PHYSICAL REVIEW D **80,** 105004 (2009)

Fundamental length in quantum theories with $\mathcal{PT}$-symmetric Hamiltonians. II. The case of quantum graphs

Miloslav Znojil*

Nuclear Physics Institute ASCR, 250 68 Řež, Czech Republic

(Received 11 September 2009; published 6 November 2009)

$\mathcal{PT}$-symmetrization of quantum graphs is proposed as an innovation where an adjustable, tunable nonlocality is admitted. The proposal generalizes the $\mathcal{PT}$-symmetric square-well models of Ref. [M. Znojil, Phys. Rev. D **80**, 045022 (2009).] (with real spectrum and with a variable fundamental length θ) which are reclassified as the most elementary quantum q-pointed-star graphs with minimal $q = 2$. Their equilateral $q = 3, 4, \ldots$ generalizations are considered, with interactions attached to the vertices. Runge-Kutta discretization of coordinates simplifies the quantitative analysis by reducing our graphs to star-shaped lattices of $N = qK + 1$ points. The resulting bound-state spectra are found real in an N-independent interval of couplings $\lambda \in (-1, 1)$. Inside this interval the set of closed-form metrics $\Theta_j^{(N)}(\lambda)$ is constructed, defining independent eligible local (at $j = 0$) or increasingly nonlocal (at $j = 1, 2, \ldots$) inner products in the respective physical Hilbert spaces of states $\mathcal{H}_j^{(N)}(\lambda)$. In this way each graph is assigned a menu of nonequivalent, optional probabilistic quantum interpretations.

DOI: 10.1103/PhysRevD.80.105004 PACS numbers: 03.65.−w, 11.10.Lm, 03.65.Ca, 03.65.Db

I. INTRODUCTION

Many nontrivial quantum systems are described via a simplified effective model. Vibrational excitations of fields, nuclei or molecules may often be represented, for example, by artificial models where a single real or virtual (quasi)particle moves along a suitable one-dimensional trajectory, finite or infinite. In paper I [1] we even analyzed a family of models where this trajectory has further been replaced, in the so called Runge-Kutta approximation, by a finite lattice of points.

Specific difficulties may survive even after a drastic reduction of the number of degrees of freedom. Typically, a quasi-one-dimensional narrow-tube trajectory may happen to be curved (causing the emergence of bound states [2]) or twisted (returning these bound states to the free-motion continuum again [3]). Other pathologies may emerge when the (quasi)particle moves along a topologically nontrivial waveguide. In the simplest thin-tube realization of the latter scenario one speaks, in general, about the motion of a quantum (quasi)particle along a *graph*, i.e., along a system of one-dimensional free-motion trajectories (called ''edges'' of the graph) connected at the so called ''vertices'' of the graph (various nontrivial interactions could be admitted at these points).

A purely phenomenological motivation of interest in quantum graphs has originally emerged in quantum chemistry where the edges were identified with the bonds between atoms in a larger organic molecule along which the electrons might move almost freely [4]. Soon, a more abstract appeal of quantum graphs prevailed offering a nontrivial quantitative picture of quantum dynamics in many arrangements ranging from the Y-shaped tree up to fractal trajectories [5]. The recent proceedings [6] can be cited as a source of updated information about the current state of the art. More than 700 pages of predominantly mathematically oriented reviews still incorporate a few physics-centered summaries of potentially appealing phenomenological consequences and applications of the theory. *Pars pro toto* we could point out Refs. [7,8]) putting more emphasis on physics and listing many related references. Today, the use of quantum graphs ranges from the analysis of photonic crystals up to the studies of thin wires and waveguides and other mesoscopic devices produced by sophisticated nanotechnologies. On theoretical level quantum graphs are increasingly popular as formal structures testing field theory [9] or describing certain important phenomena in solid-state physics [10]. Multiple concrete models serve as a laboratory of our understanding of systems with constraints [11]. Last but not least one finds quantum graphs used as benchmark systems in quantum chaos [12] and/or random walks [13].

The incessant transfer of the quantum-graph idea from its original, purely descriptive role to a more abstract theoretical framework may be expected to continue. An illustration of the emergence of new tendencies in this field may be seen, e.g., in the *complexified*, non-Hermitian boundary-supported interactions as studied, in the context of fully realistic three-dimensional lattice models, in Ref. [14]. These tendencies grew from origins which may be traced back to a few papers by Hatano and Nelson [15] and by Feinberg and Zee [16] as well as to a number of more recent studies rooted not only in solid-state physics [10] but also, say, in nuclear physics [17], field theory [18] or cosmology [19]. An intensification of interest in all of these non-Hermitian quantum systems with real spectra occurred, in particular, after the publication of influential letter [20] where the very special form of

*znojil@ujf.cas.cz

non-Hermiticity called $\mathcal{PT}$-symmetry of Hamiltonians (which is to be explained below) has been promoted as an unexpectedly productive heuristic principle. It found many concrete applications reported, e.g., in proceedings of several dedicated conferences [21]. Virtually all of these studies may be characterized as a search for a new point of optimal balance between the mathematical requirements of simplicity (and, in particular, of constructive tractability of physical models) and the natural requirements of dynamical and phenomenological relevance of new models. For illustration let us mention just the recent proposals of the tests of quantum brachistochrones (where the recent Refs. [22] summarizes the existing theoretical proposals) or of measurements over certain anomalous scattering systems [23]. The quickly developing discussion of possible measurable effects involving $\mathcal{PT}$-symmetric systems in quantum optics [24] (and, perhaps, in quantum gravity etc [25]) must also certainly be mentioned here.

The emergence of all of these new theoretical ideas motivated also our present work. Their multisided applicability persuaded us not only about an undeniable phenomenological appeal and relevance of non-Hermitian interaction models but also about the promising tractability and feasibility of many of their computational and constructive aspects. In what follows we shall propose and study, therefore, a few schematic though still nontrivial quantum-graph models based on a non-Hermitian form of interaction supported, as usual, just by certain vertices of the given graph.

The text will start from a concise outline of the inspiration and origins incorporating simple square-well models reviewed in Sec. II and their elementary Hermitian star-shaped discrete quantum-graph generalizations proposed in Sec. III. The key ideas of our present innovations will be then listed in Sec. IV followed by Sec. V where the main necessary property of our quantum-graph models, viz., the reality of their spectra will be demonstrated. Section VI will then be devoted to the presentation and explanation of the core of our message, viz., to the description of a few first nontrivial examples of nonlocal $\mathcal{PT}$-symmetric quantum graphs. Finally, our concluding remarks will be collected in Sec. VII.

II. SQUARE-WELL SCHRÖDINGER EQUATIONS

A. Runge-Kutta discretization

Let us start our considerations from the most common ordinary differential Schrödinger equation for bound states in a square well,

$$-\frac{d^2}{d\xi^2}\psi(\xi) = E\psi(\xi), \qquad \psi(\pm L) = 0 \tag{1}$$

and review a few results obtained for various modifications and perturbations of this model in the recent literature. First, let us mention the study [26] where the addition of a "sufficiently small" potential $V(\xi)$ has been shown to leave the spectrum real (i.e., in principle, observable) *irrespectively* of the detailed form of function $V(\xi)$ which can even be allowed *complex*. This result can be perceived as one of the most persuasive rigorous mathematical confirmations of the Bender's and Boettcher's conjecture [20] that in applied Quantum Mechanics there exists a broad class of complex potentials supporting *real* spectra of bound-state energies.

Bender *et al.* [27] noticed and emphasized that many Hamiltonians $H = p^2 + V(\xi) \neq H^\dagger$ can be characterized by their $\mathcal{PT}$-symmetry, i.e., by the property $H\mathcal{PT} = \mathcal{PT}H$ with parity $\mathcal{P}$ and with time reversal $\mathcal{T}$ mimicked by Hermitian conjugation [28]. Bound states in a few solvable $\mathcal{PT}$-symmetric piecewise-constant potentials were studied in Refs. [29]. The correct probabilistic interpretation of some of these potentials found its first constructive formulation in Ref. [30]. In parallel, an efficient simplification of the underlying mathematics via Runge-Kutta (RK) discretization of coordinates has been proposed in Refs. [31]. It was based on the replacement of the interval of $\xi \in (-L, L)$ by its discrete version

$$\xi_k = kh, \qquad k = 0, \pm 1, \ldots, \pm K, \qquad h > 0, \tag{2}$$

i.e., by the discrete lattice of points

$$\boxed{\xi_{-K}}\ \xi_{-K+1}\ \cdots\ \xi_{-2}\ \xi_{-1}\ \boxed{\boxed{\xi_0}}\ \xi_1\ \xi_2\ \cdots\ \xi_{K-1}\ \boxed{\xi_K}\ . \tag{3}$$

In this perspective one has to replace differential Eq. (1) by its discrete analogue or approximation

$$-\frac{\psi(\xi_{k-1}) - 2\psi(\xi_k) + \psi(\xi_{k+1})}{h^2} = E\psi(\xi_k). \tag{4}$$

A clear insight in the formal structure of the square-well eigenvalue problem is achieved. With $-K \leq k \leq K$ and $\psi(\xi_{\pm(K+1)}) = 0$ our difference Schrödinger Eq. (4) reads

$$\begin{bmatrix} 2 & -1 & 0 & \ldots & & \ldots & 0 \\ -1 & 2 & -1 & 0 & \ldots & \ldots & 0 \\ 0 & -1 & 2 & -1 & \ddots & & \vdots \\ \vdots & \ddots & \ddots & \ddots & \ddots & 0 & 0 \\ & & & -1 & 2 & -1 & 0 \\ \vdots & & & \ddots & -1 & 2 & -1 \\ 0 & \ldots & & \ldots & 0 & -1 & 2 \end{bmatrix} \begin{bmatrix} \psi(\xi_{-K}) \\ \psi(\xi_{-K+1}) \\ \psi(\xi_{-K+2}) \\ \vdots \\ \psi(\xi_{K-1}) \\ \psi(\xi_K) \end{bmatrix} = E \begin{bmatrix} \psi(\xi_{-K}) \\ \psi(\xi_{-K+1}) \\ \psi(\xi_{-K+2}) \\ \vdots \\ \psi(\xi_{K-1}) \\ \psi(\xi_K) \end{bmatrix} \tag{5}$$

i.e., it acquires the transparent matrix-diagonalization form.

B. Equivalence to a linear discrete quantum graph

Let us renumber the linear array (3) of $N = 2K + 1$ points in a slightly unusual manner which emphasizes its left-right symmetry,

$$\boxed{x_{2K-1}}\ x_{2K-3}\ \ldots\ x_3\ x_1\ \boxed{\boxed{x_0}}\ x_2\ x_4\ \ldots\ x_{2K-2}\ \boxed{x_{2K}}\ . \tag{6}$$

Our Schrödinger Eq. (5) becomes rearranged,

$$\begin{bmatrix} 2 & -1 & -1 & 0 & 0 & \ldots & 0 \\ -1 & 2 & 0 & -1 & 0 & \ddots & \vdots \\ -1 & 0 & 2 & 0 & \ddots & \ddots & \vdots \\ 0 & -1 & 0 & \ddots & \ddots & -1 & 0 \\ \vdots & \ddots & \ddots & \ddots & 2 & 0 & -1 \\ 0 & \ldots & \ddots & -1 & 0 & 2 & 0 \\ 0 & \ldots & \ldots & 0 & -1 & 0 & 2 \end{bmatrix} \begin{bmatrix} \psi(x_0) \\ \psi(x_1) \\ \psi(x_2) \\ \vdots \\ \psi(x_{2K-1}) \\ \psi(x_{2K}) \end{bmatrix} = E \begin{bmatrix} \psi(x_0) \\ \psi(x_1) \\ \psi(x_2) \\ \vdots \\ \psi(x_{2K-1}) \\ \psi(x_{2K}) \end{bmatrix}. \tag{7}$$

It may be perceived as describing a system which lives on the linear (one could also call it V-shaped) graph which consists of two wedges connected in the origin.

