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On the eigenvalues and dynamics of non-Hermitian PT symmetric Hamiltonians in finite basis spaces

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Abstract

We consider two simple examples of $\widehat{P}\widehat{T}$ symmetric non-Hermitian Hamiltonians $H(\lambda) = H_0 + i\lambda x^n$ $(n = 1, 3)$, H_0 being the harmonic oscillator Hamiltonian. Analytical and numerical estimates in finite-dimensional subspaces of the Hilbert space spanned by eigenfunctions of H_0 establish the existence of thresholds for λ (λ_c) only below which the spectrum of $H(\lambda)$ is real. We also investigate the dynamics of evolution generated by $H(\lambda < \lambda_c)$ and $H(\lambda > \lambda_c)$ in finite-dimensional subspaces looking for typical signatures of $\widehat{P}\widehat{T}$ symmetry on the dynamics. © 2001 Published by Elsevier Science B.V.

1. Introduction

It is a matter of common knowledge that a Hermitian Hamiltonian, real or complex, supports only a real eigenvalue spectrum. It is apparent that the condition $H^+ = H$ imposed on the operator restricts the spectrum to a real one. The removal of the restriction (i.e., $H^+ \neq H$) allows the operator to be non-Hermitian and the spectrum to be generally non-real. That does not mean, however, that real eigenvalues are entirely precluded—they are just not guaranteed. On the basis of numerical calculations, Bessis conjectured (henceforth referred to as Zinn-Justin–Bessis conjecture) several years ago that the spectrum of the non-Hermitian Hamiltonian $H = P^2 + x^2 + ix^3$ is real and positive [1]. Bender and Boettcher [2] noted that Bessis' Hamiltonian is a specific example of a class of non-Hermitian Hamiltonians whose spectrum may be real and positive and argued that a common feature of all such non-Hermitian Hamiltonians is their $\widehat{P}\widehat{T}$ symmetry. It implies that these Hamiltonians remain invariant under the operation defined by the product of parity $(\widehat{P})$ and time reversal $(\widehat{T})$ operators. They noted, however, that along with $\widehat{P}\widehat{T}$ symmetry, the absence of spontaneous symmetry breaking is needed for generating a real spectrum. Delabaere and Pham [3] used perturbative arguments to show that a polynomial potential *closely* resembling the harmonic oscillator potential generated real spectrum if it is $\widehat{P}\widehat{T}$ symmetric, and went on to establish [4] further that a $\widehat{P}\widehat{T}$ symmetric real anharmonic oscillator (the symmetric double-well) could generate complex eigenvalues in the presence of a small imaginary potential $(i\beta x,\ \beta > 0)$ although the perturbation does not affect $\widehat{P}\widehat{T}$ symmetry. Delabaere and Tai [5] have recently moved closer to proving a stronger version of the Zinn-Justin–Bessis conjecture (the polynomial potential need not closely resemble harmonic potential). Bender et al. [6] pro-

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posed to broaden the canonical formulation of quantum mechanics by requiring the $\widehat{P}\widehat{T}$ invariance of the Hamiltonian to replace the Hermiticity requirement. New classes of Hamiltonians with real and positive spectra could be generated by this approach. They noted, however, that Hermiticity is a far stronger condition on the Hamiltonian compared to $\widehat{P}\widehat{T}$ invariance and the reality of the spectra of non-Hermitian Hamiltonians cannot be possibly guaranteed by $\widehat{P}\widehat{T}$ invariance alone.

Several other interesting aspects of the $\widehat{P}\widehat{T}$ symmetric Hamiltonians have been analysed recently [7–9]. The point that we may not miss here is that just $\widehat{P}\widehat{T}$ symmetry alone cannot perhaps ensure reality of the spectrum of a non-Hermitian Hamiltonian, while the lack of Hermiticity alone, on the other hand, does not completely forbid the Hamiltonian to have a few real eigenvalues. In what follows, we show that for finite basis set transcriptions of the perturbed harmonic oscillator Hamiltonians of the type

$$H(\lambda) = \frac{P_x^2}{2m} + \frac{1}{2}kx^2 + i\lambda x\left(x^n\right) \quad (n = 1, 3),$$

