal{Q}, \mathcal{Q}\} = \{\tilde{\mathcal{Q}}, \tilde{\mathcal{Q}}\} = 0, \quad [\mathcal{H}, \mathcal{Q}] = [\mathcal{H}, \tilde{\mathcal{Q}}] = 0.$$

This representation may be admitted non-self-adjoint. For this purpose, we have to return to the above-introduced complex quasi-coordinates $q \in \mathbb{C}$ and to define, formally, the first-order linear differential operators $A = \partial_q + W$ and $B = -\partial_q + W$ in terms of a one-parametric complex function called superpotential,

$$W = W^{(\gamma)}(q) = q - \frac{\gamma + 1/2}{q}, \quad q = q(x) = x - ic, \quad \gamma, x, c \in \mathbb{R}. \quad (1.3.5)$$

Once we denote

$$H^{(\xi)} = -\frac{d^2}{dq^2} + \frac{\xi^2 - 1/4}{q^2} + q^2$$

we may verify that

$$H_{(\text{Left})}^{(\gamma)} = H^{(\alpha)} - 2\gamma - 2, \quad H_{(\text{Right})}^{(\gamma)} = H^{(\beta)} - 2\gamma, \quad (1.3.6)$$

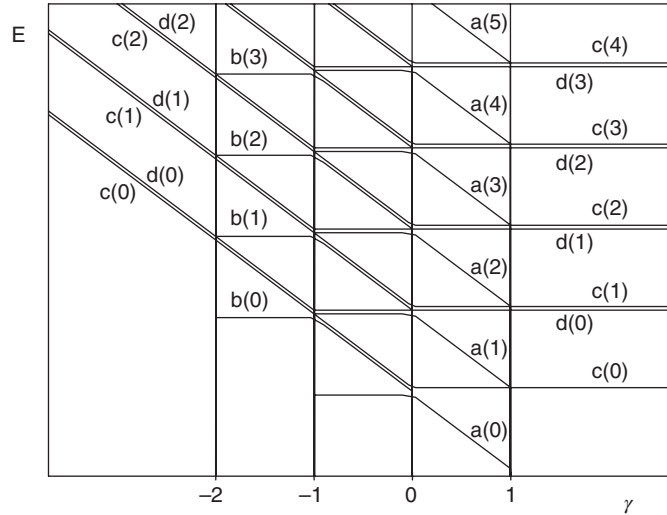


Figure 1.2 The spectrum of the non-self-adjoint harmonic-oscillator SUSY Hamiltonian \mathcal{G} of eqs (1.3.4) and (1.3.6).

provided only that we define quantities $\alpha = \alpha(\gamma) = |\gamma|$ and $\beta = \beta(\gamma) = |\gamma + 1|$ as nonnegative functions of the real input parameter γ .

As long as our benchmark SUSY Hamiltonian \mathcal{G} of eq. (1.3.4) is a direct sum of two non-self-adjoint harmonic oscillators (1.3.6), the determination of its spectrum (cf. Fig. 1.2) is straightforward. The discussion of its properties leads to interesting and unusual observations. For example, we may always treat this spectrum as an infinite sequence of quadruplets of energies that share the main index $n = 0, 1, \dots$ and that may differ just by their superscripts α or β and by their quasi-parities,

$$a(n) \leq b(n) \leq c(n) \leq d(n). \quad (1.3.7)$$

Naturally, the usual and well-known self-adjoint special case reemerges here at the unique value of $\gamma = -1/2$ for which the numbers $\alpha = \beta = 1/2$ become equal. In review (86) (see, in particular, Section 2.1 in *loc. cit.*), the corresponding self-adjoint harmonic-oscillator SUSY model with $\alpha = \beta = 1/2$ is called “linear SUSY.”

At any other $\gamma \neq -1/2$, the model ceases to be self-adjoint. Thus, at every main quantum number n , we may reinterpret the four corresponding eigen-energies as an ordered quadruplet (1.3.7). We may recall the discussion in Ref. (89) and conclude that sufficiently far from the self-adjoint special case with $\gamma = -1/2$, that is, more precisely, out of the interval of $\gamma \in (-1, 0)$, some of the energy levels of eq. (1.3.7) cease to exist.

The pattern of such a disappearance of states is made visible in Fig. 1.2. Your count of the levels is guided there by a small artificial shift of one of the levels in the



cases of the well-known SUSY-related degeneracies⁵. After the thorough inspection of the picture, we may conclude that in contrast to the dominant levels $c(N)$ and $d(N)$ that correspond to the normalizable bound states at any real $\gamma \in \mathbb{R}$, the existence of the remaining two levels $b(N)$ and $a(N)$ is restricted to the mere finite intervals of $\gamma \in (-2, 0)$ and $\gamma \in (-1, 1)$, respectively.

The phenomenon of the disappearance of levels itself is caused by the loss of normalizability of wave functions at some integer values of γ . The critical phenomenon of the disappearance always involves infinitely many states, but such a “phase transition” only occurs at one of the four privileged forbidden values of $\gamma = -2$, $\gamma = -1$, $\gamma = 0$, and $\gamma = 1$.

1.4 PROBABILISTIC INTERPRETATION OF THE NEW MODELS

1.4.1 Variational Constructions

One of the typical features of the differential operators A and B of eq. (1.3.4) is that they are unbounded. In principle, this would entail the necessity of a very careful specification of the domains on which they are defined. For this reason, it has been proposed, in the very first review (24) of the THS formalism by Scholtz et al., that whenever possible, our attention should remain restricted just to the bounded-operator Hamiltonians $H \in \mathcal{B}(\mathcal{H})$ or even to the mere truncated, N -dimensional matrix representations of all of the operators of quantum observables.

1.4.1.1 Nuclear Physics Example Under the above-mentioned constraints, many mathematical challenges would either disappear or become inessential. In particular, whenever the finite matrix-truncation dimensions $N < \infty$ are used, the sophisticated formalism of functional analysis may be replaced by the mere linear algebra. This also seems to explain why the first (viz., variational) applications of the THS strategy to heavy nuclei took place perceptibly earlier than in field theory.

In the \mathcal{PT} -symmetry studying community, a return of attention to the bounded-operator or even linear-algebraic mathematical origins came rather late. One of the important by-products of this simplification of technicalities may be seen in the subsequent opening of communication channels between different areas of physics and, in particular, in a rediscovery of the natural factorizability of the metrics, $\Theta = \Omega^\dagger \Omega$.

The introduction of the factor operator Ω (which must be, in all of the nontrivial cases of our present interest, nonunitary) is usually attributed to Freeman Dyson (see one of the footnotes earlier). In the context of nuclear physics, Janssen et al. (90) were probably the first who imagined that the nonunitarity assumption $\Omega^\dagger \neq \Omega^{-1}$ opens a truly unexplored space for possible simplification of the computing.

Let us recollect that the Dyson-inspired nuclear physics concrete choice of Ω was in fact just an intuition-guided mapping between the most common Hilbert space

⁵The illustration was prepared as a part of Ref. (89). Unfortunately, the Figure itself was not included in the printed version of *loc. cit.*, due to an inadvertent technical omission by the Editors.



$\mathcal{H}^{(P)}$ of protons and neutrons (forming a heavy atomic nucleus—the superscript $^{(P)}$ hints that the space is “physical” as well as “primary”) and another, very different (and, incidentally, much friendlier!) bosonic representation space $\mathcal{H}^{(F)}$.

In the latter space, one works with preselected and, presumably, more relevant effective degrees of freedom carried by quasi-particles called “interacting bosons” (IB). In contrast to the naive and prohibitively complicated form of the initial, strictly microscopic and realistic Hamiltonian (for the sake of clarity let us denote it by the “dedicated” lower-case symbol \mathfrak{h}), its isospectral IB partner $H = \Omega^{-1} \mathfrak{h} \Omega$ constructed via an educated guess of Ω proved, in many a respect, simpler after truncation. One should not be too surprised because the very nature of the dynamical input information about the nucleon–nucleon forces is such that it patches the fermionic nucleons to form certain correlated pairs. *A priori* these pairs may be expected to exhibit bosonic features.

