Complex Spectrum of a Spontaneously Unbroken PT Symmetric Hamiltonian

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(Dated: August 9, 2018)

PACS numbers: 03.65.Ge, 03.65.-w, 02.60.Lj

INTRODUCTION

It is one of the postulates of quantum mechanics that any operator associated with a physically measurable property is Hermitian. Hermiticity is a useful property as it guarantees the reality of the spectrum. However, it was shown in 1998 that the following non-Hermitian potential

\[ U(x) = x^2(ix)^\epsilon \quad (\epsilon \geq 0) , \tag{1} \]

have real positive spectra [1]. It was realized that although this potential is not Hermitian, it is invariant under PT transformations, where P and T are linear parity and antilinear time-reversal operator, respectively. They have the effect

\[ p \rightarrow p, \quad x \rightarrow -x, \quad i \rightarrow -i, \quad t \rightarrow -t. \tag{2} \]

Hermiticity requirement is replaced by the analogous condition of space-time reflection symmetry. It should be noted that PT symmetry can not be regarded as the fundamental property as there exist also examples with real spectra for which not even the Hamiltonian is PT symmetric. Furthermore, there are also PT-symmetric Hamiltonians that do not have a real spectrum. Neither Hermiticity nor PT symmetry serves as a sufficient condition for a quantum Hamiltonian to preserve the reality of energy spectrum.

For the case of a PT symmetric Hamiltonian, the PT operator commutes with the Hamiltonian \( H \). Because PT operator is not linear, the eigenstates of \( H \) may or may not be eigenstates of \( P T \). If all eigenfunction of a PT symmetric Hamiltonian is also an eigenfunction of the PT operator, it is said that PT symmetry of \( H \) is unbroken.

\[ [H, PT] = 0 ; \quad PT \Psi(x) = \mp \Psi(x) . \tag{3} \]

Conversely, if some of the eigenfunctions of a PT symmetric Hamiltonian are not simultaneously eigenfunctions of the PT operator, then the PT symmetry of \( H \) is spontaneously broken.

The appearances of complex eigenvalues in the spectra of PT symmetric quantum mechanical systems are usually associated with a spontaneous breaking of PT transformations. In other words, the eigenvalues are real when the Hamiltonian and its wave function remain invariant under a simultaneous parity and time reversal transformations [1, 2, 3, 4, 5]. As an example, the potential (1) is PT symmetric because it is invariant under (2). The energy spectrum is not real when \( \epsilon < 0 \). This is because \( \epsilon < 0 \) is the parametric region of broken PT symmetry [1].

In this study, in contrast with the first conjectures, we will show that unbroken PT symmetry is not sufficient to guarantee that the spectrum of a non-Hermitian Hamiltonian is real.

This paper is organized as follows. Section 2 considers a non-Hermitian Hamiltonian and finds its eigenstates and complex eigenvalues exactly. Section 3 discusses the reason for the existence of complex energy spectrum when PT symmetry is not spontaneously broken. Finally, section 4 concludes our discussion.

FORMALISM

Consider the following non-Hermitian Hamiltonian

\[ H = p^2 + x^2 + 2if(t) x , \tag{4} \]

where \( f(t) \) is a real-valued time-dependent function. The constants are set to unity for simplicity (\( \hbar^2 / 2m = \hbar = 1 \)). The Hamiltonian is invariant under PT transformations provided that \( f(-t) = f(t) \). This analytically solvable Hamiltonian allows us to investigate the relation between the reality of the energy spectrum and the broken PT symmetry.

Suppose first that \( f(t) \) is equal to a constant \( f_0 \). In this case, the eigenfunctions of the Hamiltonian can be readily found by shifting the coordinate as \( x \rightarrow x' = x + if_0 \). The potential in the primed coordinate system reads \( U(x') = x'^2 + f_0^2 \). The boundary conditions remain unchanged and the energy eigenvalues are shifted by a constant \( f_0^2 \) and given by \( E_n = 2n + 1 + f_0^2 \), where \( n = 0, 1, \ldots \). As can be seen, the energy eigenvalues are real when \( f(t) = f_0 \). As a result, it can be claimed that since PT symmetry is not spontaneously broken for this case, the energy eigenvalues are real.