which are $\widehat{P}\widehat{T}$ symmetric, a critical value of $\lambda = \lambda_c$ exists in each case only below which the eigenvalues of $H(\lambda)$ are real. The values of λ_c depend upon the nature of the perturbing potential (i.e., values of n) and the dimension of the subspace (N). A question that naturally crops up here concerns the evolution under $\widehat{P}\widehat{T}$ symmetric Hamiltonians in a parameter regime where reality of the spectrum is ensured. The basic non-Hermiticity of $H(\lambda)$ apparently demands that the evolution operator $U(\lambda)$ be non-unitary and the dynamics to be dissipative, the $\widehat{P}\widehat{T}$ invariance of $H(\lambda)$ and the reality of the spectrum not withstanding. We propose to investigate the quantum dynamics of evolution under a $\widehat{P}\widehat{T}$ symmetric $H(\lambda)$ both under adiabatic and sudden switching approximations and look for typical signature of $\widehat{P}\widehat{T}$ symmetry on the dynamics, if any.

2. The problem

Let us consider a family of non-Hermitian Hamiltonians $H(\lambda)$, where

$$H(\lambda) = \frac{P_x^2}{2m} + \frac{1}{2}kx^2 + i\lambda x^n \quad (n = 1, 2, 3). \tag{1}$$

$H(\lambda)$ is $\widehat{P}\widehat{T}$ invariant for $n = 1, 3$ and $\widehat{P}\widehat{T}$ non-invariant for $n = 2$. We may partition $H(\lambda)$ in the following manner:

$$\begin{aligned} H(\lambda) &= \left(\frac{P_x^2}{2m} + \frac{1}{2}kx^2\right) + i\lambda x^n \\ &= H_0 + i\lambda x^n \quad (n = 1, 2, 3). \end{aligned} \tag{2}$$

H_0 in Eq. (2) is the unperturbed Hermitian Hamiltonian (the harmonic oscillator Hamiltonian) and $i\lambda x^n$ is a purely imaginary perturbation ($\lambda > 0$). The problem is to predict the nature of the eigenvalues of $H(\lambda)$ as a function of λ in a finite basis space. The eigenkets and eigenvalues of $H(\lambda)$ can be found by diagonalizing $H(\lambda)$ in the basis provided by the eigenkets ($\{\phi_i^0\}$) of H_0, where $\{|\phi_i^0\rangle\}$:

$$H_0\left|\phi_i^0\right\rangle = \epsilon_i^0\left|\phi_i^0\right\rangle, \quad i = 0, 1, 2, \ldots. \tag{3}$$

We can then look for the eigenvalues that are real in the given subspace. By doing so, we are essentially trying to explore if we could make use of a finite basis space version of Zinn-Justin–Bessis conjecture for $\widehat{P}\widehat{T}$ symmetric Hamiltonians.

Let us consider the following case:

$$H_0 = \frac{P_x^2}{2m} + \frac{1}{2}kx^2 \tag{4}$$

and

$$H(\lambda) = H_0 + i\lambda x. \tag{5}$$

We choose

$$x' = x + \frac{i\lambda}{k}. \tag{6}$$

It is straightforward to see that

$$\begin{aligned} &\frac{P_x^2}{2m} = \frac{P_x'^2}{2m}, \\ &\frac{1}{2}kx^2 = \frac{1}{2}k\left(x' - \frac{i\lambda}{k}\right)^2 = \frac{1}{2}kx'^2 - \frac{\lambda^2}{2k} - i\lambda x', \\ &i\lambda x = i\lambda\left(x' - \frac{i\lambda}{k}\right) = i\lambda x' + \frac{\lambda^2}{k}. \end{aligned} \tag{7}$$

In the x' coordinate, the Hamiltonian $H(\lambda)$ given by

$$H(x', \lambda) = \frac{P_x'^2}{2m} + \frac{1}{2}kx'^2 + \frac{\lambda^2}{2k}. \tag{8}$$

We note that as $\lambda \to 0$, $x' \to x$, $H(x', \lambda) = H_0$.

