Periodic square-well potential and spontaneous breakdown of \( PT \)-symmetry

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Abstract

A particle moving on a circle in a purely imaginary one-step potential is studied in both the exact and broken \( PT \)-symmetric regime.

1 Introduction

In textbooks on quantum mechanics one finds a lot of solvable models. They mostly offer just a rough approximation to a physical situation. At the same time, their simplicity enables us to avoid some inessential technical difficulties. In this sense they provide a basic insight in physical phenomena appearing in complicated realistic systems.

Also the basic properties of \( PT \)-symmetric quantum mechanics [1] may be tested by the most elementary quantum mechanical models. One of them has been proposed in [2] as a description of a particle moving in a purely imaginary antisymmetric potential. In its time-independent Schroedinger equation

\[
H\psi = \left[-\frac{d^2}{dx^2} + iZ\frac{x}{|x|}\right]\psi(x) = E\psi(x), \quad x \in (-1, 0) \cup (0, 1)
\] (1)

the Dirichlet boundary conditions were introduced at \( x = \pm 1 \). The role of the growing non-Hermiticity \( Z \) was studied and shown to induce a spontaneous breakdown of the \( PT \)-symmetry at \( Z \approx 4.475 \) (cf. also [3]).

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An interesting application of the latter model has been found in [4] where the whole supersymmetric hierarchy of solvable potentials has been assigned to the most trivial “zeroth-term” member (1) of the family.

In the present note we intend to replace the Dirichlet boundary conditions at \(x = \pm 1\) (mimicking a simple confined motion) by their periodic alternative which would represent the slightly more sophisticated motion of the particle along a circle.

Our main motivation stems from an observation [5] that a weakening of the Hermiticity (or, in our present language, of \(T\)-symmetry [6]) to \(PT\)-symmetry may cause serious difficulties in some exactly solvable models. In [5] this problem has been revealed during a study of angular Schrödinger equations with certain potentials of a multiple-well shape over the circle. Unfortunately, even after a replacement of these potentials by their schematic square-well forms, the solution of the related bound-state problem proved more or less purely numerical.

We see the main source of the latter difficulty in an over-complicated structure of the underlying trigonometric secular equations in the “realistic” multi-square-well cases. For this reason we intend to return to the “non-realistic” single-step potential in equation (1) subject to the periodic boundary conditions. We shall show and see that a graphical analysis of such a problem remains tractable non-numerically.

2 \(PT\)-symmetric regime

Assuming that the energies are real, the solution of (1) may be sought in the form

\[
\begin{align*}
\psi_1(x) &= A_1 e^{kx} + A_2 e^{-kx}, & x \in (0, 1), \\
\psi_2(x) &= B_1 e^{k^*(x+1)} + B_2 e^{-k^*(x+1)}, & x \in (-1, 0),
\end{align*}
\]

where \(k^2 = -E + iZ\). Ambiguity in coefficients \(A_i, B_i\) will be eliminated by application of the following periodic boundary conditions

\[
\psi_1(1) = \psi_2(-1), \quad \psi_1'(1) = \psi_2'(-1), \quad \psi_1(0) = \psi_2(0), \quad \psi_1'(0) = \psi_2'(0). \quad (3)
\]

Substituting (2) into (3), we obtain a system of linear equations for unknown coefficients \(A_i, B_i\). It has non-trivial solution if and only if the determinant of its matrix \(W\) vanishes,

\[
\det W = 4e^{2k}(-1 + e^{2k})^2k^2 = 0 \quad (4)
\]
Dividing $k$ into its real and imaginary part and using the following relations

$$E = s^2 - t^2, \quad 2st = Z, \quad k = t + is,$$

we can rewrite (4) as

$$\det W' = 4e^{-2t}(-1 + e^{2t})^2t^2 + \frac{2Z^2}{t^2}(-1 + \cos\left(\frac{Z}{t}\right)) = 0. \quad (5)$$

For large $t$ the first term in (5) is dominant and exponentially grows to infinity, see Fig.1. The roots $t$ have a positive upper bound and the energy is bounded from below, consequently.

