Annals of Physics 363 (2015) 496–502

Contents lists available at ScienceDirect

Annals of Physics

journal homepage: www.elsevier.com/locate/aop

Three PT-symmetric Hamiltonians with completely different spectra

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HIGHLIGHTS

- PT-symmetric Hamiltonians exhibit real eigenvalues when PT symmetry is unbroken.
- PT-symmetric multidimensional Hamiltonians appear to show PT phase transitions.
- We study the PT-Stark effect on three different central-field models.
- They exhibit completely different spectra in terms of a parameter g.
- The spectra range from complex for all g to real for all g.

ARTICLE INFO

Article history:
Received 13 July 2015
Accepted 15 October 2015
Available online 24 October 2015

Keywords:
PT-symmetry
Central-field part
Stark effect
PT phase transition
Broken PT symmetry

ABSTRACT

We discuss three Hamiltonians, each with a central-field part H_0 and a PT-symmetric perturbation igz. When H_0 is the isotropic Harmonic oscillator the spectrum is real for all g because H is isospectral to $H_0 + g^2/2$. When H_0 is the Hydrogen atom then infinitely many eigenvalues are complex for all g. If the potential in H_0 is linear in the radial variable r then the spectrum of H exhibits real eigenvalues for $0 < g < g_c$ and a PT phase transition at g_c.

1. Introduction

It is known since long ago that some non-Hermitian operators may exhibit real eigenvalues [1,2]. This fact remained a somewhat exotic mathematical subject till Bender and Boettcher [3] suggested that those operators may exhibit unbroken parity-time (PT) symmetry. From then on the problem quickly developed into a prolific field of research [4] (and references therein).

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http://dx.doi.org/10.1016/j.aop.2015.10.011
0003-4916/

In a roughly general way we may say that most of the studied problems are represented by Hamiltonian operators of the form $H = H_0 + \lambda H'$, where H_0 is parity-invariant $PH_0P = H_0$ and H' is parity antisymmetric $PH'P = -H'$, where P is the parity operator. If $\lambda = ig$ is imaginary (where g is obviously real) then H is PT symmetric: $PTHPT = H$, where T is the time-reversal operator [5].

In the beginning, most of the models studied were mainly one-dimensional [3,4,6,7] in which case H_0 only exhibits parity symmetry and its eigenfunctions $\psi^{(0)}$ are even or odd: $P\psi^{(0)} = \pm\psi^{(0)}$ but later the researchers began to look for multidimensional examples [8–22]. It was suggested that space–time (ST) symmetry could be a suitable generalization of the PT one [23]. In this case $SH_0S = H_0$ and $SH'S = -H'$, where S is a unitary operator such that $S^\dagger = S^{-1} = S$. Most of the effort was devoted to find new multidimensional non-Hermitian Hamiltonians with real spectra.

In the multidimensional case H_0 and H may exhibit more complex symmetry that is conveniently described by means of group theory [23–25]. In this way Fernández and Garcia [26,27] and Amore et al. [28,29] found that some ST-symmetric Hamiltonians exhibit broken ST symmetry for all values of g. The main conjecture was that ST symmetry may be unbroken for some values of g provided that S is the only member of a class in the point group for H_0 [28]. This appeared to be the case when $S = P$. In particular, some of the results of Fernández and Garcia [26,27] and Amore et al. [28,29] appear to contradict the main conjecture put forward by Klaiman and Cederbaum [23].

The purpose of this paper is the discussion of three PT-symmetric Hamiltonians for which $H_0 = p^2/2 + V(r)$ exhibits central-field symmetry and $H' = z$. The resulting Hamiltonian H exhibits cylindrical symmetry and may be viewed as a kind of Stark effect with imaginary electric field. In Section 2 we outline the main ideas of PT symmetry as well as a simple argument based on perturbation theory [26–29]. In Section 3 we briefly discuss the general case. In Sections 4–6 we show that the models with $V(r) = r^2/2$, $V(r) = -1/r$, and $V(r) = r$, respectively, exhibit completely different spectra. Finally, in Section 7 we summarize the main results of the paper and draw conclusions.

