Solvable $\mathcal{PT}$–symmetric model with a tunable interspersion of non-merging levels.

Miloslav Znojil

Ústav jaderné fyziky AV ČR, 250 68 Řež, Czech Republic

Abstract

We study the spectrum in such a $\mathcal{PT}$–symmetric square well (of a diameter $L \leq \infty$) where the “strength of the non-Hermiticity” is controlled by the two parameters, viz., by an imaginary coupling $ig$ and by the distance $\ell < L$ of its onset from the origin. We solve this problem and confirm that the spectrum is discrete and real in a non-empty interval of $g \leq g_0(\ell, L)$. Surprisingly, a specific distinction between the bound states is found in their asymptotic stability/instability with respect to an unlimited growth of $g$ beyond $g_0(\ell, L)$. In our model, all of the low-lying levels remain asymptotically unstable at the small $\ell \ll L$ and finite $L$ while only the stable levels survive near $\ell \approx L < \infty$ or in the purely imaginary force limit with $0 < \ell < L = \infty$. In between these two extremes, an unusual and tunable, variable pattern of the interspersed “robust” and “fragile” subspectra of the real levels is obtained.

PACS 03.65.Ge, 03.65.Ca, 02.30.Tb, 02.30.Hq

MSC 2000: 81Q05, 81Q10, 46C20, 47B50, 34L40

\textsuperscript{1}e-mail: znojil@ujf.cas.cz
1 Introduction

Around 1992, Daniel Bessis succeeded in attracting attention of a few people to a certain toy Hamiltonian (with some relevance in quantum field theory) which appeared to produce the real and discrete spectrum of energies in spite of being manifestly non-Hermitian [1]. A few years later, Bender and Boettcher returned to his mind-boggling problem and published a numerical study [2] of the whole class of the perceivably more general one-dimensional Schrödinger equations

\[
-\frac{d^2}{dx^2} + V(x) + iW(x) \psi(x) = E \psi(x) \tag{1}
\]

where, in our present perspective, the real component of the potential was assumed spatially symmetric while its Hermiticity-violating partner was chosen as spatially antisymmetric,

\[
\mathcal{P} V(x) \mathcal{P} = V(-x) = +V(x), \quad \mathcal{P} W(x) \mathcal{P} = W(-x) = -W(x).
\]

The latter study confirmed that the similar models [exhibiting, obviously, the parity ($\mathcal{P}$) times time-reversal ($\mathcal{T}$) symmetry] may possess both the purely real and partially (or, perhaps, completely) complex spectra. The Bender’s and Boettcher’s Figure 1 (loc. cit.) illustrated the existence of the spectrum which proved “robustly real”, i.e., real in a wide range of parameters of their “massless” $\mathcal{PT}$–symmetric model. In contrast, a merely slightly modified “massive” $\mathcal{PT}$–symmetric model of their Figure 3 (loc. cit.) behaved quite differently. The values of many of its energy levels proved extremely sensitive to the very small variations of the parameters and, moreover, even the very reality of some energies proved “fragile” in the sense that after a very small change of a parameter of the model, certain energy pairs merged and disappeared forming, presumably, the complex conjugate pairs. At present, many more similar and more or less purely numerical examples exists (cf., e.g., the recent paper [3] for a sample of references).
The recent progress in our understanding of the various $\mathcal{PT}$–symmetric quantum Hamiltonians $H$ may be briefly summarized as an observation that their symmetry is important. Firstly, it was established that the time-reversal-type antilinear operator factor $\mathcal{T}$ merely mediates the Hermitian conjugation $A \rightarrow A^\dagger$ [4, 5]. The role of parity $\mathcal{P}$ is more subtle and seems to offer the main mathematical key to the study of the $\mathcal{PT}$–symmetric quantum Hamiltonians $H$ within the so called Krein-space theory (cf., e.g., ref. [6] for a nice as well as concise introduction to this language).

On the background of these mathematical observations, the formalism lost its originally highly enigmatic features in the context of physics. During the last two or three years, the use of the $\mathcal{PT}$–symmetric quantum models has in fact been accepted as just opening new horizons within the standard Quantum Mechanics. At present, virtually all the people active in the field would agree that it is only necessary to make the resulting physical picture complete by a revitalization of its probabilistic contents and tractability. This is being achieved via an introduction of the “missing” (and, in fact, quite nontrivial) metric $\eta \neq I$ in the Hilbert space of states [6, 7, 8].

The temporary doubts and puzzles related, typically, to the applicability of the formalism look, at least roughly, clarified. One feels urged to return to many recently neglected and apparently evasive and mathematically more subtle questions like the problems of the robustness/fragility of the individual energies or of a global typology of the spectra. We believe that it is time for their deeper and more technical study via, say, simplified and, first of all, non-numerically tractable models. A new one, with rather surprising properties and descriptive features of the spectrum, is to be proposed and analyzed in what follows.
1.1 Non-Hermitian square-well-type models

Within $\mathcal{PT}$–symmetric Quantum Mechanics a one-parametric non-Hermitian square well (NSW) model has been described in ref. [9]. A key merit of the NSW model lies in a combination of its straightforward mathematical solvability with an exceptional transparency of its applications. In this way, the NSW model was able to offer an insight into the mechanism of the spontaneous $\mathcal{PT}$–symmetry breaking [10]. Next, due to its elementary character, the NSW model has been selected by Bagchi et al. [11] as a starting point of a systematic supersymmetric generation of solvable non-Hermitian Hamiltonians with $\mathcal{PT}$–symmetry and real spectra. Last but not least, Mostafazadeh and Batal [7] choose the NSW model in their very recent illustrative application of the $\mathcal{PT}$–symmetric Quantum Mechanics in its present, mathematically as well as physically more or less consistent updated form (readers may consult some of the available reviews for more details [12]).

In our recent paper [13] we revealed that a certain “hidden” shortcoming of the NSW model may be seen in its “fragility”, i.e., in an instability of all the higher energy levels with respect to a certain highly speculative form of a complex-coordinate perturbation. Although such an observation does not have any immediate impact on the applications of the NSW model in refs. [7, 10, 11], certain doubts survive concerning the possible manifestations of some more serious instabilities in some of the generalized, NSW-type (NSWT) models.

For our present purposes let us vaguely characterize the latter NSWT potentials as piecewise constant. Then we may immediately recollect the existence of several “user-friendly” NSWT examples incorporating square-well models on a compact domain [14] or systems based on the use of point interactions [15]. Unfortunately, even within this class, the expectations concerning the stability of the spectrum are not always fulfilled. One may recollect, e.g., a spontaneous complexification of the high-lying
part of many NSWT spectra as detected in very early numerical studies of certain particular potentials in ref. [16]. The phenomenon looks puzzling and makes all the NSWT models worth a more detailed non-numerical study.

1.2 The choice of a specific example

In applied quantum mechanics the construction of the majority of phenomenological models relies quite heavily on the correspondence principle which tries to connect each quantum model with its classical predecessor. $\mathcal{PT}$-symmetric Quantum Mechanics offers a weakening of this connection [17]. The operator of parity $\mathcal{P}$ is indefinite so that, as we already mentioned, the formalism requires an explicit additional construction of a Hamiltonian-dependent positively definite metric $\eta > 0$ in Hilbert space. Equivalently, this may be mediated by the construction of a quasi-parity $\mathcal{Q}$ [18] or charge $\mathcal{C}$ [19], both defined as a product $\eta \mathcal{P}$. In practical calculations this means that the metric is often being introduced in a suitably factorized form [20].

It is worth adding that the quasi-parity in $\eta = \mathcal{QP}$ is easily defined in some exactly solvable examples [18] while the charge in $\eta = \mathcal{CP}$ has immediate connotations in field theory [19]. In between these two extremes the authors of ref. [7] revealed that the application of the formalism to the particular NSW model proves facilitated by a perturbative connection between the NSW model and a Hermitian square well. Their construction of $\eta^{(NSW)}$ profited from the existence of a finite-dimensional matrix approximation of the non-Hermitian part of the NSW Hamiltonian. A transition to the extended NSWT class of models looks promising and co-motivates also our present project.