The practical numerical tests of the Dyson-inspired IB models of atomic nuclei confirmed the expectations and were successful. The non-unitary-mapping-mediated transition to a definitely friendlier bosonic Hilbert space rendered the calculation of certain spectra of heavy nuclei feasible, easier and usually much more quickly convergent in the realistic limit of matrix dimension $N \rightarrow \infty$.

1.4.1.2 Quantum Theory Using Bounded Observables One of the paradoxes which resulted from the lack of a sufficiently intensive communication between mathematicians and physicists manifested itself in a deplorable mutual incompatibility of the respective vocabularies. Besides the above-mentioned parallelism and duplicity between the concepts of \mathcal{PT} -symmetry in quantum physics and Krein-space Hermiticity in operator-theory mathematics, another hidden source of possible misunderstandings may be found in the use of term “quasi-Hermiticity.” It carries, traditionally, an entirely different meaning in mathematics and physics. Thus, in the light of the definition as introduced, in 1960, by Dieudonné (91), the quasi-Hermiticity of H need not imply the quasi-Hermiticity of its adjoint H^\dagger (or, as mathematicians would write it, H^*). In the context of physics, on the contrary, such an implication is *always* required and guaranteed. Owing to the purpose-adapted and better-designed definition as promoted by Scholtz et al. (24), nuclear physicists assume that the quasi-Hermitian quantum observable H is a *bounded* operator.

Using this basic assumption, review paper (24) presented an overall theoretical framework for an update of the unitary quantum theory guaranteeing the consistent use of non-self-adjoint representations of observable quantities. We already emphasized above that in the subsequent preparatory step of the THS representation theory, once a *given* Hamiltonian H (or possibly another quantum observable represented by a non-self-adjoint operator $Q \neq Q^\dagger$ with real spectrum (92)) appears non-Hermitian in a *given* Hilbert space $\mathcal{H}^{(F)}$, the latter a space must be declared ill-chosen and unphysical, manifestly “false.”

Let us now add that in practice one preserves the topological vector space $\mathcal{H}^{(F)}$ as the *exclusive* working space. In other words, the “correct” Hilbert space $\mathcal{H}^{(S)}$ is solely present *via* its representation in $\mathcal{H}^{(F)}$. Thus, one works with the two metrics



$\Theta^{(F)} = I$ and $\Theta^{(S)} \neq I$ in parallel and solely in $\mathcal{H}^{(F)}$. In such a setting, it suffices to introduce just a new double-ket symbol or abbreviation $|\psi\rangle\rangle$ for the representation of the updated dual vectors $\Theta|\psi\rangle$, which are identified with the elements of the dual vector space $(\mathcal{H}^{(S)})'$.

Unless the metric operator itself appears unbounded (which would require a more sophisticated construction (38)), one can return to popular abbreviations. Thus, the change $\mathcal{H}^{(F)} \rightarrow \mathcal{H}^{(S)}$ is then most concisely characterized as an *ad hoc* upgrade of the inner product (11),

$$\langle\psi|\chi\rangle^{(F)} \rightarrow \langle\psi|\chi\rangle^{(S)} \equiv \langle\psi|\Theta|\chi\rangle^{(F)}. \quad (1.4.1)$$

The necessary assumptions are that the symbol $\Theta = \Theta^{(S)}$ denotes a nontrivial and self-adjoint, bounded and strictly positive operator possessing a bounded inverse in $\mathcal{H}^{(F)}$.

In a pragmatic perspective of postulates of unitary quantum theory, the consistent formulation of the idea is concise. One merely stops making the measurable predictions directly in the auxiliary Hilbert space $\mathcal{H}^{(F)}$ and replaces them by the predictions containing the metric. Then, the same operator of any quantum observable (be it a Hamiltonian or not) is made acceptable and self-adjoint (in the properly amended physical representation space $\mathcal{H}^{(S)}$) and its mean values are simply always calculated between bras and kets.

In most of the older applications of the idea, the above-mentioned mathematical condition of boundedness was not always sufficiently carefully considered. This did not necessarily imply that the construction was mathematically incorrect. For example, let us return to the “wrong-sign” quartic anharmonic oscillator Hamiltonian $H \neq H^\dagger$ of Buslaev and Grecchi (12) for which these authors found the manifestly self-adjoint “correct-sign” quartic-oscillator double-well isospectral partners $\mathfrak{h} = \mathfrak{h}^\dagger$ without any recourse to the metric.

We are now prepared to summarize the message: The abstract quantum theory using *bounded* non-Hermitian representations of its operators of observables may be perceived as a well-defined and mathematically consistent foundation of the standard quantum picture of reality. The trick is that the specific three-Hilbert-space recipe based on the use of a nontrivial metric $\Theta \neq I$ enables us to treat the “first” Hilbert space $\mathcal{H}^{(F)}$, simultaneously, as most friendly as well as manifestly unphysical. And while the advantage is simply kept unchanged, the shortcoming is easily suppressed by the metric-mediated redefinition $\mathcal{H}^{(F)} \rightarrow \mathcal{H}^{(S)}$ yielding the metric-equipped second space $\mathcal{H}^{(S)}$, which is, by construction, unitarily equivalent to the primary $\mathcal{H}^{(P)}$.

As long as we very often choose space $\mathcal{H}^{(F)}$ in the most common form $L^2(\mathbb{R}^d)$ of the space of the quadratically integrable wave functions in d dimensions (69), a truly unpleasant increase in the complexity of the necessary constructive mathematics may be expected to follow from the transition to $\mathcal{H}^{(S)}$ (i.e., to the complicated metrics Θ) in general.

Last but not least, also the development of reliable and efficient techniques of proving the reality (i.e., the observability) of the spectrum of preselected Hamiltonians H (which used to be, for any self-adjoint $H = H^\dagger$ in $L^2(\mathbb{R}^d)$, trivial) becomes a serious technical obstacle (77). In order to support such a necessity of search for updates



of mathematical methods, once more, the nice older study of the imaginary cubic anharmonicities by Caliceti et al. (73) may be recalled as an illustrative example: The reality of the energy levels has been shown there to follow from a clever modification of the usual perturbation-expansion techniques⁶.

1.4.2 Non-Dirac Hilbert-Space Metrics $\Theta \neq I$

1.4.2.1 Hilbert Space $\mathcal{H}^{(S)}$ Many non-Hermitian Hamiltonians $H \neq H^\dagger$ as sampled above are, strictly speaking, merely non-Hermitian in $\mathcal{H}^{(F)}$ but not in $\mathcal{H}^{(S)}$. In any case, these operators must be required diagonalizable (11). In the amended Dirac's notation of Ref. (23), this means that one has to solve two rather than one time-independent Schrödinger equation,

$$H |\psi_n\rangle = E_n |\psi_n\rangle, \quad H^\dagger |\psi_m\rangle = E_m^* |\psi_m\rangle, \quad m, n = 0, 1, \dots \quad (1.4.2)$$

For finite, $(N + 1)$ -dimensional Hilbert spaces $\mathcal{H}^{(F)}$ and for the Hamiltonian matrices H with real, nondegenerate and discrete spectrum⁷, this implies that the respective vectors $|\psi_n\rangle$ and $|\psi_m\rangle$ are mutually orthogonal in $\mathcal{H}^{(F)}$ for $m \neq n$. After a suitable rescaling these eigenvectors of the two respective operators in (1.4.2) will form a biorthonormal basis in $\mathcal{H}^{(F)}$. The following two spectral formulae become available,

$$I = \sum_{n=0}^N |\psi_n\rangle \langle\langle \psi_n|, \quad H = \sum_{n=0}^N |\psi_n\rangle E_n \langle\langle \psi_n|. \quad (1.4.3)$$

Under the same assumptions, we introduce an auxiliary $(N + 1)$ by $(N + 1)$ matrix, which is $(N + 1)$ -parametric, invertible, positive-definite and Hermitian,

$$\Theta = \sum_{n=0}^N |\psi_n\rangle \kappa_n^2 \langle\langle \psi_n| = \Theta^\dagger > 0. \quad (1.4.4)$$

Once we interpret this matrix as a metric operator, we obtain a new, "standard" Hilbert space $\mathcal{H}^{(S)}$. In this $(N + 1)$ -dimensional space, the Hermitian conjugation of any operator Λ becomes defined in terms of the given metric as follows,

$$\mathcal{T}_{(oper.)}^{(S)} : \Lambda \rightarrow \Lambda^\ddagger := \Theta^{-1} \Lambda^\dagger \Theta. \quad (1.4.5)$$

Thus, in the amended space $\mathcal{H}^{(S)}$, the habitual Hermitian conjugation

$$\mathcal{T}_{(oper.)}^{(F)} : \Lambda \rightarrow \Lambda^\dagger \quad (1.4.6)$$

as defined in $\mathcal{H}^{(F)}$ must be replaced by the amended definition (1.4.5).