The N-dimensional Hamiltonian with $N = 2K + 1$ as it appears in Eq. (7) has a block-tridiagonal partitioned matrix structure

$$H^{(N)} = \begin{bmatrix} u & \vec{v} & \vec{0} & \cdots & \cdots & \vec{0} \\ \vec{v}^T & 2I & -I & 0 & \ldots & 0 \\ \vec{0}^T & -I & \ddots & \ddots & \ddots & \vdots \\ \vec{0}^T & 0 & \ddots & 2I & -I & 0 \\ \vdots & \vdots & \ddots & -I & 2I & -I \\ \vec{0}^T & 0 & \cdots & 0 & -I & 2I \end{bmatrix} \tag{8}$$

with $\vec{v} = (-1, -1)$ and $\vec{0} = (0, 0)$ being two-dimensional row vectors while $u = 2$ is a number. The rest of the matrix is composed of two-dimensional unit matrices I and null-matrices 0. In the light of what has been written in Introduction the naive, discrete quantum square-well problem may be reinterpreted as one of the simplest quantum graphs, therefore.

III. STAR-SHAPED DISCRETE QUANTUM GRAPHS

The example of preceding section may be complemented by a series of its generalizations living on q-pointed star graphs with $q = 3, 4, \ldots$. In this new context the trivial example (6) + (7) indicates how this generalization can be "translated" back into the language of difference or matrix Schrödinger equations. Let us now complement this idea by a few concrete examples of its implementation.

A. Y-shaped model: $q = 3$

The simplest nontrivial discrete realization of a graph with $q = 3$ may be visualized as an Y-shaped (or, if you wish, T-shaped) N-point lattice composed of three equally long branches whose individual points will be numbered as follows,

$$\boxed{x_{N-2}}\ x_{N-5}\ \ldots\ x_5\ x_2\ \boxed{\boxed{x_0}}\ x_3\ x_6\ \ldots\ x_{N-4}\ \boxed{x_{N-1}}$$
$$x_1$$
$$x_4$$
$$\vdots \tag{9}$$
$$x_{N-6}$$
$$\boxed{x_{N-3}}$$

This lattice connects the three (framed) endpoints with the central (doubly framed) junction at x_0. The simplest version of a quantum system living on this graph may/will employ again the RK discretization of the kinetic energy [i.e., of the second derivative operator, cf. Eq. (4)]. The only exception is encountered at x_0 where our choice of an acceptable matching is more flexible (see Ref. [32]). For the sake of simplicity we shall postulate

$$-\frac{\psi(x_1)+\psi(x_2)+\cdots+\psi(x_q)-u\psi(x_0)}{h^2}=E\psi(x_0) \tag{10}$$

with a free parameter $u=u(q)$ set equal, say, to 3 at $q=3$. In the bound-state arrangement this matching condition in the origin must be complemented by the three "asymptotic" Dirichlet boundary conditions imposed at the remote ends of the edges. The bound-state energies will then coincide with the eigenvalues of the real and symmetric $(3K+1)$-dimensional matrix Hamiltonian with partitioned structure shown in Eq. (8). Wave functions will be specified by Schrödinger equation

$$\begin{bmatrix} 3 & -1 & -1 & -1 & 0 & \ldots & 0 \\ -1 & 2 & 0 & 0 & -1 & \ddots & \vdots \\ -1 & 0 & 2 & 0 & 0 & \ddots & 0 \\ -1 & 0 & 0 & \ddots & \ddots & \ddots & -1 \\ 0 & -1 & 0 & \ddots & 2 & 0 & 0 \\ \vdots & \ddots & \ddots & \ddots & 0 & 2 & 0 \\ 0 & \ldots & 0 & -1 & 0 & 0 & 2 \end{bmatrix} \begin{bmatrix} \psi(x_0) \\ \psi(x_1) \\ \psi(x_2) \\ \psi(x_3) \\ \vdots \\ \psi(x_{N-2}) \\ \psi(x_{N-1}) \end{bmatrix} = E \begin{bmatrix} \psi(x_0) \\ \psi(x_1) \\ \psi(x_2) \\ \psi(x_3) \\ \vdots \\ \psi(x_{N-2}) \\ \psi(x_{N-1}) \end{bmatrix}. \tag{11}$$

From the symmetry (i.e., Hermiticity) of the Hamiltonian one deduces that at any integer K the spectrum is real though not necessarily nondegenerate. At $N=4$, for example, we get $E^{(4)}_{2,3}=2$ while $E^{(4)}_{1,4}=5/2\mp\sqrt{13}/2$.

B. X-shaped model and its star-shaped descendants with $q \geq 4$

At $q=4$ the lattice-points should be numbered in the same manner as above,

$$\boxed{x_{N-2}}$$
$$x_{N-6}$$
$$\vdots$$
$$x_3$$
$$\boxed{x_{N-3}}\ x_{N-7}\ \ldots\ x_6\ x_2\ \boxed{\boxed{x_0}}\ x_4\ x_8\ \ldots\ x_{N-5}\ \boxed{x_{N-1}} \tag{12}$$
$$x_1$$
$$\vdots$$
$$x_{N-8}$$
$$\boxed{x_{N-4}}$$

The extension of this pattern to any positive integer q is obvious. In the corresponding Hamiltonian (8) we may keep the RK-discretization-related scalar parameter $u = u(q)$ variable or equal to its "maximum" $u(q) = q$ tractable as natural after embedding of our graph into a sufficiently high-dimensional space. We may add that at any u the degeneracy of the spectrum will grow with q. For illustration we may use the model with the smallest dimensions $N = N(q) = q + 1$ where the energy eigenvalue $E = 2$ proves $(q - 1)$-times degenerate. This is easily seen from Eq. (11) and/or from its $q > 3$ generalizations once we put there, tentatively, $\psi(x_0) = 0$. The whole set of equations then degenerates to the single constraint $\sum_{j=1}^{q} \psi(x_j) = u - 2$ with $q - 1$ linearly independent eigenvector solutions.

At the two remaining unknown energies $E = E_{1,q+1} \neq 2$ we may normalize $\psi(x_0) = 1$ and eliminate $\psi(x_j) = 1/(2 - E)$ at all $j > 0$. We arrive at the elementary Bethe-ansatz-type quadratic secular equation $q/(2 - E) = u - E$ giving the two missing roots in closed form,

$$2E_{1,q+1} = 2 + u \mp \sqrt{(2 - u)^2 + 4q}. \tag{13}$$

This is the first nontrivial q-star-graph-spectrum formula which is, of course, compatible with its above-mentioned special case computed at $u(q) = 3$ for $q = 3$.

IV. INNOVATION: TWO CHANGES OF PERSPECTIVE

The message delivered by the examples presented in preceding sections can be summarized as a recommendation that the current discrete square-well eigenvalue problem with $q = 2$ can easily be generalized to its q-pointed-star analogues with any integer $q \geq 2$. Formally these models may be characterized by the N-dimensional partitioned Hamiltonian matrices $H^{(N)}$ of Eq. (8) where we set $N = qK + 1$ and use q-dimensional row vectors $\vec{v} = (-1, -1, \ldots, -1)$ and $\vec{0} = (0, 0, \ldots, 0)$ and q-dimensional unit matrices and null-matrices I and 0, respectively. Of course, nothing really new emerges in such an elementary constructive project which requires just a routine application of the well known principles of quantum mechanics.

The situation becomes much more exciting when the purely kinetic nature of the Hamiltonian of a quantum graph is enriched by an interaction added, preferably, at the vertices. For us, this option opened a way toward two generalizations which will be described in what follows. In essence, they will be based on the thorough change

(i) of the naively Hermitian nature of the interactions (we shall advocate here the transition from the usual real and symmetric interaction matrices $H^{(\mathrm{int})}$ to their asymmetric alternatives preserving the reality of the spectrum, cf. paragraph IV A below),

(ii) of the naively realistic assumption of the strict locality of the models (this will represent a further development of the idea proposed in Ref. [1] and briefly recalled in paragraph IV B below).

A. $\mathcal{PT}$-symmetric interactions at vertices

One of the purposes of our present text is to enrich the picture of dynamics of bound states living on quantum graphs via an introduction of certain nontrivial interactions at their vertices. In a broader physical context this is the project inspired not only by Ref. [1] (on bound states) but also by some of our other papers (dealing with scattering). In the language of mathematics, the formal connections between these two physical scenarios are quite close, especially in the RK discretized models. Thus, although there is no space here for a deeper study of the scattering on the $\mathcal{PT}$-symmetric graphs, we find it meaningful to mention, briefly, at least some of the possible parallels.

1. A brief detour to scattering models

In our few recent papers on scattering [33–36] the introduction of certain elementary nearest-neighbor $\mathcal{PT}$-symmetric interactions between RK lattice points proved fruitful as a very useful and productive model-building principle. Unfortunately, there exist several obstacles for making the analogy between the bound- and scattering-state one-dimensional RK-based models sufficiently close. Firstly, one must keep in mind that in the scattering scenario the number N of the RK lattice points must be kept very large or infinite. Secondly, the very essence of the arrangement of the scattering experiments requires that the interactions themselves should preferably be localized very close to the origin [33,37]. In contrast, the bound-state arrangement of Schrödinger equations seems to prefer the transfer of the support of interactions to the remote ends of the interval of coordinates. In such a case, perceivable technical simplifications were reported not only in the one-dimensional continuous-coordinate square-well models (cf. Refs. [38]) but also in the realistic three-dimensional discrete-lattice calculations (cf. Ref. [14]).

This being said, a note on some lattice-based models of scattering may still prove approprate. Firstly we could classify them more easily in our present graph-based language. The presence of a nearest-neighbor coupling will be indicated by the insertion of symbol $\diamond$ between the corresponding two lattice points. In the scattering-inspired arrangement these points are usually chosen as lying not too far from the origin. In the first step the following modification is obtained of the discrete graph of Eq. (6),

$$\boxed{x_{2K-1}}\ x_{2K-3}\ \ldots\ x_3\ x_1\ \diamondsuit\ \boxed{\boxed{x_0}}\ x_2\ x_4\ \ldots\ x_{2K-2}\ \boxed{x_{2K}}\ . \tag{14}$$

For illustration of a quantum system living on this graph let us recall the interaction matrix of Ref. [33],

$$H^{(\mathrm{int})} = \begin{bmatrix} 0 & g & 0 & \ldots \\ -g & 0 & \ldots & \\ 0 & \ldots & & \\ \vdots & \ddots & & \end{bmatrix}. \tag{15}$$

This real and antisymmetric (i.e., $\mathcal{PT}$-symmetric [33]) matrix has to be added to the purely kinematic discrete square-well Hamiltonian (8). Unfortunately, some of the predictions of this oversimplified model are unphysical [39]. In subsequent Ref. [34] another version of $\mathcal{PT}$-symmetric interaction has been proposed, therefore. It employed the fully symmetrized localization of the nearest-neighbor interactions in the RK graph,

$$\boxed{x_{2K-1}}\ x_{2K-3}\ \ldots\ x_3\ x_1\ \diamondsuit\ \boxed{\boxed{x_0}}\ \diamondsuit\ x_2\ x_4\ \ldots\ x_{2K-2}\ \boxed{x_{2K}} \tag{16}$$

leading to the amended interaction matrix

$$H^{(\mathrm{int})} = \begin{bmatrix} 0 & g & g & 0 & \ldots \\ -g & 0 & \ldots & & \\ -g & 0 & \ldots & & \\ 0 & \ldots & \ddots & & \\ \vdots & \ddots & & & \end{bmatrix}. \tag{17}$$

In Refs. [34,36] we further shifted the diamonds $\diamondsuit$ (representing the localization of interactions) by one step in the lattice and arrived at the next graph

$$\boxed{x_{2L-1}}\ x_{2L-3}\ \ldots\ x_3\ \diamondsuit\ x_1\ \boxed{\boxed{x_0}}\ x_2\ \diamondsuit\ x_4\ \ldots\ x_{2L-2}\ \boxed{x_{2L}} \tag{18}$$

yielding the next eligible interaction matrix

$$H^{(\mathrm{int})} = \begin{bmatrix} 0 & 0 & 0 & 0 & \ldots & & \\ 0 & 0 & 0 & g & 0 & \ldots & \\ 0 & 0 & 0 & 0 & g & 0 & \ldots \\ 0 & -g & 0 & 0 & 0 & 0 & \ldots \\ 0 & 0 & -g & 0 & 0 & 0 & \ldots \\ 0 & 0 & 0 & 0 & 0 & 0 & \ddots \\ \vdots & \vdots & \vdots & \vdots & \vdots & \ddots & \ddots \end{bmatrix}. \tag{19}$$

A general pattern emerges clearly. The whole class of interactions can be realized via four nonvanishing matrix elements which are not necessarily located just in the closest vicinity of the origin. This quadruplet of off-diagonal matrix elements is allowed to move away from the origin forming a series of descendants of Eq. (19).