Within such a framework we intend to pay attention to the family of Schrödinger equations (1) where the interaction is non-Hermitian but manifestly $\mathcal{PT}$-symmetric. For the sake of definiteness we shall contemplate the less interesting real part of the
potential just in the most elementary infinitely deep square-well form,

\[
V(x) = \begin{cases} 
+\infty & \text{for } x > L \\
0 & \text{for } -L < x < L \\
+\infty & \text{for } x < -L.
\end{cases}
\tag{2}
\]

This means that all our wave functions have to vanish at its walls,

\[
\psi(-L) = \psi(L) = 0.
\tag{3}
\]

By adding any imaginary interaction we break the Hermiticity of the Hamiltonian. By doing so in the \(\mathcal{PT}\)–symmetric manner we preserve a chance and good hope of having the energies real \[2\].

For the sake of definiteness and in a way generalizing the NSW model of ref. [9] we shall assume that the Hermiticity-breaking term \(W\) is composed of two purely imaginary steps which both vanish inside a subinterval \((-\ell, \ell)\) of the interval \((-L, L)\),

\[
W(x) = \begin{cases} 
+ig, & \text{for } \Re x > \ell > 0, \\
0 & \text{for } \Re x \in (-\ell, \ell), \\
-ig & \text{for } \Re x < -\ell.
\end{cases}
\tag{4}
\]

\(A \text{ priori}\), the strength of the Hermiticity-violating imaginary force may be expected proportional to the coupling \(g > 0\) and inversely proportional to \(\ell < L\).

Our interest in the particular two-parametric model \(4\) results from the obvious need of an enhancement of flexibility of its one-parametric NSW predecessor and also from the lasting possibility of its rigorous mathematical description by means of the efficient moving-lattice method of ref. [13] (reviewed also briefly in Appendix A below). Among additional purposes of the study of the similar NSWT models one may list a search for reliable comparisons between different potentials revealing, hopefully, some new, unnoticed characteristic features of their spectra. One would like to understand, i.a., how the details of the shape of \(W(x)\) could influence the
stability of the spectrum, or how one could control the domain of parameters where all the energies remain real.

Some of the NSWT studies have been motivated by their potential capacity of mimicking the properties of unsolvable models and, in particular, of one of the most popular $\mathcal{PT}$-symmetric toy interactions $W(x) = ix^3$ [21]. Some parallels are definitely there since in the latter unsolvable case the spectrum was proved real, non-negative and discrete [22]. Of course, there are always good reasons for an introduction of more parameters in NSW. Thus, the new freedom of a weakening of the non-Hermiticity by the choice of $\ell > 0$ might simulate analogies with the Bender’s and Boettcher’s generalized $\mathcal{PT}$-symmetric family $W(x) = -(ix)^{3-\mu}$ characterized by an abrupt change of its spectral properties at $\mu = 1$ and by the spontaneous complexification of all the sufficiently high-lying energies inside the interval $\mu \in (1, 2)$ of the shape-parameter [2].

The possibility of the latter correspondence passes an easy test at $\ell = 0$ and $L = \infty$ when the general solutions of our Schrödinger eq. (1) are mere exponentials at any real $g > 0$. Once we demand that they vanish in infinity we have

$$\psi(x) = \begin{cases} B_+ \exp(-\sigma x), & \sigma^2 = ig - E, & \Re \sigma > 0, & x \in (0, \infty), \\ B_- \exp(\sigma' x), & \sigma'^2 = -ig - E, & \Re \sigma' > 0, & x \in (-\infty, 0). \end{cases} \quad (5)$$

When $x \to 0^\pm$ the coincidence of the right and left limit of $\psi(x)$ itself specifies the normalization, $B_+ = B_-$, while the second matching rule $\psi'(0^+) = \psi'(0^-)$ implies that $\sigma = -\sigma'$, i.e., equation (5) has no solutions at $g > 0$. It is of no avail to admit that $\Re \sigma \to 0$ and $\Re \sigma' \to 0$ and to employ the scattering boundary conditions since, unless $g = 0$, the matching-compatible states remain always incompatible with our differential Schrödinger equation on a half-line.

We may conclude that both the discrete and continuous spectra are empty at $\ell = 0$ for $g > 0$ and $L = \infty$. This re-confirms our above expectations since the
emptiness of the spectrum also characterizes the Bender’s and Boettcher’s toy interaction \( W(x) = -(ix)^{3-\mu} \) at the Herbst’s extreme shape parameter \( \mu = 2 \) [23]. At the same time, the spectrum abruptly ceases to be empty at \( \mu < 2 \) [2] as well as at \( \ell > 0 \) while \( L = \infty \) (cf. the proof of this assertion as given in Appendix B below).

2 The method

2.1 Wave functions and their matching

As long as our potential is piecewise constant at \( 0 < \ell < L < \infty \) we may postulate

\[
\psi(x) = \begin{cases} 
\psi_-(x) = B_- \sinh \kappa^* (L + x), & x \in (-L, -\ell), \\
\psi_0(x) = C \cos k x + i D \sin k x, & x \in (-\ell, \ell), \\
\psi_+(x) = B_+ \sinh \kappa (L - x), & x \in (\ell, L)
\end{cases}
\]

(6)

where \( \kappa = s + it, \ E = k^2 = t^2 - s^2, \ g = 2st > 0 \) and where \( s, t \) and \( k \) are assumed real and, for the sake of definiteness, positive. In the other words, we assume that within a not yet specified non-empty domain of parameters \( g \) and \( \ell \) the \( \mathcal{PT} \) symmetry of the wave functions remains unbroken. In the way proposed in ref. [9] we prescribe the phase,

\[
\psi(x) = \text{real symmetric} + \text{imaginary antisymmetric}
\]

and deduce that \( C \) and \( D \) are real. Next, we differentiate

\[
\psi'(x) = \begin{cases} 
\psi'_-(x) = \kappa^* B_- \cosh \kappa^* (L + x), & x \in (-L, -\ell), \\
\psi'_0(x) = -k C \sin k x + i k D \cos k x, & x \in (-\ell, \ell), \\
\psi'_+(x) = -\kappa B_+ \cosh \kappa (L - x), & x \in (\ell, L)
\end{cases}
\]
and write down the following four matching conditions,

\[ \psi_-(\ell) = \psi_0(-\ell), \text{ i.e., } B_- \sinh \kappa^*(L - \ell) = C \cos k \ell - i D \sin k \ell, \]

\[ \psi'_-(\ell) = \psi'_0(-\ell), \text{ i.e., } \kappa^* B_- \cosh \kappa^*(L - \ell) = k C \sin k \ell + i k D \cos k \ell, \]

\[ \psi_+(\ell) = \psi_0(\ell), \text{ i.e., } B_+ \sinh \kappa (L - \ell) = C \cos k \ell + i D \sin k \ell, \]

\[ \psi'_+(\ell) = \psi'_0(\ell), \text{ i.e., } -\kappa B_+ \cosh \kappa (L - \ell) = -k C \sin k \ell + i k D \cos k \ell. \]

Two of them define the (complex) values of \( B_\pm \) so that we are left with the pair of the matching constraints,

\[ (k C \sin k \ell + i k D \cos k \ell) \sinh \kappa^*(L - \ell) = (C \cos k \ell - i D \sin k \ell) \kappa^* \cosh \kappa^*(L - \ell) \]

\[ (k C \sin k \ell - i k D \cos k \ell) \sinh \kappa (L - \ell) = (C \cos k \ell + i D \sin k \ell) \kappa \cosh \kappa (L - \ell). \]

