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LETTER TO THE EDITOR

Generalized PT symmetry and real spectra

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Abstract
The fact that eigenvalues of **PT**-symmetric Hamiltonians **H** can be real for some values of a parameter and complex for others is explained by showing that the matrix elements of **H**, and hence the secular equation, are real, not only for **PT** but also for any antiunitary operator **A** satisfying $\mathbf{A}^{2k} = 1$ with k odd. The argument is illustrated by a 2×2 matrix Hamiltonian, and two examples of the generalization are given.

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1. Introduction

At first encounter it is surprising that any finite subset of levels of a complex-valued non-Hermitian operator is real. It is known, however, that complex-valued non-Hermitian operators invariant under parity **P** and time-reversal **T** (but not **T** alone) can have energy levels that are sometimes real and sometimes complex, depending on the value of a parameter. This happens, for example, with

$$H = p^2 + x^4 + \mathrm{i}ax \qquad (1)$$

where as a increases successively higher pairs of real levels collide and become complex (Delabaere and Trinh 2000, Bender *et al* 2001, Dorey *et al* 2001b).

Our main aim here is to demystify such behaviour by demonstrating (section 3) that for non-Hermitian Hamiltonians **H**, invariant not only under **PT** but also under a much wider class of antiunitary symmetries, it is possible to construct a basis in which the matrix elements of **H** are real. Then the secular equation $\det(E - \mathbf{H}) = 0$ is real, and it is not surprising that some energies are real and some are complex. We also give examples (section 3) of these generalized symmetries.

There also exist non-Hermitian but **PT**-symmetric Hamiltonians such as

$$H = p^2 - (\mathrm{i}x)^a \qquad (a > 2) \qquad (2)$$

for which *all* levels are known (Bender and Boettcher 1998, Bender *et al* 1999, Mezincescu 2000, Bender and Wang 2001, Dorey *et al* 2001a) to be real. Here we will not be concerned with such examples; proofs that the spectra are real seem to require methods that are special to each case.

We begin with the simplest possible example: a quantum particle inhabiting a coordinate axis that consists of just the two points $x = \pm 1$. Then $\mathbf{H}$ is a 2×2 matrix with indices $i, j = \pm 1$, and the action of $\mathbf{PT}$ is

$$(\mathbf{PTH})_{i,j} = H^*_{-i,-j}. \tag{3}$$

$\mathbf{PT}$ symmetry, that is $[\mathbf{PT}, \mathbf{H}] = 0$, means

$$H^*_{-i,-j} = \mathbf{H}_{i,j} \qquad \text{i.e.} \quad \mathbf{H} = \begin{pmatrix} a & b \\ b^* & a^* \end{pmatrix}. \tag{4}$$

This is non-Hermitian if a is complex. The secular equation is

$$E^2 - 2E\,\mathrm{Re}\,a + |a|^2 - |b|^2 = 0 \tag{5}$$

which is real. The eigenvalues

$$E = \mathrm{Re}\,a \pm \sqrt{|b|^2 - (\mathrm{Im}\,a)^2} \tag{6}$$

are real if $|\mathrm{Im}\,a| < |b|$ (including the Hermitian case $\mathrm{Im}\,a = 0$), are degenerate when $|\mathrm{Im}\,a| = |b|$ and are complex if $|\mathrm{Im}\,a| > |b|$, so this simple example encapsulates the phenomena we wish to understand.

From the form (4) of $\mathbf{H}$, it is not immediately obvious why the secular equation is real. However, it can be made obvious by representing $\mathbf{H}$ in the orthonormal basis

$$|u\rangle = \frac{1}{2}\begin{pmatrix} 1+\mathrm{i} \\ 1-\mathrm{i} \end{pmatrix} \qquad |v\rangle = \frac{1}{2}\begin{pmatrix} 1-\mathrm{i} \\ 1+\mathrm{i} \end{pmatrix} \tag{7}$$

(whose construction will be explained later) because this makes the operator real (though non-Hermitian):

$$\mathbf{H} = \begin{pmatrix} \langle u|\mathbf{H}|u\rangle & \langle u|\mathbf{H}|v\rangle \\ \langle v|\mathbf{H}|u\rangle & \langle v|\mathbf{H}|v\rangle \end{pmatrix} = \begin{pmatrix} \mathrm{Re}\,a - \mathrm{Im}\,b & -\mathrm{Im}\,a + \mathrm{Re}\,b \\ \mathrm{Im}\,a + \mathrm{Re}\,b & \mathrm{Re}\,a + \mathrm{Im}\,b \end{pmatrix}. \tag{8}$$

The non-Hermitian Hamiltonians (4) and (8) have physical significance. The operator (4) represents a spin-1/2 particle in a magnetic field whose x and y components are real but the z component is complex, corresponding to differential absorption between the spin states $s_z = \pm 1/2$. The operator (8) describes 2-beam diffraction of an atomic beam in a near-resonant laser beam, represented by a complex periodic potential (Berry and O'Dell 1998).