2. Parity-time symmetry

Let $A = PT = A^{-1}$ be the antiunitary operator given by the product of the parity P and time-reversal T operators [5,3]. The Hamiltonian operator H is said to be PT symmetric if

$$AHA^{-1} = H. \tag{1}$$

If

$$H\psi = E\psi, \tag{2}$$

then

$$AH\psi = AHA^{-1}A\psi = HA\psi = AE\psi = E^*A\psi. \tag{3}$$

If $A\psi = a\psi$, a being a complex number, then we say that PT symmetry is unbroken and $E = E^*$. It is not difficult to prove that $|a| = 1$. Fernández and Garcia [30] found a case in which $A\psi \neq a\psi$ and still E is real. They proposed the supposedly more general condition $HA\psi = EA\psi$ for the occurrence of real spectrum; that is to say, when ψ and $A\psi$ are two linearly independent eigenfunctions of H with the same eigenvalue E. This situation does not take place unless the spectrum of H is degenerate. However, further analysis reveals that both conditions are equivalent. In fact, if we choose $\varphi = c_1\psi + c_2A\psi$, where $c_2^* = ac_1$ and $c_1^* = ac_2$, then $A\varphi = a\varphi$. It is worth adding that none of these conditions is of practical utility to predict whether H will have real eigenvalues or not because one commonly ignores the effect of A on the eigenvectors of H.

Most of the examples studied so far are of the form

$$H = H_0 + \lambda H', \tag{4}$$

where

$$PH_0P = H_0, \qquad TH_0T = H_0, \qquad PH'P = -H', \qquad TH'T = H' \tag{5}$$

and $\lambda = ig$, where g is real. Since $T\lambda H'T = \lambda^* THT = -\lambda H'$ then $AHA = H$. Some useful information on the spectrum of H is given by the perturbation series

$$E = \sum_{j=0} E^{(j)} \lambda^j, \tag{6}$$

because if at least one coefficient of odd order $E^{(2i+1)}$ is nonzero then E is expected to be complex for sufficiently small g. In such a case the PT-phase transition [14] takes place at the trivial Hermitian limit $g = 0$. If we write $H(\lambda)\psi_m = E_m(\lambda)\psi_m$ then $PH(\lambda)\psi_m = PH(\lambda)PP\psi_m = H(-\lambda)P\psi_m = E_m(\lambda)P\psi_m$. If ψ_m and $P\psi_m$ are linearly dependent, then $E_m(-\lambda) = E_m(\lambda)$ and all the perturbation corrections of odd order vanish; otherwise $P\psi_m = \psi_n$, $E_m(-\lambda) = E_n(\lambda)$ and we cannot draw a conclusion so easily. The latter case may only take place when the spectrum of H is degenerate. In many cases it suffices to calculate the simplest, straightforward perturbation correction of first order $E^{(1)}$ [26–29].

3. Stark effect

Consider the Hamiltonian operator

$$H = -\frac{1}{2}\nabla^2 + V(r) + \lambda z, \tag{7}$$

where $V(r)$ is spherically symmetric (depends only on r). The eigenfunctions of $H_0 = H(\lambda = 0)$

$$H_0 \psi^{(0)}_{\nu lm} = E^{(0)}_{\nu l} \psi^{(0)}_{\nu lm}, \tag{8}$$

are also eigenfunctions of the angular momentum operators L^2 and L_z

$$\begin{aligned} L^2 \psi^{(0)}_{\nu lm} &= l(l+1)\psi^{(0)}_{\nu lm}, \\ L_z \psi^{(0)}_{\nu lm} &= m\psi^{(0)}_{\nu lm}, \\ l &= 0, 1, \ldots, \ m = 0, \pm 1, \ldots, \pm l. \end{aligned} \tag{9}$$

In spherical coordinates the eigenfunctions can be factored as

$$\psi^{(0)}_{\nu lm}(r, \theta, \phi) = R_{\nu l}(r) Y^m_l(\theta, \phi), \tag{10}$$

where $R_{\nu l}(r)$ is the radial part, $\nu = 0, 1, \ldots$, is the radial quantum number and $Y^m_l(\theta, \phi)$ are the spherical harmonics. Since the eigenvalues of H_0 do not depend on m they are at least $(2l + 1)$-fold degenerate.

The perturbation $H' = z$ breaks the degeneracy of the spectrum of H_0 but the states with $m > 0$ remain two-fold degenerate because the eigenvalues of H do not depend on the sign of the magnetic quantum number m.

Since

$$P\psi^{(0)}_{\nu lm} = (-1)^l \psi^{(0)}_{\nu lm}, \tag{11}$$

and $PzP = -z$ the matrix elements

$$z^{\nu' l' m}_{\nu lm} = \left\langle \psi^{(0)}_{\nu lm} \middle| z \middle| \psi^{(0)}_{\nu' l' m} \right\rangle, \tag{12}$$

are zero when $l - l'$ is even. The perturbation corrections of first order to the energy $E^{(1)}_{\nu lm}$ are given by the eigenvalues of the matrix with elements $z^{\nu' l' m}_{\nu lm}$. We will discuss three examples in the subsequent sections.