These two relations are complex conjugate of each other so that we have to consider just one of them, say,

\[ (k C \sin k \ell - i k D \cos k \ell) \sinh(s + it) (L - \ell) = \]

\[ = (C \cos k \ell + i D \sin k \ell) \kappa \cosh(s + it) (L - \ell). \quad (7) \]

with \( k \geq 0. \)

### 2.2 Matching equations in the \( \sigma - \tau - \varrho \) space

After we abbreviate \( \sigma = s (L - \ell), \tau = t (L - \ell) \) and \( \varrho = k \ell, \) equation (7) reads

\[ \varrho (L - \ell) (C \sin \varrho - i D \cos \varrho) [\sinh \sigma \cos \tau + i \cosh \sigma \sin \tau] = \]

\[ = (C \cos \varrho + i D \sin \varrho) [\cosh \sigma \cos \tau + i \sinh \sigma \sin \tau]. \quad (8) \]

We have to keep in mind that

\[ \tau^2 = \sigma^2 + \frac{(L - \ell)^2}{\ell^2} \varrho^2 \]
while the respective real and imaginary parts of eq. (8) have to be treated as independent equations

\[ \varrho (L - \ell) \left( C \sin \varrho \sinh \sigma \cos \tau + D \cos \varrho \cosh \sigma \sin \tau \right) = \]

\[ = \ell \left[ \sigma \left( C \cos \varrho \cosh \sigma \cos \tau - D \sin \varrho \sin \sigma \sin \tau \right) - \right. \]

\[ \left. - \tau \left( C \cos \varrho \sinh \sigma \sin \tau + D \sin \varrho \cosh \sigma \cos \tau \right) \right] \]

(9)

and

\[ \varrho (L - \ell) \left( C \sin \varrho \cosh \sigma \sin \tau - D \cos \varrho \sinh \sigma \cos \tau \right) = \]

\[ = \ell \left[ \sigma \left( C \cos \varrho \sinh \sigma \sin \tau + D \sin \varrho \cosh \sigma \cos \tau \right) + \right. \]

\[ \left. + \tau \left( C \cos \varrho \cosh \sigma \cos \tau - D \sin \varrho \sinh \sigma \sin \tau \right) \right]. \]

(10)

In the next step we notice that the latter equations form a linear algebraic homogeneous set for the two coefficients \( C \) and \( D \). They possess a nontrivial solution if and only if the secular determinant \( D \) vanishes. After we abbreviate \( \Omega = \tan \varrho \) (= a quickly oscillating function of \( \varrho \)), \( T = \tan \tau \) (= a quickly oscillating function of \( \tau \)) and \( \Sigma = \tanh \sigma \) (= a monotonous and bounded function of \( \sigma \)) we can evaluate \( D \). After a lengthy calculation the secular condition \( D = 0 \) acquires the following compact form

\[ X(\sigma) + Y(\tau) + F(R) [x(\sigma) + y(\tau)] = 0 \]

(11)

where

\[ X(\sigma) = \frac{1 + \Sigma^2}{1 - \Sigma^2} \sigma^2 = \sigma^2 \cosh 2 \sigma, \]

\[ Y(\tau) = \frac{1 - T^2}{1 + T^2} \tau^2 = \tau^2 \cos 2 \tau, \]

\[ x(\sigma) = \frac{\Sigma}{1 - \Sigma^2} \sigma = \frac{1}{2} \sigma \sinh 2 \sigma, \]

\[ y(\tau) = \frac{T}{1 + T^2} \tau = \frac{1}{2} \tau \sin 2 \tau, \]

\[ F(R) = \frac{1 - \Omega^2}{\Omega} R = \frac{2 R}{\tan 2 \varrho}, \quad \varrho = \varrho(R) = \frac{\ell}{L - \ell} R. \]
We may re-scale our coupling \( g = 2 \frac{Z}{(L-\ell)^2} \) and conclude that our \( Z \)-independent secular equation (11),

\[
\sin 2 g(R) \left[ \sigma^2 \cosh 2 \sigma + \tau^2 \cos 2 \tau \right] + R \cos 2 g(R) \left[ \sigma \sinh 2 \sigma + \tau \sin 2 \tau \right] = 0 \tag{12}
\]

only has to be complemented by the two trivial constraints

\[
\sigma \tau = Z, \quad \tau^2 - \sigma^2 = R^2. \tag{13}
\]

The triplets of roots \( R_n, \sigma_n \) and \( \tau_n \) of this triplet of equations with \( n = 0, 1, \ldots \) define all the bound-state energies \( E_n \) by the elementary formula

\[
E_n = \frac{1}{(L-\ell)^2} R_n^2 \equiv \frac{1}{(L-\ell)^2} \left( \tau_n^2 - \sigma_n^2 \right). \tag{14}
\]

In an indirect check of the recipe we may recollect its \( \ell \to 0 \) (i.e., \( g \to 0 \)) limit and conclude that our present eq. (12) degenerates smoothly and correctly back to the known secular \( \ell = 0 \) equation {cf. eq. Nr. (9) in ref. [9]}.

### 2.3 Matching in the moving-lattice representation

The basic tool for a rigorous analysis of the form of the solutions of our matching constraints is the moving-lattice method of ref. [13] as reviewed in Appendix A below. Skipping the majority of details let us only note that for an analysis of this type, one of the recommended techniques seems to be the reduction of the problem to \( \sigma - \tau \) plane. Preserving the definition of \( \tau = \tau(N,t) \) of Appendix A and replacing the definition of \( \sigma = \sigma(N,t) \) by another formula,

\[
\sigma = \sigma(N,t,K,r) = \pi \times \sqrt{[N+t]^2 + \left[ \frac{L-\ell}{2\ell} (K+r) \right]^2},
\]

we eliminate the coordinate \( R \). A shortcoming of this approach is that our matching condition (12) transferred into the \( \sigma - \tau \) plane has to be understood as the following quadratic equation for \( \tau \),

\[
\Phi(t) \tau^2 + \omega_{K,t} \tau + \Omega_{K,t}(\sigma) = 0 \tag{15}
\]
where we abbreviated

\[
\omega_{K,r,t} = \frac{(L - \ell) \pi \Psi_t}{2\ell \Xi_r} (K + r), \quad \Omega_{K,r,t}(\sigma) = \Xi_r \left[ \sigma^2 \cosh 2\sigma + \frac{\omega_{K,r,t}}{\Psi_t} \sigma \sinh 2\sigma \right].
\]

This defines \( \tau = \tau_{K,r,t}(N) \) on the lattice, the “motion” of which will be controlled not only by \( t \) and \( r \) but also, not so strongly, by \( K \). Technically, the price to be paid is still reasonable - we get the closed form of the matching-compatible function \( \tau = \tau(\sigma) \) as the two well known root formulae from eq. (15). Nevertheless, significant simplifications of the resulting picture may be mediated by the direct inspection of the equations in question.

3 Solutions

3.1 Matching equations in the \( \sigma - \tau \) plane

Building far-reaching analogies with the \( \ell = 0 \) special case would be misleading because the form of our matching constraint (12) is discontinuous in the limit \( \ell \to 0 \). Thus, let us assume that \( \ell \neq 0 \) and study eq. (12) in its full-fledged form. Firstly, we abbreviate \( \mathcal{M}(\sigma, \tau) = \sigma \sinh 2\sigma + \tau \sin 2\tau \) and \( \mathcal{N}(\sigma, \tau) = \sigma^2 \cosh 2\sigma + \tau^2 \cos 2\tau \) and re-write our matching constraint (12) as the secular equation

\[
D(\sigma, \tau, R) = Q(\sigma, \tau) + \frac{\tan 2\varphi(R)}{R} = 0, \quad Q(\sigma, \tau) = \frac{\mathcal{M}(\sigma, \tau)}{\mathcal{N}(\sigma, \tau)}.
\]

This enables us to formulate several obvious observations.