The eigenvalue equation satisfied by $H(x')$ is

$$\left(\frac{P_x'^2}{2m}+\frac{1}{2}kx'^2+\frac{\lambda^2}{2k}\right)\Psi_n(x')=E_n\Psi_n(x'),$$

or,

$$\left(\frac{P_x'^2}{2m}+\frac{1}{2}kx'^2\right)\Psi_n(x')=\left(E_n-\frac{\lambda^2}{2k}\right)\Psi_n(x') \\ =E_n'\Psi(x').$$

As $\lambda\to 0$, $H(x')\to H_0$, $\Psi_n(x')\to\Psi_n(x)$ and $E_n'=(E_n-\lambda^2/2k)\to E_n=(n+1/2)\hbar\omega$ as H_0 is the harmonic oscillator Hamiltonian. Therefore, the eigenvalues of $H(\lambda)$ are given by $E_n'=(n+1/2)\hbar\omega-\lambda^2/2k$ which are real for all n and λ, $H(\lambda)$ therefore has a real spectrum. We now turn to a finite basis set approximation to the eigenvalues of $H(\lambda)$. We consider two cases.

Case 1. Let as consider a two-dimensional orthonormal subspace of H_0 ($k=1, m=1$) spanned by ϕ_0^0 and ϕ_1^0. The diagonalization of $H(\lambda)=H_0+i\lambda x$ in the two-dimensional subspace leads to the following secular equation for the $n=1$ case:

$$\begin{pmatrix}\frac{1}{2}-\epsilon & \frac{i\lambda}{\sqrt{2}}\\ \frac{i\lambda}{\sqrt{2}} & \frac{3}{2}-\epsilon\end{pmatrix}=0. \tag{9}$$

Reality of ϵ demands then that

$$\frac{1}{4}-\frac{\lambda^2}{2}\geqslant 0,\quad\text{or}\quad \lambda\leqslant\frac{1}{\sqrt{2}}\approx 0.7071. \tag{10}$$

In the two-dimensional subspace therefore the critical value of λ ($=\lambda_c^{(2)}$) is 0.7071. For the three-dimensional basis space spanned by ϕ_0^0, ϕ_1^0 and ϕ_2^0, the corresponding secular equation for the $n=1$ case is

$$\begin{pmatrix}\frac{1}{2}-\epsilon & \frac{i\lambda}{\sqrt{2}} & 0\\ \frac{i\lambda}{\sqrt{2}} & \frac{3}{2}-\epsilon & i\lambda\\ 0 & i\lambda & \frac{5}{2}-\epsilon\end{pmatrix}=0. \tag{11}$$

Again, reality of the eigenvalues of the secular equation in this case demands that

$$\left(\frac{1}{3}-\frac{\lambda^2}{2}\right)^3-\left(\frac{\lambda^2}{4}\right)^2\geqslant 0,\quad\text{or}$$
$$\frac{\lambda^2}{6}-\frac{3\lambda^4}{16}+\frac{\lambda^6}{8}\leqslant\frac{1}{27},\quad \lambda\approx 0.55329. \tag{12}$$

In the three-dimensional subspace $\lambda_c^{(3)}=0.55329<\lambda_c^{(2)}=0.7071$.

Let us consider yet another Hamiltonian of the same family, $H(\lambda)=H_0+i\lambda x^3$. We cannot show analytically, if all the eigenvalues of this $H(\lambda)$ are real.

Case 2. In this case also we make use of the Harmonic oscillator basis set to diagonalize $H(\lambda)=H_0+i\lambda x^3$ using ϕ_0^0 and ϕ_1^0 as the basis elements. The secular equation for the two-dimensional problem in this case becomes

$$\begin{pmatrix}\frac{1}{2}-\epsilon & \frac{3i\lambda}{2\sqrt{2}}\\ \frac{3i\lambda}{2\sqrt{2}} & \frac{3}{2}-\epsilon\end{pmatrix}=0, \tag{13}$$

$$\frac{1}{4}-\frac{9\lambda^2}{8}\geqslant 0,\quad\text{i.e.,}\quad \lambda\leqslant\frac{\sqrt{2}}{3}\approx 0.4710. \tag{14}$$

So, $\lambda_c^{(2)}$ in this cases is $=0.471$. The three-dimensional analogue of the problem leads to the secular equation

$$\begin{pmatrix}\frac{1}{2}-\epsilon & \frac{3i\lambda}{2\sqrt{2}} & 0\\ \frac{3i\lambda}{2\sqrt{2}} & \frac{3}{2}-\epsilon & 3i\lambda\\ 0 & 3i\lambda & \frac{5}{2}-\epsilon\end{pmatrix}=0. \tag{15}$$

