

Reality and non-reality of the spectrum of \mathcal{PT} -symmetric operators: Operator-theoretic criteria

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Abstract. We generalize some recently established criteria for the reality and non-reality of the spectrum of some classes of \mathcal{PT} -symmetric Schrödinger operators. The criteria include cases of discrete spectra and continuous ones.

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1. Introduction

A basic fact underlying \mathcal{PT} -symmetric quantum mechanics is the existence of non-self-adjoint, and not even normal, \mathcal{PT} -symmetric Schrödinger operators which have fully real spectrum. Here we consider only the classical \mathcal{PT} symmetry: in $L^2(\mathbf{R}^d)$, $d \geq 1$, \mathcal{P} is the parity operator defined by $(\mathcal{P}\psi)(x) = \psi(-x)$, and \mathcal{T} is the (antilinear) complex conjugation operator $\mathcal{T}\psi = \bar{\psi}$, $\forall \psi \in L^2(\mathbf{R}^d)$. An operator H is \mathcal{PT} -symmetric if it commutes with the combined action of \mathcal{P} and \mathcal{T} : $[H, \mathcal{PT}] = 0$, i.e. $H(\mathcal{PT}) = (\mathcal{PT})H$. A natural mathematical question arising in this context is the determination of conditions under which \mathcal{PT} symmetry actually yields real spectrum. A classical example is the imaginary cubic anharmonic oscillator

$$H_1(g) = -\frac{d^2}{dx^2} + x^2 + igx^3, \quad g \in \mathbf{R}. \quad (1)$$

The reality of the eigenvalues of $H_1(g)$ for small $|g|$ was first proved in 1980 [1] in the framework of perturbation theory. More precisely, in [1] it was proved that the unperturbed eigenvalues, $E_n = 2n + 1$, $n = 0, 1, \dots$, of $H_1(0)$ are stable with respect to the operator family $\{H_1(g) : g \in \mathbf{R}\}$ and the Rayleigh–Schrödinger perturbation expansion (RSPE) near any E_n has the form:

$$\sum_{k=0}^{\infty} a_k^{(n)} g^k, \quad a_0^{(n)} = E_n, \quad (2)$$

where $a_k^{(n)}$ is real $\forall n, k$ and $a_k^{(n)} = 0$ if k is odd. Moreover, the RSPE (2) is divergent but Borel summable to an eigenvalue $\lambda_n(g) \in \sigma(H_1(g))$. More precisely, let $B(u)$ denote the Borel transform of the series (2), then $B(u)$ has positive radius of convergence. It can be analytically continued to a neighbourhood of \mathbf{R}^+ and there exists $g_n > 0$ such that

$$\lambda_n(g) = \int_0^\infty B(gu)e^{-u}du, \quad \text{for } |g| < g_n. \quad (3)$$

The reality of the coefficients $a_k^{(n)}$ and (3) imply the reality of $\lambda_n(g)$.

In 1985, Bessis and Zinn-Justin made the conjecture that $\sigma(H_1(g))$ is real for all $g \in \mathbf{R}$. The conjecture was proved in 2002 by Shin [2]. Prior to that, Dorey *et al* in [3] proved the reality of the spectrum of $-d^2/dx^2 + igx^3, g \in \mathbf{R}$. However, examples can be provided of Hamiltonians where a spontaneous breaking of \mathcal{PT} symmetry generates complex eigenvalues. Therefore, an important issue is to extend the class of \mathcal{PT} -symmetric operators with real spectrum, providing both criteria for the reality of the spectrum and criteria for the existence of (non-real) complex eigenvalues (or, in general, complex spectrum).

