More on Exact $\mathcal{PT}$-Symmetric Quantum Mechanics

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Abstract

In this article, we discussed certain properties of non-Hermitian $\mathcal{PT}$-symmetry Hamiltonian, and it is shown that a consistent physical theory of quantum mechanics can be built on a $\mathcal{CPT}$-symmetry Hamiltonian. In particular, we show that these theories have unitary time evolution, and conservation probability. Furthermore, transition from quantum mechanics to classical mechanics is investigate and it is found that the Ehrenfest theorem is satisfied.

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1 Introduction

It was shown that one can construct infinitely many new Hamiltonians that have PT-symmetry and it is rejected in past because they are not Hermitian. In one the first explicit studies of non-Hermitian Schrödinger Hamiltonians, have considered the imaginary cubic oscillator problem in the context of permutation theory [1]. It has recently been observed that quantum mechanical theories whose Hamiltonians are PT-symmetry have positive spectra even if the Hamiltonian is not Hermitian [2, 3, 4]. A class of such theories that has been studied extensively is defined by the Hamiltonian,

$$H = p^2 - (ix)^N \ (N \geq 2).$$

It is shown that the reality of the spectrum of (1) is due to PT-symmetry. Also, many quantum mechanical Hamiltonians have been studied in great detail by many authors[5-15]. Direct numerical evidence for reality and positivity of the spectrum of non-Hermitian Hamiltonians, can be found with great accuracy by using conventional WKB approximation, and performing a Runge-Kutta integration of the associated Schrödinger equation[2, 4]. It is well known that the class of PT-symmetry Hamiltonian is larger than real Hamiltonian, because all real symmetric Hamiltonians have time reversal symmetric and one can define the parity operator only up to unitary equivalence[3].

It is seen that the eigenfunctions of a Hamiltonians H which have PT-symmetry are simultaneously eigenfunctions of the PT operator, if the PT-symmetry of a Hamiltonian H is not spontaneously broken[3]. In fact, even if the Schrödinger equation and the corresponding equation boundary conditions are PT-symmetric, the wave function that solve the Schrödinger equation boundary value problem may not be symmetric under space-time reflection. When the solution exhibits PT-symmetry, the symmetry is unbroken, and if the solution does not the PT-symmetry, the PT-symmetry is broken.

In [19, 20], it is shown that PT-symmetric Hamiltonians are P-pseudo Hermitian and, also it is found that the necessary condition for having real spectrum is:

$$\eta H \eta^{-1} = H^\dagger,$$

where has been referred to a Hermitian linear automorphism. One can, however, show that the real spectrum and the orthogonality of the states for some complex potentials can be understood in terms of P-pseudo Hermiticity of a Hamiltonian, provided the Hermitian linear automorphism, $\eta = e^{-\alpha P}$, which affects an imaginary shift of the coordinate ($x \rightarrow x + i\alpha$)[21]. The author of [19], in some of his articles, attempt to demonstrate that PT-symmetry can be understood from the theory of pseudo Hermitian operators and, in particular, he shown [22], that the exact PT-symmetry is equivalent to Hermiticity. Also in [23], it is found that all PT-symmetric quantum theories with real eigenvalues have the same completeness relation (5) which for some especial example has been verified numerically in [10, 12].

The organization of this article is as follows. In sec.2, we offer a discussion of CPT-symmetry. In sec.3 and 4, we discus the conservation of probability, the time evolution and expectation value of an operator in non-Hermitian PT-symmetry quantum mechanics. In sec.5, we study the transition of quantum mechanic to classical mechanic and it is shown that the Ehrenfest theorem is satisfied.

2 Preliminaries

In this section we review a formal discussion of non-Hermitian Hamiltonian which passes the PT-symmetry, $[H, PT] = 0$. In quantum mechanic if a liner operator A commutes with H, then the
eigenstates of $H$ are also eigenstates of $A$. However, we know that the operator $PT$ is anti-linear, but we emphasize that the $PT$-symmetry of $H$ is unbroken, which means that the eigenfunction of $H$ is simultaneously an eigenfunction of $PT$ [17, 18]. So that

$$H \psi_n(x) = E_n \psi_n(x),$$

$$PT \psi_n(x) = \lambda_n \psi_n(x).$$

(3)