The main benefit of this series of models defined on RK lattices is threefold. Firstly, their study opens the way toward the *unitary* scattering systems described by the sufficiently elementary $\mathcal{PT}$-symmetric Hamiltonians [33]. Secondly, the physical predictions (i.e., the reflection and transmission coefficients) retain the form of closed formulas [34]. Thirdly, these models of scattering may find generalizations living on some suitable classes of nontrivial quantum graphs in the nearest future.

2. $\mathcal{PT}$-symmetric bound-state models with $q = 2$

In contrast to the scattering scenario where, typically, the matrix in Eq. (19) is infinite-dimensional, the RK version of the bound-state problem may always be considered finite-dimensional. Then, the repeatedly shifted symbol $\diamondsuit$ of the interaction must ultimately reach the ends of the V-shaped graph,

$$\boxed{x_{2L-1}} \diamondsuit x_{2L-3} \ \cdots \ x_3 \ x_1 \ \boxed{\boxed{x_0}} \ x_2 \ x_4 \ \cdots \ x_{2L-2} \diamondsuit \boxed{x_{2L}} \ . \tag{20}$$

The related exceptional Hamiltonian matrix represents the modified square well with a nontrivial $\mathcal{PT}$-symmetric interaction which is localized solely in the closest vicinity of the external vertices. The related quantum Hamiltonian acquires the partitioned $(K+1)$-dimensional tridiagonal form

$$H = H^{(N)}(\lambda) = \begin{bmatrix} u & \vec{v}^T & 0 & \cdots & \cdots & 0 \\ \vec{v} & 2I & -I & \ddots & \ddots & \vdots \\ 0 & -I & \ddots & \ddots & \ddots & 0 \\ \vdots & \ddots & \ddots & 2I & -I & 0 \\ \vdots & & \ddots & -I & 2I & c(\lambda) \\ 0 & \cdots & \cdots & 0 & c(-\lambda) & 2I \end{bmatrix} \tag{21}$$

i.e., at $q = 2$,

$$H = \left[\begin{array}{ccc|cc|ccccc} 2 & -1 & -1 & 0 & 0 & 0 & & \cdots & & 0 \\ \hline -1 & 2 & 0 & -1 & 0 & 0 & \cdots & & \cdots & 0 \\ -1 & 0 & 2 & 0 & -1 & \ddots & \ddots & & & \vdots \\ \hline 0 & -1 & 0 & 2 & 0 & \cdots & & & \ddots & \vdots \\ \vdots & \ddots & -1 & \ddots & \ddots & \ddots & \ddots & & & \\ \hline & \vdots & & \vdots & \cdots & & & 2 & -1+\lambda & 0 \\ \vdots & & & & \ddots & -1-\lambda & 0 & & 2 & 0 \\ 0 & 0 & \cdots & & \cdots & 0 & -1-\lambda & & 0 & 2 \end{array}\right] .$$

The rightmost lowest corner carries all the dependence of the Hamiltonian on the coupling (note that we changed its symbol from g to λ). This parallels the preferences recommended in Refs. [38] or [14].

B. Introduction of nonlocality via inner products

Whenever we declare a matrix [e.g., our Hamiltonian (21) considered in the RK coordinate representation] manifestly non-Hermitian, we almost always have in mind just the non-Hermiticity in the current ℓ_2-representation of the Hilbert space. This space may be denoted by the symbol $\mathcal{H}^{(F)}$ where the superscript stands for the "first" or "friendly" space (cf. also [40]). In this space the usual formula

$$\sum_{k=0}^{N-1} \psi_1^*(x_k)\psi_2(x_k) := \langle \psi_1 | \psi_2 \rangle \tag{22}$$

defines the inner product between any pair of its elements (i.e., finite- or infinite-dimensional vectors) ψ_1 and ψ_2. In this setting the authors of Ref. [17] noticed and emphasized that *the same* Hamiltonian may appear to be Hermitian in another Hilbert spaces $\mathcal{H}^{(S)}$ where our choice of the superscript stands for the "second" or "subtle" space and where *the same* set of vectors is merely assigned the following *different*, non-ℓ_2 inner product using a suitable nontrivial "metric" $\Theta \neq I$,

$$\sum_{j=0}^{N-1}\sum_{k=0}^{N-1} \psi_1^*(x_j)\Theta(x_j,x_k)\psi_2(x_k) = \langle \psi_1 | \Theta | \psi_2 \rangle := \langle\langle \psi_1 | \psi_2 \rangle\rangle. \tag{23}$$

One can always make use of this flexibility of basic definitions, keeping only in mind that the standard probabilistic interpretation can *solely* be assigned to a Hamiltonian which is Hermitian (in whatever Hilbert space). In this

sense the models described by asymmetric real Hamiltonian matrices with real spectra *do not* leave the territory of the standard formalism of quantum theory.

Although the latter idea has thoroughly been explained by several authors [17,41–43], some of its key aspects and consequences may be summarized in two brief sentences. Firstly, we must assume that the spectrum of our Hamiltonians $H = H(\lambda)$ remains real in some nonempty interval of the measures of their asymmetry λ. In the second step we have to introduce an invertible operator Ω which maps our ℓ_2 Hilbert space $\mathcal{H}^{(F)}$ onto another, unitarily nonequivalent "physical" ℓ_2 Hilbert space $\mathcal{H}^{(P)}$ which is expected unitarily equivalent to the subtle physical space $\mathcal{H}^{(S)}$ endowed with nontrivial metric and product (23).

More thoroughly, both these steps will be explained in Sec. IV B 1. Now let us only add that their practical appeal has been well illustrated in nuclear physics where $\mathcal{H}^{(P)}$ represented the textbook Hilbert space of nucleons (i.e., fermions) while both the auxiliary Hilbert spaces $\mathcal{H}^{(F,S)}$ were identified with the spaces of certain artificial, effective "interacting bosons" (cf. Ref. [17] for more details).

In Ref. [1] we also worked with the triplet of spaces $\mathcal{H}^{(F,S,P)}$ and emphasized there the deep technical *nontriviality* of the construction of the necessary metric operator $\Theta = \Theta(H)$ in terms of which our asymmetric, non-Hermitian real-matrix representations of the Hamiltonians were made Hermitian with respect to the *ad hoc* inner product (23). In particular, as long as we worked in coordinate representation, we made distinction between the models which were *local* (i.e., where $\Theta = \Theta_0(H) \neq I$ remained represented by a diagonal matrix) and *nonlocal*, i.e., characterized by the nondiagonal metrics $\Theta_1(H), \Theta_2(H), \ldots$. Moreover, the most unexpected property of the oversimplified models as studied in Ref. [1] has been revealed in the fact that, via a suitable renumbering, one could achieve that the j-th metric $\Theta_j(H)$ was represented by a very special $(2j+1)$-diagonal matrix.

In our present paper we intend to demonstrate that these results may be extended to a broad family of quantum graphs.

1. A return to (hidden) Hermiticity of observables

In the formalism described in Ref. [17] the simple but non-Hermitian Hamiltonian matrix $H \neq H^\dagger$ defined in $\mathcal{H}^{(F)}$ has been put in correspondence with its idealized isospectral partner $\mathfrak{h} = \mathfrak{h}^{(N)}(\lambda)$. The latter operator is defined in $\mathcal{H}^{(P)}$ and it may be assumed complicated. The correspondence is realized by the Dyson map,

$$\Omega\colon H \to \mathfrak{h} = \Omega H \Omega^{-1} \tag{24}$$

which is, by definition, nonunitary, $\Omega = \Omega^{(N)}(\lambda) \neq (1/\Omega)^\dagger$. Thus, we are allowed to require the Hermiticity of the isospectral partner Hamiltonian,

$$\mathfrak{h}^{(N)}(\lambda) = \Omega(\lambda) H^{(N)}(\lambda) \Omega^{-1}(\lambda) = [\mathfrak{h}^{(N)}]^\dagger(\lambda). \tag{25}$$

The latter relation can be reread as a constraint imposed upon the simpler operator $H = H^{(N)}(\lambda)$ itself,

$$\Omega H^{(N)} \Omega^{-1} = [\Omega H^{(N)} \Omega^{-1}]^\dagger = [\Omega^{-1}]^\dagger [H^{(N)}]^\dagger \Omega^\dagger.$$

In the rearranged and abbreviated form this relation coincides with the condition of a hidden Hermiticity or "quasi-Hermiticity" [17,44] of $H^{(N)}(\lambda)$,

$$[H^{(N)}]^\dagger = \Theta H^{(N)} \Theta^{-1}, \qquad \Theta = \Omega^\dagger \Omega > 0. \tag{26}$$

The closest correspondence between metric Θ of Eq. (23) and the Dyson-map Ω is established in this manner.

2. The reconstruction of the ad hoc metric $\Theta = \Theta(H)$

In any $\mathcal{PT}$-symmetric quantum model, i.e., for Hamiltonians with the property $H^\dagger = \mathcal{P} H \mathcal{P}^{-1}$ (*and* with the real spectrum) the correct physical probabilistic interpretation of bound states must be based on the reconstruction of the metric in $\mathcal{H}^{(S)}$. The matrix elements of this metric may be made available as a solution of the linear algebraic system of Eqs. (26),

$$\sum_{k=1}^{N} [(H^\dagger)_{jk} \Theta_{kn} - \Theta_{jk} H_{kn}] = 0, \qquad j, n = 1, 2, \ldots, N. \tag{27}$$

Needless to repeat that the resulting metrics are Hamiltonian-dependent and by far not unique in general, $\Theta = \Theta_j(H)$, $j = 0, 1, \ldots$. Each of them defines a new, independent Hermitian conjugation and, hence, a respective independent N-dimensional physical Hilbert space $\mathcal{H}^{(S)} \equiv \mathcal{H}_j^{(N)}$. The knowledge of the metric is substantial. The parallel availability of the factor Ω and of its conjugate $\Omega^\dagger$ remains less essential (though note their role in section V B 2 below). For this reason we shall pay our main attention here just to the constructive assignment of one or several alternative metrics $\Theta = \Theta_j^{(N)}(\lambda)$, $j = 0, 1, \ldots$ to a given, "prescribed" quantum-graph Hamiltonian $H = H^{(N)}(\lambda)$.

This project consists of fulfilling two separate subtasks. Firstly, we shall search for the metric in the form of a superposition

$$\Theta = \Theta^{(N)}_{\beta_0, \beta_1, \ldots} = \beta_0 \mathcal{P}_0^{(N)} + \beta_1 \mathcal{P}_1^{(N)} + \ldots \tag{28}$$

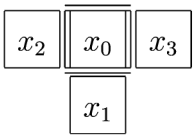
of some suitable Hermitian, sufficiently simple though not necessarily positive definite auxiliary components. Secondly, due attention must be paid to the positive definiteness of the metric (28) controlled by the appropriate choice of parameters β_j. In addition, all of the "pseudometrics" $\mathcal{P}_\mu^{(N)}$ will individually be assumed compatible with the Hermiticity condition (26),

$$\sum_{k=1}^{N}[(H^{\dagger})_{jk}(\mathcal{P}_{\mu}^{(N)})_{kn}-(\mathcal{P}_{\mu}^{(N)})_{jk}H_{kn}]=0, \qquad j,n=1,2,\ldots,N, \qquad \mu=0,1,\ldots. \tag{29}$$

In this manner our ansatz (28) will specify metrics Θ as superpositions of pseudometrics $\mathcal{P}=\mathcal{P}^{(N)}=\mathcal{P}_1^{(N)},\mathcal{P}_2^{(N)},\ldots$ which will be required to possess a sparse-matrix structure. At $q=2$ this idea has been shown productive in Ref. [1]. In our present paper we just extend this recipe to the $\mathcal{PT}$-symmetric quantum graphs with $q\geq 3$.