4. Isotropic harmonic oscillator

When

$$V(r) = \frac{1}{2} r^2 \tag{13}$$

the Schrödinger equation is exactly solvable and the eigenfunctions and eigenvalues are given by

$$\psi_{n_1\,n_2\,n_3}(x,y,z) = \varphi_{n_1}(x)\varphi_{n_2}(y)\varphi_{n_3}(z+\lambda),$$
$$E_k = \left(k+\frac{3}{2}\right) - \frac{1}{2}\lambda^2, \quad k = n_1+n_2+n_3,$$
$$n_1, n_2, n_3 = 0, 1, \ldots, \tag{14}$$

where $\varphi_n(q)$ is an eigenfunction of the one-dimensional harmonic oscillator $H_{HO} = -\frac{1}{2}\frac{d^2}{dq^2} + \frac{1}{2}q^2$.

Since

$$A\psi_{n_1\,n_2\,n_3}(x,y,z) = \psi_{n_1\,n_2\,n_3}(-x,-y,-z)^* = \varphi_{n_1}(-x)\varphi_{n_2}(-y)\varphi_{n_3}(-z+\lambda^*)$$
$$= (-1)^k\psi_{n_1\,n_2\,n_3}(x,y,z), \tag{15}$$

then the PT symmetry is unbroken for all g which accounts for the fact that the eigenvalues in Eq. (14) are real for all g.

Although in this case the approximate analysis based on perturbation theory may appear to be unnecessary we carry it out anyway merely for comparison purposes. To begin with, note that $P\psi^{(0)}_{n_1\,n_2\,n_3}(x,y,z) = (-1)^k\psi^{(0)}_{n_1\,n_2\,n_3}(x,y,z)$. The perturbation correction of first order to a given energy level $E_k^{(0)}$ is given by matrix elements of the form

$$z^{m_1\,m_2\,m_3}_{n_1\,n_2\,n_3} = \left\langle \psi^{(0)}_{n_1\,n_2\,n_3}\right| z \left|\psi^{(0)}_{m_1\,m_2\,m_3}\right\rangle, \tag{16}$$

that vanish for all degenerate states because $k = n_1+n_2+n_3 = m_1+m_2+m_3$. Therefore, $E_k^{(1)} = 0$ for all the states of the PT Stark effect in the isotropic harmonic oscillator. This result is consistent with the form of the exact eigenvalues (14) that depend on g^2.

There is another way to prove that the PT symmetry for this problem remains unbroken for all values of g. The proof is based on the fact that H can be written in terms of a similarity transformation of H_0:

$$H = UH_0U^{-1} + \frac{g^2}{2}, \qquad U = e^{-gp_z}, \tag{17}$$

where $p_z = -i\frac{d}{dz}$. Obviously, H_0 and UH_0U^{-1} are isospectral [31].

5. Hydrogen atom

The unperturbed eigenvalues for the Coulomb interaction

$$V(r) = -\frac{1}{r}, \tag{18}$$

are given by

$$E_n^{(0)} = -\frac{1}{2n^2}, \qquad n = \nu + l + 1. \tag{19}$$

Therefore, there are pairs of degenerate states $\psi^{(0)}_{\nu lm}$, $\psi^{(0)}_{\nu' l' m}$ for which $l - l' = \nu' - \nu$ is odd and the corresponding matrix elements $z^{\nu' l' m}_{\nu\, l\, m}$ (12) are nonzero. In such cases, which for real λ give rise to what is commonly known as linear Stark effect [32,33], the perturbation correction of first order is nonzero and the eigenvalues of H are complex for $g \neq 0$.

The Schrödinger equation for this problem is separable in parabolic coordinates and the exact calculation of the perturbation corrections in terms of the parabolic quantum numbers $n_1 = 0, 1, \ldots$, $n_2 = 0, 1, \ldots$ and $m = 0, \pm 1, \ldots$ is straightforward [34]. It is customary to write the perturbation series

$$E_{nq|m|} = \sum_{j=0}^{\infty} E^{(j)}_{nq|m|}\lambda^j, \tag{20}$$

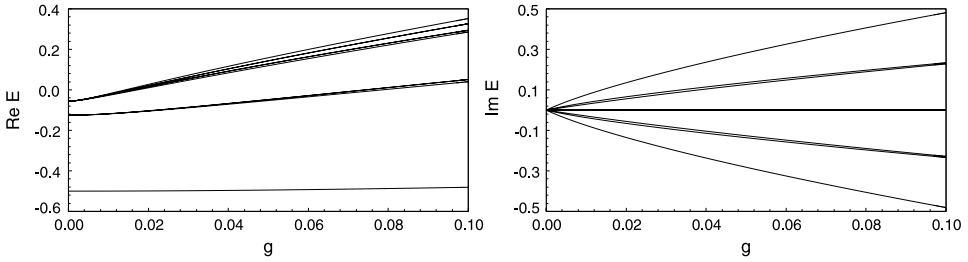

Fig. 1. Real and imaginary parts of the lowest eigenvalues of the PT-symmetric Stark effect in hydrogen.

