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#### Fundamental length in quantum theories with PT-symmetric Hamiltonians

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One-dimensional motion of a quantum point particle is usually described by its wave function  $\psi(x)$ , where the argument  $x \in \mathbb{R}$  represents a (measurable) coordinate and where the integrated probability density is normalized to one,  $\int \psi^*(x)\psi(x)=1$ . The direct observability of x may be lost in  $\mathcal{PT}$ -symmetric quantum mechanics where a "smeared" metric kernel  $\Theta_{(x,x')} \neq \delta(x-x')$  may enter the double-integral normalization  $\iint \psi^*(x)\Theta_{(x,x')}\psi(x')=1$ . We argue that such a formalism proves particularly suitable for the introduction of a nonvanishing fundamental length  $\theta>0$ , which would characterize the "smearing width" of the kernel  $\Theta_{(x,x')}$ . The technical feasibility of such a project is illustrated via a toy family of Hamiltonians  $H^{(N)}(\lambda)$  taken from Ref. [11]. For each element of this family the complete set of all the eligible metric kernels  $\Theta_{(x,x')}^{(N)}(\lambda)$  is constructed in closed form. We show that at any preselected non-negative fundamental length these metrics can be made to vanish unless  $|x-x'|\leq \theta$ . The strictly local inner product of Ref. [11] recurs at  $\theta=0$ , while the popular  $\mathcal{CPT}$ -symmetric option requires  $\theta=\infty$  in this language.

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#### I. INTRODUCTION

The introduction of a minimal length scale (denoted, say, by symbol  $\theta$ ) is tempting on empirical as well as purely pragmatic grounds. Typically, its existence would facilitate the regulation of the high energy asymptotics in field theory [1], etc. A more ambitious motivation of its introduction might be sought in M theory or string theory in their various limiting cases [2]. Connections between  $\theta > 0$  and the emergence of certain singularities with nontrivial physical meaning could further be sought in cosmological applications of quantum theory [3]. In the astrophysical context, last but not least, the fundamental length might be identified as accounting for the dark energy [4] or for the inflationary era in the early evolution of the Universe [5].

In the majority of similar considerations the fundamental length scale emerges as a free parameter. For the particular quantum dynamics of spacetime, for example, its value can be related not only to the Planck length but also, say, to a nonvanishing cosmological constant or to the vacuum energy density [6]. In the simplified context of quantum mechanics this quantity can even be treated as one of phenomenological, experimentally determined characteristics, say, of a condensed-matter system [7]. In parallel, in some more ambitious theoretical studies the introduction of a fundamental length constant is being based on a deeper principle like the stabilization requirement imposed upon relativistic algebra [8].

Many of the latter ideas are implemented using the assumption of noncommutativity of coordinates (cf. a rather nonsystematic selection [8,9] of some sample references). In what follows we intend to develop a different

theoretical concept in which the existence of fundamental length will find its origin and realization via analytic rather than algebraic considerations. We shall particularly be guided by the recent innovative interpretations of certain analytic potentials characterized by their so-called  $\mathcal{PT}$  symmetry (for a review, Ref. [10] is recommended).

More specifically, in our preparatory Sec. II we shall define  $\mathcal{P}$  and  $\mathcal{T}$  via a sample Hamiltonian H (Sec. II A) and explain why we believe that in quantum theory of similar models one of the most natural definitions of the length scale  $\theta > 0$  could be based on a suitable particular realization of the physical Hilbert space  $\mathcal{H}$ . We show, in Sec. II B, how a "smearing of coordinates" emerges as allowed by the well-known ambiguity of the physical inner products in  $\mathcal{H}$ . This enables us to conjecture that in general, one should be able to remove or at least suppress this ambiguity by the requirement that the range of the smearing of coordinates acquires precisely the preselected non-negative value  $\theta$ .

For a quantitative understanding of the similar quantum models with built-in scale  $\theta$  a family of very specific illustrative examples is introduced in Sec. III. The feasibility of their analysis is achieved not only by the use of a nonperturbative technique of solving Schrödinger equations (based on a discretization of coordinates, cf. paragraph III A) but also by the choice of a very elementary, next-to-trivial interaction (cf. Ref. [11] or Eq. (10) in Sec. III B below). In this way all our Hilbert spaces become finite dimensional, and the Hamiltonians become represented by certain 2K-dimensional matrices  $H^{(2K)}(\lambda)$  where the real parameter  $\lambda$  controls their non-Hermiticity. At the minimal Hamiltonian-matrix dimension 2K = N = 2 this renders all the eligible "physical" inner products in  $\mathcal{H}$ available in closed form (paragraph IIIC) making the discussion of the fundamental length  $\theta$  trivial.