Suppose next that \( f(t) \) depends on time explicitly. Let us now obtain the exact analytic solution and investigate...
whether the reality of energy spectrum is maintained. The corresponding Schrodinger equation reads

$$-\frac{\partial^2 \Psi}{\partial z^2} + (x^2 + 2if(t)x) \Psi = i\frac{\partial \Psi}{\partial t}, \quad (5)$$

The following coordinate transformation is introduced to solve this equation

$$z = x + ig(t), \quad (6)$$

where the real-valued time-dependent function $g(t)$ to be determined later. Under the coordinate transformation (6), the time derivative operator transforms as $\partial/\partial t \to \partial/\partial t + ig \partial/\partial z$, where dot denotes time derivation. Substitution of the equation (6) into the equation (5) yields

$$-\frac{\partial^2 \Psi}{\partial z^2} + \partial_t \Psi + (z^2 + 2i(f-g)z + (2f-g)g) \Psi = i\frac{\partial \Psi}{\partial t}. \quad (7)$$

Let us introduce

$$\Psi(z,t) = e^{\alpha(t)}z \Phi(z,t), \quad (8)$$

where $\alpha(t)$ is a time-dependent function. The equation (7) simplifies if we choose $\alpha(t)$ and $g(t)$ as

$$\alpha = \frac{g}{2}; \quad \dot{\alpha} = 2(f-g). \quad (9)$$

Substituting (8,9) into (7), we obtain

$$-\frac{\partial^2 \Phi}{\partial z^2} + \left(z^2 + (2f-g)g + \frac{g^2}{4}\right) \Phi = i\frac{\partial \Phi}{\partial t}. \quad (10)$$

Separation of variable techniques can be applied to get rid of the time-dependent part.

$$\Phi(z,t) = \exp\left(-iE_n t - i \int_0^t (2f-g)g + \frac{g^2}{4} \ dx\right) \phi(z), \quad (11)$$

Then, the equation (10) is reduced to

$$-\frac{\partial^2 \phi}{\partial z^2} + z^2 \phi = E_n \phi, \quad (12)$$

It has been shown that the time dependent part of the Schrodinger equation (5) can be eliminated and the problem is reduced to the well-known harmonic oscillator one. So, the constant $E_n$ is given by

$$E_n = 2(n + \frac{1}{2}), \quad (13)$$

where $n = 0, 1, 2, ....$. Using the eigenfunctions for the standard harmonic oscillator (12) and transforming backwards yields the exact eigenfunctions for the Hamiltonian (4)

$$\Psi_n = \exp\left(-iE_n t - i \int_0^t (2f-g)g + \frac{g^2}{4} \ dx\right) \times \exp(\alpha(x + ig) - (x + ig)^2/2) H_n(x + ig). \quad (14)$$

where $H_n(x + ig)$ are the Hermite polynomials. The first two of them are given by $H_0(x + ig) = 1$ and $H_1(x + ig) = 2(x + ig)$. Having obtained the exact analytic solution, let us find the energy eigenvalues for the time-dependent non-Hermitian Hamiltonian (4).