In perturbation theory we consider a family of \mathcal{PT} -symmetric operators of the form

$$H(g) = H_0 + igW, \quad g \in \mathbf{R} \quad (4)$$

and we ask what conditions we can assume on the unperturbed operator H_0 and on the perturbation W in order to guarantee that the spectrum of $H(g), \sigma(H(g))$, is real, at least for small $|g|$, or, vice versa, to ensure that $\sigma(H(g))$ contains complex terms. In this framework the present article aims to provide answers to these questions. In §2 we present a review of the results obtained by the authors and collaborators in the case of discrete spectrum [4-6] and we provide a more general formulation of two criteria on the reality of the spectrum of $H(g)$ for small $|g|$. More precisely, we remark that the assumption that H_0 is bounded below, introduced in [4,5], is unnecessary: in fact the proof of the results does not make use of such assumption. In §3 we complete our review presenting some recent results [7] on the reality of the spectrum of \mathcal{PT} -symmetric Schrödinger operators $H(g)$ in the case of periodic potentials with continuous band-shaped spectrum. Finally, in §4 we improve the result obtained in [7] by providing a more general condition which ensures that $\sigma(H(g))$ contains at least a pair of complex analytic arcs for small $|g|$.

2. The case of discrete spectrum

We first define the operator family $H(g)$ formally given by (4) by specifying the assumptions on H_0 and W . Let H_0 be a self-adjoint operator in $L^2(\mathbf{R}^d), d \geq 1$, on some domain D_0 , with compact resolvents and therefore discrete spectrum. Let $\sigma(H_0) = \{\lambda_n: n \in \mathbf{N}\}$ denote the set of distinct eigenvalues of H_0 . Let W be a bounded operator in $L^2(\mathbf{R}^d)$. Moreover, assume that H_0 is \mathcal{P} -even and W is \mathcal{P} -odd, i.e. $\mathcal{P}H_0 = H_0\mathcal{P}$ and $\mathcal{P}W = -W\mathcal{P}$. Furthermore, let H_0 and W be \mathcal{T} -symmetric, i.e. $\mathcal{T}H_0 = H_0\mathcal{T}$ and $\mathcal{T}W = W\mathcal{T}$. Then the operator $H(g) = H_0 + igW, g \in \mathbf{R}$,

defined on the domain D_0 is \mathcal{PT} -symmetric and has discrete spectrum. The following theorem provides a criterion for the reality of $\sigma(H(g))$.

Theorem 1. *Under the above assumptions on H_0 and W assume the following conditions:*

- (i) $\sigma(H_0)$ is simple, i.e. each eigenvalue of H_0 has multiplicity 1;
- (ii) $\delta := \frac{1}{2} \inf_{n \neq m} |\lambda_n - \lambda_m| > 0$.

Then $\sigma(H(g)) \subset \mathbf{R}$ for $|g| < \delta/\|W\|$.

Remark. The set $\{\lambda_n: n \in \mathbf{N}\}$ does not necessarily represent an increasing sequence. For example the operator $H_0 := \mathcal{P}(-d^2/dx^2 + x^2)$ is not bounded below and its eigenvalues are

$$\lambda_n = \begin{cases} 2n + 1, & \text{if } n \text{ is even} \\ -2n - 1, & \text{if } n \text{ is odd.} \end{cases}$$

Sketch of the proof of Theorem 1

The proof (see [4] where the theorem is proved under the unnecessary condition that H_0 is bounded below) is based on the stability of the unperturbed eigenvalues. Since λ_n is simple $\forall n$, near each $\lambda_n \in \sigma(H(0))$ there is one and only one eigenvalue $\lambda_n(g)$ of $H(g)$ for $|g| < g_n$ (g_n suitably small) and $\lambda_n(g) \rightarrow \lambda_n$ as $g \rightarrow 0$. Now we recall that the eigenvalues of a \mathcal{PT} -symmetric operator come in pairs of complex conjugate values. Therefore, the uniqueness of $\lambda_n(g)$ implies its reality. Moreover, $\lambda_n(g)$ can be obtained as the sum of the (convergent) RSPE near λ_n , whose radius of convergence r_n can be bounded below uniformly in n : $r_n \geq g_0 := \delta/\|W\| > 0$. Hence g_0 is a common radius of convergence and for all n and $|g| < g_0$ the following expansion holds:

$$\lambda_n(g) = \lambda_n + \sum_{k=1}^{\infty} a_k^{(n)} g^k. \tag{5}$$

Thus, for $|g| < g_0$ the spectrum of $H(g)$ contains the set of real eigenvalues $\lambda_n(g), n \in \mathbf{N}$ given by (5). Now the core of the proof consists in showing that for $|g| < g_0$ there are no other eigenvalues in the spectrum of $H(g)$ besides those generated by the above expansions, i.e. $\sigma(H(g)) = \{\lambda_n(g): n \in \mathbf{N}\}$ for $|g| < \delta/\|W\|$, and this is proved in [4] using the analyticity of the operator family $H(g)$ for $g \in \mathbf{C}$ (see also [8]).