in terms of the quantum numbers $n = n_1 + n_2 + |m| + 1$ and $q = n_1 - n_2$ [34]. All the coefficients of odd order vanish when $q = 0$ but the states with $q \neq 0$ are expected to be complex when $g \neq 0$.

The argument based on perturbation theory just outlined is sufficient to conclude that this model exhibits complex eigenvalues when $g \neq 0$ and that the PT phase transition [14] takes place at the trivial Hermitian limit $g = 0$. Nevertheless, we will show some numerical results to illustrate the point. Here we choose the most efficient method of Benassi and Grecchi [35] that is based on the separation of the Schrödinger equation in squared-parabolic coordinates. Since the details of this approach have been given elsewhere [35–37], here we just show the results. Fig. 1 shows the real and imaginary parts of the lowest eigenvalues. It is clear that the PT phase transition takes place at the trivial Hermitian limit as already argued above.

The remarkable difference between the spectra of this problem and the previous one can be traced back to the symmetry of H_0. The general central-field model is invariant under the group O(3) while, on the other hand, the hydrogen atom is invariant under the group O(4) [38]. Such higher symmetry is due to the conservation of the Runge–Lenz vector in the latter model. Thus, the higher symmetry of H_0 appears to be the reason why the PT symmetry is broken for all g in the perturbed hydrogen atom. While the kth harmonic-oscillator eigenvalue $E_k^{(0)}$ is $\frac{(k+1)(k+2)}{2}$-fold degenerate, the nth eigenvalue of the hydrogen atom $E_n^{(0)}$ is n^2-fold degenerate. The greater degeneracy of the latter model allows the appearance of nonzero matrix elements $z_{\nu\, l\, m}^{\nu' l' m}$ and nonzero perturbation corrections of first order.

6. Linear potential

As a nontrivial example we consider the linear potential

$$V(r) = r. \tag{21}$$

In this case we cannot solve the eigenvalue equation for H_0 exactly but we can nevertheless calculate the perturbation correction of first order to any energy level $E_{\nu\, l}^{(0)}$ because it is determined by matrix elements of the form

$$z_{\nu\, l\, m}^{\nu\, l\, m'} = \left\langle \psi_{\nu\, l\, m}^{(0)} \middle| z \middle| \psi_{\nu\, l\, m'}^{(0)} \right\rangle, \tag{22}$$

which vanish for all sets of quantum numbers as argued in Section 3. Therefore, $E_{\nu\, l\, |m|}^{(1)} = 0$ and there is a chance that PT symmetry may be unbroken for sufficiently small g.

We can calculate approximate eigenvalues by means of diagonalization of a suitable matrix representation of the Hamiltonian. For simplicity, here we choose the nonorthogonal Slater-type basis set

$$B = \left\{ r^n e^{-\alpha r} Y_l^m(\theta, \phi), n, l, |m| = 0, 1, \ldots \right\}. \tag{23}$$

Present numerical results show that this problem exhibits the usual spectral pattern common to most PT-symmetric Hamiltonians studied by other authors; that is to say, unbroken PT symmetry for $0 < g < g_c$. For sufficiently small values of g the eigenvalues are real. As g increases two eigenvalues approach each other, coalesce at an exceptional point [39–42] $g_i \geq g_c$ becoming a pair of

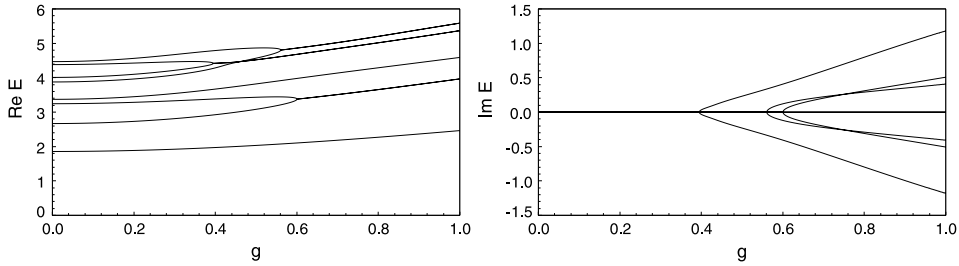

Fig. 2. Lowest eigenvalues with $m = 0$ for the potential $V(r, z) = r + igz$.