Using the facts that $(PT)^2 = 1$ and $P$ and $T$ commute with each other, also. We can conclude that $\psi_n(x) = \lambda_n^* \lambda_n \psi_n(x)$, which means that $\lambda = e^{i\alpha}$ for some $\alpha \in \mathbb{R}$. Thus it is seen that one can replace the $\psi_n(x)$ by $e^{i\alpha/2} \psi_n(x)$, in which its eigenvalue under the operator $PT$ is 1.

$$PT \psi_n(x) = \psi_n(-x)^* = \psi_n(x).$$

(4)

Whereas $[H, PT] = 0$, it is easily seen that the eigenvalue $E_n$ is real, $E_n = E_n^*$ [18]. The completeness relation of these eigenfunctions, $\psi_n(x)$, in coordinate-space statement for all $PT$-symmetric quantum theories with real eigenvalues is [23].

$$\sum_n (-1)^n \psi_n(x_1) \psi_n(x_2) = \delta(x_1 - x_2),$$

(5)

for all $x,y \in \mathbb{R}$. This completeness relation has been verified numerically with great accuracy for some particular cases of $PT$-symmetric Hamiltonians in [10, 12]. Introducing the $PT$ inner product for functions $f(x)$ and $g(x)$ as:

$$<f(x)|g(x)>_{PT} := \int_c dx |PT f(x)| g(x),$$

(6)

where $c$ is an infinite contour in the complex-$x$ plane, which the boundary conditions on the eigenfunctions are that $\psi(x) \to 0$ exponentially rapidly as $|x| \to \infty$ on the contour. It is clearly seen that the eigenfunction are normalized to 1 as follows [17]

$$<\psi_n(x)|\psi_m(x)>_{PT} = (-1)^n \delta_{mn},$$

(7)

where shows that the $PT$-norm is not positive definite. It is found that in any quantum mechanical theory having an unbroken $PT$-Symmetry, there exists a symmetry of the Hamiltonian connected with the fact that there are equal number of positive-norm and negative-norm states. For this purpose, the authors of[16], construct a linear operator, which denoted by $C$, as:

$$C(x_1, x_2) = \sum_n \psi_n(x_1) \psi_n(x_2),$$

(8)

where $\psi_n(x)$ is an eigenfunction of $H$. The operator $C$ has properties such as: i) $C^2 = 1$, ii) the inner product is defined as:

$$<f(x)|g(x)>_{CPT} := \int_c dx |CPT f(x)| g(x),$$

(9)

whose associated norm is positive, because $C$ contribute 1(-1) when it acts on states with positive(negative) $PT$ norm, and the completeness relation (5), rewritten as:

$$\sum_n |CPT \psi_n(x)|^2 \psi_n(y) = \delta(x - y),$$

(10)

which is valid for all $PT$-symmetric Hamiltonians [22, 23].
3 Conservation of Probability

The time dependence Schrödinger equation of one dimensional non-relativistic quantum theory is:

\[ i\hbar \frac{\partial \Psi(x,t)}{\partial t} = H \Psi(x,t), \]  

(11)

and for the CPT-symmetry Hamiltonian, H, we have

\[ H(x) = H^*(-x). \]  

(12)

According to Born’s postulate (one of the postulate of Hermitian quantum mechanical theory), we define the probability of finding the particle at time \( t \) within the volume element \( dx \) about the point \( x \) for the case which the Hamiltonian is CPT-symmetry as:

\[ P(x,t)dx = [\mathcal{CPT} \Psi(x,t)]\Psi(x,t)dx. \]  

(13)

Here we assume that the particle is described by a wave function \( \Psi(x,t) \). By using of (7) and (10) it is seen that:

\[ \int_c P(x,t)dx = 1, \]  

(14)

where \( c \) is the contour in complex-\( x \) plane. It is clear that, this probability is conserved, and at any arbitrary time the wave function is normalized. In other hand, it is found that:

\[ \frac{\partial}{\partial t} \int_c P(x,t)dx = \int_c \left( \frac{\partial}{\partial t} [\mathcal{CPT} \Psi(x,t)] \right) \Psi(x,t)dx + \int_c [\mathcal{CPT} \Psi(x,t)] \frac{\partial \Psi(x,t)}{\partial t} dx. \]  

(15)

Using (11) and its CPT-Conjugate, we have

\[ -i\hbar \frac{\partial}{\partial t} \left( \mathcal{CPT} \Psi(x,t) \right) = H^*(-x) \left( \mathcal{CPT} \Psi(x,t) \right). \]  

(16)

