Spontaneous breakdown of $\mathcal{PT}$ symmetry in the solvable square-well model

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Abstract

Apparently, the energy levels merge and disappear in many $\mathcal{PT}$ symmetric models. This interpretation is incorrect: In square-well model we demonstrate how the doublets of states in question continue to exist at complex conjugate energies in the strongly non-Hermitian regime.

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1 Introduction

In their pioneering work which dates back to the late seventies, Caliceti et al\cite{1} have noticed that, rather unexpectedly, non-Hermitian Hamiltonians of certain type could generate the resonances with the strictly vanishing width (i.e., the stable bound states with strictly real energies). Rigorously (using a summability of perturbation series), they proved that the energy levels remain real for the sufficiently weak cubic anharmonicity \textit{with the purely imaginary coupling constant}. This result remained virtually unnoticed even after Buslaev and Grecchi\cite{2} discovered, independently, that also the spectra of certain non-Hermitian versions of the more current quartic anharmonic oscillators remain real and bounded below even far beyond the mere perturbative regime.

The decisive and abrupt increase of interest in all the similar non-Hermitian Hamiltonians (characterized, usually, by the property $H = \mathcal{P}\mathcal{T}H\mathcal{P}\mathcal{T}$ of the so called $\mathcal{PT}$ symmetry, with the parity $\mathcal{P}$ and the complex conjugation $\mathcal{T}$) has only been initiated by Bender and Boettcher in the late nineties\cite{3}. Using the so called delta expansions and quasi-classical techniques they emphasized the possible relevance of this particular type of the non-Hermiticity for the phenomenological physics and field theory\cite{4,5}. They also conjectured\cite{6} the possible existence (and mathematical consistence) of an alternative, $\mathcal{PT}$ symmetric quantum mechanics.

The most important (and, sometimes, counterintuitive) properties of the latter quickly developing formalism are most easily clarified via solvable examples\cite{7}-\cite{17}. Within this framework, special attention has been paid to the existence and properties of the critical strengths of the interaction at which the $\mathcal{PT}$ symmetry becomes spontaneously broken \cite{18,19}. One of the conclusions seems to be an unexplained difference between the numerical and exactly solvable models. In the former case (illustrated, say, on the popular quartic anharmonic oscillator in ref.\cite{20}), the breakdown of the $\mathcal{PT}$ symmetry seems to take place at more steps. This means that there exist many separate critical couplings $Z_n^{\text{crit}}$ where at most a finite number of the energies “merges” and disappears.

In the light of our recent study\cite{21} the pattern looks different for many exactly solvable models. We found that within their shape-invariant subclass, the critical
coupling $Z_n^{(\text{crit})}$ proves *always n-independent* and remains unique. In the other words, all the energy levels stay real up to the point beyond which we find no real energy at all.

Our present short note offers the resolution of the latter apparent puzzle which proves to be an artifact of the choice of the class of models in ref. [21]. We shall pick up a different solvable model (viz., the $\mathcal{PT}$ symmetric “square well” of ref. [22]) and show that the set of its critical points $Z_n^{(\text{crit})}$ remains very large (presumably, infinite).

An important additional merit of our new construction of solutions lies in its extremely elementary nature. We would like to emphasize that as an illustrative example, the $\mathcal{PT}$ symmetric square well proves at least as relevant as its standard Hermitian predecessor. We would expect, in particular, that the exceptional transparency of its solutions with broken symmetry could clarify several open problems which still exist within $\mathcal{PT}$ symmetric quantum mechanics involving, e.g., the necessary modification of the concept of Hermiticity [23, 24] and of the norm [25, 26] as well as the pseudo-unitarity of the time evolution [27] and the various Sturm-Liouville oscillation theorems [28].