3. Nonlocal metrics: their sample construction at $N=4$

For quantum systems living on the smallest Y-shaped discrete graph



(30)

no space is left for the end point additional interactions since we do not wish that the matching point x_0 gets involved. Thus, our present $N=4$ Y-shaped quantum graph will remain purely kinematic. Its spectrum of energies will coincide with the eigenvalues of the four-dimensional matrix Hamiltonian

$$H^{(4)}(0)=\begin{bmatrix}3&-1&-1&-1\\-1&2&0&0\\-1&0&2&0\\-1&0&0&2\end{bmatrix}. \tag{31}$$

The latter particular matrix is real, symmetric (i.e., Hermitian) and positive definite. These properties (plus its natural commutativity with itself) make this matrix eligible as an admissible metric. Further metrics compatible with their implicit algebraic definition (26) can be sought as arbitrary polynomial functions of Hamiltonian (31),

$$\Theta^{(4)}=\Theta^{(4)}_{\{c_0,c_1,\ldots\}}=c_0I+c_1H^{(4)}(0)+c_2[H^{(4)}(0)]^2+\cdots. \tag{32}$$

The recipe is quick since the necessary explicit construction of the integer powers of the Hamiltonian is straightforward yielding

$$\Theta^{(4)}_{\{0,0,1,\ldots\}}=[H^{(4)}(0)]^2=\begin{bmatrix}12&-5&-5&-5\\-5&5&1&1\\-5&1&5&1\\-5&1&1&5\end{bmatrix} \tag{33}$$

etc. Unfortunately, the construction of metrics via Eq. (32) cannot be transferred to non-Hermitian matrices $H\neq H^{\dagger}$. Another unpleasant feature of the metrics sampled by Eq. (33) lies in their nonsparse, full-matrix form. For both of these reasons a return is recommended to the methods of paragraph IV B 2. Their results are universal—for example, metric Eq. (33) appears as a special case of formula (38) [cf. Sec. VI A below] at $a=12$, $b=-5$ and $f=j=k=1$.

V. THE PROOFS OF THE REALITY OF ENERGIES

At any integer number q the energy spectrum of our quantum graphs is partially degenerate at $\lambda=0$. This leaves the specification of a complete basis ambiguous. Another ambiguity emerges via the non-Dirac metrics $\Theta_j\neq I$, $j=0,1,\ldots$. We may construct several alternative, *nonequivalent* representations of the respective "correct" or "selected" Hilbert space of states $\mathcal{H}^{(N)}(\lambda)=\mathcal{H}_j^{(N)}(\lambda)$, $j=0,1,\ldots$. In the respective inner products (23) one encounters mutually nonequivalent metrics $\Theta_j^{(N)}(\lambda)$ sampled in paragraph IV B 3 above. The discovery of such a new freedom of making the choice between alternative inner products can be perceived as belonging to the most important recent achievements in quantum physics, with impact ranging from the new flexibility of the interacting boson models in nuclear physics [17] and from formulations of several new theoretical ideas in quantum mechanics [42] up to the emergence of the new classes of phenomenological Lagrangians in quantum field theory [41] where, e.g., the presence of ghosts can successfully be eliminated in some cases [45] and where even the concept of integrability acquired an updated meaning [43]. The use of the varying non-Dirac metrics $\Theta\neq I$ also opened the way toward new challenges connected, e.g., with the description of bound states in time-dependent systems [46] or in the relativistic kinematical regime [47]. In some phenomenological models of scattering the variability of Θ has been suggested as a guarantee of the causality and/or unitarity of the process [33,34,37,39].

In our present treatment of the ambiguity of $\Theta=\Theta_j$, $j=0,1,\ldots$ we shall be guided by the approach of paper [1]. We considered there the standard coordinate representation $\langle x|\Theta|x'\rangle$ of the metric operator and required that a suitable measure of its "nonlocality" [i.e., of its deviation from the Dirac's "local" delta function $\delta(x-x')$] should be identified with the postulate of the existence of fundamental length θ which characterizes the physical system in question. The same philosophy will also be accepted in our present text. We shall assume that the appeal of the concept of fundamental length survives the transition to the discrete-graph Hamiltonians of any dimension $N=qK+1$ with $K\geq 1$. We feel that partially nonlocal models with nonvanishing elementary lengths might find a very natural area of applicability in quantum graphs since the experimental waveguides and other nanotechnological realiza-

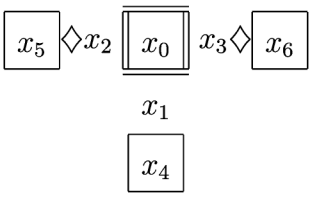
tions of quantum graphs almost certainly contain an uncertainty in the localization related to the degree of idealization of the real physical system in question [48]. In addition, the observability of the coordinate in a quantum graph may prove overridden by the transfer of emphasis to some other measured quantities (cf., e.g., the famous question ''Can one hear the shape of a graph?'' as asked in Refs. [49]).

A. Numerical proofs

We believe that even the oversimplified discrete quantum graphs with not too large q and/or N can offer a new source of entirely abstract elementary models with, say, an unusual or anomalous parameter-dependence of their spectra tractable by numerical techniques. Having this purely descriptive ambition in mind let us now study the first few $q = 3$ models in some detail, emphasizing that a key to all of the above-sampled applications of non-Dirac metrics $\Theta \neq I$ lies in the demonstration of the reality of the spectrum of the initial Hamiltonian H which is non-Hermitian, $H \neq H^\dagger$ in $\mathcal{H}^{(F)}$.

1. The Y-shaped discrete quantum graph with $N = 7$

The first nontrivial discrete $q = 3$ graph



(34)

leads to the seven-dimensional one-parametric family of Hamiltonians

$$H^{(7)} = \begin{bmatrix} 3 & -1 & -1 & -1 & 0 & 0 & 0 \\ -1 & 2 & 0 & 0 & -1 & 0 & 0 \\ -1 & 0 & 2 & 0 & 0 & -1+\lambda & 0 \\ -1 & 0 & 0 & 2 & 0 & 0 & -1-\lambda \\ 0 & -1 & 0 & 0 & 2 & 0 & 0 \\ 0 & 0 & -1-\lambda & 0 & 0 & 2 & 0 \\ 0 & 0 & 0 & -1+\lambda & 0 & 0 & 2 \end{bmatrix}. \tag{35}$$

They exhibit a particularly tight mutual interaction between the endpoints. The analysis of the energy spectrum pertaining to $H^{(7)}(\lambda)$ may rely on the construction of the secular polynomial which appears factorized into its quadratic and quintic component. Thus, two of the levels are prescribed by explicit formulas, $E_{2,5} = 2 \mp \sqrt{1-\lambda^2}$, while the remaining ones follow from the reduced secular equation,

$$E^5 - 11E^4 + (\lambda^2 + 43)E^3 - (7\lambda^2 + 72)E^2 + (14\lambda^2 + 48)E - 7\lambda^2 - 9 = 0.$$

This confirms that the energy levels of our seven-point Y-shaped quantum graph remain real in the interval of couplings $\lambda \in (-1, 1)$. Its endpoints coincide with the position of the Kato's ''exceptional points'', i.e., of the values at which the first merger and complexification of a pair of energies takes place.

The overall λ-dependence of energies is displayed in Fig. 1. We see there that the spectrum has four fragile (i.e., asymptotically complex) and three robust (i.e., never complexifying) components. This observation fits the pattern predicted by the generic tunable $\mathcal{PT}$-symmetric model of Ref. [50].

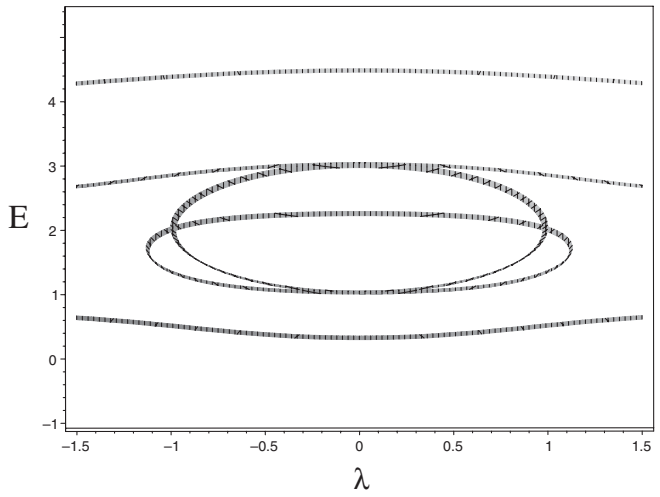
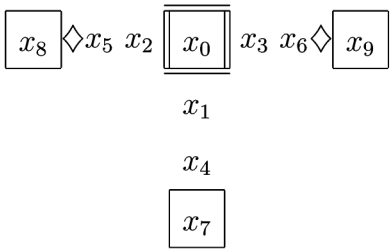


FIG. 1. The spectrum of $H^{(7)}(\lambda)$.

2. The next, $q = 3$ model with $N = 10$

On the ten-point graph-lattice



(36)

our Hamiltonian $H^{(10)}(\lambda)$ acquires the matrix form

$$\begin{bmatrix} 3 & -1 & -1 & -1 & 0 & 0 & 0 & 0 & 0 & 0 \\ -1 & 2 & 0 & 0 & -1 & 0 & 0 & 0 & 0 & 0 \\ -1 & 0 & 2 & 0 & 0 & -1 & 0 & 0 & 0 & 0 \\ -1 & 0 & 0 & 2 & 0 & 0 & -1 & 0 & 0 & 0 \\ 0 & -1 & 0 & 0 & 2 & 0 & 0 & -1 & 0 & 0 \\ 0 & 0 & -1 & 0 & 0 & 2 & 0 & 0 & -1+\lambda & 0 \\ 0 & 0 & 0 & -1 & 0 & 0 & 2 & 0 & 0 & -1-\lambda \\ 0 & 0 & 0 & 0 & -1 & 0 & 0 & 2 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & -1-\lambda & 0 & 0 & 2 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & -1+\lambda & 0 & 0 & 2 \end{bmatrix}.$$

The set of its eigenvalues comprises the constant and doubly degenerate doublet $E_{5,6} = 2$, the two explicit roots $E_{3,8} = 2 \pm \sqrt{2-\lambda^2}$ and the six implicit nodal zeros of the reduced secular polynomial

$$E^6 - 13E^5 + (\lambda^2 + 63)E^4 - (9\lambda^2 + 140)E^3 + (25\lambda^2 + 141)E^2 - (22\lambda^2 + 56)E + 5\lambda^2 + 6 = 0.$$

The λ-dependence of these energies is displayed in Fig. 2 where the thickness of the middle straight line emphasizes that the exceptional constant-energy level $E = 2$ is doubly degenerate.

B. Nonnumerical proof

The most straightforward rigorous proof of the reality of the energies [i.e., of the reality of the spectrum of Hamiltonian $H^{(N)}(\lambda)$] may proceed via the explicit constructive demonstration of existence of at least one metric $\Theta = \Theta(H) \neq I$ which makes this Hamiltonian Hermitian in $\mathcal{H}^{(S)}$.

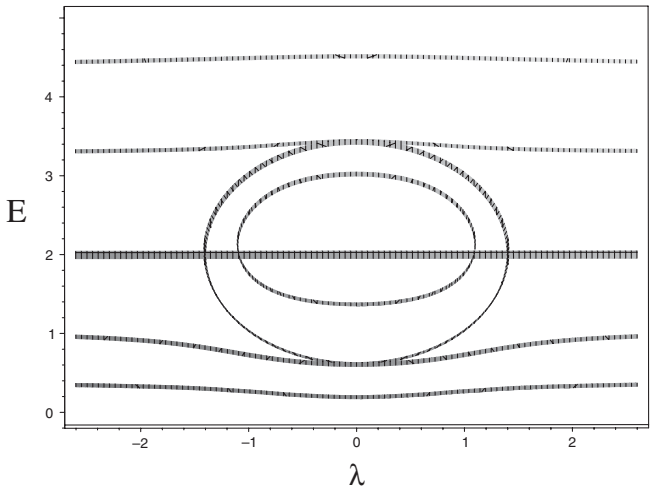


FIG. 2. The spectrum of $H^{(10)}(\lambda)$.