[O1] The shape of both the functions \( \mathcal{M}(\sigma, \tau) \) and \( \mathcal{N}(\sigma, \tau) \) of two variables is easily deduced using their separability, \( \mathcal{X}(\sigma, \tau) = \mathcal{X}(\sigma, 0) + \mathcal{X}(0, \tau), \mathcal{X} = \mathcal{M}, \mathcal{N} \).

[O2] The smoothness of the \( \sigma \)– and \( \tau \)–dependence of the denominator \( \mathcal{N}(\sigma, \tau) \) facilitates also the determination of the shape of \( \mathcal{F}(\sigma, \tau) = 1/\mathcal{N}(\sigma, \tau) \).
In $\sigma - \tau$ plane we may visualize the shape of the second fraction in (16) as a function which is constant along hyperbolas $R(\sigma, \tau) = \sqrt{\tau^2 - \sigma^2} = \text{fixed}$.

All these innocent-looking observations have several far-reaching though not always obvious consequences and form in fact a background for a rigorous analysis of the spectrum.

### 3.2 A rigorous graphical interpretation of $Q(\sigma, \tau)$

In more detail, observation [O1] means that the surfaces defined by the two non-negative function(s) $\mathcal{X}(\sigma, 0) \geq 0$ have the form of the two only slightly different parabolic valleys with the same degenerate minimum (= zero) which coincides with the axis $\sigma = 0$. The pertaining second components $\mathcal{X}(0, \tau)$ differ more from each other but both are adding a structurally similar perpendicular set of infinitely many parallel hills and valleys possessing a steadily increasing (though always finite) amplitude. As an obvious result of the superposition, both the resulting surfaces $\mathcal{X}(\sigma, \tau)$ cross the zero plane merely along certain ovals $O_n^\mathcal{X}$, and both of them only get negative in their interior.

The precise shape of these ovals (numbered by $n = 0, 1, \ldots$) may fully rigorously be determined using the moving-lattice method (cf. Appendix A) but even without any use of the moving lattices the qualitative character of their shape is obvious and we may conclude that the zero lines of $\mathcal{M}(\sigma, \tau)$ and $\mathcal{N}(\sigma, \tau)$ form the families of ovals $O_n^\mathcal{M}$ and $O_n^\mathcal{N}$ located within the stripes of $\tau \in [(n + 1/2)\pi, (n + 1)\pi]$ and $\tau \in [(n + 1/4)\pi, (n + 3/4)\pi]$, respectively. All of them are symmetric with respect to the reflection $\sigma \rightarrow -\sigma$ and their size in the $\sigma$ direction increases with $\tau$.

Examples of these structures may be found in both refs. [9] and [13] and another illustration appears in Figure 1 here. In fact, the Figure displays another surface $Q(\sigma, \tau) = \mathcal{M}(\sigma, \tau)/\mathcal{N}(\sigma, \tau)$ (within a narrow window of $0 \leq Q \leq 0.05$) but the
shape of the curve where $\mathcal{M}$ vanishes ($O_{1}^{M} \equiv V_{1}$) appears there clearly since the denominator $F(\sigma, \tau) = 1/N(\sigma, \tau)$ has its zeros, generically, elsewhere (cf. observation [O2]). Besides the oval $V_{1}$ (and a part of $O_{0}^{M} \equiv V_{0}$) the picture displays another oval $O_{1}^{N} \equiv D_{1}$ of the zeros of the denominator $N$. Incidentally it lies within the chosen interval of $\tau \in (3, 7)$ and remains visible due to a numerical artifact of a spurious projection of an infinite discontinuity of the function $F(\sigma, \tau)$.

Although the visibility of the discontinuities reflects just an imperfection of the graphical representation of the surface, in will prove useful in what follows.

3.3 The role of the second component of $D[\sigma, \tau, R(\sigma, \tau)]$

The presence of the subsurface generated by the second, $R-$dependent component $D_{(R)}[R(\sigma, \tau)]$ in eq. (16) does not violate the separation between $\sigma$ and $\tau$ too much (cf. observation [O3]). At the smallest absolute values of $\sigma$ we may safely return to the approximation of $D_{(R)}[R(\sigma, \tau)]$ by a function of a single variable, $\left[\tan 2\phi(R)/R \approx \left[\tan 2\ell \tau/(L - \ell)\right]/\tau\right]$. This picture only becomes deformed, at the larger $\sigma$, by being bent to the right, i.e., along hyperbolas $R(\sigma, \tau) = constant$.

A clear understanding of the $\tau-$dependence of the whole surface $D[\sigma, \tau, R(\sigma, \tau)]$ will be obtained when we distinguish between the domain of the “small $\tau$” {where $\left[\tan 2\ell \tau/(L - \ell)\right]/\tau \approx 2\ell/(L - \ell)$ is positive and virtually constant}, “medium $\tau$” {with the repeated quick growth of the curve $\left[\tan 2\ell \tau/(L - \ell)\right]/\tau$ from minus infinity up to plus infinity within each interval of the constant length $\Delta \tau = \pi (L - \ell)/2\ell$} and “large $\tau$” {where the values of $D_{(R)}[R(\sigma, \tau)] \approx 1/\tau$ become very small up to the very thin layers near the singularity hyperbolas $H_{n}$}. Due to the local dominance of the latter singularities $H_{n}$ at any $n = 0, 1, \ldots$ it is easy to imagine that the sign of the whole function $D[\sigma, \tau, R(\sigma, \tau)]$ is positive and negative in their left and right vicinity, respectively. This “rule of thumb” enables us to deduce the sign of the whole
function $D[\sigma, \tau, R(\sigma, \tau)]$ in all our Figures.

### 3.4 The left-moving hyperbolic discontinuities $H_n$

In the domain of the small shifts $\ell \ll 1$ the numerical values of the $R-$dependent component $D_{(R)}[R(\sigma, \tau)]$ of eq. (16) remain almost constant and small. In this regime the above-mentioned “small-$\tau$” constraint $\tau \ll (L-\ell)/\ell$ is not particularly restrictive so that the matching-compatible roots of equation $D = 0$ remain very similar to their $\ell = 0$ predecessors in quite a large leftmost portion of the $\sigma - \tau$ plane. In our notation, the first few ovals $O_{D}^{n} \equiv V_{n}$ of the zeros of the secular determinant stay only perturbatively shifted and deformed by an increase of $\ell \ll 1$.

With the growth of $\ell$ or $\lambda = \ell/(L-\ell)$ the leftmost discontinuity-hyperbola $H_0$ of the surface $D[\sigma, \tau, R(\sigma, \tau)]$ moves to the left and emerges in the right half of Figure 2 where we choose the scale-independent parameter $\lambda = 11/40$ which corresponds to $\ell = 11 L/51$. This means that we are just leaving the domain of the small shifts $\ell \ll 1$ so that the deformation of the nodal oval $O_{1}^{D} \equiv V_{1}$ becomes perceivable, caused by the closeness of $H_0$ to the $\ell-$independent discontinuity oval $D_1 \equiv O_{1}^{N}$ inherited from the never-vanishing factor $F(\sigma, \tau) = 1/N(\sigma, \tau)$.

In a way which generalizes the illustrative Figure 2, each hyperbolic singularity $H_k$ (defined by the equation $R(\sigma, \tau) = (L-\ell)(k+1/2)\pi/\ell$ with $k = 0, 1, \ldots$) moves to the left with the growth of $\ell$ and $\lambda$. Once it gets close to the $N-$th singularity oval $D_{N-1}$, it touches it at a point with the coordinates $\sigma_{(in)}^{(N,k)} = 0$ and $\tau_{(in)}^{(N,k)} = (N-1/4)\pi$ at the critical value $\lambda = 2\ell/(L-\ell) = (4k+2)/(4N-1) \equiv \lambda_{(in)}^{(N,k)}$ of the shift.

