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Nimrod Moiseyev
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1

Different formulations of quantum mechanics

This book is dedicated to the non-Hermitian formalism of quantum mechanics. In this chapter we wish to give the motivation and the rational for developing a non-Hermitian formalism to quantum mechanics. Therefore this chapter will not explain how non-Hermitian calculations are carried out or in what way the non-Hermitian formalism is analogous to the standard (Hermitian) formalism of quantum mechanics. It is important to emphasize that there is no (known) transformation which enables one to map results which were obtained using one formalism to the other one. Yet, the same physical results should be obtained by studying the same phenomenon using the two formalisms. If this is the case, why should one bother to develop an alternative formalism to the standard Hermitian formalism of quantum mechanics?

There are several reasons for doing this and here we shall focus on five of those reasons.

(1) *There are phenomena which can be explained in a straightforward fashion using the non-Hermitian formalism but are very hard and often impossible to explain within the framework of the standard (Hermitian) formalism of quantum mechanics.*
In particular in Chapter 9 we will describe several physical phenomena which are associated with the self-orthogonality where two or more degenerate resonance states are coalesced.

(2) *There are physical phenomena which one might not immediately associate with quantum behavior where the quantum language can be used to describe the physics.*
The studied problem may be, for example, in systems described in terms of classical statistical mechanics, diffusion in biological systems, or propagation of light in waveguides (WG). In such cases the Hamiltonians are not Hermitian since the system at hand is open to interaction with its environment. For example, when light is propagated in an optical WG within the paraxial approximation the scalar Maxwell equation is like the time-dependent Schrödinger equation with a time-independent Hamiltonian. The square of the index of refraction (with a minus sign) serves as a potential

energy term in quantum mechanics. The propagation axis Z serves as time in quantum mechanics. The imaginary part of the complex index of refraction indicates the amount of absorption loss of the propagated light when it passes through the wave guide. The complex potential renders the Hamiltonian non-Hermitian and therefore such systems can be only studied within the framework of the non-Hermitian formalism discussed here.

(3) *Simplification of numerical propagation of wave packets in time.*
The propagation of matter waves by the Schrödinger equation and the propagation of light in waveguides in the paraxial approximation are associated with two different physical phenomena but they obey the same mathematical equation. The numerical propagation of wave packets is much more simple when taken within the framework of the non-Hermitian formalism of quantum mechanics rather than in the standard (Hermitian) formalism. This is due to the inclusion of a reflection-free complex absorbing potential (RF-CAP) in the Hamiltonian which attains non-zero values only in the non-interacting region in the coordinate space where the physical potentials vanish. This approach enables one to avoid the artificial reflections from the edge of the numerical grid when a finite number of grid points (or a finite number of basis functions) are used to describe a propagated wave-packet. By adding the complex non-Hermitian potential to the Hamiltonian one can carry out numerical calculations using a finite number of grid points or a finite number of basis functions (after all, our computers are finite) and have a numerically exact propagated wave-packet in the region where the RF-CAPs vanish. By numerically exact, we mean that the wave-packet which is obtained by introducing a RF-CAP into the calculations, is exactly as the wave-packet which would be calculated (if it were possible) by computers which are infinite (i.e. infinite capacity, memory and computational power). The derivation of RF-CAPs by carrying out a smooth exterior scaling transformation of the spatial coordinates is presented in Chapter 5.

(4) *Another numerical example for the advantage of the use of the non-Hermitian formalism over the standard one is when the dynamics of a given system can be described by a small number of resonance states.*
Often it is enough to describe the dynamical process and to calculate all possible measurable quantities just from a single resonance state. See, for example, in Chapter 8, the calculations of the high-harmonic-generation (HHG) spectra (i.e. the emitted high frequency radiation) and the calculations of the above-threshold-ionization (ATI) spectra from a single quasi-energy photo-induced resonance state when atoms or molecules interact with strong laser fields.