In order to prove the reality of the perturbed eigenvalues $\lambda_n(g)$ in the proof of Theorem 1, a crucial role is played by the simplicity of the unperturbed eigenvalues. Therefore, a natural question arises at this point regarding what can be said in the degenerate case, i.e. when the multiplicity of an eigenvalue $\lambda_n \in \sigma(H(0))$, $m(\lambda_n)$, is greater than one. The answer is not *a priori* obvious; in fact now near λ_n there are $m(\lambda_n) > 1$ eigenvalues of $H(g)$ and among them there might be pairs of complex conjugate values. A result that takes care of this question is stated in the following theorem, proved in [5].

Theorem 2. Let H_0 and $W \in L^\infty(\mathbf{R}^d)$ satisfy the assumptions stated at the beginning of the section. Let δ be defined as in Theorem 1. Assume the following conditions:

(A₁) $\delta > 0$;

(A₂) for each n , all the eigenfunctions of λ_n have the same parity: they are either all \mathcal{P} -even or all \mathcal{P} -odd.

Then for $|g| < \delta/\|W\|_\infty$, the spectrum of $H(g)$ is purely real.

Example (Perturbations of resonant harmonic oscillators)

Let

$$H_0 = \frac{1}{2} \sum_{k=1}^d \left[-\frac{d^2}{dx_k^2} + \omega_k^2 x_k^2 \right], \quad \omega_k \in \mathbf{R}. \quad (6)$$

First of all it is easy to see that in order to ensure condition (A₁) it is necessary and sufficient to assume that the frequencies ω_k are rational multiples of the same frequency, i.e. we must assume that they have the form

$$\omega_k = \frac{p_k}{q_k} \omega, \quad k = 1, \dots, d,$$

where p_k, q_k are relatively prime natural numbers. In turn, condition (A₂) is guaranteed if p_k, q_k are odd $\forall k$. More precisely the following result is proved in [5].

Corollary 3. Let H_0 be defined by (6) and $W \in L^\infty(\mathbf{R}^d)$. If p_k, q_k are both odd $\forall k$, then $H(g) = H_0 + igW$ has a purely real spectrum for $|g| < \delta/\|W\|_\infty$.

Assumption (A₂) is also a necessary condition for the reality of the spectrum of $H(g)$ for small $|g|$, when the degeneracy of the unperturbed eigenvalues is double. More precisely the following criterion for the existence of complex eigenvalues holds (see [4] for the proof).

Theorem 4. Let λ be an eigenvalue of H_0 with multiplicity $m = 2$ with eigenvectors ψ_1, ψ_2 with opposite parity, i.e. $\mathcal{P}\psi_1 = \psi_1$ and $\mathcal{P}\psi_2 = -\psi_2$. Let $W \in L^\infty_{\text{loc}}(\mathbf{R}^d)$ be relatively bounded with respect to H_0 , i.e. there exist $a, b > 0$ such that

$$\|Wu\| \leq a\|u\| + b\|H_0u\|, \quad \forall u \in D(H_0) \subset D(W).$$

Moreover, let $\langle W\psi_1, \psi_2 \rangle \neq 0$. Then there exists g_0 such that $H(g) = H_0 + igW$ has a pair of (non-real) complex conjugate eigenvalues near λ for $|g| < g_0$.

The criteria provided so far for the reality of the spectrum require that the perturbation W is bounded. A criterion that applies to a class of unbounded perturbations is given in the following theorem, proved in [6].

Theorem 5. Let $H(g)$ be the closed operator in $L^2(\mathbf{R})$ defined by the differential expression

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$$H(g) = -\frac{d^2}{dx^2} + V(x) + igW(x), \quad g \in \mathbf{R},$$

on the domain $H^2(\mathbf{R}) \cap D(V)$. Here V is a real valued even polynomial: $V(-x) = V(x), \forall x$, of degree $2p$, diverging positively at infinity, and W is a real valued odd polynomial: $W(-x) = -W(x), \forall x$, of degree $2q - 1$. Assume that $p > 2q, q \geq 1$. Then there exists $g_0 > 0$ such that $\sigma(H(g)) \subset \mathbf{R}$ for $|g| < g_0$.