With the further growth of $\lambda$ the intersection of the hyperbola with the standing oval moves to the left and disappears, curiously enough, at a certain pair of points with the “last-contact” $|\sigma| = |\sigma_{(out)}^{(N,k)}| > 0$ and $\tau = \tau_{(out)}^{(N,k)} < (N-3/4)\pi$. The latter value lies slightly below the oval’s end. Let us skip here the proof of this subtlety as
3.5 A completion of the list of the nodal lines

We are now prepared to detect all the nodal curves of $\mathcal{D}[\sigma, \tau, R(\sigma, \tau)]$ and to determine their qualitative $\ell-$dependence in all the interval of $\ell \in (0, L)$ and/or of $\lambda = \lambda(\ell) \in (0, \infty)$. For the first inspiration we return to Figure 2 where the oval of zeros $O_1^P \equiv V_1$ cannot be interpreted as a mere small perturbation of $O_1^M$ in spite of the fact that the singularity hyperbola $H_0$ still did not touch the singularity oval $O_1^N \equiv D_1$ since $\lambda = 0.275 < \lambda_{(in)}^{(2,1)} = 2/7 \approx 0.286$.

Still, the much more important observation made in Figure 2 concerns the emergence of the new curve $W_0$ of the new zeros of the function $\mathcal{D}$. At the chosen $\lambda$ this curve just entered Figure 2 at its right side. Our next Figure 3 confirms that the new nodal curve $W_0$ moves to the left and gets deformed in a way reflecting the presence of a steep oval dip in $Q(\sigma, \tau)$ below $\tau = 2\pi$. We choose $\lambda = 0.355$ which is still safely smaller than the lower estimate $(4k - 2)/(4N - 3) = 0.4$ of the singularity hyperbola’s “jumped-over” parameter $\lambda_{(out)}^{(2,1)} \approx 0.403$.

The “next-step snapshot” of Figure 4 at $\lambda = 0.395$ shows how the same dip deforms the shape of the oval $O_1^P \equiv V_1$ in the domain where the function of $R$ is small. In the subsequent Figure 5 we finally see how the two curves of the zeros merge while a topologically new situation is created and sampled at $\lambda = 0.415 > \lambda_{(out)}^{(2,1)}$.

We may summarize that for the growing $\lambda$ the motion of the singular component $\tan 2\varphi(R)/R$ of our secular determinant $\mathcal{D}(\sigma, \tau)$ to the left gives a clear guide how to keep the $\ell-$dependence of its zero lines under full control. The emergence and the asymptotically hyperbolic shape of the new (and, in fact, not quite expected) non-oval curves $W_m$ of zeros follows immediately from the asymptotic smallness of the positive component $Q(\sigma, \tau) \sim 1/\sigma^2$ of $\mathcal{D}(\sigma, \tau)$ at the larger $|\sigma| \gg 1$. 

not too relevant.
Due to the reasonably elementary character of the function $D(\sigma, \tau)$ we are able to understand that the pattern sampled by the Figures 2 - 5 is entirely universal. Always, step by step, the nodal ovals $V_n$ as well as their asymptotically hyperbolic nodal-line partners $W_m$ become deformed by the existence of the dip in the numerator function $M(\sigma, \tau)$.

Of course, after the hyperbola of singularities $H_k$ as well as its strongly deformed trailing nodal curve $W_k$ “creep” over the fixed singularity oval $D_j$ (as well as over its attached and strongly deformed zero curve $V_j$), the smoother shapes of both the nodal curves $W_k$ and $V_j$ are more or less recovered, and only their ordering remains permanently reversed. In spite of the apparent nonlinearity of the “creeping-over” effects, their details might again be analyzed algebraically, using an adapted version of the moving-lattice method of section 2.3.

The most important reward compensating an increase in complexity of the latter recipe is that one becomes able to treat one of the two roots of eq. (15), say, as a “non-perturbative” solution at the small $\ell$. The most important example of its role are the hyperbolic nodal curves $W_m$ which move to the right in $\tau$ with the decrease of $\ell$ and which disappear in infinity in the NSW limit of $\ell \to 0$.

4 Energies

4.1 Graphical representation and classification

On the background of the preceding material, what remains for us to do is a combination of the above-described knowledge of the nodal lines of $D[\sigma, \tau, R(\sigma, \tau)]$ with the coupling-dependence constraint $\sigma \times \tau = Z = (L - \ell)^2 g/2$. A sample of the intersections of this type (i.e., of a typical final solution) is offered in Figure 6 where $\lambda = 2.40$ is neither small nor large and where we choose $Z = Z^{(a)} = 1.00$ and $Z = Z^{(b)} = 2.24$
(= the critical “exceptional-point” value of ref. [9]) for illustration. The conclusions
which are illustrated by this graph have a general validity:

- We always have $\tau > \sigma > 0$ which means that all the real bound-state energies
  $E_n$ remain positive at $Z > 0$.

- Some of the energies remain real at any value of $Z > 0$. They correspond to
  the intersections of the hyperbola $\sigma = Z/\tau$ with the hyperbolic nodal lines $W_m$
  and may be called “stable”, $E = E_m^{(s)}$.

- All the other energies $E = E_n^{(u)}$ correspond to the intersections of the hyper-
  bola $\sigma = Z/\tau$ with the nodal ovals $V_k$. At a sufficiently small $Z$ the latter
  intersections remain real (see the line (a) with $Z = 1$ in Figure 6).

- We may call the latter energies “unstable” as they merge in pairs and form
  complex conjugate doublets [4] beyond certain “exceptional-point” [24] values
  of $\ell$ and $Z$ (illustration: the line (b) in Figure 6).

The decomposition of the spectrum into its stable and unstable parts varies with $\ell$ or
$\lambda = \ell/(L-\ell)$ in an obvious manner. Hence, the stability pattern in the spectrum will
be entirely different at the small and large $\lambda$ since in the former case the hyperbolic
curves $W_n$ only generate the high-lying energies and vice versa.

4.2 Numerical construction

After all our previous detailed analysis of the qualitative features of the spectrum
the numerical determination of energies becomes fully routine. Indeed, as long as we
know $\tau = Z/\sigma$, the rule $\tau^2 - \sigma^2 = R^2$ leads immediately to the definition of

$$\sigma = \sigma(R) = \sqrt{\frac{2Z^2}{R^2 + \sqrt{R^4 + 4Z^2}}}.$$ (17)
In parallel to such an introduction of the closed function $\sigma = \sigma(R)$ of $R$ we may return once more to the recipe $\tau = Z/\sigma(R)$ and re-read it as another explicit definition of the second auxiliary function $\tau(R) = Z/\sigma(R)$ of $R$.

In such a setting, the purely numerical determination of the bound-state energies is reduced to the search for the roots $R_n$ of eq. (12), i.e., of the zeros of the secular determinant

$$\hat{D}(R) = \left[ \sigma^2(R) \cosh 2\sigma(R) + \tau^2(R) \cos 2\tau(R) \right] \sin 2\lambda R +$$

$$+ R \left[ \sigma(R) \sinh 2\sigma(R) + \tau(R) \sin 2\tau(R) \right] \cos 2\lambda R$$

(converted now in the function of the single variable $R \sim \sqrt{E}$). An illustration of such a search is given in Figure 7 at a fixed choice of $Z = 2$. The quadruplet of the graphs of the secular determinant $\hat{D}(R) = \mathcal{D}[\sigma(R), \tau(R), R]$ is presented there at the four different values 1.25, 1.35, 1.45 and 1.55 of $\lambda$ (indicated along the vertical axis). In each of these graphs we magnified the vertical units near $\hat{D}(R) \approx 0$ and compressed them to a single point representing all the bigger values of $|\hat{D}(R)| \geq \varepsilon$. In this way the picture samples the left-hand side of eq. (18) solely near its zeros. Our magnification of the vertical dimension marks these zeros by the virtually straight parts of the curve which are seen as practically perpendicular to the horizontal axis.