(5) *Within the framework of the non-Hermitian formalism of quantum mechanics, one can get a better understanding of different methods and theories developed in the standard (Hermitian) formalism of quantum mechanics.*
The first example is the Rayleigh–Schrödinger perturbation theory where the full Hamiltonian is defined as $\hat{H} = \hat{H}_0 + \lambda \hat{V}$, where λ is the perturbation strength parameter. The interesting non-trivial cases occur when $\hat{H}_0$ and $\hat{V}$ do not commute. The radius

of convergence of the perturbation expansion for the eigenvalues and the eigenfunctions is $|\lambda_{\text{bp}}|$, where λ_{bp} is a complex branch point associated with a self-orthogonal state where several (usually only two) eigenfunctions of the full Hamiltonian coalesce. The nature of these branch points and a method to calculate them and thereby to determine the radius of convergence of a perturbational series expansion of the eigenvalues and eigenfunctions is described in Chapter 9. Another example is the calculations of the poles of the scattering matrix for many-body problems. Within the framework of the standard formalism of quantum mechanics it is very difficult, if not impossible (by the available computational facilities), to calculate the poles of the scattering matrix for many-electron atomic or molecular systems. This is particularly true when considering the electronic correlations which are missing in mean field approximations (e.g. Hartree Fock calculations for fermions and Hartree calculations for bosons). In the non-Hermitian formalism the poles of the scattering matrix can be directly obtained by calculating the complex eigenvalues of the non-Hermitian Hamiltonian, as described in Chapters 4 and 5, for time-independent and time-dependent Hamiltonians.

1.1 Hermitian operators: a brief review

A fundamental postulate in standard quantum mechanics is that any measurable dynamical quantity is represented by a Hermitian operator. This postulate results from another postulate in quantum mechanics which states that the quantities we observe are the eigenvalues of operators which represent the measurable quantities. Since measurable quantities such as the momentum of free particles or the energy of stable atoms and molecules are real quantities, the operators which represent them should be Hermitian operators. For example, the x-component of the momentum, $\hat{p}_x$, is represented by $-i\hbar\partial/\partial x$, the Hamiltonian is represented by $\hat{H}$, etc. However, these operators, $\hat{O}$, which represent measurable dynamical quantities, are Hermitian provided that they operate on functions which belong to the Hilbert space $\mathcal{H}$ of square integrable functions such that if f and g are square integrable functions, $f, g \in L_2(\mathbb{R}) = \mathcal{H}$, or have asymptotes which are periodic functions, they satisfy

$$\langle f|\hat{H}|g\rangle = \langle g|\hat{H}|f\rangle^* . \qquad (1.1)$$

As a consequence of this postulate there are a series of theorems that serve milestones in the formalism of quantum mechanics. The eigenvalues of Hermitian operators are real and expectation values of any measurable quantity are real. The eigenfunctions of Hermitian operators can serve as a complete set in the series expansion of any wavepacket (including time-dependent wavepackets) that represent the system under study. That is, $|\Psi\rangle = \sum_j c_j|j\rangle$, where $\hat{O}|j\rangle = o_j|j\rangle$. The

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absolute value of any one of the expansion coefficients, $|c_j|^2$, is the probability of measuring a specific quantity, o_j.

Exercise 1.1

Since the standard formulation of quantum mechanics defines physical operators as Hermitian we have to stress here that **the Hermitian property of an operator is heavily dependent on the basis set which is used to represent a dynamical variable by matrices of infinite order**. It is commonly assumed that these matrices obey the usual laws valid for finite matrices. However, it is obvious that this is not necessarily always true. Show that $\hat{p}_x^3 = (-\mathrm{i}d/dx)^3 \equiv \mathrm{i}d_x^3$ is not Hermitian when particle-in-a-box eigenfunctions, $\{\phi_n(x)\}_{n=1,2,\ldots}$, are used as a basis set. Associate it with the fact that $\mathbf{P}\mathbf{P}^2 \neq \mathbf{P}^2\mathbf{P}$, where $\mathbf{P}$ is an infinite order Hermitian matrix that represents the momentum operator for a particle in a box, and its square $\mathbf{P}^2$ is well defined and diagonal.

We should emphasize here that the kind of non-Hermiticity of an operator demonstrated in Ex. 1.1 which is associated with the momentum operator is **not** the type which we commonly discuss in this book. **All the non-Hermitian properties of the Hamiltonian which will be discussed in this book result from the potential energy term in the Hamiltonian**. There are two different types of local potential energy term which render the Hamiltonian of the studied system non-Hermitian. The first type are potentials that in standard (Hermitian) formalism of quantum mechanics support a continuous spectrum. The second type of potentials are complex local potentials.