Japaridze (2002) and Mostafazadeh (2002) have also discussed general features of $\mathbf{PT}$ symmetry, including those we consider here, though with a different emphasis.

2. Generalization

The key observation is that $\mathbf{PT}$ is an antiunitary operator (Porter 1965). The defining property for any such operator $\mathbf{A}$ is that, for arbitrary states $|\psi\rangle$ and $|\phi\rangle$,

$$\langle \mathbf{A}\phi|\mathbf{A}\psi\rangle = \langle \phi|\psi\rangle^*. \tag{9}$$

Any antiunitary operator can be represented in the form

$$\mathbf{A} = \mathbf{UK} \tag{10}$$

where $\mathbf{U}$ is a unitary operator (e.g., $\mathbf{P}$) and $\mathbf{K}$ is a complex conjugation (e.g., $\mathbf{T}$ in position representation).

Now consider Hamiltonians with antiunitary symmetry, that is $[\mathbf{A}, \mathbf{H}] = 0$, for which $\mathbf{A}$ has the form

$$\mathbf{A}^{2k} = 1 \qquad k \text{ odd} \tag{11}$$

($\mathbf{PT}$ corresponds to $k = 1$). We will show that for any such $\mathbf{A}$ it is possible to construct a basis in which the matrix elements of $\mathbf{H}$ are real, so that the secular equation determining the eigenvalues of $\mathbf{H}$ is real. The argument is a slight generalization of that applied in quantum chaology (Robnik and Berry 1986), which itself slightly generalized arguments (Porter 1965) from nuclear physics; the previous applications were to Hermitian operators, but remain valid for the non-Hermitian operators we consider here.

For the basis $|n_A\rangle$ in which $\mathbf{H}$ is real, we use the term $\mathbf{A}$-adapted; $|n_A\rangle$ is defined to have the property

$$\mathbf{A}^k|n_A\rangle = |n_A\rangle. \tag{12}$$

We construct the $\mathbf{A}$-adapted basis $|n_A\rangle$ from any orthonormal basis $|n\rangle$ by writing

$$|n_A\rangle = |n\rangle + \mathbf{A}^k|n\rangle. \tag{13}$$

It is easily verified that $|n_A\rangle$ satisfies (12), and application of a standard orthonormalization procedure will ensure that $\langle m_A|n_A\rangle = \delta_{m,n}$.

The proof that $\mathbf{H}$ is real goes as follows:

$$\begin{aligned}\langle n_A|\mathbf{H}|m_A\rangle &= \langle \mathbf{A}^k n_A|\mathbf{A}^k\mathbf{H}m_A\rangle^* && \text{(antiunitarity)}\\ &= \langle \mathbf{A}^k n_A|\mathbf{H}|\mathbf{A}^k m_A\rangle^* && \text{(antiunitarity symmetry)}\\ &= \langle n_A|\mathbf{H}|m_A\rangle^* && (\mathbf{A}\text{-adapted basis}).\end{aligned} \tag{14}$$

Evidently the proof applies when $\mathbf{A} = \mathbf{PT}$. For the simple example in the last section, the $\mathbf{A}$-adapted basis (7) follows (after normalization) from the prescription (13) with $k = 1$, starting from the basis $\mathrm{col}(1, \pm\mathrm{i})$, because

$$\begin{pmatrix}1\\ \mp\mathrm{i}\end{pmatrix} + \mathbf{PT}\begin{pmatrix}1\\ \mp\mathrm{i}\end{pmatrix} = \begin{pmatrix}1\pm\mathrm{i}\\ 1\mp\mathrm{i}\end{pmatrix}. \tag{15}$$

For a $\mathbf{PT}$-symmetric differential operator on the axis $-\infty < x < +\infty$, the analogous $\mathbf{A}$-adapted basis is

$$\begin{aligned}|u(x)\rangle &= \tfrac{1}{2}((1+\mathrm{i})|x\rangle) + ((1-\mathrm{i})|-x\rangle)\\ |v(x)\rangle &= \tfrac{1}{2}((1-\mathrm{i})|x\rangle) + ((1+\mathrm{i})|-x\rangle).\end{aligned} \tag{16}$$

It is easy to confirm that in this representation the eigenequation for the operator

$$H = p^2 + V(x) \qquad \text{where} \quad V(x) = V^*(-x) \tag{17}$$

decouples into two real differential equations on the positive axis $0 \leqslant x < +\infty$.

