Quantum star-graph analogues of $\mathcal{PT}$–symmetric square wells. II: Spectra.

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Abstract

For non-Hermitian equilateral $q$–pointed star-shaped quantum graphs of paper I [Can. J. Phys. 90, 1287 (2012), arXiv 1205.5211] we show that due to certain dynamical aspects of the model as controlled by the external, rotation-symmetric complex Robin boundary conditions, the spectrum is obtainable in a closed asymptotic-expansion form, in principle at least. Explicit formulae up to the second order are derived for illustration, and a few comments on their consequences are added.

PACS

03.65.Ca (Formalism), 03.65.Db (Functional analytical methods), 03.65.Ta (Foundations of quantum mechanics; measurement theory) and 03.70.+k (Theory of quantized fields)
1 Introduction

In paper I [1] we recalled the recent growth of popularity of the study of quantum systems in their $\mathcal{PT}$–symmetric *alias* pseudo-Hermitian representations (cf., e.g., review papers [2] and [3], respectively). In this broader context we summarized briefly the basic characteristics of one of the exactly solvable illustrative examples of such a quantum system. We emphasized that the model proposed in [4] proved useful, as a mathematically consistent methodical laboratory, in a few subsequent publications (cf., e.g., their summaries in [5]). Next, we reinterpreted the latter toy model (which lives on a finite real interval $(−L, L)$) as one of the most elementary (viz., two-pointed-star-shaped) exemplifications of a non-Hermitian quantum graph [6]. We felt inspired by the friendly nature and tractability of the model and we proposed one of its most natural $q$–pointed star-shaped generalizations with $q > 2$ (cf. the first nontrivial sample graph in Fig. 1).

![Figure 1: Star-shaped-graph coordinates running inwards ($q = 3$).](image)

The main result of paper I was the derivation of a universal and compact form of the secular equation which defined the spectra in implicit form. We also added a few mathematics- as well as physics-oriented overall comments on the spectrum and, in particular, we employed a brute-force, purely numerical method in order to demonstrate that at $q > 2$, some of the energies may prove complex in general.

In the present brief completion of paper I we intend to pay more attention to the symmetries of the model. In essence, we shall be able to reveal that the formal and algebraic boundary-condition symmetries as carried by the Hamiltonian really exhibit a nontrivial connection with certain approximate symmetries of the geometry of certain
subsets of the energy roots in complex plane.

2 The model

Let us accept the convention that the family of the star-shaped graphs \( G^{(q)} \) is numbered by an integer \( q = (2, 3, 4, \ldots) \) and that in each member of this family the \( j \)-th edge is parametrized by the respective coordinate \( y_j \). Let us also set this coordinate equal to zero at the external end of the edge, and let it grow up to value \( y_j = L \) at the central vertex (cf. Fig. 1 where \( q = 3 \)).

For the whole family of the equilateral star-shaped non-Hermitian quantum graphs \( \mathbb{G}^{(q)} \) we postulated, in paper I, a Laplace-type operator on the graphs in the form which generalizes the Hamiltonian of Ref. [4] and which was introduced via a \( q \)-plet of its ordinary differential free-motion components,

\[
- \frac{d^2}{dy_j^2} \psi_j(y_j) = k^2 \psi_j(y_j), \quad y_j \in (0, L), \quad j = 0, 1, \ldots, q - 1.
\]

The Kirchhoff’s continuity law was imposed to match the flows and wave functions at the central vertex,

\[
\sum_{m=0}^{q-1} \partial_{y_m} \psi_m(L) = 0, \quad \psi_j(L) = \psi_0(L), \quad j = 1, 2, \ldots, q - 1.
\]

At the outer ends of the edges we picked up the manifestly non-Hermitian boundary conditions

\[
\partial_{x_j} \psi_j(0) = i\alpha e^{i\varphi} \psi_j(0), \quad j = 0, 1, \ldots, q - 1, \quad \varphi = 2\pi/q, \quad \alpha > 0
\]

exhibiting, at any fixed \( q \), a constant growth of phase with a move \( j \to j + 1 \) to the neighboring edge.