1.2 Non-Hermitian potentials which support a continuous spectrum

The potentials of open systems describe ionization or dissociation or any other phenomenon where the system under study breaks up into freely moving non-interacting subsystems. When a system is in a metastable state (so called a resonance state) it has enough energy to break up into several subsystems. A given system can arrive at a metastable resonance state in a full collision process where the target and the projectiles form an “activated complex” as they collide, which can be considered as a system that has the energy to break up into subsystems. A more natural way to create a system in a metastable resonance state is in a half collision process. In half collision processes the energy can be pumped into the system by many different ways. For example, by applying a static field, by exposing the system under study to weak or strong lasers, by using accelerators, or by heating. The systems can be, for example: nuclei, atoms, molecules, solids, nano-structured materials, and condensates. The subsystems might contain elementary particles and/or neutral or negative/positive charged atomic or molecular ions. Systems where dynamical behavior is controlled by resonances can be, for example, as small as protonium or helium atoms or as large as proteins.

Different situations where energy is pumped into a system giving it enough energy to break up into subsystems are described in the next chapter. We focus in the next chapter on resonance phenomena which are associated with systems that do not break up immediately into subsystems although they have the energy to do so, but rather remain stable for long periods of time. As time passes the outgoing subsystems reach a detector where the energy and momenta can be measured precisely. Since the momenta are eigenvalues of the momentum operator it seems that the detectors measure the wave-vectors of plane waves, $\{\mathbf{k}_j\}_{j=1,2,\dots}$, where the measured momentum vector of the j-th particle/subsystem is given by $\hbar\mathbf{k}_j$. Therefore, it is very natural to associate the metastable resonance states of the system with ***stationary*** *solutions of the* ***time-independent*** *Schrödinger equation with* ***outgoing*** *asymptotes rather than with non-stationary wavepacket solutions of the time-dependent Schrödinger equation*. We will show in the following chapters that, even when the system interacts with time periodic electromagnetic fields, resonances can be associated with quasi-stationary solutions.

Exercise 1.2

Often in experiments the detectors measure the momenta of the outgoing particles/subsystems. Because of the uncertainty relation in quantum mechanics we know that it is impossible to measure precisely both the positions and the momenta of the outgoing particles/subsystems. However, it is possible to build detectors (antennas) that measure precisely the momenta of the outgoing particles/subsystems. Is there violation of the uncertainty "principle" since we know precisely the location of the antenna that measures the momenta of the outgoing particles/subsystems?

Here we are coming to a critical point in our discussion of the resonance phenomena. By imposing outgoing boundary conditions on the eigenfunctions of the time-independent Hamiltonian (we will extend this approach also to the time-dependent Hamiltonian in Chapter 4) two kinds of solutions are obtained. The first type of solution is the bound states. The second type of solution is the resonance states which are associated with complex eigenvalues and eigenfunctions which are **not in the Hermitian sector of the domain of the physical Hamiltonian**.

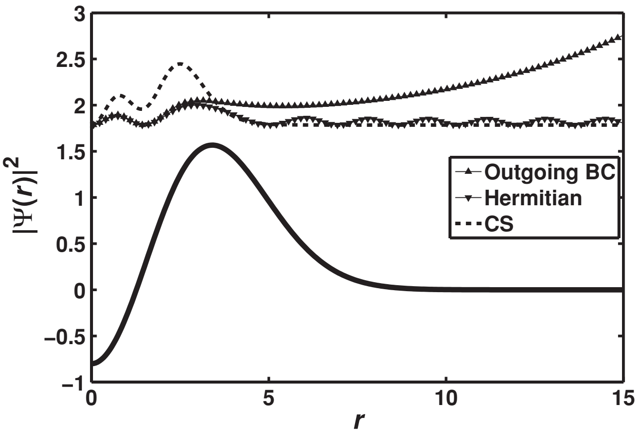

Figure 1.1 The *second* longest living resonance state for a spherical potential, $V(r) = (r^2/2 - 0.8)\exp(-0.1r^2)$, obtained by carrying out three different types of calculation. The model potential is plotted using a full dark line.