One can use the properties of cubic equations to show that the reality of the solutions (ϵ) is ensured if $\lambda\leqslant 0.17032$ which yields $\lambda_c^{(3)}=0.1703$. It is simple to show in a similar manner that for $H(\lambda)=H_0+i\lambda x^n$, $n=2$, which is not $\widehat{P}\widehat{T}$ invariant, the solutions of the corresponding secular equation in a two-dimensional basis space are always complex no matter what the value of λ is. Apparently, $\widehat{P}\widehat{T}$ invariance imposes some restrictions on the eigenvalues of certain classes of non-Hermitian Hamiltonians in finite-dimensional subspaces but cannot ensure reality of the spectrum of $H(\lambda)=H_0+i\lambda x^n$ ($n=1,3,\cdot$) for the entire range of λ. *The spectrum is real only if λ is below a critical value* (λ_c). The critical value apparently depends upon the dimensionality of the basis space (N) and the index of the power n. We have already seen that $\lambda_c^{(3)}<\lambda_c^{(2)}$ for both $n=1$ and 3. One may be curious to know how $\lambda_c^{(N)}$ would behave, if $N\to\infty$ for $n=1$ or 3. We have investigated this question numerically by diagonalizing $H(\lambda)$ for different values of N, and checking out for each N the threshold value of λ below which all the eigenvalues are real. It turns out that $\lambda_c^{(N)}$ becomes vanishingly small as $N\to\infty$ [10]. This result, however, echoes the perturbative result obtained by Delabaere and Pham [4].

It further appears that larger the value of λ, smaller is the fraction of real eigenvalues for a given N, the dimensionality of the basis set [10]. It could be that the harmonic oscillator basis is inadequate to represent the $\widehat{P}\widehat{T}$ symmetric complex non-Hermitian Hamiltonians. Very little is known about the completeness of the eigenfunctions of non-Hermitian operators. The present analysis suggests that we must look into the problem more closely. Further analysis is in progress and we hope to return to the problem in the near future [10].

Dynamics with $H(\lambda)$. Since

$$H^{+}(\lambda) \neq H(\lambda),$$

$U_\lambda = e^{-iH(\lambda)t}$ is non-unitary although $H(\lambda)$ may be $\widehat{P}\widehat{T}$ symmetric. However, if $H(\lambda)$ is $\widehat{P}\widehat{T}$ symmetric U_λ is $\widehat{P}\widehat{T}$ symmetric, too. Does the $\widehat{P}\widehat{T}$ invariance of U_λ confer any special character on the dynamics of evolution under U_λ? In what follows, we demonstrate that for $\lambda < \lambda_c$, adiabatic switching in finite-dimensional subspaces allows the unperturbed eigenstate of $H_0 = P_x^2/2m + (1/2)kx^2$ to evolve into the corresponding eigenstate of the $\widehat{P}\widehat{T}$ invariant $H = H_0 + i\lambda_c x^n$ $(n = 1, 3)$. For $\lambda > \lambda_c$, adiabatic switching fails to achieve this transition.

Let us define a time-dependent Hamiltonian $H(t) = H_0 + S(t)[H(\lambda) - H_0]$, where

$$H(\lambda) = H_0 + i\lambda x^n \quad (n = 1),$$
$$H_0 = \frac{P_x^2}{2m} + \frac{1}{2}kx^2.$$

$S(t) = 0$ at $t = 0$ and 1 at $t = t_0$, where t_0 is the switching time. With the given choice for $S(t)$, $H(t) = H_0$ at $t = 0$ and $H(t) = H(\lambda)$ at $t = t_0$. Let us first consider a special $S(t)$ which approximately satisfies the required conditions; for example, if we take

$$S(t) = e^{-\gamma(t-t_0)^2}$$

with appropriate choices for γ and t_0, $H(t)$ can be made to evolve very slowly and $S(0) \approx 0$ and $S(t) = 1$. Alternatively, we may choose $S_1(t) = t/t_0$ so that $S_1(0) = 0$ and $S_1(t_0) = 1$. We start with the ground eigenstate of H_0 and allow the system Hamiltonian to evolve into $H(\lambda < \lambda_c)$. Fig. 1(a) shows the evolution profile of $E(t)$ with $S(t)$ as the switching function ($\gamma = 0.000000007$, $t_0 = 50000$ a.u.) while Fig. 1(b) displays the corresponding profile when $S_1(t_0 = 50000$ a.u.) is used as the switching function. During the entire span of the switching time, the norm of the evolving wave function remains practically conserved. The final energy which is real is independent of the mode of switching and corresponds to the lowest eigenvalue $\widehat{P}\widehat{T}$ symmetric Hamiltonian