2.1 Secular equation

Due to the simplicity of Eq. (3) we were able to prove, in paper I, the existence of infinitely many bound states of the system \( \mathbb{G}^{(q)} \) with real energies. In implicit form,
these energies were defined via the real roots $\kappa = kL$ of secular equation
\[
\frac{\kappa^{p+2} + (i\beta)^{p+2} \tan^{p} \kappa}{\kappa^{p+2} - (i\beta)^{p+2} \tan^{p+2} \kappa} \tan \kappa = 0, \quad \beta = \alpha L, \quad p = q - 2 = 0, 1, \ldots \tag{4}
\]
For non-trivial quantum stars with positive $p$ the implicit energy formula (4) was the main result of paper I. We also showed there that although the two free parameters $L$ and $\alpha$ of the model were chosen real and positive, some of the energy roots might still be admitted complex in general, $\kappa \in \mathbb{C}$.

In paper I there was no space left for a more detailed analysis of the $p > 0$ spectra. In what follows we intend to fill the gap and to turn attention to the open questions of the existence, type and parametric dependence of all of the roots $\kappa_n(\beta)$ of Eq. (4), real or complex.

### 2.2 Two sets of the roots of secular equation

A subset of the roots of Eq. (4) will originate from the zeros of function $\tan \kappa$ (via the second factor of the left-hand-side expression) and from the poles of function $\tan \kappa$ [due to the higher power (viz., $p + 2$) of this function in the denominator of the first factor of the left-hand-side expression]. This subset is real, $\beta$–independent, equidistant and may be superscripted,
\[
\kappa = \kappa^{[1]}_n = n\pi/2, \quad n = 1, 2, \ldots \tag{5}
\]
The remaining, $\beta$–dependent and, in general, complex roots $\kappa = \kappa^{[2]}(\beta) = \lambda$ should be then sought via the remaining, reduced part of the secular equation,
\[
\tan^p \lambda = -\left(\frac{\lambda}{i\beta}\right)^{p+2}. \tag{6}
\]
At any positive $p = 1, 2, \ldots$ the latter transcendental relation is equivalent to the $p$–plet of simpler equations
\[
\tan \lambda_{[n]} = \left(\frac{\lambda_{[n]}}{\beta}\right)^{1+2/p} \quad \text{e}^{i\pi \left(-\frac{1}{2} + \frac{2n}{p}\right)}, \quad n = 0, 1, \ldots, p - 1. \tag{7}
\]
In spite of the scepticism as expressed in paper I (cf. also a few complementary comments on the localization of non-real roots in proceedings [7]), this equation is still amenable to non-numerical analysis. This will be our present key observation.
3 The second, complex subset of the roots

3.1 Non-numerical localization

At a fixed $\beta > 0$ and at the larger values of the imaginary part of $\lambda_{[n]}$ the absolute value of the left-hand-side function lies very close to one so that the absolute value of $\lambda_{[n]}$ cannot in fact be too large. *Vice versa*, at the larger absolute values of $\lambda_{[n]}$ the roots of Eq. (7) cannot lie too far from the real axis and, in particular, from the poles of the left-hand-side function. Thus, it makes sense to reparametrize

$$\lambda_{[n]} = \kappa_{[n]}^{[p]}(\beta) = \frac{2M + 1}{2} \pi + \varepsilon_{[n]}(\beta, M), \quad M = 0, 1, \ldots . \quad (8)$$

Whenever the auxiliary integer $M$ is chosen sufficiently large, quantities $\varepsilon_{[n]}(\beta, M)$ may be assumed small. Such an assumption is not inconsistent since after the $M$–dependent change $\lambda \to \varepsilon$ of our variables one obtains another form of secular Eqs. (7),

$$\tan \varepsilon_{[n]} = \left( \frac{\beta}{(M + 1/2)\pi + \varepsilon_{[n]}} \right)^{1+2/p} e^{-i\pi\left(\frac{1}{2} + \frac{2\pi}{p}\right)}, \quad n = 0, 1, \ldots, p - 1. \quad (9)$$

From this exact implicit relation we may derive explicit approximate formula

$$\varepsilon_{[n]} = \left( \frac{\beta}{(M + 1/2)\pi} \right)^{1+2/p} e^{-i\pi\left(\frac{1}{2} + \frac{2\pi}{p}\right)} \left[ 1 + \mathcal{O}\left( \frac{1}{M^{1+2/p}} \right) \right] \quad (10)$$

or, on the next level of precision and with an amended error factor,

$$\varepsilon_{[n]} = \frac{(M + 1/2)\pi}{1 + 2/p + \beta^{-1-2/p}[M + 1/2]^{2+2/p} e^{i\pi\left(\frac{1}{2} + \frac{2\pi}{p}\right)}} \left[ 1 + \mathcal{O}\left( \frac{1}{M^{3+4/p}} \right) \right]. \quad (11)$$

These estimates imply that in certain complex discs centered at real axis we could solve Eq. (9) by iterations.