Remark. Further investigations in the more general case of unbounded perturbation W , including the case when H_0 is \mathcal{PT} -symmetric and not self-adjoint, have led to weaker results (see [9,10]) that can be summarized as follows:

1. The perturbed eigenvalues of $H(g)$, generated by the stability of the unperturbed simple eigenvalues are real for $|g|$ small.
2. Complex eigenvalues cannot accumulate to finite points, i.e. if complex eigenvalues occur they diverge to infinity as $g \rightarrow 0$.

3. The case of continuous spectrum: Schrödinger operators with periodic potentials

One basic assumption for the criteria provided in the previous section is the discreteness of the spectrum of the unperturbed Hamiltonian (and consequently of the whole family $H(g), \forall g$, since the perturbation is assumed to be bounded or relatively bounded with respect to $H(0)$). In this section we will examine the case of continuous spectrum, again with the aim to obtain criteria for the reality of $\sigma(H(g))$ for small $|g|$. Although the setting may appear quite different from the previous one, we will actually deal with operators whose spectrum is given by the union of discrete spectra, and we will be able to extend the perturbation theory techniques described in the previous section to a class of operators with continuous spectrum.

We deal with the Schrödinger operator in $L^2(\mathbf{R})$

$$H\psi = \left(-\frac{d^2}{dx^2} + V \right) \psi, \quad (7)$$

where the potential V is complex-valued, \mathcal{PT} -symmetric and 2π -periodic, already considered by several authors (see e.g. [11–16]). If V is real-valued under mild regularity assumptions the spectrum of H is absolutely continuous on \mathbf{R} and band shaped (see e.g. [17]). Then a natural question is whether there exist periodic potentials generating Schrödinger operators with real band spectrum. The question has been examined in [11–15] by a combination of numerical and WKB techniques in several particular examples. In [16] it is proved that the occurrence of complex spectra cannot be excluded, and a condition has been isolated under which H admits complex spectrum consisting of a disjoint union of analytic arcs. In this section we illustrate a criterion for the reality of the spectrum for a class of \mathcal{PT} -symmetric Schrödinger operators with periodic potentials, obtained in [7].

Let us now specify the assumptions on H which will be again of the form $H = H(g) = H(0) + gW$, since the framework is once again that of perturbation theory.

Let $q(x) \in H_{loc}^{-1}(\mathbf{R})$ be a real-valued tempered distribution, 2π -periodic and \mathcal{P} -symmetric. Moreover, assume that the quadratic form generated by q is bounded relative to that generated by the kinetic energy, with relative bound $b < 1$, i.e. there exist $a, b > 0, b < 1$ such that

$$\int_{\mathbf{R}} q(x)|u(x)|^2 dx \leq b \int_{\mathbf{R}} |u'(x)|^2 dx + a \int_{\mathbf{R}} |u(x)|^2 dx, \quad \forall u \in H^1(\mathbf{R}).$$

Let $H(0)$ denote the self-adjoint realization in $L^2(\mathbf{R})$ of the differential expression

$$H(0) = -\frac{d^2}{dx^2} + q(x).$$

It is known [18] that the spectrum of $H(0)$ is continuous and band-shaped. More precisely, there exist two sequences $\alpha_n, \beta_n, n = 0, 1, \dots$, such that

$$0 \leq \alpha_0 \leq \beta_0 \leq \beta_1 \leq \alpha_1 \leq \alpha_2 \leq \beta_2 \leq \beta_3 \leq \alpha_3 \leq \alpha_4 \leq \dots$$

and $\sigma(H(0))$ is given by the union of the bands

$$B_{2n} := [\alpha_{2n}, \beta_{2n}], \quad B_{2n+1} := [\beta_{2n+1}, \alpha_{2n+1}], \quad n = 0, 1, \dots$$

Then

$$\Delta_n :=]\beta_{2n}, \beta_{2n+1}[, \quad]\alpha_{2n+1}, \alpha_{2n+2}[, \quad n = 0, 1, \dots$$

are the gaps between the bands. Let $|\Delta_n|$ denote the width of the gap $\Delta_n, n = 0, 1, \dots$. Now we introduce the perturbation term W . Let $W \in L^\infty(\mathbf{R})$ be a 2π -periodic, \mathcal{PT} -symmetric function, $\overline{W(-x)} = W(x), \forall x$.