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The N=2 conclusions encouraged us to develop and employ a linear-algebraic algorithm of the construction of metrics applicable at any even Hilbert-space dimension N=2K. The symbolic-manipulation results are sampled, in Sec. IV, at the two subsequent integers K=2 and 3. The availability as well as unexpectedly transparent matrix structure of the resulting matrices of the metric proved crucial for our present fundamental-scaling purposes. In essence we revealed that the set of  $\Theta^{(N)}$  appears composed of subsets in which the matrices  $\Theta^{(N)}$  acquire a bandmatrix structure. The elementary length  $\theta$  (i.e., the range of the smearing of coordinates in the inner product) is then identified with a measure of nondiagonality (i.e., with the ratio between the number of diagonals and dimension) of these matrices.

In Sec. V we turn our attention, first of all, to the next few higher dimensions  $N \geq 8$  at which the computer-assisted brute-force determination of *all* of the eligible physical inner products in  $\mathcal{H}$  still remains feasible. Of course, the very enumeration of the N-parametric sets of the resulting matrices  $\Theta^{(N)}$  becomes clumsy. For this reason we developed a recurrent technique of their description, which offers their compact classification as well as their explicit and compact description at any dimension N = 2K.

The phenomenological core of our present message lies in several observations formulated in several separate subsections of Sec. VI. We point out here that our present choice of the family of Hamiltonians  $H^{(2K)}(\lambda)$  looks particularly suitable for illustrative purposes since the bound-state energies remain real in a dimension-independent interval  $\lambda \in (-1,1)$ . One finds out that at a fixed dimension N=2K the phenomenologically motivated fundamental length  $\theta$  can equally well be perceived as a means of classification of eligible metrics. This feature of our solvable model becomes particularly useful when a fixed choice of the fundamental length  $\theta > 0$  is analyzed in the continuous-coordinate limit  $N \to \infty$ .

Our last, summary Sec. VII re-emphasizes the importance of the exact, nonperturbative solvability of our schematic benchmark example, which admits the exhaustive and exact construction of the *complete menu* of matrices  $\Theta^{(N)}$  of the metrics at a given N. In the future, having such a transparent methodical guide at our disposal we may expect that all the prospective transitions to the more realistic interaction models will be facilitated and/or more easily mediated via approximate (e.g., perturbation theory) techniques.

#### II. NONLOCAL INNER PRODUCTS

#### A. PT-symmetric models

Our main source of inspiration can be traced back to the discoveries of existence of the *real* spectra of energies generated by non-Hermitian one-dimensional Hamil-

tonians [12,13]. For illustration let us recollect just the Buslaev's and Grecchi's (BG, [13]) Hamiltonian  $H = p^2 + V(x) \neq H^{\dagger}$  of this type containing the asymptotically quartic "wrong-sign" potential

$$V(x) = V^{(\mathrm{BG})}(x) = -(x - \mathrm{i}\varepsilon)^4 + \mathcal{O}(x^2) \neq V^*(x),$$
  
$$x \in (-\infty, \infty), \qquad \varepsilon > 0.$$

The distinguishing feature of this non-Hermitian Hamiltonian (studied, later, also by Jones *et al.* [14]) is that it is characterized by its  $\mathcal{P}\mathcal{T}$  symmetry  $\mathcal{P}\mathcal{T}H = H\mathcal{P}\mathcal{T}$  where the operators  $\mathcal{P}$  and  $\mathcal{T}$  stand for the parity and time reversal, respectively.

The essential merit of the BG model is that the asymptotically dominant parts of the general solutions  $\psi_{1,2}^{(\mathrm{BG})}(x)$  of the related differential Schrödinger equation near the respective endpoint coordinates  $x_{1,2}=\pm\infty$  are easily deduced,

$$\psi_{1,2}^{(\text{BG})}(x) = c_{+}^{(1,2)} \psi_{+}^{(\text{BG})}(x) + c_{-}^{(1,2)} \psi_{-}^{(\text{BG})}(x),$$
  
$$\psi_{+}^{(\text{BG})}(x) = e^{\pm (1/3)ix^{3} \pm \varepsilon x^{2} + \mathcal{O}(x)}.$$

As long as  $\varepsilon>0$  we can set  $c_+^{(1,2)}=0$  guaranteeing that the resulting functions  $\psi_{1,2}^{(\mathrm{BG})}(x)$  will asymptotically vanish,  $\psi_1^{(\mathrm{BG})}(+\infty)=0$  and  $\psi_2^{(\mathrm{BG})}(-\infty)=0$ . After analytic continuation their matching near the origin gives the physical bound-state solution which is analytic at all  $x\in(-\infty,\infty)$  and quadratically integrable, i.e.,  $\psi_n^{(\mathrm{BG})}(x)\in\mathbb{L}^2(\mathbb{R})$  or

$$\int_{\mathbb{R}} dx [\psi_n^{(\mathrm{BG})}(x)]^* \psi_n^{(\mathrm{BG})}(x) < \infty. \tag{1}$$

It has also rigorously been proved in [13] that the energies  $E = E_n$  are all real, nondegenerate and growing with the main quantum number  $n = 0, 1, \ldots$ 

From our present point of view, it is more important that the related wave functions remain mutually nonorthogonal. This means that the physical information carried by these wave functions remains unclear. In order to restore the physical probabilistic interpretation of such a  $\mathcal{PT}$ -symmetric model one must modify the inner product [10,15]. Usually, this goal is achieved by the replacement of the unphysical Hilbert space  $\mathbb{L}^2(\mathbb{R}) := \mathcal{H}^{(F)}$  (where F stands for "first" or "friendly" or "false") by its amendment  $\mathcal{H}^{(S)} \neq \mathbb{L}^2(\mathbb{R})$  where S means "second" or "standard" and where the bound states become mutually orthogonal [16].