⁶Chapter 4 of the present book should be read as a topical review of the freshest updates of these efforts.

⁷For more general cases, a few relevant comments may be found in (93).



The main consequence of the introduction of metric (1.4.4) is that Hamiltonian H becomes, by construction, self-adjoint in $\mathcal{H}^{(S)}$. The new Hilbert space $\mathcal{H}^{(S)}$ may be declared physical. We have $H = H^\ddagger$ so that in the new space the time evolution generated by H becomes unitary. In parallel, the original, “friendly” Hilbert space $\mathcal{H}^{(F)}$ in which the time evolution generated by H remains manifestly nonunitary must be declared unphysical and “false.”

On this linear-algebraic methodical background, one may decide to move to the more usual separable, infinite-dimensional Hilbert spaces. In some cases, it proves sufficient to set simply $N = \infty$ in the above-listed formulae. Unfortunately, there exist only too many models in which much more mathematical care is needed and necessary. Perhaps, this is one of the key reasons why the present book had to be written.

1.4.2.2 The Reasons for Factorization of the Metrics Let us recall the family of quantum models exhibiting \mathcal{PT} -symmetry *alias* parity-pseudo-Hermiticity $H^\dagger \mathcal{P} = \mathcal{P} H$. For them, we immediately see the link between the empirical observation of the reality of their spectra and a general mathematical framework offered by the THS formalism. In one direction, the reality of the spectrum gets explained as a consequence of the Hermiticity of H in some not yet known Hilbert space $\mathcal{H}^{(S)}$. In opposite direction, the knowledge of the Dyson-type mapping between upper-case operator H and lower-case operator \mathfrak{h} leads immediately to the identification of the metric Θ with the superposition of the Dyson’s mapping with its conjugate,

$$\Theta = \Omega^\dagger \Omega. \quad (1.4.7)$$

In the unitary-mapping extreme, one would have $\Omega^\dagger = \Omega^{-1}$ so that the whole THS-represented quantum theory would degenerate to its textbook special case in which one never needs to work with any auxiliary unphysical Hilbert space $\mathcal{H}^{(F)}$ and with any non-self-adjoint representation H of the Hamiltonian.

The overall belief in applicability of nontrivial metrics Θ proved amazingly productive in a number of phenomenological and heuristic considerations. The approach helped to clarify, first of all, the consistent probabilistic tractability of the relativistic quantum-mechanical Klein–Gordon systems with spin zero (44). Secondly, formal analogs of Klein–Gordon systems were found in the gravity-quantizing Wheeler-De-Witt equations (43). Finally, very similar conclusions were achieved for the less known Proca systems with spin one (94), and so on.

For a number of \mathcal{PT} -symmetric systems, a key to the progress in applications was found in a simplification of the factorization of the metric in which it has been assumed that $\Theta = \Omega_s^\dagger \Omega_s$ where $\Omega_s = \Omega_s^\dagger$. This assumption may be reread as formula $\Omega_s = \sqrt{\Theta}$ that defines a special Dyson map Ω_s and removes a part of the ambiguity from the correspondence between Hilbert spaces $\mathcal{H}^{(F)}$ and $\mathcal{H}^{(P)}$ for a given Hamiltonian H .

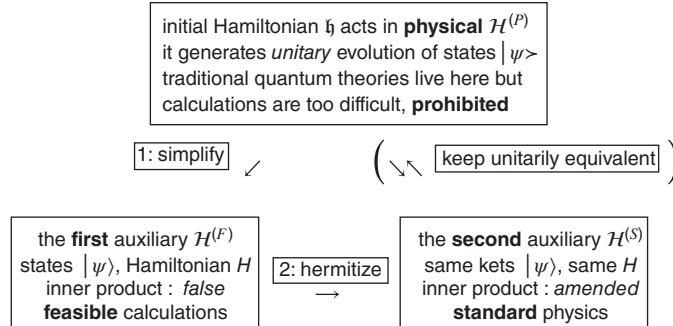


1.5 INNOVATIONS IN MATHEMATICAL PHYSICS

1.5.1 Simplified Schrödinger Equations

From the knowledge of the triplet of operators H , Θ , and Ω , one may reconstruct the primitive physical Hamiltonian $\mathfrak{h} = \Omega^{-1}H\Omega$, which is assumed prohibitively complicated (otherwise, the whole THS machinery would not be needed at all). The latter operator is still, by construction, kept self-adjoint in its own Hilbert space, that is, $\mathfrak{h} = \mathfrak{h}^\dagger$ in $\mathcal{H}^{(P)}$. As long as the inner product is postulated trivial in $\mathcal{H}^{(P)}$, the mathematically and computationally much more complicated representation \mathfrak{h} of the Hamiltonian often offers, paradoxically, the most natural background for the physical interpretation of the results of calculations. The vital point of the whole THS recipe is that two Hilbert spaces $\mathcal{H}^{(S)}$ and $\mathcal{H}^{(P)}$ are unitarily equivalent. This makes them indistinguishable from the point of view of physical predictions so that one can work in more friendly $\mathcal{H}^{(S)}$.

1.5.1.1 Starting from an Overcomplicated, Hermitian Schrödinger Equation As we already mentioned, the general abstract pattern of quantum theory as it emerges from such a THS arrangement found its important application in nuclear physics (24). The implementation of the ideas started from an introductory step in which one defines effective non-self-adjoint matrix $H \neq H^\dagger$ (of any dimension $N + 1 \leq \infty$) as a simplified isospectral partner of a realistic input (i.e., known but prohibitively complicated) Hamiltonian \mathfrak{h} . As long as the details of the construction may be found in Ref. (24), let us merely summarize the pattern as the following THS flowchart,



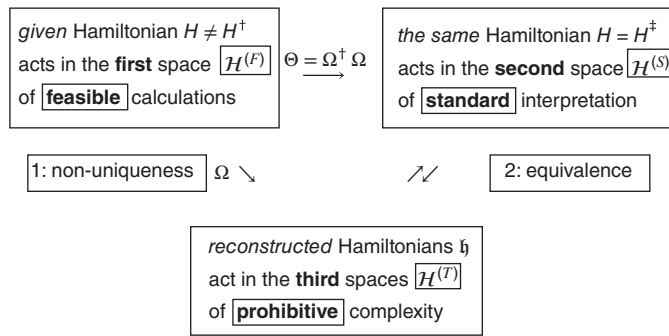
It is necessary to add that while $\mathcal{H}^{(F)}$ and $\mathcal{H}^{(S)}$ were, in the nuclear physics implementation, the perceivably simpler Hilbert spaces of bosons (called “interacting bosons” in the related extensive literature), the “initial” space $\mathcal{H}^{(P)}$ was the most common Hilbert space of fermionic nucleons. For this reason, the definition of the “prohibitively complicated” Hamiltonian \mathfrak{h} was more or less routine (i.e., based on the principle of correspondence). In contrast, the choice of the innovative, *nonunitary* form of the mapping Ω between spaces (defined via formula $|\psi\rangle = \Omega |\psi\rangle$) required a truly ingenious insight in the underlying physics.