1. The local versions of the discrete quantum graphs

For our Y-shaped graphs the dimension $N = 3K + 1$ is finite so that we may search for special solution Θ_0 of Eq. (27) using a diagonal matrix ansatz and some computer-assisted symbolic manipulations. In this way we verified that at $N = 7$ the diagonal solution is positive definite and, up to an overall factor, unique,

$$\Theta^{(7)}_{(\text{diagonal})} = \begin{bmatrix} 1 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 1 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 1 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 1 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & \frac{1-\lambda}{1+\lambda} & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & \frac{1+\lambda}{1-\lambda} \end{bmatrix}.$$

At any $N = 3K + 1$ with $K = 3, 4, \ldots$ we then revealed that the verification of the absence of any nondiagonal elements in the difference $\Theta^{(7)}_{(\text{diagonal})} - I$ can be performed non-numerically. Finally, using the assumption of diagonality we reduced the matrix difference $H^\dagger\Theta - \Theta H$ in Eq. (27) to the mere pair of equations which specified the last two missing matrix elements in our ultimate solution compatible with Eq. (27) at any integer K,

$$\Theta^{(3K+1)}_{(\text{diagonal})} = \begin{bmatrix} 1 & 0 & 0 & \cdots & \cdots & 0 \\ 0 & 1 & 0 & \ddots & & \vdots \\ \vdots & \ddots & \ddots & \ddots & & \\ & & & 1 & \ddots & \vdots \\ \vdots & & & \ddots & \frac{1-\lambda}{1+\lambda} & 0 \\ 0 & \cdots & & \cdots & 0 & \frac{1+\lambda}{1-\lambda} \end{bmatrix}. \quad (37)$$

Obviously, this matrix is invertible, Hermitian and positive definite so that it may play the role of the metric inside the whole interval of couplings $\lambda \in (-1, 1)$. This confirms that our Hamiltonian $H^{(N)}(\lambda)$ becomes Hermitian in the *ad hoc* Hilbert space $\mathcal{H}^{(S)}$ where the diagonal metric (37) is employed. Thus, we may modify our notation, write $\Theta^{(3K+1)}_{(\text{diagonal})} = \Theta^{(N)}_0(\lambda)$ and $\mathcal{H}^{(S)} \equiv \mathcal{H}^{(N)}_0(\lambda)$ and reread

the latter statement as the rigorous proof of the reality of the energies for $\lambda \in (-1, 1)$.

2. Equivalent Hermitian Hamiltonians

Our constructive proof of existence of the (unique) diagonal metric $\Theta = \Theta_0^{(N)}(\lambda)$ given by Eq. (37) implies the survival of the observability of the RK coordinates in both our (unitarily equivalent) physical Hilbert spaces $\mathcal{H}^{(P)}$ and, in an amended notation, $\mathcal{H}^{(S)} \equiv \mathcal{H}_0^{(N)}(\lambda)$. As long as the diagonality of $\Theta_0^{(N)}(\lambda)$ is specified in coordinate representation, the usual multiplicative operator of coordinates remains Hermitian in the *same* Hilbert space $\mathcal{H}_0^{(N)}(\lambda)$ as the Hamiltonian $H^{(N)}(\lambda)$, indeed.

In such an exceptional case it makes sense to recollect the Dyson-mapping-related factorization $\Theta = \Omega^\dagger \Omega$ of our diagonal metric and to restrict our attention to the positive definite and diagonal operator factors $\Omega = \sqrt{\Theta}$. Their knowledge enables us to recall definition (25) and, for illustration, to evaluate the related Hermitian isospectral partner Hamiltonian $\mathfrak{h} = \mathfrak{h}^{(N)}(\lambda)$, say, at $N = 7$,

$$\mathfrak{h} = \begin{bmatrix} 3 & -1 & -1 & -1 & 0 & 0 & 0 \\ -1 & 2 & 0 & 0 & -1 & 0 & 0 \\ -1 & 0 & 2 & 0 & 0 & -\sqrt{1-\lambda^2} & 0 \\ -1 & 0 & 0 & 2 & 0 & 0 & -\sqrt{1-\lambda^2} \\ 0 & -1 & 0 & 0 & 2 & 0 & 0 \\ 0 & 0 & -\sqrt{1-\lambda^2} & 0 & 0 & 2 & 0 \\ 0 & 0 & 0 & -\sqrt{1-\lambda^2} & 0 & 0 & 2 \end{bmatrix}.$$

The block-tridiagonal generalization of this formula to all dimensions $N = 3K + 1$ is obvious.

VI. MANIFESTLY NON-LOCAL QUANTUM GRAPHS

Our general quantization recipe described in paragraph IV B admits the transition from the diagonal metric Θ_0 [exemplified by Eq. (37) at $q = 3$] to its arbitrary non-equivalent alternative (28). This means that in the spirit of trivial examples studied in Ref. [1] we are allowed to violate the locality also in all the other $\mathcal{PT}$-symmetric quantum graphs. Moreover, we can demand that the sequence of the not necessarily unique nondiagonal metrics $\Theta_1, \Theta_2 \ldots$ is partially ordered with respect to their increasing degree of nonlocality defined, in a way suggested in Ref. [1], as a suitable growing function $\theta = \theta_j$ of subscript j which is proportional, say, to the number of nonzero diagonals in the matrices or metrics Θ_j.

Expansion (28) of each individual Θ_j combines, in principle, several indefinite pseudometrics $\mathcal{P} = \mathcal{P}(H)$. In this sense, our main task is twofold: Firstly we have to find at least one solution of Eq. (29), the nonlocality of which saturates the number θ_j. Secondly we must guarantee the positivity of the resulting multiparametric sum Θ_j.

A. Sparse-matrix pseudometrics at $N = 4$

For our model (31) the brute-force solution of Eq. (27) leads to the following most general and exhaustive five-parametric formula for the (pseudo)metric,

$$\Theta^{(4)}(a, b, f, j, k) = \begin{bmatrix} a & b & b & b \\ b & b - f - j + a & f & j \\ b & f & b - f - k + a & k \\ b & j & k & b - j - k + a \end{bmatrix}. \tag{38}$$

The variability of one of the parameters is spurious since it merely signals the double degeneracy of one of the eigenvalues. The fifth degree of freedom may immediately be interpreted, therefore, as an inessential angle of rotation in the two-dimensional subspace spanned by the corresponding pair of eigenvectors. The remaining four real parameters are independent and their presence reflects the well known ambiguity of the assignment of the metric Θ to a given Hamiltonian (for a thorough discussion of this mathematical subtlety with serious physical consequences cf., e.g., Ref. [17]).

1. Positive-definite cases (metrics)

The apparent simplicity of formula (38) is slightly misleading because the interpretation of the matrix $\Theta^{(4)}(a, b, f, j, k)$ as a metric requires that we guarantee its positive-definite status [17]. At $N = 4$, this property would be equivalent to the positivity of all of its four

eigenvalues $\tau_j > 0$, $j = 0, 1, 2, 3$,

$$\tau_{0,1} = a + b/2 \pm b\sqrt{13}/2,$$
$$\tau_{2,3} = a + b - f - j - k \pm \sqrt{f^2 + j^2 + k^2 - fj - fk - kj}. \quad (39)$$

We see that the positivity of the metric (i.e., of the norm) is guaranteed by the specification of the allowed domain $\mathcal{D}$ of our quintuplet of parameters. This is particularly easy when we restrict our attention to the subdomain of $\mathcal{D}$ where $f = j = k = 0$ and where

$$\Theta^{(4)}(a, b, 0, 0, 0) = \begin{bmatrix} a & b & b & b \\ b & b+a & 0 & 0 \\ b & 0 & b+a & 0 \\ b & 0 & 0 & b+a \end{bmatrix}.$$

We obtain the complete positivity constraint

$$2a > |b|(\sqrt{13} + 1), \qquad b \le 0,$$
$$2a > b(\sqrt{13} - 1), \qquad b > 0.$$

This means that the allowed values of b belong to an interval which grows with $a > 0$. As long as this guarantees the positivity of $\tau_{0,1}$ at all f, j, k, the specification of the allowed domain of parameters will be completed by the inequality

$$f + j + k + \sqrt{f^2 + j^2 + k^2 - fj - fk - kj} < a + b. \quad (40)$$

Out of the doublet of constraints $\tau_{2,3} > 0$ this is equivalent to the stronger one. We see that neither of the three parameters f, j, k will be allowed to get too large in comparison with a.

2. Indefinite cases (generalized parities $\mathcal{P}$)

Elementary $N = 4$ example looks particularly well suited for illustrative purposes. Thus, in a search for the simplest possible *parity-type* pseudometrics $\mathcal{P}^{(4)}(a, b, f, j, k)$ we have to construct such a solution of Eq. (29) which *is* invertible but which *is not* positive definite. This matrix may be represented by the same formula as the metric $\Theta^{(4)}(a, b, f, j, k)$ but at least one of the positivity constraints (39) must be violated. In such a setting the requirement of maximal simplicity may start from the elimination of b which is exceptional in occurring 9 times in Eq. (38). At $b = 0$ we may also normalize $a = 1$ [$\mathcal{P}^{(4)}(a, 0, f, j, k)$ would not be invertible at $a = 0$] and have

$$\mathcal{P}^{(4)}(1, 0, f, j, k) = \begin{bmatrix} 1 & 0 & 0 & 0 \\ 0 & 1-f-j & f & j \\ 0 & f & 1-f-k & k \\ 0 & j & k & 1-j-k \end{bmatrix}. \quad (41)$$

For a maximal simplicity of this matrix we leave just one of its parameters nonzero and get, say,

$$\mathcal{P}^{(4)}(1, 0, 0, 0, 1) = \begin{bmatrix} 1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & 0 & 1 \\ 0 & 0 & 1 & 0 \end{bmatrix}. \quad (42)$$

In $\mathcal{PT}$-symmetric models this matrix can play the role of parity $\mathcal{P}$. Geometrically, it realizes the left-right reflection of our Y-shaped graph (30).

B. Block-tridiagonal pseudometrics

1. Solutions of Eq. (29) at $N = 7$ and $N = 10$

The main source of insight in the structure of metrics and pseudometrics lies in the natural partitioning of Hamiltonians $H^{(N)}$ in q-dimensional submatrices. At $q = 3$ the first two nontrivial though still sufficiently sparse matrix solutions were obtained by the straightforward computer-assisted symbolic manipulations with Eq. (29). The results

$$\mathcal{P}^{(7)}_1(\lambda) = \begin{bmatrix} -1 & 1 & 1 & 1 & 0 & 0 & 0 \\ 1 & 0 & 0 & 0 & 1 & 0 & 0 \\ 1 & 0 & 0 & 0 & 0 & 1-\lambda & 0 \\ 1 & 0 & 0 & 0 & 0 & 0 & 1+\lambda \\ 0 & 1 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 1-\lambda & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 1+\lambda & 0 & 0 & 0 \end{bmatrix} \quad (43)$$

and

$$\mathcal{P}_1^{(10)}(\lambda) = \begin{bmatrix} -1 & 1 & 1 & 1 & 0 & 0 & 0 & 0 & 0 & 0 \\ 1 & 0 & 0 & 0 & 1 & 0 & 0 & 0 & 0 & 0 \\ 1 & 0 & 0 & 0 & 0 & 1 & 0 & 0 & 0 & 0 \\ 1 & 0 & 0 & 0 & 0 & 0 & 1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 & 0 & 0 & 0 & 1 & 0 & 0 \\ 0 & 0 & 1 & 0 & 0 & 0 & 0 & 0 & 1-\lambda & 0 \\ 0 & 0 & 0 & 1 & 0 & 0 & 0 & 0 & 0 & 1+\lambda \\ 0 & 0 & 0 & 0 & 1 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 1-\lambda & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 1+\lambda & 0 & 0 & 0 \end{bmatrix} \tag{44}$$

open the way toward extrapolations.