In the vicinity of $t = 0$ the determinant in (5) exhibits oscillations caused by the dominance of the non-positive second term. Still, a positive perturbation caused by the first term implies the existence of the infinitely many real and non-degenerate nodal doublets in each oscillation at the sufficiently small $t$. Empirically, this feature has been observed in [5] but its essence lied hidden in the complicated form of the determinant.

To study the spectrum for infinitesimally small $Z (= 2st)$, it is convenient to rewrite (4) in its alternative $s$-representation

$$8s^2(-1 + \cos(2s)) + e^{-\frac{Z}{s}}\left(-1 + e^{\frac{Z}{s}}\right)^2\frac{Z^2}{s^2} = 0 \quad (6)$$

Obviously, in the hermitian limit $Z \to 0$ the energies coincide with the spectrum of the circular oscillator, $E_n = s^2 = \pi^2n^2$. We can ask how these
“unperturbed” energies will be effected by a very small perturbation \( Z > 0 \). It can be expected that there will appear correction terms in energy description. The secular equation (11) can be rewritten as

\[
(t \sinh t + s \sin s)(t \sinh t - s \sin s) = 0.
\] (7)

We expect the correction to the hermitian case in the following form

\[
s = n\pi + \rho(t), \quad \rho = \sum_{0}^{\infty} A_i t^i.
\] (8)

Substituting the ansatz into (7) and comparing coefficients at the corresponding powers of \( t \), we get

\[
\rho_\pm = \pm \frac{(-1)^n}{n\pi} t^2 + \left( -\frac{1}{n^3\pi^3} \pm \frac{(-1)^n}{n\pi} \right) t^4 + \cdots
\]

(9)

In contrast to unperturbed spectrum of infinite square-well, the energies of \( PT \)-symmetric square-well are divided into two families. They are

\[
E^+_n = (n\pi + \rho_+)^2 - t^2, \quad E^-_n = (n\pi + \rho_-)^2 - t^2.
\] (10)

\section{Violation of \( PT \)-symmetry}

It has been observed in [3] that as the coupling \( Z \) rises over a critical value \( Z^{(\text{crit})} \), two lowest energy levels of the infinite square-well coalesce and become complex conjugate simultaneously. This happens repeatedly as the coupling rises, so that there exists a sequence of critical values

\[
Z_0^{(\text{crit})} < Z_1^{(\text{crit})} < Z_2^{(\text{crit})} < \ldots < Z_{\nu}^{(\text{crit})}
\] (11)

for which the corresponding energy pair \( \{E_{2\nu}, E_{2\nu+1}\} \) merges and becomes complex.

We can observe the very same situation in the case of periodic boundary conditions. In Fig.2, an intersection of \( Z = \text{const} \) with the boarders of black and white area determines the root of (15). Merging of the highest roots for rising coupling \( Z \) is then quite transparent.

In order to study the system in the broken \( PT \)-symmetry regime, we make the following ansatz of the wave function associated with energy \( E^+ = E + i\epsilon \)

\[
\psi_1(x) = A_1 \sinh k(1 - x) + A_2 \cosh k(1 - x), \quad x \in (0, 1)
\]
Figure 2: Determinant vanishes on the border curve of black and white area.

\[ \psi_2(x) = B_1 \sinh l^* (1 + x) + B_2 \cosh l^* (1 + x), \quad x \in (-1, 0) \quad (12) \]

where \( k^2 = -E + i\epsilon - iZ \) and \( l^2 = -E - i\epsilon - iZ \). In analogy with exact PT-symmetry case, we substitute (12) into the boundary conditions and get a system of linear equations. The corresponding secular equation

\[ 2k(1 - \cosh k \cosh l^*) - \frac{k^2 + l^2}{l^*} \sinh k \sinh l^* = 0 \quad (13) \]

is complex valued and contains two complex parameters that are mutually related

\[ k = s - it, \quad l = p - iq \Rightarrow E = t^2 - s^2 = p^2 - q^2, \quad \epsilon = pq - st. \]