The ground state energy is computed as

$$<0|E|0> = \frac{\int_{-\infty}^{\infty} \Psi_0^* H \Psi_0 \ dx}{\int_{-\infty}^{\infty} |\Psi_0|^2 dx} = 1 + g^2 + \alpha^2 + 2i\alpha f. \quad (15)$$

and the energy eigenvalue for the first excited state is given by

$$<1|E|1> = \frac{E_{11} + 2i\alpha f(3 + 2\alpha^2 + 2g^2)}{1 + 2g^2 + 2\alpha^2}, \quad (16)$$

where $E_{11} = 3 + 7g^2 + \alpha^2 + 4\alpha^2 g^2 + 2(\alpha^4 + g^4)$ is the real part of the numerator. The energy eigenvalues for the excited states can also be found exactly. As it can be seen from (15,16), the energy eigenvalues for the ground and the first excited states are real if and only if either $f(t)$ or $\alpha(t)$ is equal to zero. The former one is trivial since the Hamiltonian (4) becomes a Hermitian operator when $f(t)$ is zero. The latter case is surprising. The time-dependent function $\alpha(t)$ is equal to zero if $f(t)$ is a constant (Suppose $f(t) = f_0$, then using (9) we get $g(t) = f_0$ and $\alpha(t) = 0$). So, the energy spectrum for the non-Hermitian Hamiltonian is not real unless $f(t) = 0$ or $f(t) = f_0$.

If $\alpha(t)$ does not vanish ($f(t)$ depends on time explicitly) then the corresponding energy eigenvalues are not real any more. As an example, let the non-Hermitian potential be given by $V(x) = x^2 + 2itx$. In this case, $f(t) = t$ and using (9) we get $g(t) = t$ and $\alpha = 1/2$. Substitution these into (14), we get the exact wave function

$$\Psi_n = e^{-2i(n+\frac{1}{2})t - i(\frac{t^2}{4} + \frac{g}{2}) + (x+it)^2/2} \times H_n(x + it) \quad (17)$$

The energy eigenvalues for the ground and the first excited states are given by

$$<0|E|0> = t^2 + \frac{5}{4} + it. \quad (18)$$

As a second example, let us choose $f(t) = t^2$. If we solve (9), we obtain $g(t) = t^2 - 1/2$ and $\alpha = t$. The exact wave function for the non-Hermitian potential $V(x) = x^2 + 2it^2x$ reads

$$\Psi_n(x,t) = \exp\left(t(x + i(t^2 - \frac{1}{2})) - \frac{1}{2}(x + i(t^2 - \frac{1}{2}))^2\right) \times e^{-2i(n+\frac{1}{2})t - i(\frac{t^2}{4} + \frac{g}{2})} H_n\left(x + i(t^2 - \frac{1}{2})\right). \quad (19)$$
This example is of great importance since PT symmetry is not spontaneously broken for this case. It was conjectured that the reality of the spectrum was due to the unbroken PT symmetry of the non-Hermitian Hamiltonians. So, one expects that the energy spectrum is real since the Hamiltonian and its eigenfunction \( (20) \) are both invariant under PT operations. However, the energy eigenvalue for the ground state is not real as can be seen below

\[
< 0 | E | 0 > = t^4 + \frac{5}{4} t^2 + 2 i t^3 . \quad (21)
\]

One can run Mathematica program to calculate the energy eigenvalues for the excited states. They are also not real. The general idea that the energy eigenvalues are real for unbroken PT symmetric Hamiltonian does not hold for this example.

In the next section, we will explain why complex eigenvalues appear for the non-Hermitian Hamiltonian for which PT symmetry is not spontaneously broken.

**SYMMETRY**

As has been shown, the condition \( (3) \) to guarantee the reality of energy spectrum does not always work. So, we need a more general condition to explain the reason for the existence of complex energy eigenvalues when PT symmetry of a Hamiltonian \( H \) is not spontaneously broken.

Let a Hamiltonian be given by

\[
H = \frac{p^2}{2m} + U^R + i U^I ,
\]

where the real-valued functions \( U^R(x, t), U^I(x, t) \) are the real and the imaginary parts of the Hamiltonian \( H \), respectively. It was suggested in \( [6] \) that the energy spectrum for this non-Hermitian Hamiltonian is real if the expectation value of its imaginary part, \( < U^I > \), is equal to zero

\[
< U^I > = \int |\Psi|^2 U^I d^3 x = 0 , \quad (22)
\]

where the integral is taken over all space.