1.5.1.2 Starting Directly from a Non-Hermitian Schrödinger Equation In a broader methodical perspective, the success of simplification $\mathfrak{h} \rightarrow H = \Omega \mathfrak{h} \Omega^{-1}$ may be rephrased as an acceptability of non-Hermiticity during practical model



building. As long as the main purpose of the mapping lies in the feasibility of the determination of the spectrum, one can also proceed in opposite direction, trying to deal with a given Hamiltonian operator $H \neq H^\dagger$. This operator living in an auxiliary Hilbert space $\mathcal{H}^{(F)}$ should only be assumed maximally elementary, at the expense of being allowed manifestly non-self-adjoint.

Such an operator H may then be related, via a suitable *family of the operators* $\Omega = \Omega(H)$, to a *multiplet* of its eligible isospectral partners $\mathfrak{h} = \mathfrak{h}^\dagger$. The individual members of the latter family live in the respective metric-dependent (i.e., different) “third” Hilbert spaces $\mathcal{H}^{(T)}$. The overall THS flowchart should be rearranged and redirected as follows:



Just one of the reconstructed “third” scenarios should be selected as representing the expected observable physical phenomena, $\mathcal{H}^{(T)} \rightarrow \mathcal{H}_0^{(T)} \equiv \mathcal{H}^{(P)}$. The ambiguity of the mapping Ω to the third space implies the nonequivalence of the alternative physical interpretations compatible with the initial information about the quantum system in question. Formally, all of the options are equally acceptable while admitting very broad variability of their phenomenological and observable consequences. More information about the system must necessarily be provided (see the extensive discussion of this point in Ref. (24)).

1.5.1.3 The Concept of Charge \mathcal{C} An introduction of a *privileged and unique* physical operator \mathfrak{h}_0 assigned to a given toy-model Hamiltonian H belongs to the most impressive merits of the very specific \mathcal{PT} -symmetric quantum theory as summarized by Bender (10). This formalism makes *two additional* assumptions by asking for the existence of a charge \mathcal{C} (yielding the unique special metric $\Theta_0 = \mathcal{P}\mathcal{C}$) and for the unique self-adjoint specification $\Omega_{s,0} = \sqrt{\Theta_0}$ of the preferred Dyson-type mapping. These two physics-determining postulates imply a complete suppression of the ambiguity of the reconstruction of the isospectral self-adjoint representation \mathfrak{h}_0 of the Hamiltonian for the conservative systems and in the finite-dimensional Hilbert spaces at least⁸.

The essence of the uniqueness of the reconstruction $H \rightarrow \mathfrak{h}_0$ in \mathcal{PT} -symmetric quantum mechanics is closely connected to another, implicit assumption that a generic \mathcal{PT} -symmetric quantum system with Hamiltonian $H = p^2 + V(x)$ lives, in general, on a *complex* curve of coordinates x . In other words, the values of x cannot

⁸cf. following paragraph.



certainly be treated as eigenvalues of an operator, Hermitian or crypto-Hermitian, of an observable, anymore. Thus, the concept of locality is lost. For compensation, in a way inspired by quantum field theory, one introduces the CPT -symmetry of H plus the observability status of the operator C called charge. Review paper (10) may be recommended as one of the most exhaustive physics-oriented comprehensive accounts of the related technical and interpretation details.

1.5.2 Nonconservative Systems and Time-Dependent Dyson Mappings

In the THS notation of review (23), one marks each element ϕ of the primary physical Hilbert space by the “spiked” ket symbol, $|\phi\rangle \in \mathcal{H}^{(P)}$. In parallel, the representants of the same state in both the first and second auxiliary Hilbert spaces may remain marked by the same, usual ket symbol, $|\phi\rangle \in \mathcal{H}^{(F,S)}$. The conjugate or bra-vector symbols retain their traditional forms just in the two spaces, with $\langle\phi| \in (\mathcal{H}^{(P)})'$ and with $\langle\phi| \in (\mathcal{H}^{(F)})'$. Thus, the notation convention only remains unclear for the dual *alias* Hermitian-conjugate elements within the second physical Hilbert space $\mathcal{H}^{(S)}$.

In the current THS-related literature, the apparent puzzle is easily resolved by keeping the latter Hilbert space “absent,” that is, *exclusively* present *just* via its representation in $\mathcal{H}^{(F)}$. For the purpose, one merely changes, whenever necessary, the inner product. In other words, the transitions $\mathcal{H}^{(F)} \leftrightarrow \mathcal{H}^{(S)}$ are mediated by the mere replacements of the metric operators, $\Theta^{(F)} (= I = \Theta^{(Dirac)}) \leftrightarrow \Theta^{(S)} (= \Theta \neq I)$. Thus (93), the linear functionals *alias* bra-vector elements of the third dual vector space $(\mathcal{H}^{(S)})'$ may always be chosen and defined, inside the friendly representation space $\mathcal{H}^{(F)}$ and in terms of the *ad hoc* metric Θ , as products $\langle\phi|\Theta \in (\mathcal{H}^{(S)})'$. In fact, while staying in $\mathcal{H}^{(F)}$, we are permitted to abbreviate the related (i.e., F -space conjugate) ket-vector products $\Theta|\phi\rangle$ by a dedicated double-ket symbol, $\Theta|\phi\rangle := |\phi\rangle\rangle$, with the F -space conjugate $\langle\langle\phi| = \langle\phi|\Theta$ as long as $\Theta = \Theta^\dagger$ by construction.

1.5.2.1 Paradox of Two Hamiltonians In the above-mentioned notation, it is very easy to extend the THS scheme to cover the cases where the Hamiltonian is allowed to be time dependent in the primary physical Hilbert space $\mathcal{H}^{(P)}$. Naturally, the prohibitively complicated time-dependent Schrödinger equation

$$i \partial_t |\varphi(t)\rangle = \mathfrak{h}(t) |\varphi(t)\rangle \quad (1.5.1)$$

is still correct and it determines the unitary evolution of the wave functions of the system. In contrast, one encounters a thorough weakening of the physical relevance of the eigenvalues of $\mathfrak{h}(t)$ because the very concept of observable energy only retains its full physical sense and meaning in adiabatic approximation. Secondly, also the role of the general time-dependent isospectral “Hamiltonian” operator $H(t) = \Omega^{-1}(t)\mathfrak{h}(t)\Omega(t)$ becomes influenced by the emergence of time dependence in the Dyson mapping, $\Omega = \Omega(t)$.

According to Ref. (23), the combined effect of time dependence in $\mathfrak{h} = \mathfrak{h}(t)$ and in $\Omega = \Omega(t)$ only manifests itself via the non-Hermitian operator

$$G(t) = H(t) - i\Omega^{-1}(t)\dot{\Omega}(t),$$



where the over-dot represents the derivative with respect to time t . Precisely this operator plays the role of the generator of the time evolution of wave functions, that is, of the ket vector and its Hermitian conjugate bra dual vector in the “standard” physical Hilbert space $\mathcal{H}^{(S)}$. For this reason, we have to replace eq. (1.5.1) by the doublet of the time-evolution equations

$$i\partial_t|\Phi(t)\rangle = G(t)|\Phi(t)\rangle, \quad (1.5.2)$$

$$i\partial_t|\Phi(t)\rangle\rangle = G^\dagger(t)|\Phi(t)\rangle\rangle \quad (1.5.3)$$

represented and to be solved in the friendly Hilbert space $\mathcal{H}^{(F)}$ as usual.

1.5.2.2 Heisenberg-like Frames Naturally, also in the manifestly time-dependent scenario, one may try to proceed in opposite direction, from G to \mathfrak{h} . In such a case, the usual self-adjoint Hamiltonian $\mathfrak{h}(t)$ acting in a primary Hilbert space $\mathcal{H}^{(P)}$ (where, typically, the principle of correspondence may form the background of the preparation of measurements) is not known in advance. In principle, it must be reconstructed from a given and, necessarily, *particularly elementary* non-self-adjoint generator $G(t)$ defined as acting in an auxiliary, preselected but manifestly unphysical Hilbert space $\mathcal{H}^{(F)}$ via eqs (1.5.2) and (1.5.3).