The set of graphs in Figure 7 illustrates the $\lambda$–dependence of the bound-state roots $R_n$. We see that a pair of the unstable energies may merge and cease to be real after a fine-tuned growth of $\lambda$. This illustrates the complexification of the unstable energies which is not caused by the growth of $Z$ but rather by the growth of $\lambda$. At the first sight this phenomenon looks like a paradox because we are now weakening the non-Hermiticity in fact. Fortunately, this paradox is still easily understood once we imagine (and check, say, in the spirit of Figures 2 or 3) that the growth of $\lambda$ “pushes” all the zeros (including of course also the nodal oval in question) to the left. Of course, this oval cannot get prolonged in the $\sigma$ direction because the function
$\mathcal{M}(\sigma, \tau)$ itself grows too quickly with $\sigma$. This implies that the two real intersections of the oval with the hyperbola $\sigma = Z/\tau$ disappear because the latter curve grows to the left.

In the light of an additional scaling in eq. (14) one may only admire the subtlety of the phenomenon, the verification of which very much profits from the exact solvability of the model. An independent confirmation of the absence of any contradictions may be also offered via a further simplification of mathematics. This inspires us to pay particular attention to the “most counterintuitive” limiting case where $L \to \infty$. Such an analysis may be of an independent interest as it simulates, very roughly, the shape of the most popular antisymmetric and purely imaginary potential $V(x) \sim ix^3$ with real spectrum [22]. As long as this discussion already lies somewhat beyond the scope of the present text, it is moved to the Appendix B.

## 5 Conclusions

After more than ten years of an intensive research many people now seem to believe that we now better understand the key problems related to the so called $\mathcal{PT}$–symmetric as well as to many other similar non-Hermitian models or, in the more rigorous terminology, to all the models where the metric remains nontrivial, $\eta \neq I$ [25]. By the way, not all the related results are new. For example, Scholz et al [26] (inspired, presumably, by a few earlier mathematical as well as physical publications) studied the similar $\eta \neq I$ models more than ten years ago (!) and coined the name “quasi-Hermitian” for them.

Still, one cannot deny that during the last cca seven years, a new and intensive excitement has been caused by the discoveries of the reality of the spectra in many $\mathcal{PT}$–symmetric models. The emphasis of the research has been shifted, typically, to the explicit constructions of the charge $\mathcal{C}$ [20] or to the more detailed analysis of
what happens at the “exceptional” points where the reality of the spectrum is being lost [24, 27]. A few unusual features exhibited by our present model seem to offer another welcome and clear intuitive guidance in this area.

We found our results interesting since the merger and subsequent spontaneous complexification of some “twin” pairs $E^{(\pm\text{twin})}$ of the energies cannot be easily described within the usual textbook models where the metric is “trivial”, $\eta(\text{trivial}) = I$. It is also in this context where considerations based on our present model could lead to a deeper insight in the underlying mechanisms and mathematics, not only because our model is solvable but also because it proves able to provide different “twin-merging” patterns in the spectrum. Indeed, by the choice of the shape parameter $\ell$ we may, up to a large extent, prescribe which particular excitations (say, in the low-lying spectrum) should remain robustly stable and which ones should form the unstable, fragile “twins” merging at some sufficiently large couplings $g(\text{critical})$.

In the similar constructions and studies, one might feel hesitant whether his/her models should be simpler or more realistic. We believe that one should transfer the insight gained in the solvable models (like in the present one) to all the more realistic applications where just some approximate methods can be used. In this sense we already mentioned a parallelism between the role of the shift $\ell$ in our solvable model and of the exponent $\mu$ in the power-law potentials with $\mathcal{PT}$—symmetry.

It is encouraging to see that a certain nontrivial enrichment of the merging pattern has been detected, more or less in parallel, within the class of the power-law forces [27]. In this comparison, our present model’s merit lies in its exact solvability. Definitely, it proves able to offer a comparably rich pattern of the mergers of the levels.

This being said, the key phenomenological and “model-building” specific merit of our present new version of the $\mathcal{PT}$—symmetric square-well model is still to be
seen in the “global” structure of its spectrum. There, one observes that the “fragile” and the “robust” levels seem to form the two sets which may be moved with respect to each other as a whole. Thus, the whole spectrum becomes “almost completely robust” in one extreme (which is “almost Hermitian”) and “almost all fragile” in another extreme which is, near $\ell \approx 0$, “maximally non-Hermitian”.

Acknowledgment

Partially supported by GA AS in Prague, contract No. A 1048302.

Figure captions

Figure 1. A thin slice through the surface $Q(\sigma, \tau) = \mathcal{M}/\mathcal{N}$.

Figure 2. A thin slice through the surface of the secular determinant $D(\sigma, \tau)$ at $\lambda = \ell/(L-\ell) = 0.275$.

Figure 3. Same as Figure 2, $\lambda = 0.355$.

Figure 4. Same as Figure 2, $\lambda = 0.395$.

Figure 5. Same as Figure 2, $\lambda = 0.415$.

Figure 6. Solutions at $Z^{(a)} = 1.00$ and $Z^{(b)} = 2.24$, intersections marked by circles, $\lambda = 2.4$.

Figure 7. Four re-scaled graphs of the function $\hat{D}(R)$.

Figure 8. Graphical solution of eq. (28) ($y = \omega_N/2, T = 1$)
References

[1] D. Bessis and C. M. Bender, private communication

[2] C. M. Bender and S. Boettcher, Phys. Rev. Lett. 80 (1998) 5243.

[3] U. Günther, F. Stefani and M. Znojil, math-ph/0501069, J. Math. Phys., in print.

[4] A. Mostafazadeh, J. Math. Phys. 43 (2002) 205 and 2814.

[5] A. Mostafazadeh, A Critique of PT-Symmetric Quantum Mechanics (arXiv: quant-ph/0310164, unpublished);
   C. M. Bender, D. C. Brody and H. F. Jones, Phys. Rev. Lett. 92 (2004) 119902 (erratum).

[6] H. Langer and C. Tretter, Czechosl. J. Phys. 54 (2004) 1113.

[7] A. Mostafazadeh and A. Batal, J. Phys. A: Math. Gen. 37 (2004) 11645.

[8] C. M. Bender, D. C. Brody and H. F. Jones, Am. J. Phys. 71 (2003) 1095;
   A. Mostafazadeh, Czech. J. Phys. 54 (2004) 1125;
   M. Znojil, PT-symmetry, ghosts, supersymmetry and Klein-Gordon equation (arXiv: hep-th/0408081), in “Symmetry Methods in Physics”, Ed. Č. Burdík et al on CD with ISBN 5-9530-0069-3 (JINR, Dubna, 2004).

[9] M. Znojil, Phys. Lett. A. 285 (2001) 7.

[10] M. Znojil and G. Lévai, Mod. Phys. Lett. A 16 (2001) 2273.

[11] B. Bagchi, S. Mallik and C. Quesne, Mod. Phys. Lett. A17 (2002) 1651.
[12] P. A. M. Dirac, Proc. Roy. Soc. London A 180 (1942) 1;
W. Pauli, Rev. Mod. Phys. 15 (1943) 175;
M. Znojil, What is PT symmetry? preprint quant-ph/0103054v1, unpublished;
M. Znojil, Conservation of pseudo-norm in PT symmetric quantum mechanics, 
preprint math-ph/0104012, unpublished;
R. Kretschmer and L. Szymanowski, The Interpretation of Quantum-Mechanical 
Models with Non-Hermitian Hamiltonians and Real Spectra, preprint quant-
ph/0105054, unpublished;
B. Bagchi, C. Quesne and M. Znojil, Mod. Phys. Letters A 16 (2001) 2047;
A. Mostafazadeh, J. Math. Phys. 43 (2002) 3944 and 6343.
B. Bagchi and C. Quesne, Phys. Lett. A 300 (2002) 18;
A. Ramírez and B. Mielnik, Rev. Fis. Mex. 49S2 (2003) 130;
Z. Ahmed and S. R. Jain, Phys. Rev. E 67 (2003) 045106(R);
A. Mostafazadeh, Czech. J. Phys. 53 (2003) 1079;
F. Kleefeld, in “Hadron Physics, Effective Theories of Low Energy QCD”, AIP 
Conf. Proc. 660 (2003) 325.
C. M. Bender, Czech. J. Phys. 54 (2004) 13.