These complex resonance eigenvalues are associated with the complex poles of the scattering matrix derived within the framework of the standard (Hermitian) formalism of quantum mechanics. We will explain the properties of the resonance complex eigenvalues and eigenfunctions in detail in Chapters 4–6. As we will show in this book, the use of the resonance states as a basis set in describing full collision and half collision processes has both conceptual and numerical advantages over the standard approach. First, in many cases the dynamical process can be described as a linear combination of a small number of resonance eigenstates (i.e. solutions of the time-independent Schrödinger equation obtained by imposing outgoing boundary conditions). Often only one resonance state dominates the dynamics. In such cases, even without doing any computations one can find out what the potential parameters are which should be varied in order to control the dynamics. The variation of potential parameters can be done by selecting different type of atomic, molecular or mesoscopic systems, or by varying the structure of the system as in the case of quantum dots, quantum wells and waveguides or by varying the laser parameters when photo-induced dynamics is under study. For instance, it is quite difficult and often impossible to explain the results of experiments where the electronic and nuclear coordinates are strongly coupled to one another, such as in the case of scattering of electrons from molecules or in the scattering of anti-protons from atoms. As we will show in Chapters 4–9, within the framework of the non-Hermitian formalism of quantum mechanics we can explain the results of such experiments.

In order to illustrate the advantages in using non-Hermitian quantum mechanics for studying the resonance phenomenon, we show here in Fig. 1.1 the metastable resonance states for a particle in a spherically symmetric potential barrier given by

$$V(r) = (r^2/2 - 0.8)\mathrm{e}^{-0.1r^2} \qquad \{0 \le r \le \infty\}\,. \tag{1.2}$$

Note that the cross section of this potential in any given direction supports two barriers separated by a potential well. The s-waves eigenfunctions which are associated with the resonance phenomenon were calculated numerically by three different approaches: (1) using the Hermitian formalism of quantum mechanics; (2) using the non-Hermitian formalism by imposing outgoing boundary conditions (BC) on the solutions of the time-independent Schrödinger equation; (3) using the complex scaling method (CS) where the Hamiltonian becomes non-Hermitian due to rotation of the coordinate into the complex plane, i.e., $r \to r\exp(+\mathrm{i}\theta)$. In this method we calculate the square-integrable eigenfunctions which decay to zero as $r \to \infty$. These functions are associated with complex eigenvalues which are θ-independent (provided that θ gets to sufficiently large values). In this case the Hamiltonian is non-Hermitian due to the use of the complex scaling technique and not because of the requirement of outgoing boundary conditions.

The non-Hermitian methods for the calculations of resonance energies and wavefunctions will be described briefly in this chapter and in greater detail in Chapters 4–5. The resonance phenomenon in this case is related to the fact that a wavepacket which is initially localized inside the potential well remains localized for quite a long period of time. The different types of physical resonance phenomenon in nature are described in detail in the next chapter since resonances are one of the most interesting phenomena in physical sciences.

We now closely examine the manifestation of the resonance phenomenon in each of the approaches described above.

(1) In the first approach we calculated the s-wave continuum eigenfunctions of the Hamiltonian $\hat{H} = -0.5\partial_r^2 + (r^2/2 - 0.8)\exp(-0.1r^2)$ within the framework of the standard formalism of quantum mechanics. In Figs. 1.1 and 1.2 we show the results obtained by the Hermitian calculations for $E = \mathrm{Re}(E_{\mathrm{res}})$, where E_{res} are complex poles of the scattering matrix. To avoid the relatively complicated calculations of the scattering matrix (we discuss this approach in Chapter 3) we first evaluated the poles of the scattering matrix using the non-Hermitian formalism of quantum mechanics. Knowing the relevant values we proceeded to calculate the relevant continuum functions for two energies. One case is when $E = \mathrm{Re}(E_1^{\mathrm{res}}) = 1.784582$ au and the other case is when $E = \mathrm{Re}(E_2^{\mathrm{res}}) = 2.455696$ au. As one can see from the results presented in Fig. 1.1 for the first case, the Hermitian continuum function is localized inside the potential well and has only very weak oscillations outside the potential barrier. However, in the second case, shown in Fig. 1.2, the situation is very different and it is hard to distinguish between the continuum function $\Psi^{QM}_{E=2.455696}(r)$ which is obtained by the