The general scenario has only been discussed in unpublished preprint (95) (cf. also (96)). The simplest choice with time-independent $G(t) = G(0)$ was recently introduced, in (97), as an immediate generalization of the usual fundamental and universal Heisenberg representation of quantum systems. In such a special case, the explicit respective solutions

$$|\phi(t)\rangle = \exp(-iG(0)t)|\phi(0)\rangle, \quad |\phi(t)\rangle\rangle = \exp(-iG^\dagger(0)t)|\phi(0)\rangle\rangle \quad (1.5.4)$$

of non-Hermitian Schrödinger equations (1.5.2) and (1.5.3) degenerate immediately to the common (69) Heisenberg representation rule at the trivial choice of $G^{(Heis.)}(0) = 0$.

1.6 SCYLLA OF NONLOCALITY OR CHARYBDIS OF NONUNITARITY?

The message of traditional textbooks on quantum mechanics may be read as a declaration of necessity of avoiding the nonunitarity of the evolution in time by all means including even the acceptance of a nonlocality of the interactions. This immediately reminds us about the Homer’s story about the six-headed monster Scylla which, together with the all-destroying whirlpool of Charybdis controlled the pass through the Strait of Messina. No surprise that in the mythology of old Greeks the fabulous Odysseus followed the advise by Kirke and that, in order to avoid the deadly Charybdis, he rather sacrificed six of his men to Scylla while saving the rest. In this sense, the “acceptable evil” of Scylla finds its traditional quantum analog in nonlocality. The “Charybdis” of nonunitarity was perceived much more deadly a danger.



Certainly so before the year 1998. For this reason, the Bender's and Boettcher's proposal (5) of working with non-Hermitian generators H of evolution in quantum physics looked, initially, so courageous and counter-Kirke-ish. Still, even their proposal finds a support and parallels in the same old myth. In fact, the message sent by old Greeks is not as straightforward as it might have seemed since during his second trip, Odysseus changed his mind and, having kept safely out of the reach of the Scylla, he still managed to navigate out of Charybdis without any losses at all.

In the present analogy with the story of non-Hermitian Hamiltonians in quantum physics, the second message is certainly encouraging: It allows us to reclassify the Bender's and Boettcher's apparent acceptance of the Charybdis-resembling evils of nonunitarity in 1998 as a promising and well-working strategy.

Of course, it is true that a highly nonstandard care is needed to get through, especially when the most traditional local-potential interactions are used as a dynamical input. These days (i.e., the additional 15 years later, in the year 2013) an updated conventional wisdom still reconfirms that the local models need not necessarily be the most easily tractable ones.

The first signs of a return of pendulum and the first words of warning against too stubborn an insistence on the locality of interactions already appeared around the second, metric-ambiguity crisis in 2004. The threat of the Scylla-resembling nonlocality of the interaction was circumvented and appeared tractable as well. In the influential letter (28), the status of the main energy-complementing physical observable has been transferred from the coordinate x to another quantity C carrying all of the characteristics of a *global, delocalized* charge.

On a higher level of analysis, the dilemma of the choice between the Scylla of nonlocality and the Charybdis of nonunitarity has been reopened. It also reappeared at the very core of the third crisis in 2007 and the fifth crisis in 2013.

1.6.1 Scattering Theory

In the years 1998–2007, we witnessed a virtually uninterrupted success of physics-oriented studies of \mathcal{PT} -symmetric quantum systems defined by non-self-adjoint toy-model quantum Hamiltonians of the traditional form $H = p^2 + V(x)$. During the dedicated series of international conferences “Pseudo-Hermitian Hamiltonians in Quantum Physics” (PHHQ, (16)), people reported the reality of bound-state spectra for a surprising number of various local complex potentials $V(x) \in \mathbb{C}$ defined along suitable complex curves of $x \in \mathbb{C}$. An exhaustive list of these results would have ranged from the original field-theory-inspired models with forces $V(x) = x^2(ix)^\delta$ using an arbitrary nonnegative exponent δ (5, 10) up to an amazingly extensive family of their simplified alternatives (39, 42) including even supersymmetric generalizations (98), many-body systems (99), and deformed-symmetry dynamics (52).

It is rather surprising that during the first years of the study of such a quantum-theory-enriching class of toy-model interactions $V \neq V^\dagger$, practically nobody⁹ paid

⁹i.e., up to a few marginal exceptions (100, 101)



attention to the parallel problem of scattering. Naturally, in a longer perspective, such an omission was untenable.

1.6.1.1 Cross-Shaped-Matrix Metrics and the Loss of Causality Keeping in mind the enormous heuristic success of the concept of \mathcal{PT} -symmetric bound states, it was necessary to turn attention to the phenomenological as well as theoretical aspects of possible further extensions of the theory beyond bound states. Not quite expectedly, a number of new problems emerged.

A definite failure of the theory took place commencing with the remarkable lecture by Jones during PHHQP VI in London in 2007 ((102); cf. also his two subsequent publications (29)). He pointed out that the description of a *unitary* scattering process caused by a *local* \mathcal{PT} -symmetric interaction potential, for example, a complex square well $V(x)$ presents a quantum theory with a dilemma. Either one changes the experimental setting *nonlocally* (i.e., in fact, everywhere), or one must accept (like, typically, the authors of Ref. (45)) that the probability is not conserved.

For the needs of theoretical physicists, the Jones' argument has been based on the Mostafazadeh's choice and study of one of the simplest possible toy-model interactions, namely, of its delta-function form $V(x) \sim \delta(x - x_0)$ (11, 103). This rendered possible an approximate spectral-method construction of the related metric (or rather metrics) Θ . The result appeared enormously important because the construction led to the metric operators, which were *all* strongly nondiagonal in the most common coordinate representation.

The use of such a representation was, naturally, vital for the Jones' considerations about scattering in which such a diagonal plus antidiagonal (i.e., "cross-shaped") matrix form of the metric implied that in the most elementary one-dimensional arrangement of the scattering experiment the two separate asymptotic regions (viz., with $x \ll -1$ and $x \gg +1$, respectively) appeared mutually coupled by the above-introduced matrices Θ (of the metric) and/or Ω (of the Dyson-type mapping), which enter the physical mean values and the measurable scattering cross sections.

Consequently, the causality of the scattering process appeared strongly violated. Such a conclusion requalified all metrics *or* all local potentials $V(x)$ as unacceptable in the scattering models exhibiting \mathcal{PT} -symmetry. In other words, it was necessary to reclassify all of the models based on a local $V(x)$ as deeply nonunitary. For experimental physicists, this simply meant that these models can only be used as "effective" in the sense that the information about the dynamics remains, in general, incomplete.

Up to now, a fully satisfactory way out of such a quandary has not been found. One of the most promising keys to the resolution of the puzzle has been found using a discretization of the coordinates in papers (30). It has been demonstrated there that the theory may remain unitary (i.e., the probability may remain conserved) provided only that one allows for a suitable *restricted, short-ranged* form of nonlocality in the underlying \mathcal{PT} -symmetric interaction potential.

1.6.2 Giving up the Locality of Interaction

The emergence of mathematical difficulties with \mathcal{PT} -symmetric scattering proves intimately related to the necessity of an overall upgrade of the specification of what we



mean by locality and unitarity in scattering experiments. One has to keep in mind, first of all, the mutual connection between the traditional time-independent formulation of the scattering theory and its proper time-dependent upgrades (cf. (23, 104) for an outline of some most relevant technicalities in the latter case).

In the nearest future, the very concept of quantum scattering must be, after transition to generalized, non-self-adjoint forms of the Hamiltonians, duly and thoroughly rethought and modified, therefore. Up to now, the latter problem has only been tackled either from the “extremely sceptical” point of view (sampled by Ahmed (45) and giving up unitarity) or from the nondifferential, discrete-coordinate, “drastically simplified” point of view of Ref. (30).

In the current literature, the majority of papers seems to prefer the preservation of the locality of $V(x)$ to the unitarity of the process. Certainly, for a consistent build-up of the unitary theories, it will be necessary to pay *simultaneous* attention to the judicious specification of a minimally nonlocal interaction as well as to the construction and selection of such a nontrivial metric operators, which would allow us to return to the properly generalized position and momentum observables. Their operators should certainly retain at least a part of their role of observable quantities, in the remote, asymptotic spatial domain at least¹⁰.