It seems worth adding that the asymptotic-estimate nature of formulae (10) or (11) leaves the question of the exhaustive description of the complex roots in a non-asymptotic domain (of $M$) open to further analysis. Perhaps, the comparatively elementary nature of our secular Eq. (4) might provoke a mathematician to provide a fully rigorous proof of the results of our present, large–$M$ approximative analysis.
3.2 Asymptotic series

A concrete implementation of the iteration recipe could proceed either numerically or via algebraic, computer-assisted symbolic manipulations. In both cases, the qualitative messages delivered by the construction will be very similar, showing that our non-Hermitian quantum graphs $G^{(p+2)}$ support the existence of $p$–plets of large complex eigenvalues with small imaginary parts which lie on approximate circles with very small radii.

A more explicit characteristics of these circles of eigenvalues may be deduced from our asymptotic formulae (10) or (11) as well as, if necessary, from their higher-order asymptotic-series descendants. One may immediately see that these circles are centered at the odd real eigenvalues $\kappa_{2M+1}^{[1]}$. Far from the origin we could even assign every such a $p$–plet a shared integer index $M$ and re-subscript the eigenvalues yielding $\lambda_{[M,m]}$ with $m = 0, 1, \ldots, p - 1$.

With the decrease of $M$ the radii and deformations of the circles may cease to be small. Their description becomes numerical. The rate of convergence of their numerical localization may systematically be amended via higher-order asymptotic formulae for $\varepsilon$. During the derivation of these formulae one should keep in mind that in exact formula (9) the game is entered by the value of $p = q - 2$. This leads to the necessity of more careful algebraic manipulations.

First of all, the left-hand-side Taylor series must be constructed in the odd powers of $\varepsilon_{[n]} = O\left(1/M^{1+4/5}\right)$ yielding the sequence of corrections $O\left(1/M^{3+6/5}\right), O\left(1/M^{5+10/5}\right)$, etc. The resulting expression must then match the right-hand-side Taylor series in the integer powers of $\varepsilon_{[n]}/[(M + 1/2)\pi] = O\left(1/M^{2+4/5}\right)$ so that another, different sequence of corrections emerges, of the orders of magnitude $O\left(1/M^{4+4/5}\right), O\left(1/M^{5+6/5}\right)$, etc.

In principle, the resulting dedicated double-series semi-numerical recipe is feasible and straightforward and the resulting formulae may be easily stored in the computer. Its only unpleasant feature is that the formulae become too long to be displayed in print. Nevertheless, in Refs. [11] and [17] we pointed out that for the practical numerical purposes of localization of individual roots $\varepsilon_{[n]}$ at the smallest $M$, even the generic, non-dedicated numerical algorithms are also able to provide satisfactory results.
4 Discussion

4.1 The generalized Robin boundary conditions

One of the features which made the exactly solvable $q = 2$ model $G^{(2)}$ of Ref. [4] truly important in the context of quantum theory was the $\mathcal{PT}$-invariance of its Hamiltonian $H$ with parity $\mathcal{P}$, time reversal $\mathcal{T}$ and symmetry relation $H \mathcal{PT} = \mathcal{PT} H$. In paper I we just pointed out that even such an elementary $q = 2$ model illustrates, in parallel, also several important features of a non-Hermitian quantum graph. Thus, taking the $q = 2$ quantum model $G^{(2)}$ as a guide to its $q > 2$ generalization, we replaced the original Schrödinger equation of Ref. [4] (living on an interval) by its two-subinterval version, with a single oriented edge ($\to$) replaced by two edges, ($\to, \to$). Besides such an oriented-graph reinterpretation it was necessary to add the explicit Kirchhoff’s condition of smoothness of wave functions in the origin. Finally, we came to the $q = 2$ graph $G^{(2)} = (\to, \leftarrow)$ of the present paper via a re-orientation of one of the edges/subintervals.