2. Extrapolation to any $N = 3K + 1$

The knowledge of the nontrivial solutions (43) and (44) of Eq. (29) inspires the proposal of the following block-partitioned ansatz

$$\mathcal{P}_1^{(3K+1)}(\lambda) = \begin{bmatrix} w & \vec{v}^T & 0 & \cdots & \cdots & 0 \\ \vec{v} & 0 & -I & \ddots & \ddots & \vdots \\ 0 & -I & \ddots & \ddots & \ddots & 0 \\ \vdots & \ddots & \ddots & 0 & -I & 0 \\ \vdots & & \ddots & -I & 0 & d(\lambda) \\ 0 & \cdots & \cdots & 0 & d(\lambda) & 0 \end{bmatrix}. \tag{45}$$

Using the Hamiltonian of Eq. (21) in its $q = 3$ version

$$\begin{bmatrix} 3 & -1 & -1 & -1 & 0 & 0 & \cdots & & \cdots & 0 \\ -1 & 2 & 0 & 0 & -1 & 0 & \ddots & & & \vdots \\ -1 & 0 & 2 & 0 & 0 & -1 & \ddots & & & \\ -1 & 0 & 0 & 2 & 0 & \ddots & \ddots & 0 & \vdots & \vdots \\ 0 & -1 & 0 & 0 & 2 & \ddots & \ddots & -1 & 0 & 0 \\ \vdots & 0 & -1 & 0 & 0 & \ddots & \ddots & 0 & -1+\lambda & 0 \\ & & \ddots & \ddots & \ddots & \ddots & \ddots & 0 & 0 & -1-\lambda \\ & & \cdots & 0 & -1 & 0 & 0 & 2 & 0 & 0 \\ \vdots & & & \cdots & 0 & -1-\lambda & 0 & 0 & 2 & 0 \\ 0 & \cdots & & \cdots & 0 & 0 & -1+\lambda & 0 & 0 & 2 \end{bmatrix}$$

(were only the right low corner is coupling-dependent) and performing the appropriate insertions one readily verifies that Eq. (29) becomes an identity provided only that the unknown submatrix $d(\lambda)$ is defined by the elementary formula $d(\lambda) = -c(\lambda)$ [cf. Eq. (21)] which remains the same at all integers $K = 2, 3, \ldots$.

Naturally, our block-tridiagonal ansatz (45) as well as its verification and subsequent conclusions may immediately be extended to the other star graphs with $q = 4, 5, \ldots$. The details are left to the reader. In what follows we shall address, instead, the other two questions, viz., a transition from the block-tridiagonal pseudometrics (45) to their block-pentadiagonal and higher descendants (cf. paragraph VI C below) and a transition from the indefinite pseudometric matrices [exemplified here by Eq. (45)] to the acceptable and positive definite band-matrix metrics ex-

pressed by the first nonlocal formula

$$\Theta = \Theta^{(N)}_{[\beta]} = \beta\Theta^{(N)}_0 + \mathcal{P}^{(N)}_1 \tag{46}$$

[cf. the paragraph VI D below and note that the latter expression is just the two-term truncated version of the general expansion (28)].

C. Block-pentadiagonal pseudometrics

The appeal of finding a block-pentadiagonal pseudometric (denoted by the symbol $\mathcal{P}^{(N)}_2$ here) would lie in its possible insertion in the next truncated version of formula (28),

$$\Theta = \Theta^{(N)}_{[\beta,\gamma]} = \beta\Theta^{(N)}_0 + \gamma\mathcal{P}^{(N)}_1 + \mathcal{P}^{(N)}_2. \tag{47}$$

This formula may be used to define the more smeared, block-pentadiagonal nonlocal metrics.

Once we leave the positivity questions aside and choose $N = 10$, the application of the computer-assisted direct-solution algorithm produces the pseudometric solution $\mathcal{P}^{(10)}_2(\lambda)$ of Eq. (29) in the form

$$\begin{bmatrix}
0 & 0 & 0 & 0 & 1 & 1 & 1 & 0 & 0 & 0 \\
0 & -1 & 1 & 1 & 1 & 0 & 0 & 1 & 0 & 0 \\
0 & 1 & -1 & 1 & 0 & 1 & 0 & 0 & 1-\lambda & 0 \\
0 & 1 & 1 & -1 & 0 & 0 & 1 & 0 & 0 & 1+\lambda \\
1 & 1 & 0 & 0 & -1 & 0 & 0 & 1 & 0 & 0 \\
1 & 0 & 1 & 0 & 0 & -\lambda^2-1 & 0 & 0 & 1-\lambda & 0 \\
1 & 0 & 0 & 1 & 0 & 0 & -\lambda^2-1 & 0 & 0 & 1+\lambda \\
0 & 1 & 0 & 0 & 1 & 0 & 0 & -2 & 0 & 0 \\
0 & 0 & 1-\lambda & 0 & 0 & 1-\lambda & 0 & 0 & \frac{-2+2\lambda-\lambda^2+\lambda^3}{1+\lambda} & 0 \\
0 & 0 & 0 & 1+\lambda & 0 & 0 & 1+\lambda & 0 & 0 & \frac{-2-2\lambda-\lambda^2-\lambda^3}{1-\lambda}
\end{bmatrix}.$$

In a way recommended at $q = 2$ in Ref. [1]) this $q = 3$ solution has been made unique by the requirement of having a minimum of nonvanishing matrix elements in the first row. In our present case the optimality of such a requirement is less obvious. Indeed, as long as we have to optimize the sum (47) rather than its individual components we may feel dissatisfied by the comparatively high number (= 39) of nonvanishing matrix elements in $\mathcal{P}^{(10)}_2(\lambda)$ [and, among them, 12 manifestly λ-dependent items]. In such a case we may contemplate $\mathcal{P}^{(10)}_{2a}(\lambda)$ given by the formula

$$\begin{bmatrix}
2 & -1 & -1 & -1 & 1 & 1 & 1 & 0 & 0 & 0 \\
-1 & 0 & 1 & 1 & 0 & 0 & 0 & 1 & 0 & 0 \\
-1 & 1 & 0 & 1 & 0 & 0 & 0 & 0 & 1-\lambda & 0 \\
-1 & 1 & 1 & 0 & 0 & 0 & 0 & 0 & 0 & 1+\lambda \\
1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\
1 & 0 & 0 & 0 & 0 & -\lambda^2 & 0 & 0 & 0 & 0 \\
1 & 0 & 0 & 0 & 0 & 0 & -\lambda^2 & 0 & 0 & 0 \\
0 & 1 & 0 & 0 & 0 & 0 & 0 & -1 & 0 & 0 \\
0 & 0 & 1-\lambda & 0 & 0 & 0 & 0 & 0 & \frac{-1+\lambda-\lambda^2+\lambda^3}{1+\lambda} & 0 \\
0 & 0 & 0 & 1+\lambda & 0 & 0 & 0 & 0 & 0 & \frac{-1-\lambda-\lambda^2-\lambda^3}{1-\lambda}
\end{bmatrix}.$$

containing just a minimum—30 pieces—of the nonvanishing matrix elements. We may also ask for the absence of fractions at a cost of having 32 nonvanishing matrix elements in

$$\mathcal{P}^{(10)}_{2b}(\lambda) = \begin{bmatrix}
3+\lambda^2 & -1 & -1 & -1 & 1 & 1 & 1 & 0 & 0 & 0 \\
-1 & 1+\lambda^2 & 1 & 1 & 0 & 0 & 0 & 1 & 0 & 0 \\
-1 & 1 & 1+\lambda^2 & 1 & 0 & 0 & 0 & 0 & 1-\lambda & 0 \\
-1 & 1 & 1 & 1+\lambda^2 & 0 & 0 & 0 & 0 & 0 & 1+\lambda \\
1 & 0 & 0 & 0 & 1+\lambda^2 & 0 & 0 & 0 & 0 & 0 \\
1 & 0 & 0 & 0 & 0 & 1 & 0 & 0 & 0 & 0 \\
1 & 0 & 0 & 0 & 0 & 0 & 1 & 0 & 0 & 0 \\
0 & 1 & 0 & 0 & 0 & 0 & 0 & \lambda^2 & 0 & 0 \\
0 & 0 & 1-\lambda & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\
0 & 0 & 0 & 1+\lambda & 0 & 0 & 0 & 0 & 0 & 0
\end{bmatrix}.$$

Another option could be based of the compromising choice of

$$\mathcal{P}^{(10)}_{2c}(\lambda) = \begin{bmatrix} 3 & -1 & -1 & -1 & 1 & 1 & 1 & 0 & 0 & 0 \\ -1 & 1 & 1 & 1 & 0 & 0 & 0 & 1 & 0 & 0 \\ -1 & 1 & 1 & 1 & 0 & 0 & 0 & 0 & 1-\lambda & 0 \\ -1 & 1 & 1 & 1 & 0 & 0 & 0 & 0 & 0 & 1+\lambda \\ 1 & 0 & 0 & 0 & 1 & 0 & 0 & 0 & 0 & 0 \\ 1 & 0 & 0 & 0 & 0 & 1-\lambda^2 & 0 & 0 & 0 & 0 \\ 1 & 0 & 0 & 0 & 0 & 0 & 1-\lambda^2 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 1-\lambda & 0 & 0 & 0 & 0 & 0 & -\lambda^2\frac{1-\lambda}{1+\lambda} & 0 \\ 0 & 0 & 0 & 1+\lambda & 0 & 0 & 0 & 0 & 0 & -\lambda^2\frac{1+\lambda}{1-\lambda} \end{bmatrix}$$

with some elementary fractions but with minimum (= 8 pieces) of λ-dependent matrix elements.

D. Metrics as positive definite superpositions of pseudometrics

1. Positivity constraint at $N = 7$

The results of preceding paragraph have to be complemented by the empirical observation that the candidate for the metrics which is chosen in the one-parametric block-tridiagonal form $\Theta^{(N)}_{[\beta]} = \beta \times \Theta^{(N)}_0 + \mathcal{P}^{(N)}_1$ need not necessarily be positive definite. This may numerically be confirmed not only at vanishing $\beta = 0$ but also at the positive values of β which are not sufficiently large. For illustration we selected $\beta = 1/10$ and found that in dependence on the value of λ, three or four eigenvalues of $\Theta^{(7)}_{[1/10]}(\lambda)$ remained negative.

One must be careful even if the candidate matrix $\Theta^{(7)}_{[\beta]}(\lambda)$ looks dominated by its diagonal and safely positive-definite metric component. This is illustrated in Fig. 3 where we displayed the three lowest eigenvalues of $\Theta^{(N)}_{\beta}$ at $\beta = 2$. In the picture we also see that there already exists just single eigenvalue which breaks the positivity and stays negative inside the whole interval of $\lambda \in (-1, 1)$.

Our subsequent Fig. 4 illustrates the situation in which $\beta = 3$ is sufficiently large. Similar pictures can offer a comparatively reliable graphical confirmation of the positivity of any candidate (28) for the metric. Thus, in our particular illustration we see that for $\Theta^{(7)}_{[\beta]}(\lambda)$ considered in the whole interval of $\lambda \in (-\lambda^{(\text{numerical})}(\beta), \lambda^{(\text{numerical})}(\beta))$ it is sufficient to choose $\beta = 3$. Then our picture also leads to the graphical estimate of $\lambda^{(\text{numerical})}(3) \approx 1$. As long as the dimension $N = 7$ is small, this estimate may be replaced by the rigorous identification of $\lambda^{(\text{numerical})}(3) = 1$. By means of elementary algebra it is easy to show that this value coincides not only with the singularity (i.e., with the point of divergence) of the maximal eigenvalue of $\Theta^{(7)}_{[3]}(\lambda)$ but also with the zero of the minimal eigenvalue of the same matrix.

The λ-dependence of the minimal eigenvalue of $\Theta^{(7)}_{[\beta]}(\lambda)$ is of particular relevance in the regime where the value of β decreases below it value used in Fig. 4. In our next Fig. 5 we use $\beta = 5/2$ and see that the loss of the positive-definiteness of $\Theta^{(7)}_{[\beta]}(\lambda)$ may be expected to occur at

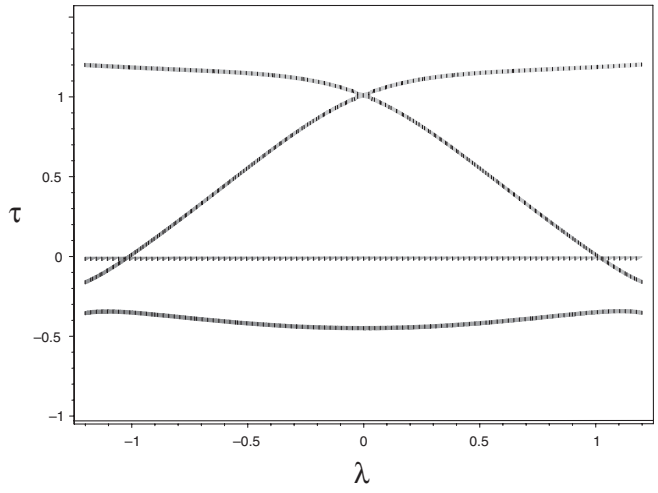


FIG. 3. The three lowest eigenvalues of the matrix $2\Theta^{(7)}_0 + \mathcal{P}^{(7)}_1$.