[13] M. Znojil, J. Math. Phys. 45 (2004) 4418.

[14] M. Znojil, J. Phys. A: Math. Gen. 36 (2003) 7825;
V. Jakubský, Czech. J. Phys. 54 (2004) 67;
V. Jakubský and M. Znojil, Czech. J. Phys. 54 (2004) 1101.

[15] S. Albeverio, S. M. Fei and P. Kurasov, Lett. Math. Phys. 59 (2002) 227;
M. Znojil, J. Phys. A: Math. Gen. 36 (2003) 7639;
S. M. Fei, Czech. J. Phys. 54 (2004) 43.

[16] C. M. Bender, S. Boettcher and P. N. Meisinger, J. Math. Phys. 40 (1999) 2201.

[17] M. Znojil, Czech. J. Phys. 54 (2004) 151.

[18] M. Znojil, Phys. Lett. A 259 (1999) 220 and 264 (1999) 108;
    G. Lévai and M. Znojil, J. Phys. A: Math. Gen., 33 (2000) 7165;
    B. Bagchi, S. Mallik and C. Quesne, Int. J. Mod. Phys. A 17 (2002) 51;
    C. S. Jia, S. C. Li, Y. Li and L. T. Sun, Phys. Lett. A 300 (2002) 115;
    A. Sinha, G. Lévai and P. Roy, Phys. Lett. A 322 (2004) 78.

[19] C. M. Bender, D. C. Brody and H. F. Jones, Phys. Rev. Lett. 89 (2002) 270401.

[20] C. M. Bender, Czech. J. Phys. 54 (2004) 1027;
    H. F. Jones, Czech. J. Phys. 54 (2004) 1107;
    E. Caliceti, F. Cannata, M. Znojil and A. Ventura, Phys. Lett. A 335 (2005) 26;
    B. Bagchi, A. Banerjee, E. Caliceti, F. Cannata, H. B. Geyer, C. Quesne and
    M. Znojil, hep-th/0412211, Int. J. Mod. Phys. A, in print.

[21] E. Caliceti, S. Graffi and M. Maioli, Commun. Math. Phys. 75 (1980) 51;
    G. Alvarez, J. Phys. A: Math. Gen. 27 (1995) 4589;
    E. Delabaere and D. T. Trinh, J. Phys. A: Math. Gen. 33 (2000) 8771;
    G. A. Mezincescu, J. Phys. A: Math. Gen. 33 (2000) 4911;
    C. R. Handy, Czech. J. Phys. 54 (2004) 57;
    M. Bentaiba, S. A. Yahiaoui and L. Chetouani, Phys. Let. 231 (2004) 175.
[22] P. Dorey, C. Dunning and R. Tateo, J. Phys. A: Math. Gen. 34 (2001) 5679;
    K. C. Shin, Commun. Math. Phys. 229 (2002) 543.

[23] I. Herbst, Commun. Math. Phys. 64 (1979) 279.

[24] C. Dembowski et al, Phys. Rev. Lett. 86 (2001) 787;
    W. D. Heiss and H. L. Harney, Eur. Phys. J. D 17 (2001) 149;
    U. Günther and F. Stefani, J. Math. Phys. 44 (2003) 3097;
    W. D. Heiss, Czech. J. Phys. 54 (2004) 1091.

[25] cf. two special issues of Czechosl. J. Phys. 54 (2004), pp. 1 - 156 and 1005 - 1148.

[26] F. G. Scholtz, H. B. Geyer and F. J. W. Hahne, Ann. Phys. (NY) 213 (1992) 74.

[27] P. Dorey, A. Milican-Slater and R. Tateo, J. Phys. A: Math. Gen. 38 (2005) 1305.
Appendix A: The method of moving lattice

Secular eq. (12) and its descendants contain quickly oscillating trigonometric functions of arguments $2\tau$ and $2\varrho$. In the spirit of ref. [13] it makes sense to re-parametrize both these variables according to the rules

$$\tau = \tau(N,t) = \pi N + \pi t, \quad N = 0, 1, \ldots, \quad t \in (0, 1),$$

$$\varrho = \pi K + \pi r, \quad K = 0, 1, \ldots, \quad r \in (0, 1)$$

which separate their “large” change (by an integer multiple of the period $2\pi$ so that the trigonometric function itself remains unchanged) from a “small” change [within one period $(0, 2\pi)$]. Thus, once we define

$$\Psi = \sin 2\tau = \sin 2\pi t, \quad \Phi = \cos 2\tau = \cos 2\pi t,$$

$$\Xi = -\tan 2\varrho = -\tan \pi r,$$

all our trigonometric functions in question become independent of both the integer variables. Thus, once we decide to work, say, in the $\sigma-R$ plane, we simply introduce a lattice $\mathcal{L}_{t,r}$ of points with coordinates

$$\sigma = \sigma(N,t) = \frac{Z}{\tau(\sigma)} = \frac{Z}{\pi N + \pi t}$$

and

$$R = \frac{L - \ell}{\ell} \varrho(R) = \frac{\pi (L - \ell)}{2\ell} (K + r)$$

where $t \in (0, 1)$ and $r \in (0, 1)$ are fixed while $N = 0, 1, \ldots$ and $K = 0, 1, \ldots$ remain variable. Our secular equation (12) then becomes more easily analyzed at the fixed $t \in (0, 1)$ and $r \in (0, 1)$ when it may be re-read as a simplified mapping $\sigma \to R$ with

$$R = R_{t,r}(\sigma) = \Xi_r \times \frac{\sigma^4 \cosh 2\sigma + Z^2 \Phi_t}{\sigma^3 \sinh 2\sigma + Z \Psi_t}, \quad (19)$$
i.e., $R_{t,r} \approx \Xi_r |\sigma|$ at $|\sigma| \gg 1$ while

$$R_{t,r} \approx \frac{Z}{\sigma} \times \frac{\Phi_t \Xi_r}{\Psi_t}$$

at $|\sigma| \ll 1$ etc. In the subsequent step, remembering that the latter formulae hold on the lattice $\mathcal{L}(t, r)$ only, we must let this lattice move with the variation of $t$ and/or $r$. Within each box numbered by the pair $(N, K)$ of non-negative integers we would be able to re-derive all the qualitative geometric considerations of section 3 in an alternative, quantitative manner.
Appendix B: Shallow well

In the infinite-size limit $L \to \infty$ our model degenerates to a purely imaginary square well with asymptotic boundary conditions

$$\psi(\pm \infty) = 0$$

and with the $\mathcal{PT}$ symmetric matching conditions in the origin,

$$\psi(0) = 1, \quad \partial_x \psi(0) = i G.$$  \hspace{1cm} (21)

This means that we have the general solution

$$\psi(x) = \begin{cases} 
\cos k x + B \sin k x, & x \in (0, \ell), \quad k^2 = E, \\
(L + i N) \exp(-\sigma x), & x \in (\ell, \infty), \quad \sigma^2 = iT^2 - k^2, 
\end{cases}$$  \hspace{1cm} (22)

with $T = \sqrt{g}$ and with the purely imaginary constant $B = i G/k$.