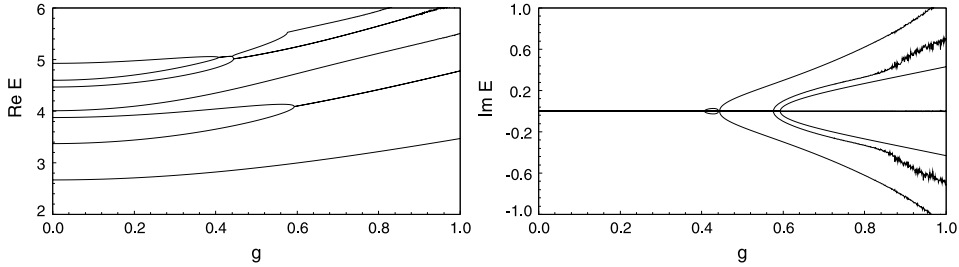

Fig. 3. Lowest eigenvalues with $m = 1$ for the potential $V(r, z) = r + igz$.

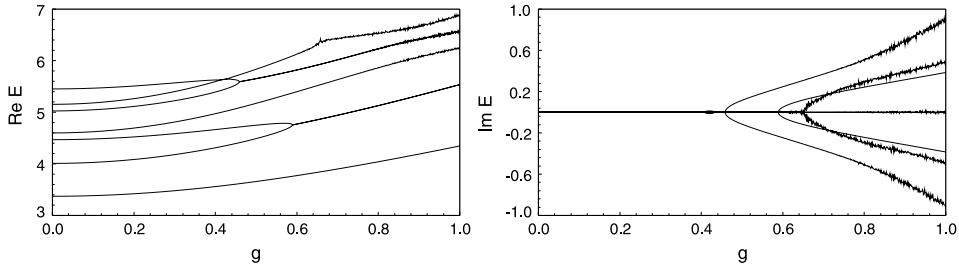

Fig. 4. Lowest eigenvalues with $m = 2$ for the potential $V(r, z) = r + igz$.

complex conjugate numbers for $g > g_i$. This behaviour is illustrated by Figs. 2–4, for $m = 0, 1, 2$, respectively. Those results were obtained by diagonalization of the matrix representation of the Hamiltonian operator in the Slater basis set (23) with $\alpha = 2$. The irregular lines reflect errors in the calculation of the eigenvalues originated in the quasi linear dependence of the basis set. This shortcoming of the present approach becomes more noticeable as the number of radial basis functions increases. Although our numerical results are not extremely accurate and are restricted to the lowest eigenvalues for the reason just indicated, they appear to suggest that the smallest exceptional point g_c may be nonzero and that there is a PT phase transition at such point. We think that a more accurate calculation is not necessary to illustrate the difference between this model and the other two ones discussed above.

7. Conclusions

In this paper we have discussed three Hamiltonians given by three different central-field Hermitian parts and the same non-Hermitian PT-symmetric perturbation. Although at first sight they appear to be similar, they exhibit completely different spectra. In the case of the isotropic harmonic oscillator the PT symmetry is unbroken and the spectrum is real for all g. The reason is that H and H_0 are related by the similarity transformation (17). On the other hand, the PT symmetry is broken for all g in the

case of the hydrogen atom. Quite in between the linear radial potential appears to exhibit unbroken PT symmetry for all $0 < g < g_c$ and a phase transition at some g_c that we were unable to determine.

The remarkable difference among the spectra of such seemingly similar Hamiltonians is due to the symmetry of H_0. As a general rule the higher the symmetry of H_0 the more likely the occurrence of complex eigenvalues and the Hamiltonian for the hydrogen atom exhibits the greatest symmetry by far. We have already discussed the effect of symmetry in earlier papers [26–29] but we have not seen such a remarkable difference in the behaviour of the non-Hermitian Hamiltonians.

In closing we want to stress the fact that perturbation theory provides a useful hint about the nature of the spectra of a given non-Hermitian Hamiltonian. If a perturbation correction of odd order (we typically look for the first one) is nonzero then we know that the spectrum is complex for all values of g (or at least for sufficiently small g). If all the available perturbation corrections of odd order are zero then there is a chance of finding real spectrum for some values of g. Obviously, this case should be investigated by more accurate calculations. As the symmetry of H_0 increases, then also increases the dimension of its eigenspaces and, consequently, the dimension of the matrix representation of the perturbation in those eigenspaces. As a result it also increases the chance of nonzero perturbation corrections of first order.

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