$$H(\lambda) = \frac{P_x^2}{2m} + \frac{1}{2}kx^2 + i\lambda x^n \quad (\lambda < \lambda_c)$$

obtained by direct diagonalization. For $\lambda > \lambda_c$, no such adiabatic evolution seems possible, however, slow the switching may be. If the switching is sudden (with $\lambda \leqslant \lambda_c$) the response of the system is Rabi-like oscillations between two real energy values (Fig. 2). For $\lambda > \lambda_c$, sudden switching predicts absurd results. In either case, norm of $\Psi(t)$ is not conserved.

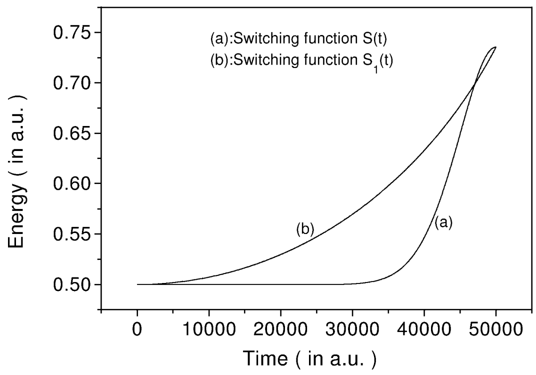

Fig. 1. (a) Profile of $E(t)$ as a function of switching time with the switching function $S(t)$. (b) The same for another choice $S_1(t)$ of the switching function for the $n = 1$ case.

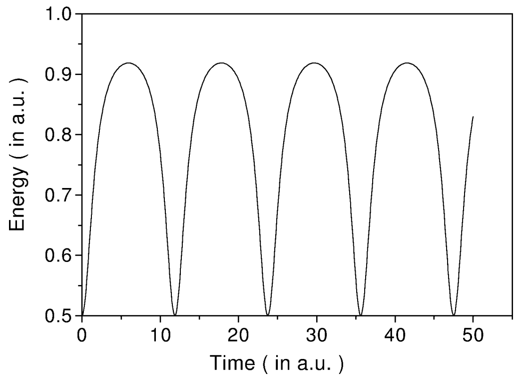

Fig. 2. Energy profile as a function of time in case of sudden switching with $\lambda < \lambda_c$.

3. Conclusion

In finite-dimensional subspaces of the Hilbert space spanned by the eigenkets of the harmonic oscillator Hamiltonian, $\widehat{P}\widehat{T}$ symmetric non-Hermitian Hamiltonians of the type $H = H_0 + i\lambda x^n$ ($H_0 \equiv$ harmonic oscillator Hamiltonian, $n = 1, 3$) have real eigenvalues only when $\lambda < \lambda_c$. The critical value of $\lambda = \lambda_c$ depends upon the basis size (N) and the nature of perturbing term $(i\lambda x^n)$. One should be cautions therefore to make use of the Zinn-Justin–Bessis conjecture while working within the limits of a finite basis set approximation. The quantum evolution dynamics from an eigenstate of a Hermitian H_0 to that of a $\widehat{P}\widehat{T}$ symmetric non-Hermitian $H(\lambda < \lambda_c)$ under adiabatic switching condition preserves the quantum number as long as $\lambda < \lambda_c$, while switching from $H_0 \to H(\lambda > \lambda_c)$ fails to do so.

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References

[1] D. Besis, as cited in Ref. [2].
[2] C.M. Bender, S. Boettcher, Phys. Rev. Lett. 80 (1998) 5243.
[3] E. Delabaere, F. Pham, Phys. Lett. A 250 (1998) 25.
[4] E. Delabaere, F. Pham, Phys. Lett. A 250 (1998) 29.
[5] E. Delabaere, T.D. Tai, J. Phys. A 33 (2000) 8741.
[6] C.M. Bender, S. Boettcher, P.N. Meisinger, J. Math. Phys. 40 (1999) 2201.
[7] M. Znojil, Phys. Lett. A 259 (1999) 220.
[8] A. Khare, B.P. Mondal, Phys. Lett. A 272 (2000) 53.
[9] M. Znojil, J. Phys. A: Math. Gen. 33 (2000) 161.
[10] C.K. Mondal, K. Maji, S.P. Bhattacharyya, in preparation.