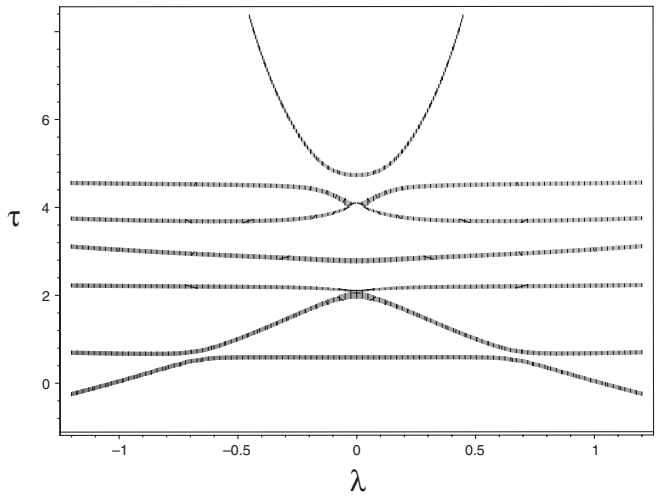


FIG. 4. The spectrum of the metric $\Theta^{(7)}_{[3]} = 3\Theta^{(7)}_0 + \mathcal{P}^{(7)}_1$.

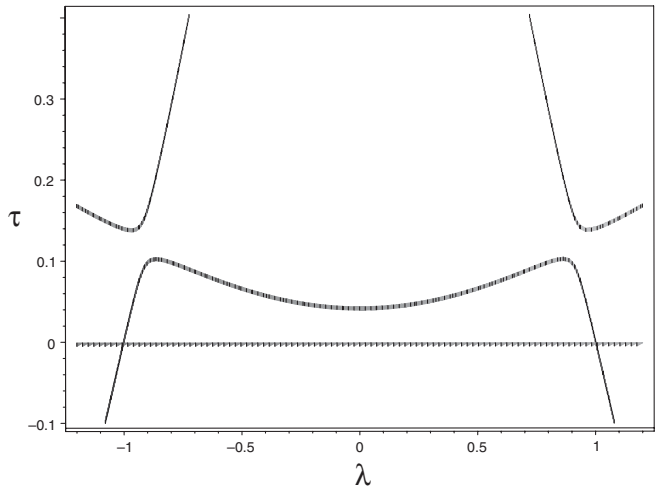


FIG. 5. The lowest two numerical eigenvalues of metric $\Theta^{(7)}_{[5/2]}(\lambda)$.

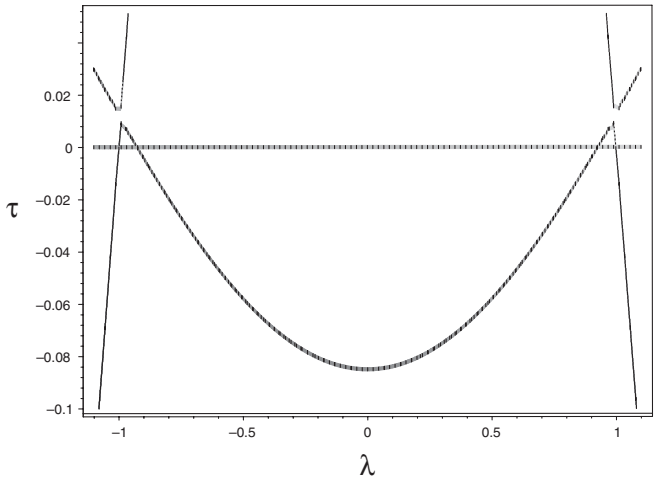


FIG. 6. The lowest two numerical eigenvalues of matrix $\Theta^{(7)}_{[38/16]}(\lambda)$.

$\lambda = 0$ where the lowest eigenvalue would vanish. Of course, as long as the dimension of our illustrative model is small, it is very easy to find the corresponding critical value of

$$\beta_{\text{minimal}} = \frac{1}{3} + \frac{1}{6}\sqrt[3]{44 + 36i\sqrt{107}} + \frac{26}{3}\,\frac{1}{\sqrt[3]{44 + 36i\sqrt{107}}}. \tag{48}$$

This quantity lies, in rational arithmetics, inside interval $(39/16, 5/2)$ and is numerically approximated by ~ 2.46050487. In a few complementary tests we found that the positivity of the metrics $\Theta^{(7)}_{[\beta]}(\lambda)$ is still reliably confirmed at $\beta = 149/60 \sim 2.483333333$ since in the standard precision of computer arithmetics the related minimum ~ 0.02 of the lowest numerical eigenvalue is still safely positive at $\lambda = 0$.

Matrix $\Theta^{(7)}_{[\beta]}(\lambda)$ retains its applicability as a metric also for βs which lie slightly below their universal, λ-independent bound (48). In these cases one must restrict the admissible variability of the coupling λ to intervals $\lambda \in (-1, -\lambda^{(ad\ hoc)}(\beta))$ and $\lambda \in (\lambda^{(ad\ hoc)}(\beta), 1)$. For explicit numerical illustration of such a conditional, λ-dependent positivity of the metric below the critical boundary (48) we choose $\beta = 39/16 = 2.4375$ and revealed that the lowest numerical eigenvalue of Θ (with the minimum $\sim -0.02 < 0$ at $\lambda = 0$) remained negative in the interval of $\lambda \in (-\lambda^{(ad\ hoc)}, \lambda^{(ad\ hoc)})$ where $\lambda^{(ad\ hoc)} \sim 0.5$ at our sample value of $\beta = 39/16$. It is necessary to keep in mind that $\lambda^{(ad\ hoc)}(\beta)$ quickly converges to one with the decrease of $\beta < \beta_{\text{minimal}}$. This is well illustrated by our last Fig. 6 where we obtained $\lambda^{(ad\ hoc)} \sim 0.94$ at $\beta = 38/16 = 2.375$.

2. *The positivity constraint at* $N = 3K + 1 \geq 10$

For the ten-dimensional metric candidates for the metric with the same block-tridiagonal structure, e.g., for $\beta = 3$ in

$$\Theta^{(10)}_{[3]}(\lambda) = \begin{bmatrix} 2 & 1 & 1 & 1 & 0 & 0 & 0 & 0 & 0 & 0 \\ 1 & 3 & 0 & 0 & 1 & 0 & 0 & 0 & 0 & 0 \\ 1 & 0 & 3 & 0 & 0 & 1 & 0 & 0 & 0 & 0 \\ 1 & 0 & 0 & 3 & 0 & 0 & 1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 & 3 & 0 & 0 & 1 & 0 & 0 \\ 0 & 0 & 1 & 0 & 0 & 3 & 0 & 0 & 1-\lambda & 0 \\ 0 & 0 & 0 & 1 & 0 & 0 & 3 & 0 & 0 & 1+\lambda \\ 0 & 0 & 0 & 0 & 1 & 0 & 0 & 3 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 1-\lambda & 0 & 0 & 3\frac{1-\lambda}{1+\lambda} & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 1+\lambda & 0 & 0 & 3\frac{1+\lambda}{1-\lambda} \end{bmatrix}$$

very similar results were obtained supporting the applicability of our above-presented considerations to all the sequence of metric candidates $\Theta^{(N)}_{[\beta]}(\lambda)$ with sufficiently large parameters $\beta > \beta_{\text{minimal}}(N)$ and with unconstrained dimensions $N = 3K + 1 = 13, 16, \ldots$.

VII. DISCUSSION AND SUMMARY

In a way emphasized by several authors [37,51] one should, strictly speaking, distinguish between the x-dependence in the wave function $\psi(x)$ and the x-dependence in the potential $V(x)$ since in these two functions the concept of locality has a different mathematical background as well as physical meaning. Usually, the variable x entering wave functions $\psi(x)$ is treated as a measurable (i.e., real) quantity while the choice of the local $V(x)$ may be treated just as a very special case of its possible generalized, equally admissible nonlocal alternatives.

The more widespread use of the ''nonlocal'' wave functions $\psi(x)$ (where x need not be an observable real coordinate) only occurred during the growth of popularity of differential-operator Hamiltonians $H_{(PT)} = p^2 + V_{(PT)}(x)$ where x has been considered complex [41]. A not too dissimilar nonlocality also characterizes our present nonlocal versions of $\mathcal{PT}$-symmetric discrete quantum graphs where we left the physical meaning of the spatial coordinate unspecified, citing only the related thorough discussion of this question available in our preceding paper Ref. [1].

We may summarize our present results by saying that we transferred the concept of $\mathcal{PT}$-symmetry to the class of quantum systems living on graphs. These graphs generalize the usual real line of coordinates in one dimension. Several non-Hermitian, $\mathcal{PT}$-symmetric versions of these structures have been studied. On technical level we found one of the most vital mathematical sources of encouragement in a few older papers [52] whose authors demonstrated the practical viability of an approximative reduction of the graph edges to discrete lattices of points and *vice versa*. On this background we succeeded in combining the existing quantum-graph concepts with the very fresh formalism using $\mathcal{PT}$-symmetric Hamiltonians which are only made Hermitian via a comparatively complicated *ad hoc* inner product.

The technical feasibility of such a synthesis had several independent reasons. First of all, the spectra of energies proved real for the range of couplings λ which stayed independent of the changes of the dimension N of the lattice. Second, our choice of the model proved lucky in the sense that in the current coordinate basis one of the *constructed* metric matrices $\Theta \neq I$ happened to remain strictly diagonal. Together with the elementary form of matrix elements of this particular metric $\Theta = \Theta_0$ this not quite expected result made the necessary rigorous proof of the reality of the energies virtually trivial.

As the first by-product of this circumstance one of the eligible physical interpretations of our apparently non-Hermitian quantum-graph system remained trivial in the sense that it just required an inessential modification of the concept of observables and that it enabled us to construct its spectrally equivalent representation characterized by the Hamiltonian which is Hermitian in the current sense (cf. operator $\mathfrak{h}$ in paragraph V B 2 above).

In the same theoretical framework the second important consequence of the existence of the well-defined interval of admissible couplings may be seen in the emergence of new freedom in the choice of alternative, *different* physical interpretations of the same quantum-graph Hamiltonian $H(\lambda)$. We were, once more, lucky in revealing that there exists an extremely natural partial ordering of these interpretations dictated merely by the degree of their nonlocality or, in other words, by the extent of the smearing of the coordinate (the degree of this smearing or, if you wish, fundamental length θ_j) grew with the subscript j of the selected closed-form metric Θ_j).

On descriptive side let us reemphasize the minimality of our interactions which were not supported by the whole graph but just by the closest vicinity of its endpoints. This also contributed to the feasibility of our constructions for which we had to develop several computer-assisted auxiliary symbolic-manipulation techniques and adaptive algorithms. Fortunately, the explicit calculations which were performed at the smallest dimensions usually generated the output which admitted an extrapolation. Hence, the subsequent adaptation of the algorithms often degenerated to the mere verification of the extrapolated ansatz.

During these constructions we completely avoided the unnecessarily complicated direct construction of the nondiagonal Dyson-map matrices Ω and restricted our attention just to the metrics. Moreover we revealed that these metrics can be decomposed into sums of certain sparse pseudometrics, i.e., matrices with a sufficiently large portion of matrix elements equal to zero. This facilitated our calculations at higher dimensions.

Our requirement of a fixed nonlocality does not make the resulting metric $\Theta = \Theta(H)$ unique. The constructive analysis of this metric-ambiguity problem in the specific quantum-graph setting can be perceived as an extension of several recent nongraph (or trivial-graph, $q = 2$) studies assigning several nonequivalent probabilistic interpretations to a given Hamiltonian [53]. A partial correspondence can be then seen to the standard transitions between the coordinate and momentum representations of wave functions $\psi(x)$ where the role of the (unitary) Fourier transformation of Hilbert space is being taken over by the manifestly nonunitary Dyson mapping Ω. In such a setting we made use of the fact that the argument x of wave functions need not necessarily carry the direct physical meaning of an (arbitrarily precisely observable) coordinate. In terms of measurements the immediate connection between the coordinate x and its observability is, therefore, weakened. The coordinates can be interpreted as ''smeared'' [35]. In the context of topologically nontrivial quantum graphs the prospective utilization of such a feature of phenomenological models looks particularly promising.