Hermiticity and PT symmetry conditions can be derived from \( (22) \) as special cases. Trivially, when a Hamiltonian is Hermitian, \( U^I = 0 \), then \( (22) \) is satisfied. The latter one will be derived in the next section.

Let us calculate \( < U^I > \) for the Hamiltonian \( (4) \). It is given by

\[
< U^I > = 2 f(t) \int_{-\infty}^{\infty} \Psi^* x \Psi \ dx . \quad (23)
\]

If we use the exact wave function \( (14) \), we get

\[
2 f \int_{-\infty}^{\infty} e^{-x^2 + 2 \alpha x} H_n(x - ig) H_n(x + ig) \ dx . \quad (24)
\]

Since the product of the Hermite polynomials \( H_n(x - ig) \) \( H_n(x + ig) \) is even for all \( n \), the above integration is equal to zero when \( \alpha = 0 \). This is because the integral of an odd function on a symmetric interval is zero.

\[
< U^I > = 2 f(t) < x > = 0 , \quad \text{if} \quad \alpha = 0 \quad (25)
\]

Note that \( \alpha = 0 \) when \( f(t) = 0 \) or \( f(t) = f_0 \). It is concluded that the energy spectrum is real if \( f(t) \) does not depend on time explicitly since \( < U^I > \) vanishes for these cases. When \( \alpha \neq 0 \) the odd character of the integrand is lost and the integral is not in general equal to zero. Hence, the energy spectrum is not real any more. The theorem given in \( [6] \) successfully explains the reason of getting complex energy eigenvalues when \( f(t) = t \) and \( f(t) = t^2 \). PT symmetry condition is not successful to explain the complex energy eigenvalues for \( f(t) = t^2 \).

**CONCLUSION**

A question arises. Is there a condition that guarantees that \( < U^I > \) vanishes for a given Hamiltonian. We will conclude our study by showing the existence of such a condition. Let us replace the PT symmetry condition \( (3) \) by the following ones.

\[
U^I(-x, t) = -U^I(x, t) ; \quad | \Psi(-x, t) |^2 = | \Psi(x, t) |^2 . \quad (26)
\]

Let us now find the expectation value \( < U^I > \) for this case. It is given by

\[
< U^I > = \int_{-\infty}^{\infty} | \Psi(x, t) |^2 U^I(x, t) \ dx . \quad (27)
\]

Let us change the variable \( x \) in the integral \( (27) \) to \( -x \). It can be seen that the function in the integral is an odd function of \( x \). Since the integral of an odd function on a symmetric interval is zero, \( < U^I > = 0 \). So, it is concluded that if \( (26) \) is satisfied than the corresponding energy eigenvalues are real for the non-Hermitian Hamiltonians.

All spontaneously unbroken PT symmetric Hamiltonians satisfy the condition \( (26) \) if the potential is time-independent. This is why PT symmetry condition works for the time-independent non-Hermitian Hamiltonians. On the contrary, they make difference for the Hamiltonians which explicitly depend on time \( [2,8] \). Even if the Hamiltonian and the corresponding wave function \( \Psi(x, t) \) are invariant under PT transformations, they don’t necessarily satisfy the above condition \( (26) \). For example, the potential \( V(x) = x^2 + 2 i t^2 x \) and the exact wave function \( (20) \) are both invariant under PT transformations, but they fail to satisfy the above condition \( (26) \). So, the
energy spectrum is not real for that case. To sum up, $PT$ symmetry requirement coincides with the condition $\text{[26]}$ for the time-independent potential fields. So far, we have considered that the interval (boundaries) is symmetrical. If it is not so, the energy spectrum may not be real even the equation $\text{[26]}$ is satisfied. So, for the investigation of the reality of energy eigenvalues for a non-Hermitian Hamiltonian, it is better to use the condition $\text{[22]}$.

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