1.6.2.1 The First Trick: Equidistant Discretization of the Real Line of x In a methodical *Gedankenexperiment* aimed at a recovery of unitarity, one would have to consider a one-dimensional quantum scattering mediated by a real and slightly nonlocal, integral-operator scatterer U . The underlying integro-differential Hamiltonian $H = -\Delta + \int U(x, \cdot)$ will be admitted non-Hermitian, say, in the conventional Hilbert space $L^2(\mathbb{R}) := \mathcal{H}^{(F)}$, $H \neq H^\dagger$. In the light of Ref. (30), these operators might probably be studied as limits of their discrete approximations. We would expect that one can still keep the scattering unitary via a suitably self-consistent delocalization or “smearing trick” leading to an integral operator $U \neq U^\dagger$. The smearing itself should be short ranged, that is, achieved, in general, via an *ad hoc* replacement $V \rightarrow U$ of the conventional local-interaction operator $V(x, x') = \delta(x - x')V(x)$ by its nonlocal generalization $U(x, x')$ such that, roughly speaking, the value of the latter function of two real variables becomes small whenever the distance $|x - x'|$ becomes large.

Up to now, the problem remains open. From the isolated source (30), we merely know that the related constructive considerations (based, say, on a systematic refinement of the grid) will not be easy in general. In *loc. cit.*, the work was decisively simplified via the replacement of the real axis of coordinates by keeping the distance h between “coordinate grid points” x_n of the *infinite* and equidistant discrete lattice fixed. In the next step, one should allow this distance to shrink to zero, $h \rightarrow 0$, while guaranteeing still the unitarity of the scattering.

1.6.2.2 The Second Trick: the Use of Two-center Bidiagonal Interactions In order to see the whole setting in a more concrete form, let us now add a few details on the construction with fixed h . Firstly, let the kinetic energy operator be represented

¹⁰The authors of Chapters 2 and 3 will say more in this context.

by the conventional negative discrete Laplacian, that is, by the tridiagonal, doubly infinite matrix T with just three nonvanishing constant diagonals,

$$T_{nn} = 2, \quad T_{n,n+1} = T_{n+1,n} = -1, \quad n = \dots, -2, -1, 0, 1, 2, \dots \quad (1.6.1)$$

In such a discretization approximation, the fundamental requirement of the unitarity of the quantum evolution has been decisive during the successful search for several scattering-unitarity-supporting crypto-Hermitian Hamiltonians $H = T + U = H^\ddagger$.

Recalling the results of our paper (105) for illustration, the aim has been reached by studying a class of tridiagonal matrix interactions U , which varied with a single coupling g and which mimicked the existence of the two interaction centers that were separated by a positive distance $\sim 2M$. Naturally, a guarantee of the necessary mutual compatibility between the two nonlocal operators $H \neq H^\dagger$ and $\Theta = \Theta^\dagger > 0$ then became a true technical challenge. Fortunately, after an ample use of computer-assisted symbolic-manipulation experiments, we were able to satisfy all the requirements using the following family of interaction matrices of the (suitably partitioned) form

$$U = \begin{pmatrix} \ddots & & & & & & \\ \ddots & & & & & & \\ & 0 & & & & & \\ & & -g & & & & \\ & & g & & & & \\ & & & 0 & & & \\ & & & \ddots & & & \\ & & & \ddots & & 0 & \\ & & & & 0 & g & \\ & & & & \underbrace{\hspace{2cm}} & -g & 0 \\ & & & & 2M-3 & & 0 \\ & & & & \text{columns} & & 0 & \ddots & \\ & & & & & & & & \ddots \end{pmatrix}. \quad (1.6.2)$$

Let us just summarize the main steps of the construction. First of all, Hamiltonian and metric were required to satisfy a doubly infinite set of linear algebraic relations $H^\ddagger \Theta = \Theta H$. In parallel, according to Jones (29), we had to eliminate the obstinate causality-violating antidiagonal components out of the metric. Finally, what was truly nontrivial was the implementation of the asymptotic causality constraint requiring that the nonnegligible matrix elements of the doubly infinite matrix Θ_{ij} of the metric only occurred in a band of indices such that $|i - j| < K$ at some finite positive integer K and at all of the sufficiently large absolute values of subscripts, namely, at $|i| \gg 1$ and $|j| \gg 1$.

Owing to the lack of space, let us skip the abstract recurrence relations analysis and, instead, let us jump directly to the supportive ‘‘proof by example’’ as provided by Ref. (105). Its essence lies in the choice of an elementary although still sufficiently flexible doubly infinite ansatz for the metric, which would make our Hamiltonian crypto-Hermitian, $H = H^\ddagger$. For this purpose, we first picked up $M = 1$ and obtained



1.6.3 The Threat of the Loss of Unitarity

Mathematically slightly different difficulties emerge in connection with *bound states* generated by differential-operator Hamiltonians $H = T + V(x) \neq H^\dagger$. The obvious phenomenological relevance of the rigorous proofs of reality of the energy spectra of these operators has already been emphasized earlier. The same care must be devoted to the analysis of spectra of candidates Q for other observables (e.g., coordinates). We need not feel bothered by the non-self-adjoint nature of Q s in the false Hilbert space $\mathcal{H}^{(F)}$ where $Q \neq Q^\dagger$ in general. Nevertheless, during the building of a consistent quantum model living in the standard Hilbert space $\mathcal{H}^{(S)}$ with metric Θ , all of these candidates Q must pass the test of reacquired Hermiticity, $Q = Q^\ddagger := \Theta^{-1}Q^\dagger\Theta$.

In paper (24) which may be read as the basic complement of the current textbooks on quantum theory, it has been emphasized that by far the most visible challenge is found in the necessity of the construction of the metric Θ compatible with the Hermitization of *all* of the given set of operators of observables Q . Thus, one cannot perceive the construction of the necessary (and, in practice, rarely easy) *concrete* representations of the underlying standard physical observables as just a technical exercise.

By physics community, it is widely being accepted that the successful use of a diagonalizable non-self-adjoint operator H with real spectrum in quantum theory requires just a successful transition from the false, unphysical Hilbert space $\mathcal{H}^{(F)}$ to its physical amendment $\mathcal{H}^{(S)}$. Although such a step requires a technically complicated assignment of a Hermitizing metric $\Theta^{(S)}$ to the given, possibly even non-self-adjoint observable $H \neq H^\dagger$, physicists generally believe in the feasibility and applicability of such an approach.

The word of strong warning is due. First of all, one should get reminded of the key role of the well-known principle of the classical-quantum correspondence. This is connected with the necessity of an interpretation of measurements. On mathematical side, the loss of Hermiticity of H and all Q s in $\mathcal{H}^{(F)}$ may immediately lead to the necessity of a certain weakening of our requirements of the direct and sharp observability of the coordinate and/or the momentum. *Vice versa*, whenever we insist on the observability status of the coordinate, specific mathematical difficulties may arise¹¹.

1.6.3.1 Metrics May Be Unbounded The possibility of a generic occurrence of metric-related class of conceptual difficulties has been first mentioned, in their unpublished note from 2001, by Kretschmer and Szymanowski (106). They noticed the existence of an inconsistency in the model-building strategy based on the brute-force redefinition (1.4.1) of the inner products. They emphasized that in only too many concrete toy models the formal inner-product-modification and metric-assignment $H \rightarrow \Theta^{(S)}$ leads to unbounded operators $\Theta^{(S)}$. They pointed out that such a choice is in sharp contradiction with the requirements of quantum theory and functional analysis.

¹¹Chapter 3 will throw more light on the problem from the algebraic point of view, with emphasis on the role of the canonical commutation (or anticommutation) relations.



These authors recommended that at least some of the serious technical problems of this type could have been circumvented via the above-mentioned formal factorization of the metrics $\Theta = \Omega^\dagger \Omega$. In our present notation, such a recommendation would imply the necessity of the replacement of H , given as acting in $\mathcal{H}^{(S)}$, by \mathfrak{h} , which is to be constructed as acting in $\mathcal{H}^{(P)}$. Naturally, the merits of working in “standard space” $\mathcal{H}^{(S)}$ or even “friendly space” $\mathcal{H}^{(F)}$ (i.e., with simpler initial H) would be lost. At the same time, this loss would only concern the toy models H for which the physical Hilbert-space representation $\mathcal{H}^{(S)}$, strictly speaking, does not exist at all.