2 Wave functions with broken $\mathcal{PT}$ symmetry

The $\mathcal{PT}$ symmetric square well model considered, say, on a finite interval $(-1, 1)$ is characterized by the boundary conditions

$$\psi(\pm 1) = 0.$$  \hspace{1cm} (1)

The general $\mathcal{PT}$ symmetric piece-wise constant interaction will be represented here by its most elementary form

$$V(x) = i Z \quad \text{Re} \ x < 0$$

$$V(x) = -i Z \quad \text{Re} \ x > 0.$$  \hspace{1cm} (2)

In the regime with unbroken symmetry the solution of this problem is virtually trivial [22] and obeys the rule

$$\text{Im} \ E_n = 0, \quad n = 0, 1, \ldots$$  \hspace{1cm} (3)
provided only that $|Z| < 4.48$. In the other words, all the wave functions remain $\mathcal{PT}$ symmetric in this weakly non-Hermitian regime,

$$ |\psi_n\rangle = \mathcal{PT}|\psi_n\rangle. \quad (4) $$

In ref. [22] the question of what happens beyond $Z_0^{(\text{crit})} \approx 4.48$ has been skipped as apparently speculative. One can partially understand the neglect of complex energies as they mimic the collapse of the system into singularity in the Hermitian limit [8]. Still, in the light of the new interpretation and generalization of the $\mathcal{PT}$ symmetry [23], such an interpretation is to be changed. Indeed, via the concept of pseudo-Hermiticity [24], one can deal with the wave functions with the broken and unbroken $\mathcal{PT}$ symmetry on equal footing [27]. Mathematically, a natural transition point from the real spectrum to the states with complex energies is provided by the unavoided level crossings, well illustrated by the symmetric (harmonic [8]) as well as asymmetric (Morse [10]) Laguerre-solvable one-dimensional oscillators.

2.1 Construction

The spontaneous breakdown of $\mathcal{PT}$ symmetry in square well beyond the above-mentioned lowest critical coupling $Z_0^{(\text{crit})}$ does not mean that the lowest pair of the energy levels $E_0$ and $E_1$ “merges and disappears” as conjectured (erroneously) in ref. [22]. These two energies rather move in the complex plain,

$$ E_0 = E - i \varepsilon, \quad E_1 = E + i \varepsilon, \quad Z > Z_0^{(\text{crit})} \quad (5) $$

and merely the rule (4) becomes violated. In this regime of broken $\mathcal{PT}$ symmetry, our Schrödinger square-well equation reads

$$ \psi''_n = \begin{cases} 
[k_n^{[+]}]^2 \psi_n, & x > 0 \\
[k_n^{-1}]^2 \psi_n, & x < 0 
\end{cases} \quad (6) $$

and remains easily solvable. Let us pick up just $n = 0$ and $n = 1$ and abbreviate

$$ [k_0^{[+]}]^2 = -E + i \varepsilon - i Z = \kappa^2 = (s - it)^2, $$

$$ [k_0^{[+]}]^2 = -E - i \varepsilon - i Z = \lambda^2 = (p - iq)^2, $$

$$ [k_0^{-1}]^2 = -E + i \varepsilon + i Z = [\lambda^*]^2, $$

$$ [k_1^{-1}]^2 = -E - i \varepsilon + i Z = [\kappa^*]^2. \quad (7) $$
Then, the general solution of eq. (6) may be written in the well known hyperbolic-function form $\psi \sim a \cosh kx + b \sinh kx$. Its specification compatible with the boundary conditions (1) is immediately available,

$$
\psi_0(x) = K_p \sinh \kappa (1 - x), \quad x > 0,
\psi_0(x) = K_n \sinh \lambda^* (1 + x), \quad x < 0,
\psi_1(x) = L_p \sinh \lambda (1 - x), \quad x > 0,
\psi_1(x) = L_n \sinh \kappa^* (1 + x), \quad x < 0.
$$

The necessary continuity of the logarithmic derivatives in the origin has the form of the four matching conditions at $x = 0$,

$$
L_p \sinh \lambda = L_n \sinh \kappa^*,
\lambda L_p \cosh \lambda = -\kappa^* L_n \cosh \kappa^*,
K_p \sinh \kappa = K_n \sinh \lambda^*,
\kappa K_p \cosh \kappa = -\lambda^* K_n \cosh \lambda^*.
$$