In the language of mathematics our present family of discrete quantum-graph models proved exceptionally friendly. Their choice enabled us to disentangle the hidden Hermiticity constraints (26) and to find closed formulas for the sparse-matrix metrics. The resulting availability of their generic multiparametric forms has been interpreted as a new freedom of a phenomenology-friendly choice among alternative inner products specifying the nonequivalent physical Hilbert spaces of states $\mathcal{H}_j^{(N)}$, $j = 0, 1, \ldots$. Whenever asked for, an extension of our present particular quantitative and illustrative results on $\mathcal{PT}$-symmetric quantum graphs to the higher degrees of nonlocality and/or beyond their equilateral q-point-star special class with small $q = 3, 4, \ldots$ looks comparatively easy and straightforward.

In the context of physics our present results are unexpectedly encouraging. A new flexibility of the model-building has been achieved here, first of all, via extension of the class of eligible interactions and, secondly, via the related innovative control of a degree of nonlocality reflected by the introduction of the ''tunable'' inner products. A deeper investigation of these possibilities seems to form a new and promising quasi-Hermitian-graph project filling a certain gap in the broader context of existing directions of the study of quantum theory on graphs.

ACKNOWLEDGMENTS

The support by the Institutional Research Plan AV0Z10480505, by the MŠMT ''Doppler Institute'' project LC06002 and by GAČR grant No. 202/07/1307 is acknowledged.

[1] M. Znojil, Phys. Rev. D **80**, 045022 (2009).
[2] P. Exner and P. Šeba, J. Math. Phys. (N.Y.) **30**, 2574 (1989).
[3] T. Ekholm, H. Kovařík, and D. Krejčiřík, Arch. Ration. Mech. Anal. **188**, 245 (2008).
[4] illustrative pictures are available on address http://en.wikipedia.org/wiki/Quantum_graph.
[5] V. Nekrashevych and A. Teplyaev, ''Groups and analysis on fractals'', review paper in proceedings [6].
[6] P. Exner, J. P. Keating, P. Kuchment, and A. Teplyaev, *Analysis on Graphs and Its Applications* (AMS, Rhode Island, 2008).
[7] P. Kuchment, Waves Random Media **14**, S107 (2004); J. Phys. A: Math. Gen. **38**, 4887 (2005); Quantum graphs: an introduction and a brief survey, review paper in proceedings [6], p. 291.
[8] P. Exner, Leaky Quantum Graphs: A Review, review paper in proceedings [6], p. 523.
[9] E. Ragoucy, J. Phys. A: Math. Theor. **42**, 295205 (2009).
[10] N. M. Shnerb and D. R. Nelson, Phys. Rev. Lett. **80**, 5172 (1998); J. Feinberg and A. Zee, Phys. Rev. E **59**, 6433 (1999); R. A. Janik, M. A. Nowak, G. Papp, and I. Zahed, Acta Phys. Pol. B **30**, 45 (1999); J. Heinrichs, Phys. Rev. B **63**, 165108 (2001).
[11] D. C. Brody, A. C. T. Gustavsson, and L. P. Hughston, J. Phys. A: Math. Theor. **42**, 295303 (2009).
[12] T. Kottos and U. Smilansky, Phys. Rev. Lett. **79**, 4794 (1997); S. Gnutzmann and U. Smilansky, Adv. Phys. **55**, 527 (2006); U. Smilansky, J. Phys. A: Math. Theor. **40**, F621 (2007).
[13] T. Huillet, J. Phys. A: Math. Theor. **42**, 275001 (2009).
[14] L. G. Molinari, J. Phys. A: Math. Theor. **42**, 265204 (2009).
[15] N. Hatano and D. R. Nelson, Phys. Rev. Lett. **77**, 570 (1996).
[16] J. Feinberg and A. Zee, Nucl. Phys. **B504**, 579 (1997).
[17] F. G. Scholtz, H. B. Geyer, and F. J. W. Hahne, Ann. Phys. (N.Y.) **213**, 74 (1992).
[18] C. M. Bender and K. A. Milton, Phys. Rev. D **55**, R3255 (1997) **57**, 3595 (1998); C. M. Bender, D. C. Brody, and H. F. Jones, Phys. Rev. Lett. **89**, 270401 (2002); M. C. Ogilvie and P. N. Meisinger, SIGMA **5**, 047 (2009) arXiv:0812.0176.
[19] A. A. Andrianov, F. Cannata, and A. Y. Kamenshchik, J. Phys. A: Math. Gen. **39**, 9975 (2006).
[20] C. M. Bender and S. Boettcher, Phys. Rev. Lett. **80**, 5243 (1998).
[21] *Proceedings of the Workshop on Pseudo-Hermitian Hamiltonians in Quantum Physics, Prague, 2003*, edited by M. Znojil [Czech. J. Phys. 54, No. 1 (2004)], dedicated issue; *Proceedings of the Workshop on Pseudo-Hermitian Hamiltonians in Quantum Physics II, Prague, 2004*, edited by M. Znojil [Czech. J. Phys. 54, No. 10 (2004)], dedicated issue;*Proceedings of the Workshop on Pseudo-Hermitian Hamiltonians in Quantum Physics III, Istanbul, 2005*, edited by M. Znojil [Czech. J. Phys. 55, No. 9 (2005)], dedicated issue; *Proceedings of the Workshop on Pseudo-Hermitian Hamiltonians in Quantum Physics IV, Stellenbosch, 2005*, edited by H. Geyer, D. Heiss, and M. Znojil [J. Phys. A: Math. Gen. 39, No. 32 (2006)], dedicated issue; *Proceedings of the Workshop on Pseudo-Hermitian Hamiltonians in Quantum Physics V, Bologna, 2006*, edited by M. Znojil [Czech. J. Phys. 56, No. 9 (2006)], dedicated issue; *Proceedings of the Workshop on Pseudo-Hermitian Hamiltonians in Quantum Physics VI, London, 2007*, edited by A. Fring, H. Jones, and M. Znojil [J. Phys. A: Math. Theor. 41, No. 24 (2008)], dedicated issue; *Proceedings of the Workshop on Pseudo-Hermitian Hamiltonians in Quantum Physics VII, Benasque, 2008*, edited by A. Andrianov *et al.* [SIGMA, 5 (2009)], http://www.emis.de/journals/SIGMA/PHHQP2008.html, dedi-

cated issue; *Proceedings of the VIIIth Conference on Non-Hermitian Hamiltonians in Quantum Physics, Mumbai, 2009*, edited by S. R. Jain and Z. Ahmed [Pramana J. Phys. 73, Nos. 2 and 3 (2009), dedicated issues.
[22] U. Guenther and B. F. Samsonov, Phys. Rev. A **78**, 042115 (2008); Phys. Rev. Lett. **101**, 230404 (2008).
[23] A. Mostafazadeh, Pramana J. Phys. **73**, 269 (2009).
[24] Z. H. Musslimani *et al.*, Phys. Rev. Lett. **100**, 030402 (2008); M. V. Berry, J. Phys. A: Math. Theor. **41**, 244007 (2008); O. Bendix, R. Fleischmann, T. Kottos, and B. Shapiro, Phys. Rev. Lett. **103**, 030402 (2009).
[25] B. Bagchi and A. Fring, arXiv:0907.5354v1.
[26] H. Langer and C. Tretter, Czech. J. Phys. **54**, 1113 (2004).
[27] C. M. Bender, S. Boettcher, and P. N. Meisinger, J. Math. Phys. (N.Y.) **40**, 2201 (1999).
[28] C. M. Bender, D. C. Brody, and H. F. Jones, Phys. Rev. Lett. **92**, 119902 (2004).
[29] M. Znojil, Phys. Lett. A **285**, 7 (2001); M. Znojil and G. Lévai, Mod. Phys. Lett. A **16**, 2273 (2001); B. Bagchi, S. Mallik, and C. Quesne, Mod. Phys. Lett. A **17**, 1651 (2002); B. Bagchi, H. Bíla, V. Jakubský, S. Mallik, C. Quesne, and M. Znojil, Int. J. Mod. Phys. A **21**, 2173 (2006).
[30] A. Mostafazadeh and A. Batal, J. Phys. A: Math. Gen. **37**, 11645 (2004).
[31] S. Weigert, Czech. J. Phys. **55**, 1183 (2005); M. Znojil, J. Phys. A: Math. Gen. **39**, 10247 (2006); E. Ergun, SIGMA **5**, 007 (2009) arXiv:0901.2916.
[32] V. Kostrykin and R. Schrader, J. Phys. A: Math. Gen. **32**, 595 (1999).
[33] M. Znojil, Phys. Rev. D **78**, 025026 (2008).
[34] M. Znojil, J. Phys. A: Math. Theor. **41**, 292002 (2008).
[35] M. Znojil, Phys. Rev. D **80**, 045009 (2009).
[36] M. Znojil, SIGMA **5**, 085 (2009) arXiv:0908.4045.
[37] H. F. Jones, Phys. Rev. D **76**, 125003 (2007).
[38] D. Krejčiřík, H. Bíla, and M. Znojil, J. Phys. A: Math. Gen. **39**, 10143 (2006); D. Krejčiřík, J. Phys. A: Math. Theor. **41**, 244012 (2008).
[39] H. F. Jones, Phys. Rev. D **78**, 065032 (2008).
[40] M. Znojil, SIGMA **5**, 001 (2009) arXiv:0901.0700.
[41] C. M. Bender, Rep. Prog. Phys. **70**, 947 (2007).
[42] A. Mostafazadeh, J. Math. Phys. (N.Y.) **43**, 205 (2002); **43**, 2814 (2002); A. Mostafazadeh, arXiv:0810.5643.
[43] P. Dorey, C. Dunning, and R. Tateo, J. Phys. A: Math. Theor. **40**, R205 (2007); Pramana J. Phys. **73**, 217 (2009).
[44] J. Dieudonne, *Proc. Int. Symp. Lin. Spaces* (Pergamon, Oxford, 1961), p. 115; J. P. Williams, Proc. Amer. Math. Soc. 20, 121 (1969).
[45] C. M. Bender, S. F. Brandt, J.-H. Chen, and Q. Wang, Phys. Rev. D **71**, 025014 (2005); C. M. Bender and P. D. Mannheim, Phys. Rev. Lett. **100**, 110402 (2008).
[46] F. C. Figueira de Morisson and A. Fring, J. Phys. A: Math. Gen. **39**, 9269 (2006); A. Mostafazadeh, Phys. Lett. B **650**, 208 (2007); M. Znojil, Phys. Rev. D **78**, 085003 (2008).
[47] A. Mostafazadeh and F. Zamani, Ann. Phys. (N.Y.) **321**, 2183 (2006); **321**, 2210 (2006); V. Jakubský and J. Smejkal, Czech. J. Phys. **56**, 985 (2006).
[48] D. Krejčiřík and M. Tater, J. Phys. A: Math. Theor. **41**, 244013 (2008).
[49] B. Gutkin and U. Smilansky, J. Phys. A: Math. Gen. **34**, 6061 (2001); R. Band, T. Shapira, and U. Smilansky, J. Phys. A: Math. Gen. **39**, 13999 (2006).
[50] M. Znojil, J. Math. Phys. (N.Y.) **46**, 062109 (2005).
[51] A. Mostafazadeh, J. Phys. A: Math. Gen. **39**, 10171 (2006).
[52] P. Exner and K. Němcová, J. Phys. A: Math. Gen. **36**, 10173 (2003); J. F. Brasche and K. Ožanová, arXiv: math-ph/0511029; K. Ožanová, J. Phys. A: Math. Gen. **39**, 3071 (2006).
[53] D. P. Musumbu, F. G. Scholtz, and H. B. Geyer, J. Phys. A: Math. Theor. **40**, F75 (2007); C. Quesne, J. Phys. A: Math. Theor. **41**, 244022 (2008).