For an explicit illustration of the latter idea, one could recall examples (although, usually, just the ones working with the finite-dimensional matrices H), which may even prove tractable in closed form. There even exists an infinite-dimensional illustration that connects H and $\mathcal{H}^{(S)}$ with \mathfrak{h} and $\mathcal{H}^{(P)}$ in constructive manner. It has been described in the older study (12) where the authors studied the quartic anharmonic oscillator possessing the wrong sign in the asymptotic $|x| \gg 1$ domain, with $V(x) = -x^4 + \mathcal{O}(x^3)$. Owing to the simplicity of the model, the authors were able to choose operators Ω in a next-to-elementary Fourier plus change-of-variables form. The self-adjoint partner Hamiltonian $\mathfrak{h} = \mathfrak{h}^\dagger$ in $\mathcal{H}^{(P)}$ has been then obtained in a closed form of another *local* quartic oscillator. Finally, the correct physical content of the model was fairly easy to specify (cf. a rediscovery of the methodical merits of this model in Ref. (75)).

1.6.3.2 The Metric’s Inverse May Be Unbounded Excluding the models without bounded metric as incomplete, the formal, purely mathematical sources of the possible failure of the whole three-Hilbert-space recipe remain threefold. Firstly, in purely technical sense, even the most popular (i.e., typically, the most common linear differential second-order) input-physics operators $H \neq H^\dagger$ may fail to admit the *feasible* construction of *any* sufficiently tractable S -space metric. For illustration see, for example, the constructions presented in Ref. (107) where even for the most elementary toy-model choices of H , the representations of $\Theta = \Theta(H)$ remain over-complicated and formal, not sufficiently clearly defined.

Secondly, in phenomenological context, even a truly extreme simplicity of the toy-model H enabling one to find some (or even all—cf. (108)) eligible metrics in a tractable form encounters the challenging ambiguity of the assignment $H \rightarrow \Theta(H)$. This point (i.e., a true physical background of the model in question) is usually not discussed with due care. In principle, an additional information about the dynamics is *always* required (24).

Thirdly, even if one deals with a theory in which the *pair* of operators H (= observable) and Θ (= physical Hilbert-space metric) is given as a complete dynamical information input in advance, one has to verify the compatibility of these operators with several *mathematical* postulates as imposed by functional analysis. As we saw earlier, it is not even so easy to prove the necessary reality and semi-bounded nature of the spectrum of H itself¹². In parallel, a double trouble occurs when one must add a

¹²Cf., in this respect, refer Chapters 4 and 5.



more subtle guarantee of the positivity and the boundedness of the metric operator Θ and its inverse.

During the eleventh PHHQP meeting in Paris in 2012 (109), the attention of attendees happened particularly intensively concentrated on the latter set of difficulties. Consequently, after circa 15 years of an apparently peaceful coexistence of the PT-symmetry-studying mathematicians and physicists, the idyll definitely ended. The community of specialists became split in the group of “traditional optimists” and “deep sceptics.” During 2012, the latter group took the initiative.

The rigorous treatment of the above-mentioned questions resulted into a new and particularly deep crisis in the field. In particular, Siegl and Krejčířík (36) discovered a very subtle although utterly decisive gap in the habitual description of the imaginary cubic oscillator, that is, of one of the most popular and appealing benchmark illustrations of the theory. Using the rigorous tools of operator theory, these authors revealed and demonstrated that their critique applies to many other popular physical examples, based on the use of the *local* \mathcal{PT} -symmetric interactions when considered from the semi-classical-analysis point of view. In the language of mathematics, the main source of such a subtle criticism of multiple apparently crypto-Hermitian Hamiltonians lies in the innocent-looking violation of the condition of the bounded nature of the inverse-metric operator Θ^{-1} . At present, the true consequences of such an observation are still to be explored¹³.

1.7 TRENDS

Immediately after the PHHQP 2012 meeting in Paris, it became clear that it would be truly necessary to initiate an intensification of communication between mathematicians and physicists. A few months later, our present book has been designed, therefore, as a project which could sufficiently efficiently map the theoretical terrain and which could reunify the community while emphasizing the rigorous interpretation and resolution of the existing problems.

At present, a new round of attempted amendments of the formulation of the theory started (cf., e.g., (37) or (38)). Currently, we are witnessing a new wave of quick developments in the area¹⁴.

1.7.1 Giving Up Metrics

One of the almost amusing paradoxes which paralleled the emergence of the above-listed mathematical difficulties with ill-defined metrics may be seen in a few parallel declarations of their almost negligible relevance and impact on practical applications of quantum theory. For illustration, let us recall a few samples of such “heresies,” starting from many-body quantum physics again.

¹³An updated account of the current situation may be found described in Chapters 6 and 7.

¹⁴In this sense, Chapter 7 may be read as sampling a few new horizons for future research.



1.7.1.1 Coupled-Cluster Variational Method Naturally, the IB Dyson-inspired mappings Ω are amenable to various generalizations. Even in the comparatively narrow domain of nuclear physics, the IB model-building pattern based on the use of non-self-adjoint Hamiltonians finds a nonequivalent analog in the so-called coupled-cluster method (CCM, cf. Ref. (110) for a truly thorough review and for an extensive list of older references).

Besides a partial parallelism in the assumptions (the CCM approach also starts from the knowledge of \mathfrak{h} defined in $\mathcal{H}^{(P)}$), the main differences lie in the purpose. The CCM calculations seem less ambitious—their first aim is a maximally precise determination of the ground state of a given many-body quantum system. In such a sense, the CCM calculations are less universal. They offer an algorithm that merely requires an elementary input guess of the ground-state eigenket of the prospective non-Hermitian operator H (i.e., of $|0\rangle \neq |0\rangle\rangle$). The rest of the CCM construction proceeds via a systematic reconstruction of an optimal Dyson-resembling map Ω . As long as the latter operator is sought via a specific exponential ansatz $\Omega = \exp S$, the method is often called “exp S method” in the literature.

1.7.1.2 Non-Hermitian Proto-Metrics $\tilde{\Theta} \neq \Omega^\dagger \Omega$ The high and well-tested practical numerical efficiency of the CCM approach seems more than compensated by several of its theoretical shortcomings. One of them may be seen in the fact that the method puts too heavy an emphasis on the optimal Hamiltonian-adapted reconstruction of the operator $\Omega^{(CCM)} = \exp S$. This is achieved at a cost of just very rough and approximate reconstruction of a far-from optimal operator \tilde{S} playing, in effect, the role of the metric, $\tilde{S} = \Theta^{(CCM)} \neq I$.

From the abstract and consequent THS point of view, the latter metric is not sufficiently well defined. Still, the numerical efficiency of the CCM recipe leads us to the belief that there must exist a way out of the difficulty. For this purpose, it would be necessary to circumvent, first of all, the obstacles represented by the manifest non-Hermiticity of the CCM “proto-metric” $\tilde{S} \neq \tilde{S}^\dagger$. A return to Hermiticity of this operator may be perceived as one of the most important challenges in the further development of the CCM formalism (111).

1.7.2 Giving Up Unitarity

In 2010, the weakening of emphasis on the explicit constructions of metrics Θ led, in parallel, to a certain loss of concentration on the problem of the stable quantum systems and to a perceivable growth of activities in the neighboring areas of physics and mathematics. In the latter, mathematical context, more attention has been paid to the subtleties of differences between the role and behavior of bases and operators in finite- and infinite-dimensional Hilbert spaces \mathcal{H} . Some of the emerging new ideas may be found, for example, in recent reviews (53) or (112).