Let $H(g)$ denote the closed operator in $L^2(\mathbf{R})$ formally given by

$$H(g) = -\frac{d^2}{dx^2} + q(x) + gW(x), \quad g \in \mathbf{R}$$

on the domain $D(H(0))$. Then $H(g)$ is \mathcal{PT} -symmetric. We are now ready to state the main result of this section (see [7] for the proof and more details).

Theorem 6. *Assume that all the gaps Δ_n of $H(0)$ are open (i.e., non-empty): $\alpha_n < \beta_n < \beta_{n+1} < \alpha_{n+1}, \forall n$ and*

$$d := \frac{1}{2} \inf_{n \in \mathbf{N}} |\Delta_n| > 0.$$

If $|g| < \frac{d^2}{2(1+d)\|W\|_\infty} := \bar{g}$ there exist real-valued sequences $\alpha_n(g), \beta_n(g), n = 0, 1, \dots$ such that $0 \leq \alpha_0(g) < \beta_0(g) < \beta_1(g) < \alpha_1(g) < \alpha_2(g) < \beta_2(g) < \beta_3(g) < \dots$, and

$$\sigma(H(g)) = \bigcup_{n \in \mathbf{N}} B_n(g),$$

where

$$B_{2n}(g) := [\alpha_{2n}(g), \beta_{2n}(g)], \quad B_{2n+1}(g) := [\beta_{2n+1}(g), \alpha_{2n+1}(g)], \quad \forall n.$$

In particular $\sigma(H(g))$ is real and band-shaped for $|g| < \bar{g}$.

Example (Perturbations of the Kronig–Penney model). The distribution

$$q(x) = \sum_{n \in \mathbf{Z}} \delta(x - 2\pi n)$$

fulfills the above conditions (see [7] for details). Hence if W is a bounded, 2π -periodic and PT -symmetric function, the operator

$$H(g) = -\frac{d^2}{dx^2} + \sum_{n \in \mathbf{Z}} \delta(x - 2\pi n) + gW(x)$$

has real band-shaped spectrum for $g \in \mathbf{R}, |g| < \bar{g}$.

Sketch of the proof of Theorem 6

By the Floquet–Bloch theory (see e.g. [17,19]), $\lambda \in \sigma(H(g))$ if and only if the equation

$$H(g)\psi = \lambda\psi \tag{8}$$

has a non-constant solution ψ . In turn all such solutions have the form $\psi_p(x) = e^{ipx}\phi_p(x)$, $p \in]-\frac{1}{2}, \frac{1}{2}]$ (the Brillouin zone), and ϕ_p is 2π -periodic. Then ψ_p solves (8) if and only if ϕ_p solves $H_p(g)\phi_p = \lambda\phi_p$ where $H_p(g)$ is the operator in $L^2(0, 2\pi)$ formally given by

$$H_p(g)u = \left(-i\frac{d}{dx} + p\right)^2 u + qu + gWu, \quad u \in D(H_p(g)), \tag{9}$$

with periodic boundary conditions. Then

$$\sigma(H(g)) = \bigcup_{p \in]-1/2, 1/2]} \sigma(H_p(g)).$$

Since the spectrum of $H_p(g)$ is discrete $\forall p$, $\sigma(H_p(g)) = \{\lambda_n(g; p) : n = 0, 1, \dots\}$, it suffices to prove the reality of the eigenvalues $\lambda_n(g; p), \forall n, \forall p$. So we apply perturbation theory to the family $H_p(g)$ for each fixed $p \in]-1/2, 1/2]$, where

$$H_p(0) = \left(-i\frac{d}{dx} + p\right)^2 + q(x).$$

The technique is similar to the former one for operators with discrete spectrum (as anticipated at the beginning of the section), plus a control on the uniformity of the results on the Brillouin zone. For instance, the requirement $\delta(p) := \inf_{n \neq m} |\lambda_n(0, p) - \lambda_m(0, p)| > 0, \forall p$ has to be satisfied uniformly in p . This is guaranteed if the width $|\Delta_n|$ of the gaps does not vanish as $n \rightarrow \infty$, as assumed in the theorem. For more details, see [7].