The first consequence of such a change of the traditional presentation of the model was that the action of the parity $\mathcal{P}$ has been simplified, mediating just a mutual interchange of the two edges of the graph. This operator may be easily generalized to $\mathcal{P}^{(q)}$ which replaces each edge $e$ by its left neighbor, i.e., with $e_j \to e_{j+1}$ and $e_{q-1} \to e_0$ at the end of course.

The above-mentioned $\mathcal{PT}$-symmetry of the $q = 2$ model may be traced back to its specific Robin boundary conditions

$$\psi_{0,1}^\prime(0) = \pm i\alpha \psi_{0,1}(0), \quad q = 2$$

in which one may compensate the mutual interchange of the two edges (i.e., the action of $\mathcal{P}^{(2)}$) by the action of an operator of time reversal $\mathcal{T} = \mathcal{T}^{(2)}$. The latter action may be realized either as complex conjugation ($\mathcal{T}i = -i$) or, in the spirit of Refs. [8], as the 180-degrees rotation in the complex plane of the parameter, ($\mathcal{T} \alpha = -\alpha$). In paper I the above-defined graphs $\mathcal{G}^{(q)}$ were proposed precisely as one of the most natural realizations of the idea of the $\mathcal{P}^{(q)}\mathcal{T}^{(q)}$-invariance in its generalization from $q = 2$ to all $q > 2$.

In paper I the latter symmetry idea has not in fact been mentioned at all. One
of the main reasons was that at $q > 2$, the alternative definitions of $T^{(q)}$ cease to be equivalent. In this sense the present results on the spectra may be perceived as a support of the most easily graph-adapted complex-rotation-operator definition. When accepted, operators $T^{(q)}$ would just cause a clockwise rotation in the complex plane of $\alpha$ by the $q$–dependent angle $\varphi = 2\pi/q$.

Under this convention the idea of rotations is shared by both its kinematical implementations (via $P^{(q)}$ which realize the spatial maps between edges) and its dynamical realization (via $T^{(q)}$ which is a complex rotation of coupling constants $\alpha$). Thus, purely formally, we could still keep speaking about a generalized $\mathcal{PT}$–symmetry in principle, although, incidentally, it appeared to remain spontaneously broken in all of our present specific toy-model quantum graphs. Moreover, in contrast to the involutive character of the parity at $q = 2$ (meaning that its square is identity, $[P^{(2)}]^2 = I$ so that we can treat it as a reflection), we only have the weaker rule $[P^{(q)}]^q = I$ in general. This means that the mathematical importance of parity $P$ (playing the role of a Krein-space metric at $q = 2$) and of the $\mathcal{PT}$–symmetry of the $q = 2$ Hamiltonian $H$ (meaning that $H$ is assumed self-adjoint in such a Krein space) are both lost at $q > 2$.

4.2 Methodical aspects of the model

In our present paper we found that one of the most unexpected features of the whole family of the nontrivial, genuine non-line graph-shaped choices of paper I is the wealth of the complex energy roots of the secular equation. This discovery should be interpreted as a word of warning because for $q > 2$ the model should be treated as a sample of a gain-loss system in optics (where the complex eigenvalues keep carrying a physical meaning) rather than as a sample of a quantum system with resonances.

One should notice that the majority of the complex energy roots of our model lies in a very close vicinity of the real line. In the language of physics, this feature of the spectrum could be perceived as a possibility of a comparatively weak violation of the stability and of the unitarity of the evolution, but a detailed analysis of these interpretation possibilities lies beyond the scope of the present paper.

In the conceptual setting, the present discovery of the wealth of the complex eigenval-
ues may be read both as disappointing and as promising. What is disappointing is that one cannot treat our present family of quantum graphs as a certain discrete guide to a reduction of technical difficulties during transition from the popular ordinary differential non-Hermitian Hamiltonians to their more sophisticated partial differential descendants [10].

On positive side, our present non-Hermitian quantum graphs $G$ still may be perceived as belonging to the simplest nontrivial non-numerically tractable quantum models. Their conceptual transparency makes their study rewarding and productive since several exceptional exact-solvability features of the $q = 2$ special case (and, in particular, the real part of the spectrum) still survived the generalization to $q > 2$.

In a historical perspective one can reveal analogies between the present and other graph-based discretizations of a more-dimensional phase space, say, with the central-symmetry-based reduction of the three-dimensional hydrogen atom description to an ordinary radial Schrödinger equation with a local effective interaction $V_{(\text{Coul})}(r) \sim 1/r$ which lives on a semi-infinite interval of the radial coordinate $r \in (0, \infty)$.