1.7.2.1 Open Quantum Systems In spite of a strict concentration of the forthcoming chapters of this book on the rigorous mathematical study of problems *inside* quantum theory of stable systems, the potential future impact of these results will



involve, paradoxically, also several other branches of physics *outside* such a restricted area. Such an effect is well known in all of the science and it certainly will apply also in the present, narrower “hidden Hermiticity” context. In this chapter, unfortunately, we were only able to devote a very limited space to a few comments and references concerning the open quantum systems possessing, typically, complex spectra (cf. Section 1.3).

1.7.2.2 Resonances This being said, it still makes sense to add that already as early as during the third PHHQP meeting in 2005 (113) the interdisciplinary appeal of the concepts of \mathcal{PT} -symmetry and/or pseudo-Hermiticity attracted attention of nonspecialists. The first consequence was that the traditional participants of this series of meetings were complemented by mathematicians and/or physicists who were mainly interested in the apparently remote fields of nonreal spectra and/or the unstable, resonant quantum states, respectively.

The progress in the research certainly profited from the resulting cooperations and from the extension of the field¹⁵.

1.7.2.3 Phase Transitions Once the attention of the community has been reattracted to the intriguing possibility of simulation of phase transitions caused by the loss of the reality of spectrum during a *smooth* variation of couplings or some other parameters that control the dynamics, a new field of research has been opened. In the language of mathematics, many Hamiltonians H and many other operators Q of quantum observables may lose the reality of their eigenvalues. By definition, this occurs at the Kato’s (56) exceptional-point value of the parameter. In the context of quantum physics, the very new and very important distinctive feature of the use of manifestly non-self-adjoint operators of observables $Q = Q(\lambda) \neq Q^\dagger$ is that such a phase-transition-mediating exceptional point value of parameter may prove *real*, that is, in principle, accessible to manipulations and to an *ad hoc* variation in experimental setups.

1.7.3 Giving Up Quantization

While the (real or complex) variable parameter λ crosses an exceptional-point value $\lambda^{(\text{EP})}$ for a realistic quantum Hamiltonian $H = H(\lambda)$, we may speak about the transmutation of bound states into resonances. As long as such a step returns us back to the huge area of traditional quantum phenomenology, it is not too surprising that in quantum physics, the specialists did not see much difference between the real and complex values of $\lambda^{(\text{EP})}$. Thus, many people admitted that the complexification of the spectrum of energies may keep the underlying quantum system phenomenologically interesting in spite of the obvious fact that the evolution of the system in time ceased to be unitary.

¹⁵cf. the proceedings of the third PHHQP conference which were published as a special issue of the Czech Journal of Physics in September 2005 (18).



Unexpectedly, the phenomenon of the system's crossing the EP boundary attracted the attention of experimentalists who found a new and fairly exciting field for *simulations* of the phenomenon in *classical*, nonquantum systems.

1.7.3.1 Interdisciplinary Aspects of Exceptional Points In the motivating and experiment-related context of physics and phenomenology, people always paid attention to the detailed analyses of various quantum and nonquantum systems in a close vicinity of their exceptional-point singularities. Still, in a way inspired by an unprecedented increase in popularity of quantum systems exhibiting \mathcal{PT} -symmetry during the past 15 years, many older studies of the physics near exceptional points acquired, suddenly, an entirely new relevance (cf., e.g., the talks for a dedicated Workshop, in NiTheP in Stellenbosch, in 2010 (57)). Mutual connections were found between the behavior of the atoms and molecules in external fields as produced, say, by lasers. In addition, the states of the classical electromagnetic field in a microwave billiard were found to share the same mathematical structures (114). The control of the schematic classical models of magnetohydrodynamics (115) was found similar to the quantum models of phase transitions, and so on.

The theoretical study of exceptional points acquired an undeniably interdisciplinary character. At random, an introductory review of a randomly selected sample of references may start, say, in the domain of classical optics. A strict formal analog of the usual quantum Schrödinger equations has been found there, shortly after the PHHQ 2007 meeting in London (116), in the so-called paraxial version of the classical equation for the diffraction, say, in two dimensions (117) (one should also refer to the older paper (101) in this respect). In the role of a \mathcal{PT} -symmetric quantum potential $V(x)$, one finds here, typically, a position-dependent complex refractive index $n(x)$, which remains constant along the z -axis (this axis mimics the time in Schrödinger equation) while exhibiting a suitable elementary gain-or-loss spatial structure along the transverse, "spatial" x -axis.

In this comparison, the classical electric-field envelope of the laser beam (which is, clearly, observable) plays the role of the quantum wave function (which was, naturally, NOT observable). It is not too surprising, therefore, that one immediately arrives at the entirely new observable features of the beam including the double refraction patterns and their power oscillations as well as nonreciprocal diffractions.

What followed the first papers and simulations in the field led not only to an experimental heyday (for a randomly selected sample of references cf. (118)) but also to the inspiration and feedback for the quantum theory of nuclei (119) and for quantum electronics (120), and so on. In addition, the search for a reunification of vocabularies of mathematics and physics continued. People moved, spontaneously, beyond the rather restricted area of study of non-self-adjoint operators with real spectra. After the complexity of the energies was admitted, one of the most natural phenomenological targets for extension of the projects has been found in an extensive search for non-quantum analogs of the traditional unstable quantum systems. The reasons for staying restricted to the field of quantum physics faded away. A number of applications of new project-setting ideas has been published, during the past 3 or 4 years, in the subdomains of physics as remote as quantum condensed-matter physics or classical optics.

Once we return back to mathematics, the quick growth of the overlap between the pragmatically and theoretically oriented studies implied an improvement of our understanding of the properties of the self-adjoint operators in the Krein or Pontriagin spaces. The contemporary forms of the applied functional analysis and spectral theory proved useful for the purpose. Thus, nowadays one finds a true challenge in presenting the new physics in the fully rigorous language of standard mathematics.

1.7.3.2 Outlook The quantum interpretation of the Kato's exceptional points as the values of parameters at which the unitarity of the evolution gets lost initiated multiple new theoretical studies beyond quantum physics. In most of these cases, such a loss of stability is still being interpreted, in the newly invented terminology, as a manifestation of the spontaneous breakdown of PT symmetry.

It is not surprising that under the new name, the old phenomenon immediately attracted new attention. Thus, experimentalists are currently trying to simulate such a form of phase transitions in multiple traditional contexts. At present, the subject of these studies ranges from optical absorbers (121) to Bose–Hubbard dimers (122) to spin chain models (123) or, if you wish, from quantum lattice models (124) to higher derivative Hamiltonians (125), and so on. In the literature, one even finds applications using the concepts of pomeron (126) or of the coupling of reaction channels (127), and so on.

The study of related mathematical methods received an equally strong impulse for the development of new ideas about coherent-state quantization techniques (128) and about their path-integral realizations (129). The rotation-operator analogs of parity (130) were studied, and the updated view of the role of the transfer matrices was presented in Ref. (131). Other methodical proposals involved also the density matrices in thermodynamics (132) or the random matrix ensembles in stochastic systems (133), and so on.

New perspectives were opened and the related upgrade of the research in mathematics blossomed. Besides the innovative new applications of the traditional Krein-space theory (134), people made a successful use of the formalism of Moyal products (135) and the ideas of the canonical classical-quantum correspondence (136). Needless to add that the applicability-oriented support of the latter efforts remained strong and broadening. New demand of rigorous background is now coming from classical electrodynamics and from the theory as well as increase in sophistication of lasers (cf. (137)), and so on. Once one admits, in mathematical formulation, the admissibility of the loss of the robust reality of the spectrum of an operator, the notion of a quantum bound state must be replaced, in quantum-theory setting, by phenomenologically more appropriate concepts that need not originate just from the needs of quantum physics.

At present, unfortunately, the global scientific community remains often separated into multiple narrow-minded subcommunities. This may be noticed to lead to a slow loss of a stable unifying communication ground and common language. Typically, having separated physicists into groups of “theoretical physicists” and “mathematical physicists,” Roman Kotecký, in his essay (138), tried to analyze the points of contact between similar subcommunities and he emphasized the need of their collaboration. We share this view. Besides the collaboration between mathematicians and physicists

during conferences (16), there exists a hope that these two subcommunities will often break the traditional isolationistic bad habits and that they will keep communicating, in the future, also via some shared publication efforts sampled by this book.

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