4. A criterion for the existence of complex continuous spectra

In this section we provide a criterion for the existence of complex continuous spectra for PT -symmetric Schrödinger operators with periodic potentials which sharpens

the result of Shin [16] and improves the one provided in [7]. More precisely let $W \in L^\infty(\mathbf{R})$ be a 2π -periodic function and

$$W(x) = \sum_{n \in \mathbf{Z}} w_n e^{inx}, \quad w_n = \frac{1}{2\pi} \int_{-\pi}^{\pi} W(x) e^{-inx} dx$$

its Fourier expansion. Consider the operator $K(g)$ formally given by

$$K(g) = -\frac{d^2}{dx^2} + gW, \quad D(H(g)) = H^2(\mathbf{R}), \quad g \in \mathbf{R}.$$

Then we have

Theorem 7. *Let W be \mathcal{PT} -symmetric, i.e. $\overline{W(-x)} = W(x)$. Then*

- (i) $\bar{w}_n = w_n, \forall n \in \mathbf{Z}$;
- (ii) *If $\exists k \in \mathbf{N}$ such that $w_k w_{-k} < 0$, then there is $g_0 > 0$ such that for $|g| < g_0$ the spectrum of $K(g)$ contains at least a pair of complex conjugate (non-real) analytic arcs.*

Remarks

1. This theorem sharpens the results of Shin [16]: here the assumptions are explicit, because they involve only the given potential $W(x)$, while those of [16] involve some conditions on the Floquet discriminant of the equation $K(g)\psi = E\psi$. This requires some *a priori* information on the solutions of the equation itself.
2. The criterion provided by Theorem 7(ii) improves that of [7] where it is required that the index $k \in \mathbf{N}$ such that $w_k w_{-k} < 0$ is odd.
3. Explicit examples of potentials fulfilling the above conditions are

$$W(x) = i \sin^{2k+1} nx, \quad k = 0, 1, \dots; \quad n \in \mathbf{N}.$$

Sketch of the proof of Theorem 7

For the proof of (i) see [7]. As for (ii), the argument is similar to the one used in [7] to prove Theorem 1.2(ii). So we will only point out the differences. As in the proof of Theorem 6 above we have $\sigma(K(g)) = \bigcup_{p \in [0, 1/2]} \sigma(K_p(g))$ where $K_p(g)$ is the operator in $L^2(0, 2\pi)$ formally given by

$$K_p(g) = \left(-i \frac{d}{dx} + p \right)^2 + gW, \quad \forall p \in [0, 1/2]$$

with periodic boundary conditions. $K_p(g)$ has discrete spectrum $\forall p$, and the proof of (ii) is based on the stability of the degenerate eigenvalues of $K_p(0)$ with respect to the family $K_p(g)$, $g \in \mathbf{R}$, for $p = 0$ and $p = 1/2$. More precisely the eigenvalues of $K_p(0)$ are $\lambda_n(0, p) = (n + p)^2, n \in \mathbf{Z}$ with the corresponding eigenfunctions $u_n := \frac{1}{\sqrt{2\pi}} e^{inx}$. All eigenvalues are simple except for $\lambda_n(0, 0) = \lambda_{-n}(0, 0) = n^2 = (-n)^2, \forall n \neq 0$, and for $\lambda_n(0, 1/2) = \lambda_{-n-1}(0, 1/2) = (n + 1/2)^2 = (-n - 1 + 1/2)^2, \forall n$, which are degenerate with multiplicity 2. In [7]

assertion (ii) is proved under the assumption that the index $k \in \mathbf{N}$ is odd using the degeneracy of $\lambda_n(0, 1/2), \forall n$. With a similar argument, using this time the degeneracy of $\lambda_n(0, 0), \forall n \neq 0$, the assertion can be proved in the case of even k . We omit the elementary details.

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