3. Examples

An alternative to parity is the inversion operator $\mathbf{Q}$, under which $x \to 1/x$; clearly $\mathbf{Q}^2 = 1$. A complex non-Hermitian operator invariant under $\mathbf{QT}$ is

$$H = -(1+x^4)\left(\frac{\mathrm{d}}{\mathrm{d}x}\right)^2 - 2x^3\frac{\mathrm{d}}{\mathrm{d}x} - (\mathrm{i}x)^a - (\mathrm{i}x)^{-a} \qquad (2 < a < 4). \tag{18}$$

Elementary numerical analysis gives the energy levels as shown in figure 1, which are real, and construction of the $\mathbf{A}$-adapted basis according to the prescription of the last section confirms that the matrix elements of (18) are real.

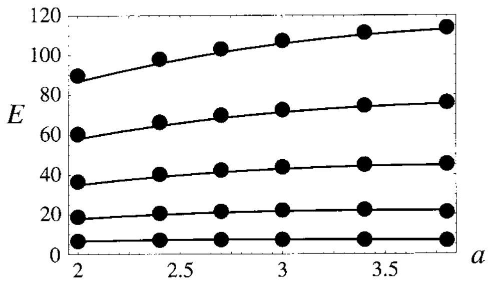

Figure 1. Dots: numerically-computed eigenvalues of the operator (18); curve: approximate eigenvalues computed from (20).

It is interesting to check that the approximate secular equation given by WKB asymptotics is also real. For this it is convenient to transform (18) to eliminate the first-order derivative, thus obtaining a non-Hermitian operator of Schrödinger form. The turning points X satisfy

$$\frac{3}{(X^2+X^{-2})} - (\mathrm{i}X)^a - (\mathrm{i}X)^{-a} = E \tag{19}$$

and (except for those on the unit circle) come in pairs X, $1/X^*$.

Consideration of the asymptotics of (18) near $x = 0$ and $x = \infty$ indicates that the appropriate path for the Bohr–Sommerfeld quantization is between turning points $1/X^*$ and X in the lower half-plane. Thus, the eigenvalues E are given by

$$\begin{aligned}\left(n+\tfrac{1}{2}\right)\pi &\approx \int_{1/X^*}^{X} \mathrm{d}x \sqrt{\frac{E+(\mathrm{i}x)^a+(\mathrm{i}x)^{-a}-3/(x^2+x^{-2})}{1+x^4}} \\ &= 2\mathrm{Re}\int_{1}^{X} \mathrm{d}x \sqrt{\frac{E+(\mathrm{i}x)^a+(\mathrm{i}x)^{-a}-3/(x^2+x^{-2})}{1+x^4}}\end{aligned} \tag{20}$$

where the second equality follows from the **QT** symmetry of the integrand after deforming the path to pass through $x = 1$. As figure 1 shows, the solutions of this real secular equation accurately reproduce even the low-lying levels.

This example is somewhat contrived, because **Q** becomes **P** under the transformation $x = \exp(y)$. A generalized antiunitary operator of the class (11), whose symmetry is not reducible to **PT**, describes a particle in the plane with a complex two-dimensional potential $V(r, \theta)$ invariant under

$$\mathbf{A} = \mathbf{R}_{\pi/k}\mathbf{K} \qquad (k \text{ odd}) \tag{21}$$

where $\mathbf{R}_\alpha$ denotes rotation by α. Such an operator is

$$H = p_x^2 + p_y^2 + V_0(r) + \mathrm{i}\sum_{l\,\text{odd}} a_l r^{kl}\cos(kl\theta+\phi_l). \tag{22}$$

From the usual angular momentum basis

$$\langle\theta|l\rangle = \exp(\mathrm{i}(l\theta+\alpha_l)). \tag{23}$$

The **A**-adapted basis constructed from (13) is

$$\langle\theta|l_A\rangle = \begin{cases}\cos(l\theta+\alpha_l) & (l \text{ even})\\ \mathrm{i}\cos(l\theta+\alpha_l) & (l \text{ odd}),\end{cases} \tag{24}$$

and it is easy to show that the matrix elements of (13) are real.

With the choice $V = r^2$, a simple form for $k = 1$ is

$$H = p_x^2 + p_y^2 + x^2 + y^2 + \mathrm{i}x \tag{25}$$

which separates into harmonic oscillators in x (shifted by $\mathrm{i}/2$) and y, both of which have real spectra. That the restriction to k odd in (11) is necessary can be seen by choosing $k = 2$, which gives

$$H = p_x^2 + p_y^2 + (x^2 + y^2) + \mathrm{i}a(x^2 - y^2) \qquad (a < 1). \tag{26}$$

Again this separates into two harmonic oscillators, but now the frequencies are complex, and the levels

$$E_{m,n} = (2m + 1)\sqrt{1 + \mathrm{i}a} + (2n + 1)\sqrt{1 - \mathrm{i}a} \tag{27}$$

are also complex unless $m = n$.

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