B.1. Matching conditions at $x = \ell$

Let us split $\sigma = p + iq$ in its real and imaginary part with $p, q \geq 0$. This gives the rules $p^2 + k^2 = q^2$ and $2pq = T^2$, easily re-parameterized in terms of a single variable $\alpha$,

$$p = q \cos \alpha, \quad k = q \sin \alpha, \quad q = \frac{T}{\sqrt{2 \cos \alpha}}, \quad \alpha \in (0, \ell/2).$$

The standard matching at the point of discontinuity is immediate,

$$\cos k \ell + B \sin k \ell = (L + i N) \exp(-\sigma \ell),$$

$$-\sin k \ell + B \cos k \ell = -\frac{\sigma}{k} (L + i N) \exp(-\sigma \ell).$$

After we abbreviate $\sigma/k = -\tan \Omega \ell$, we get an elementary complex condition of the matching of logarithmic derivatives at $x = \ell$,

$$G = -i k \tan(k + \Omega) \ell.$$
Its real part defines our first unknown parameter, \( G = G(\alpha) \). Due to our normalization conventions, the imaginary part of the right-hand-side expression must vanish, \( \text{Re}[\tan(k + \Omega)\ell] = 0 \). An elementary re-arrangement of such an equation acquires the form of an elementary quadratic algebraic equation for \( X = \tan k\ell \). Its two explicit solutions read

\[
X_1 = \frac{p + q}{k}, \quad X_2 = \frac{p - q}{k}
\]  

or, after all the insertions,

\[
\tan \left[ \frac{\ell T \sin \alpha^{(\pm)}}{\sqrt{2} \cos \alpha^{(\pm)}} \right] = \tan \left[ \frac{\ell - \alpha^{(\pm)}}{2} \right],
\]  

\[
\tan \left[ \frac{\ell T \sin \alpha^{(-)}}{\sqrt{2} \cos \alpha^{(-)}} \right] = \tan \left[ -\frac{\alpha^{(-)}}{2} \right].
\]

These equations specify, in implicit manner, the two respective infinite series of the appropriately bounded real roots \( \alpha = \alpha_n^{(\pm)} \in (0, \ell/2) \).

**B.2. Energies**

For \( \alpha \in (0, \ell/2) \) the left-hand-side arguments in eqs. (26) and (27) run from zero to infinity and the functions oscillate infinitely many times from minus infinity to plus infinity. In contrast, the limited variation of the argument \( \alpha \) makes both the right-hand side functions monotonic, very smooth and bounded, \( \tan[(\ell - \alpha^{(\pm)})/2] \in (1, \infty) \) and \( \tan[\alpha^{(-)}/2] \in (0, 1) \). This indicates that our roots \( k = k(\alpha_n^{(\pm)}) \) will all lie within well determined intervals,

\[
k_n^{(\pm)} \in \left( n + \frac{1}{4}, n + \frac{1}{2} \right), \quad n = 0, 1, \ldots,
\]

\[
k_m^{(-)} \in \left( m + \frac{3}{4}, m + 1 \right) \quad m = 0, 1, \ldots.
\]

An additional merit of parametrization (23) lies in an unambiguous removal of the tangens operators from both eqs. (26) and (27). This gives

\[
k_n^{(\pm)} = n + \frac{1}{2} - \frac{\omega_n^{(\pm)}}{4}, \quad k_m^{(-)} = m + 1 - \frac{\omega_m^{(-)}}{4}, \quad \omega_n^{(\pm)} = \frac{2\alpha_n^{(\pm)}}{\ell} \in (0, 1).
\]
After a change of notation with $\omega_n^+ = \omega_{2n}$ and $\omega_n^- = \omega_{2n+1}$, we may finally combine the latter two rules in the single secular equation

$$\sin \left( \frac{\ell}{2} \omega_N \right) = \frac{2N + 2 - \omega_N}{4T} \cdot \sqrt{2 \cos \left( \frac{\ell}{2} \omega_N \right)} \quad N = 0, 1, \ldots, \quad (28)$$

In a graphical interpretation this equation represents an intersection of a tangens-like curve with the infinite family of parallel lines. This is illustrated in Figure 8. The equation generates, therefore, an infinite number of real roots $\omega_N \in (0, 1)$ at all the non-negative integers $N = 0, 1, \ldots$. The discrete spectrum is unbounded from above and remains constrained by the inequalities

$$\frac{(N + 1/2)^2}{4} \leq E_N \leq \frac{(N + 1)^2}{4} \quad (29)$$

independently of the coupling $T$.

**B.3. Wave functions**

Equation (24) in combination with eqs. (26) and (27) determines the real parameter

$$G = G'(\pm) = -\frac{k^2}{q \pm p} \quad (30)$$

responsible for the behaviour of the wave functions near the origin [remember that $B = iG/k$ in eq. (22)]. For its deeper analysis let us first introduce an auxiliary linear function of $\omega$ and $N$,

$$\sqrt{R(\omega_N, N)} = \frac{2N + 2 - \omega_N}{4T} \in \left( \frac{N + 1/2}{2T}, \frac{N + 1}{2T} \right)$$

and re-interpret our secular eq. (28) as an algebraic quadratic equation with the unique positive solution,

$$\cos \left( \frac{\ell}{2} \omega_N \right) = \frac{1}{\sqrt{R(\omega_N, N)} + \sqrt{R^2(\omega_N, N) + 1}} \quad (31)$$
This is an amended implicit definition of the sequence $\omega_N$. As long as the right hand side expression is very smooth and never exceeds one, the latter formula re-verifies that the root $\omega_N$ is always real and bounded as required.

In the weak coupling regime (i.e., in the domain of the large and almost constant $R \gg 1$ with the small square-well height $T$ or at the higher excitations), our new secular equation (31) gives a better picture of our bound-state parameters $\omega_N = 1 - \eta_N$ which all lie very close to one. The estimate

$$\frac{\ell}{2} \eta_N = \arcsin \frac{1}{R + \sqrt{R^2 + 1}} \approx \frac{1}{2R} - \frac{5}{48 R^3} + \ldots$$

represents also a quickly convergent iterative algorithm for the efficient numerical evaluation of the roots $\omega_N$. One can conclude that in a way compatible with our \textit{a priori} expectations, the value of $p = p_N = \text{Re} \sigma \approx q/2R$ is very close to zero and, as a consequence, the asymptotic decrease of our wave functions remains slow. We have $q = q_N = \text{Im} \sigma \approx k$ so that, asymptotically, our wave functions very much resemble free waves $\exp(-ikx)$. In the light of eq. (30) we have also $\psi(x) \approx \exp(-ikx)$ near the origin.

In the strong coupling regime (i.e., for very small $R$ representing, say, the low-lying excitations in a deep well with $T \gg 1$) we get an alternative estimate

$$\frac{\ell}{4} \omega_N = \arcsin \sqrt{\frac{1}{2} \left[ R - \left( \sqrt{1 + R^2} - 1 \right) \right]} \approx \frac{1}{2} R - \frac{1}{4} R^2 + \ldots \ll \frac{\ell}{4}.$$ 

In the extreme of $R \to 0$ the present spectrum of energies moves towards (and precisely coincides with) the well known levels of the infinitely deep Hermitian square well of the same width $I = (-\ell, \ell)$. In this sense, the “complex-rotation” transition from the Hermitian well to its present non-Hermitian $\mathcal{PT}$ symmetric alternative proves amazingly smooth.

The wave functions exhibit the similar tendency. In the outer region, they are proportional to $\exp(-px)$ and decay very quickly since $p = \mathcal{O}(R^{-1/2})$. The parameter
$G^{(\pm)}$ becomes strongly superscript-dependent,

$$G^{(+)} = -\frac{k^2}{q + p} = \mathcal{O}(R^{3/2}), \quad G^{(-)} = -(q + p) = \mathcal{O}(R^{-1/2}).$$

This means that in the interior domain of $x \in (-\ell, \ell)$, the wave functions with the superscript $(+)$ and $(-)$ become dominated by their spatially even and odd components $\cos kx$ and $\sin kx$, respectively. In this sense, the superscript mimics (or at least keeps the trace of) the quantum number of the slightly broken spatial parity $\mathcal{P}$. 