It is convenient to make further re-parametrization

\[ s = K \sinh \alpha, \quad t = K \cosh \alpha, \quad p = K \sinh \beta, \quad q = K \cosh \beta \]

Imaginary part of the energy is

\[ \epsilon = \frac{K^2}{2} (\sinh 2\beta - \sinh 2\alpha) \]

where \( K = \sqrt{\frac{Z}{\sinh 2\alpha + \sinh 2\beta}} \). The parameters \( \alpha \) and \( \beta \) are solution of (13). Their values obtained numerically for several fixed \( Z \) can be found in Tab.1.
Table 1: Dependence of $E$ on the coupling $Z$ in the vicinity of the first two critical values $Z_0^{(\text{crit})}$, $Z_1^{(\text{crit})}$. The first values of interaction correspond to preserved $PT$-symmetry so that parameters $\alpha$ and $\beta$ coincide. As the interaction grove over the critical value, the parameters diverse.

| $Z$         | $\alpha$ | $\beta$ | $\text{Re}E$ |
|-------------|-----------|---------|--------------|
| 5.542309    | 0.474944  | 0.474944| 5.041586     |
| 5.542310    | 0.474653  | 0.474870| 5.044077     |
| 5.54232     | 0.474125  | 0.475399| 5.044078     |
| 5.54240     | 0.472878  | 0.476652| 5.044080     |
| 5.55        | 0.457619  | 0.492438| 5.044371     |
| 6           | 0.358129  | 0.622216| 5.062183     |
| 6.5         | 0.318347  | 0.693565| 5.083353     |
| 17.90123    | 0.325829  | 0.325829| 25.61820     |
| 17.90124    | 0.325575  | 0.326139| 25.60761     |
| 17.90126    | 0.325540  | 0.326356| 25.60762     |
| 17.90200    | 0.323724  | 0.328189| 25.60769     |
| 17.95       | 0.308679  | 0.344308| 25.61228     |
| 19          | 0.253831  | 0.422062| 25.71469     |

Comparing $\alpha$ and $\beta$, we can estimate the critical values of interaction quite precisely. The first five values are

\[ Z_0^{(\text{crit})} \in (5.542309, 5.542310), \quad Z_1^{(\text{crit})} \in (17.90123, 17.90124) \]
\[ Z_2^{(\text{crit})} \in (33.54495, 33.54495), \quad Z_3^{(\text{crit})} \in (51.20617, 51.20618) \]
\[ Z_4^{(\text{crit})} \in (70.3093, 70.3095). \]  \hspace{1cm} (14)

We can compare these results with infinite square-well. In [3], the first two members of the sequence (11) were determined as $Z_0^{(\text{crit})} \in (4.4748, 4.4754)$, $Z_1^{(\text{crit})} \in (12.80154, 12.80156)$. In our case of periodic boundary conditions, the critical values of the coupling seem to be risen. We propose that periodic boundary conditions strengthen $PT$-symmetry of the system.

4 Discussion and Outlook

The paper was intended as a connection between [2], [3] and [5]. To meet this intention, we studied solutions of (1) with periodic boundary conditions.

On one hand, the simpler choice of the potential allowed a deeper insight into spectral behavior of periodic square-well, which was the missing link
in [5]. We made a basic analytical observation and found approximation of energies for very small couplings $Z$. On the other hand, we could compare our results with the ones corresponding to the infinite square-well [2], [3]. This was interesting mainly in the regime of broken $PT$-symmetry. After the comparison, one concludes that $PT$-symmetry is weakened by Dirichlet boundary conditions or vice versa, it is strengthened in the circular domain.

There is a lot of opened questions. One can ask how is the energy dependence of the critical interaction values. The similar task has been solved in [7] for quartic harmonic oscillator $H = -\frac{p^2}{2} + x^4 + Aix$. It was shown that the relation $a = |A|E^{-\frac{1}{2}}$ holds asymptotically for a certain constant $a$.

Similarly to [5], (1) can be seen as an angular Schroedinger equation of more dimensional problem. The presented results could be also understood as a preliminary step to more-dimensional models.

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