Substitute (16) and (11) in (15) and using this fact that \( \psi(x) \to 0 \) exponentially rapidly as \( |x| \to \infty \) on the contour, we have

\[ \frac{\partial}{\partial t} \int_c P(x,t)dx + \int_c \frac{\partial j}{\partial x} dx = 0, \]  

(17)

where

\[ j(x,t) = \frac{\hbar}{2mi} \left\{ \left[ \mathcal{CPT} \Psi(x,t) \right] \frac{\partial \Psi(x,t)}{\partial x} - \left( \frac{\partial}{\partial x} \left[ \mathcal{CPT} \Psi(x,t) \right] \right) \Psi(x,t) \right\}. \]  

(18)

is the probability current density in CPT-symmetric quantum theory, which for stationary states is independent of \( x \) and \( t \).
4 The Time Evolution and Expectation Values

Since the non-relativistic quantum theories with any arbitrary Hamiltonians is a first-order differential equation in time (11), so one may introduce an evolution operator such as:

\[ \Psi(t) = U(t, t_0)\Psi(t_0), \]  

(19)

where \( U(t, t_0) = 1 \) and \( \Psi(t_0) \) is an initial wave function belonging to the Hilbert space with the \( CPT \) inner product and spanned by the energy eigenfunctions. Conservation of probability requires that:

\[ <\Psi(t)|\Psi(t)>_{CPT} = <\Psi(t_0)|\Psi(t_0)>_{CPT}, \]

\[ = <\Psi(t_0)|U^2(t, t_0)U(t, t_0)\Psi(t_0)>_{CPT}, \]  

(20)

hence

\[ U^t(t, t_0)U(t, t_0) = I, \]  

(21)

where \( U^t(t, t_0) \) is \( CPT \)-conjugate of \( U(t, t_0) \). This shows that

\[ U^2(t, t_0) = U^{-1}(t, t_0). \]  

(22)

By instituting (19) in (11), it is found that:

\[ i\hbar \frac{\partial}{\partial t}U(t, t_0) = HU(t, t_0). \]  

(23)

Let us consider the particular case for which \( \frac{\partial H}{\partial t} = 0 \). A solution of (23), which satisfying the initial condition is given by:

\[ U(t, t_0) = e^{-i/\hbar H(t-t_0)}, \]  

(24)

where

\[ U^t(t, t_0) = e^{i/\hbar H^*(t-t_0)}, \]

\[ = e^{i/\hbar H(t-t_0)}, \]

\[ = U^{-1}(t, t_0), \]

\[ = U(t_0, t). \]  

(25)

Thus a formal solution of the time-dependent Schrödinger equation for a time independent \( PT \)-symmetry Hamiltonian is given by

\[ \Psi(t) = e^{-i/\hbar H(t-t_0)}\Psi(t_0). \]  

(26)

5 Transition From Quantum Mechanics to Classical Mechanics

According to the principle of correspondence, we aspect that the motion of a wave packet should agree with that of the corresponding classical particle whenever the distances and momenta involved
in describing the motion of the particle are so large that uncertainty principle may be ignored. Let us $\hat{A}$ be a linear operator which associated with a dynamical variable in this version of quantum theory. It acts in a complex vector space. For the case that $\hat{A}$ is a proper physical quantity, we want the $<\hat{A}>$ or the eigenvalues of it be real. We call this quantity as physical observable of theories. So the reality of $<\hat{A}>$ or eigenvalues of it follows that, $\hat{A}$ commute with nonlinear invertible operator $\mathcal{PT}$ [19, 20]. Therefore, it is necessary that $\hat{A}$ has been an un-broken $\mathcal{PT}$-symmetry. Also with pseudo operators points of view, it is necessary that $\hat{A}$ be a pseudo operator, which is related to a Hermitian operator $A$ by a similarity transformation, as

$$\hat{A} = \eta^{-1} A \eta,$$  

where $\eta$ is a linear invertible operator in Hilbert space of the quantum system. Hence, whereof, the $\mathcal{PT}$-symmetric quantum theory is $\mathcal{P}$-pseudo hermitian quantum theories [19, 20] and these theories (exact $\mathcal{PT}$-symmetry) is equivalent to a Hermitian quantum theories, so we may introduce a proper observable of this observable in the state $|\Psi>$, normalized to unity, for a $\mathcal{PT}$-symmetry quantum mechanical theory, is define as follows:

$$<\hat{A}>_{\mathcal{CPT}}=\langle \Psi |\hat{A}|\Psi >_{\mathcal{CPT}},$$  

(28)

where $<|$ is $\mathcal{CPT}$-conjugate of $|\rangle$. The rate of change of this expectation value is therefore

$$\frac{d}{dt} <\hat{A}>_{\mathcal{CPT}} = \frac{d}{dt} <\Psi |\hat{A}|\Psi >_{\mathcal{CPT}},$$  