It is worth adding that the most elementary hydrogen-atom model did also serve methodical purposes in $\mathcal{PT}$-symmetric quantum mechanics (cf., e.g., [11]). At the same time, the friendly tractability of its Hamiltonian $\mathfrak{h}$ is lost in the majority of the modern applications of quantum theory. Incidentally, precisely this also motivated the acceptance of non-Hermitian Hamiltonians. For heavy nuclei, for example, a complicated non-unitary isospectral preconditioning of the realistic Hamiltonian

$$\mathfrak{h} \to H = \Omega^{-1} \mathfrak{h} \Omega \neq H^\dagger$$

appeared necessary for keeping the diagonalization of non-Hermitian $H$ feasible. This requirement also led to the theoretical formulation of the recipe of the Hermitization in quantum mechanics [12].

4.3 Symmetries

One of the main surprises provided by our present results is that the expected parallels between the $q > 2$ and $q = 2$ non-Hermitian star-shaped quantum graphs $G^{(q)}$ appeared
practically non-existent. The main difference between the $q > 2$ and $q = 2$ models was found in the nontriviality of the split of the spectrum in two infinitely large groups in the former case. Besides the expected, infinitely many real, dynamics-independent eigenvalues $\kappa_m^{[1]}$, $m = 1, 2, \ldots$ which kept existing in both cases, the single real eigenvalue which appeared dynamics-dependent (i.e., $\alpha-$dependent) at $q = 2$ [4] was replaced, at any $q > 2$, by infinitely many eigenvalues $\kappa^{[2]}(\beta)$. which were dynamics-dependent and, up to exceptions, complex.

Such a result was utterly unexpected. We also found that whenever the absolute values of the latter quantities $\kappa^{[2]}(\beta)$ prove sufficiently large, we may visualize them as forming approximatively circular complex $p-$plets [5] which encircle every odd (and sufficiently large) real eigenvalue $\kappa^{[1]}_{2M+1}$. Hence, asymptotically at least, we may number these roots $\kappa^{[2]}(\beta)$ by a pair of integers $M \gg 1$ and $m \ (= 0, 1, \ldots, p - 1)$. At a fixed $M$, differences $\varepsilon_{[M,m]}(\beta) = \kappa^{[2]}_{[M,m]}(\beta) - \kappa^{[1]}_{2M+1}$ remain small and, in leading order, $m-$independent, $\varepsilon_{[M,m]}(\beta) = O \left( \frac{1}{M^{1+2/p}} \right)$.

Let us now emphasize that this result leads to an interesting generalization of the concept of $\mathcal{PT}$—symmetry as exhibited by the present quantum graphs $\mathcal{G}^{(q)}$. This generalization is based on the fact that the action of the “generalized time reversal” $\mathcal{T}^{(q)}$ changes the Robin boundary conditions, i.e., in effect, it causes a rotation of the supporting graph $\mathcal{G}^{(q)}$. Nevertheless, this action may be also perceived as compensating the opposite rotation of the supporting graph $\mathcal{G}^{(q)}$ as caused by the “generalized spatial reversal” $\mathcal{P}^{(q)}$. Thus, in a purely formal setting we may summarize that a combined action of product $\mathcal{P}^{(q)}\mathcal{T}^{(q)}$ of our above-defined operators leaves the supporting graph $\mathcal{G}^{(q)}$ invariant.

*Simultaneously and approximatively*, the action of $\mathcal{P}^{(q)}\mathcal{T}^{(q)}$ (or, better, of $\mathcal{T}^{(q)}$ — because $\mathcal{P}^{(q)}$ itself has no effect) also rotates the discrete, $p-$point asymptotic complex circles of the second-subset leading-order eigenvalues and leaves them invariant. This observation follows from formula (10) which defines the approximate solution at a fixed $M \gg 1$ and implies that

\[
\text{transformation } \alpha \to \mathcal{T}^{(q)}\alpha = \alpha e^{-2\pi i/q} \quad \text{implies transformation } \varepsilon_{[n]} \to \varepsilon_{[n+1]}.
\]
In other words, the asymptotically dominant part of the effect of the rotation $\mathcal{T}^{(q)}$ will just cause the change of the subscript (or, if you wish, of the phase) of the individual complex roots $\varepsilon_{[n]}$. 
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