Two of them define the coefficients $K_p$ and $L_p$ (in terms of arbitrary $K_n$ and $L_n$). What remains are the two complex conjugations of the same complex equation

$$
\lambda \coth \lambda + \kappa^* \coth \kappa^* = 0.
$$

We may summarize: The real and imaginary components of $\kappa$ and $\lambda$ (i.e., the four unknown parameters $s$, $t$, $p$ and $q$) define the real and imaginary part of the energies in a way which depends implicitly on $Z = pq + st$,

$$
E = t^2 - s^2 = q^2 - p^2, \quad \varepsilon = pq - st.
$$

This enables us to re-parametrize

$$
s = k \sinh \alpha, \quad t = k \cosh \alpha, \quad p = k \sinh \beta, \quad q = k \cosh \beta
$$

and eliminate

$$
k = \sqrt{\frac{2Z}{\sinh 2\alpha + \sinh 2\beta}}.
$$

As a byproduct, one gets the definition

$$
\varepsilon = \frac{k^2}{2} (\sinh 2\beta - \sinh 2\alpha).
$$

Our solutions are completely determined by the two free parameters $\alpha$ and $\beta$ from real domain $\mathbb{R}$. Their values have to satisfy the two transcendental equations, viz. the real and imaginary part of eq. (1).

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2.2 Graphical analysis

The explicit values of the complex conjugate energy doublets have to be sought by a suitable computer routine. The numerical proof of their existence and completeness can be delivered easily by their explicit evaluation using MAPLE\textsuperscript{29}. A sample of the underlying real parameters $\alpha$ and $\beta$ is given in Table 1 for several couplings $Z$ near $Z_0^{(\text{crit})}$.

Similar computation can be performed in any range of $Z$, giving the second series of roots for $Z > Z_1^{(\text{crit})}$ etc. A sample of results is presented in Table 2 which lists the roots and the real part of the energy $E$ near the second critical point of the symmetry breaking. The value of the second critical coupling constant is determined as $Z_1^{(\text{crit})} \approx 12.80155$.

The first halves of our Tables document and cross-check the reliability of the numerical method. They reproduce the first and second excited state and re-confirm the expected coincidence of the respective roots $\alpha_{1,2} = \beta_{1,2}$ in the $\mathcal{PT}$ symmetric regime. Table 1 improves the estimate of the critical coupling $Z_0^{(\text{crit})} \approx 4.48$ as obtained in ref.\textsuperscript{22}. This estimate is consistent with its alternative determination in ref.\textsuperscript{23} using a direct evaluation of the pseudo-norm which changes its sign at $Z_0^{(\text{crit})} \approx 4.475$.

3 Summary

In the standard, Hermitian quantum mechanics the observables are represented by operators $\mathcal{O}$. Their mean values $\langle \psi | \mathcal{O} | \psi \rangle$ are given the well known probabilistic interpretation\textsuperscript{30}. We have noted that at least a part of this scheme can be extended to certain non-Hermitian and, in particular, $\mathcal{PT}$ symmetric operators\textsuperscript{24}. In the literature, the main source of interest in this alternative is the possible reality of the energies of the related bound states. This relationship is not too robust and the first counterexamples appeared in the very letter\textsuperscript{3} on the anharmonic potentials $V(x) = m^2 x^2 - (ix)^N$ at the sub-harmonic powers $N < 2$. Moreover, one can work, alternatively, with the non-standard bra-vectors\textsuperscript{25}

$$\langle \psi \rangle \rightarrow Q \cdot \langle \psi | \mathcal{P} \equiv Q \langle \psi \rangle, \quad Q = \pm 1 \quad (15)$$

admitting that the norm can be formally indeterminate\textsuperscript{26}. This reflects the non-Hermiticity of the Hamiltonians and facilitates also the perturbative $\mathcal{PT}$ symmetric
The latter considerations leave the consequent interpretation of the $\mathcal{PT}$ symmetry still open. At the same time, its use already inspired several studies in field theory where the choice of the symbol $\mathcal{T}$ indicates an intimate connection of our symmetry with time reversal.