(29)

$$= \langle \frac{\partial \Psi}{\partial t} |\hat{A}|\Psi >_{\mathcal{CPT}} + \langle \Psi |\frac{\partial \hat{A}}{\partial t} |\Psi >_{\mathcal{CPT}} + \langle \Psi |\hat{A} x \hat{A} |\Psi >_{\mathcal{CPT}}.$$  

(30)

then, one can use of (11), (12) and (16) arrive at:

$$\frac{d}{dt} <\hat{A}>_{\mathcal{CPT}}= \left(\frac{-i}{\hbar}\right) \langle \frac{\partial \Psi}{\partial t} |\hat{A}|\Psi >_{\mathcal{CPT}} + \langle \Psi |\frac{\partial \hat{A}}{\partial t} |\Psi >_{\mathcal{CPT}} + \langle \Psi |\hat{A} x \hat{A} |\Psi >_{\mathcal{CPT}}.$$  

(31)

Since $H$ is a $\mathcal{PT}$-symmetry, $H=H^\ast (-x)$, so the first matrix element on the right hand of (31) may be written as $\langle \Psi |HA|\Psi >$. Therefore we have

$$\frac{d}{dt} <\hat{A}>_{\mathcal{CPT}}= \left(\frac{i}{\hbar}\right) \langle \frac{\partial \Psi}{\partial t} |\hat{A}|\Psi >_{\mathcal{CPT}} + \langle \Psi |\frac{\partial \hat{A}}{\partial t} |\Psi >_{\mathcal{CPT}}.$$  

(32)

We assume that $\hat{A} = \hat{x}$, where is a position operator in $\mathcal{PT}$-symmetry quantum theory that acts in a complex vector space, which it may be a similarity transformation of $x_\hbar$ as $\hat{x} = e^{-i\alpha} x_\hbar e^{i\alpha} = x_\hbar + i\alpha$ ($\alpha$= constant and $\hbar :=$ Hermitian). So $\frac{\partial \hat{x}}{\partial t} = 0$ and also it is clearly seen that for any $\mathcal{PT}$-Symmetry Hamiltonian such as (11), the commutative $[H, \hat{x}]$ is equal to:

$$[H, \hat{x}] = -i\hbar \frac{\hat{p}}{m}.$$  

(33)

Then, from (29),

$$\frac{d}{dt} <\hat{x}>_{\mathcal{CPT}}= \frac{\langle \hat{p} >_{\mathcal{CPT}}}{m},$$  

(34)
and also for the case \( \hat{A} = \hat{p} \), in which, \( \hat{p} = e^{-\alpha p} \hat{p} e^{\alpha p} = \hat{p}_h \), one can arrive at:

\[
\frac{d}{dt} < \hat{p} >_{\text{CPT}} = - < \frac{\partial V}{\partial x} >_{\text{CPT}}.
\]

These two equations ((34) and (35)) show that in non-Hermitian \( \mathcal{PT} \)-symmetry quantum mechanics, the Ehrenfest theorem is satisfied exactly such as standard formulation of quantum mechanics in term of Hermitian Hamiltonians.

### 6 Conclusion

During the past five years there have appeared dozens of publications exploring the properties of the \( \mathcal{PT} \)-symmetric Hamiltonians. It is found that a consistent physical theory of quantum mechanics can be built on a non-Hermitian Hamiltonian, which satisfies the less restrictive and more physical condition of space-time reflection symmetry. Considering some aspect of these theories, it is shown that these theories are a consistence physical quantum mechanic theory. In particular it is found that the time-evolution of these theories is unitary and the probability is conserved. Also by defining the expectation value of observable with respect to \( \mathcal{CPT} \)-inner product, it is shown that the rate of expectation value is similar to rate of expectation value in standard Hermitian quantum mechanics. At last, by considering the Ehrenfest theorem, it is seen that transition from \( \mathcal{PT} \)-symmetric quantum mechanic to classical mechanic is satisfied.
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