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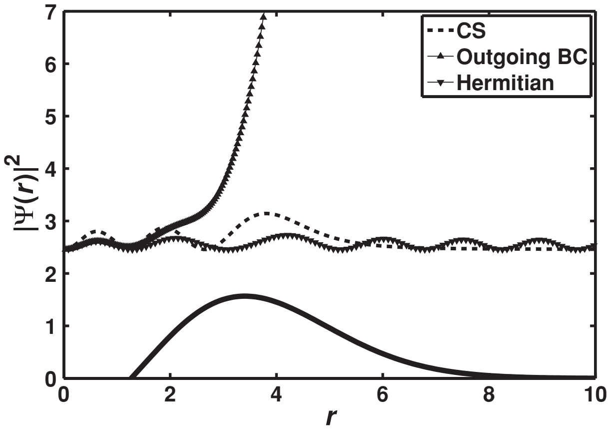

Figure 1.2 The *third* longest living resonance for a spherical potential, $V(r) = (r^2/2 - 0.8)\exp(-0.1r^2)$, obtained by carrying out three different types of calculation. The top of the potential barrier is plotted using a full dark line.

standard (Hermitian) quantum mechanical calculations and any other continuum solution which typically has a larger amplitude in the external region than in the internal region (i.e., inside the potential well). Therefore, within the Hermitian formalism of quantum mechanics the continuum functions associated with energy-eigenvalues which are equal to the real parts of the complex resonance poles are not necessarily localized in the interaction region and are not necessarily very different in their nature from other continuum functions. Note that even for the first case where the Hermitian continuum function is localized inside the potential well there are infinitely many other continuum eigenfunctions that have the same structure. Roughly speaking, any eigenfunction which is associated with an energy-eigenvalue E of the Hermitian Hamiltonian in the range

$$\mathrm{Re}(E_1^{\mathrm{res}}) - \Gamma_1^{\mathrm{res}}/2 < E < \mathrm{Re}(E_1^{\mathrm{res}}) + \Gamma_1^{\mathrm{res}}/2\,, \tag{1.3}$$

where $\Gamma_1^{\mathrm{res}} = 2\mathrm{Im}(E_1^{\mathrm{res}}) = 0.34750$ au, looks similar to the Hermitian continuum function shown in Fig. 1.1. This is the reason that within the framework of the standard formalism of quantum mechanics the resonance phenomenon is associated with the dynamical behavior of wavepackets rather than with a single stationary solution of the time-dependent Schrödinger equation.

(2) Now we repeat the calculations while imposing outgoing boundary conditions on the solutions of the time-independent Schrödinger equation. That is, we demand that $\psi(r \to \infty) = C\exp(+ikr)$. As mentioned above and as will be discussed in detail in Chapter 4, in this case the eigenfunctions are not in the Hermitian sector of the domain of the Hamiltonian and E will attain complex discrete values, E_n^{res}, where here, for example, $E_1^{\mathrm{res}} = 1.784582 - 0.173750\mathrm{i}$ au and $E_2^{\mathrm{res}} = 2.455696 - 1.111399\mathrm{i}$ au. Note

that the inverse of $\Gamma_n^{\text{res}} \equiv -2\text{Im}(E_n^{\text{res}})$ provides the lifetime of the nth resonance state. As Γ_n^{res} increases the lifetime of the metastable state is shorter. The calculations are simple and straightforward. Figures 1.1 and 1.2 show the second and third longest living resonance states obtained by the non-Hermitian quantum mechanical calculations. Their asymptotes diverge exponentially and therefore neither of the resonance wavefunctions are embedded in the Hermitian sector of the domain of the Hamiltonian. That is clear in spite of the fact that when outgoing boundary conditions are imposed the resonance states are uniquely defined and can be easily evaluated for one-dimensional, one-particle problems. However, it is hard to develop a coherent quantum mechanical theory using functions which are not bounded and can not be expanded by orthonormal square integrable functions (embedded in the Hilbert space).