Within the formalism an increasingly important role is played by the wave functions which lose the $\mathcal{PT}$ symmetry “spontaneously”. A byproduct is the complexification of the energies. This possibility, whenever encountered, has been considered “exotic” in the recent past. Only after one innovates the bra vectors in accord with eq. it becomes clear that one should work with the doublets of solutions and that the sign $Q$ in eq. plays the role of a quasi-parity. This concept did already find a natural extension to more dimensions and to the exactly solvable many-body systems.

Let us repeat that our choice of the square-well explicit example has been dictated by several reasons. Firstly, it enables us to recover a lot of new analogies between the standard and $\mathcal{PT}$ symmetric quantum mechanics. Secondly, in contrast to the purely numerical studies, the graphical solution of the square well problem remains entirely transparent. Thirdly, in a way complementing the illustrative harmonic oscillator example of ref. the square well model seems more realistic (or at least less degenerate) in exhibiting the merger of $E_{2n}$ and $E_{2n+1}$ at the different critical couplings $Z_{0}^{(\text{crit})} < Z_{1}^{(\text{crit})} < \ldots$, which form a “naturally” ordered increasing sequence.

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Table 1. Transition from the $\mathcal{PT}$—symmetric regime of ref. [22] (with equal roots $\alpha = \beta$) to the symmetry-breaking solutions with non-equal parameters $\alpha > \beta$ in the domain of $Z \approx Z^{(\text{crit})}_0$.

| coupling $Z$ | $\alpha$       | $\beta$       |
|--------------|----------------|----------------|
| 4            | 0.3879114341   | 0.3879114341   |
| 4.4          | 0.3549674685   | 0.3549674685   |
| 4.46         | 0.3395406749   | 0.3395406749   |
| 4.47         | 0.3340437385   | 0.3340437385   |
| 4.474        | 0.3299988242   | 0.3299988242   |
| 4.4748       | 0.3284804301   | 0.3284804301   |
| 4.4754       | 0.3274947400   | 0.3244090140   |
| 4.476        | 0.3302221779   | 0.3217353463   |
| 4.478        | 0.3344402377   | 0.3176964766   |
| 4.48         | 0.3372106009   | 0.3151052359   |
| 4.49         | 0.3461603724   | 0.3070500670   |
| 4.5          | 0.3523980314   | 0.3017053291   |
| 5            | 0.4640173242   | 0.2326877241   |
Table 2. The emergence of the next series of non-equal roots $\alpha > \beta$ in the vicinity of the next critical value of $Z \approx Z_{1}^{(\text{crit})} \approx 12.80155$.

| coupling $Z$ | $\alpha$       | $\beta$       | energy (real part) |
|--------------|----------------|----------------|--------------------|
| 12.8         | 0.202064800    | 0.202064800    | 30.8270139         |
| 12.801       | 0.201694378    | 0.201694378    | 30.8890887         |
| 12.8014      | 0.201428174    | 0.201428174    | 30.9330671         |
| 12.8015      | 0.201301113    | 0.201301113    | 30.9538785         |
| 12.80154     | 0.201191776    | 0.201191776    | 30.9716960         |
| 12.80156     | 0.201372370    | 0.200912853    | 30.9797156         |
| 12.80158     | 0.201489113    | 0.200796634    | 30.9797173         |
| 12.8016      | 0.201575523    | 0.200710750    | 30.9797190         |
| 12.8018      | 0.202071953    | 0.200219572    | 30.9797353         |
| 12.802       | 0.202384800    | 0.199911977    | 30.9797517         |
| 12.9         | 0.220635091    | 0.184230076    | 30.9878260         |
| 13           | 0.229622933    | 0.177852160    | 30.9961877         |
| 14           | 0.281083389    | 0.151889620    | 31.0861845         |