(3) The third approach we use here, which will be described in detail in Chapter 5, is in a sense a "trick" to change the asymptotical behavior of the non-Hermitian resonance wavefunctions by rotating the coordinates into the complex plane. For example, the simplest way to perform such a procedure is by taking $r \to r\exp(i\theta)$. The complex scaled resonance eigenfunction which has been obtained by imposing outgoing boundary conditions on the solutions of the time-independent Schrödinger equation is a square integrable eigenfunction of the complex scaled Hamiltonian. The mathematical justification for the use of this type of non-unitary transformation and its limitations will be discussed in Chapter 5. At this time we wish to point out the motivation for using this approach. The results presented in Figs. 1.1 and 1.2 show that upon complex scaling both of the short-living resonance wavefunctions are square integrable and decay exponentially to zero as $r \to \infty$. Therefore, due to the rotation of the coordinate into the complex plane, both of the resonances are embedded in the generalized Hilbert space and can be expanded by a set of orthonormal square-integrable basis functions. This property enables us to develop a non-Hermitian quantum mechanical theory and computational methods for calculating resonance energies, lifetimes and cross sections. From the results presented in Section 1.1 one might get the (wrong) impression that in the Hermitian and non-Hermitian pictures the resonance wavefunctions look alike. However, they are very different in their nature. The non-Hermitian resonance eigenfunction is associated with a complex eigenvalue whereas the Hermitian solution is associated with a real eigenvalue. The asymptote of the non-Hermitian complex scaled resonance function decays to zero whereas the Hermitian resonance wavefunction oscillates. The results obtained from the Hermitian and the non-Hermitian (complex scaling) calculations for the third longest living metastable (resonance) state in Fig. 1.2 are very different. This resonance has a very short lifetime since $1\,\text{au} = 2.419 \cdot 10^{-17}$ s and life-time $= 1/(2 \times 1.111399)$ au in our case. While the Hermitian wavefunction can not be distinguished from any other continuum state, the non-Hermitian resonance function has a sharp and clear nodal structure at the interaction region (inside the potential well), it decays exponentially to zero and therefore it is a square-integrable function which is embedded in the generalized Hilbert space.

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More information

We can summarize this by stating that the resonance states are well defined in quantum mechanics within the framework of the non-Hermitian formalism. In non-Hermitian quantum mechanics a resonance is associated with a *single* eigenstate of the Hamiltonian and not with a collection of continuum states (i.e., wavepacket) which is the case in Hermitian quantum mechanics.

1.3 Complex local potentials

In these cases the Hamiltonian is non-Hermitian despite the fact that the eigenfunctions of the time-independent Schrödinger equation are square integrable. The potentials are complex for different reasons. One example is when complex absorbing potentials are introduced in the propagation of waves solving either the Scrödinger equation (or the scalar Maxwell equation in the paraxial approximation) or the vector Maxwell equations. The motivation to introduce complex reflection-free absorbing potentials is to avoid the non-physical interferences which are introduced in conventional calculations by the reflections of the tail of the propagated wave packet from the edge of the grid used in the numerical computations. Physical reasons for introducing complex potentials may arise in optics (due to a complex index of refraction), field theory, and even in cases where the quantum language is used to describe the physics when the studied problems are associated with classical statistical mechanics or with diffusion in biological systems.

As an example of a non-Hermitian Hamiltonian that is not related to the resonance phenomena, let us mention the Hamiltonian that becomes non-Hermitian due to the inclusion of purely imaginary external fields, e.g., $\mathrm{i}gx^3$, where g is a real parameter and the Hamiltonian commutes with the symmetry operator: $x \to -x$ and $\mathrm{i} \to -\mathrm{i}$. This symmetry operator, is known as the $\mathcal{PT}$ symmetry operator, where $\mathcal{P}$ is the parity operator, i.e., $\mathcal{P}x\mathcal{P}^{-1} = -x$ and $\mathcal{T}$ is the time-reversal symmetry operator where $\mathrm{i} \to -\mathrm{i}$, i.e., $\mathcal{T}\mathrm{i}\mathcal{T}^{-1} = -\mathrm{i}$. Note in passing that $\mathcal{T}$ is an anti-linear operator while the Hamiltonian is a linear operator.

Exercise 1.3

Show by using semiclassical arguments that the spectrum of non-Hermitian Hamiltonian $\hat{H} = \hat{p}^2 + \mathrm{i}gx^3$ is real and positive for any value of $g \neq 0$ provided the solution eigenfunctions are defined on the whole real line.

In analogy to quantum-mechanical theory, quantum field theories for such non-Hermitian Hamiltonians possess special properties. The Hamiltonians which commute with the $\mathcal{PT}$ symmetry operator hold additional special properties. For