#### B. Fundamental length $\theta$ as a measure of nonlocality

During the return to the standard Hilbert space  $\mathcal{H}^{(S)}$  one reveals that our illustrative potential  $V^{(\mathrm{BG})}(x)$  is an extremely "user-friendly" interaction. In this sense many of its properties appear rather exceptional (cf. [13] where one finds that the transition to  $\mathcal{H}^{(S)}$  leaves the interaction local). For this reason it makes sense to recall also several

other illustrative models. In order to make the picture comparatively complete one must recollect, e.g., the imaginary cubic oscillator of Bessis and Zinn-Justin [17] and/or the whole one-parametric family of its generalizations with  $V(x)/x^2 = (ix)^{\delta}$  where  $\delta \geq 0$  (cf. [10] for more details). In all of these cases the transition to  $\mathcal{H}^{(S)}$  makes the interaction strongly nonlocal (for illustration we recommend to check the details, e.g., via their perturbative illustration at  $\delta = 1$  in Ref. [18]).

Let us emphasize that the necessary condition of the possibility of the transition from the unphysical Hilbert space  $\mathcal{H}^{(F)}$  to its physical parallel  $\mathcal{H}^{(S)}$  lies in the reality of the spectrum of the "non-Hermitian" Hamiltonian in question. Once this condition is satisfied, the most common realization of the correspondence  $\mathcal{H}^{(F)} \to \mathcal{H}^{(S)}$  usually (cf. Ref. [10]) proceeds under the assumption that the space  $\mathcal{H}^{(S)}$  remains spanned by the same wave functions and that only the inner products are redefined as nonlocal [19]. Here, we shall follow the same recipe. Without getting too deeply in the underlying mathematics let us only recollect that for all the sufficiently elementary Hamiltonians the inner product used in  $\mathcal{H}^{(S)}$  may be understood as leading to the generalized, double-integral orthonormalization rule

$$\int_{\mathbb{R}^2} dx dx' \, \psi_m^*(x) \Theta_{(x,x')} \psi_n(x') = \delta_{mn}, \tag{2}$$

where  $\delta_{mn}$  is the Kronecker symbol. For the Hamiltonians that are "trivially" Hermitian in  $\mathcal{H}^{(F)}$  the standard textbook scenario characterized by the Dirac's metric  $\Theta_{(x,x')} = \delta(x-x')$  leads merely to the degenerate version Eq. (1) of Eq. (2). *Vice versa*, Dirac-non-Hermitian Hamiltonians  $H \neq H^{\dagger}$  with real spectra necessitate a selection of a Hamiltonian-dependent metric kernel  $\Theta_{(x,x')} \neq \delta(x-x')$  in Eq. (2). One just replaces the elementary Dirac's Hermitian conjugation

$$\mathcal{T}^{(F)}$$
:  $\psi(x) \to \psi^*(x)$ 

by its nonlocal, more complicated version

$$\mathcal{T}^{(S)}$$
:  $\psi(x) \to \int_{\mathbb{R}} dz \, \psi^*(z) \Theta_{(z,x)}$ . (3)

There exist examples (based on a sufficiently elementary choice of Hamiltonian H—cf., e.g., [20]) where the metric  $\Theta_{(x,x')}$  itself can even be constructed exactly, nonperturbatively.

In this language our present key message is that our Eqs. (2) and (3) may be complemented by the phenomenologically motivated limited-range constraint

$$\Theta_{(x,x')} \neq 0$$
 only if  $|x - x'| \leq \theta$  (4)

using any preselected real quantity  $\theta > 0$ . One must keep in mind that this quantity is just an elementary upper estimate of nonlocality imposed upon the metric in  $\mathcal{H}^{(S)}$ . Its size may be perceived as a measure of the "smearing" of the coordinate x, which is due to the loss

of the direct physical meaning and measurability of the real variable x in  $\mathcal{H}^{(F)}$ .

Strictly speaking one should not even call quantity  $\theta>0$  a "length." At the same time, one feels that once the range of the smearing of the metric kernel is assumed restricted by Eq. (4), the effect of this smearing will quickly decrease when the measured distances exceed the preselected "fundamental" value  $\theta$ . This observation may be also read as a core of our present project specifying a class of models where the smearing is guaranteed to be safely short ranged in  $\theta$ -scaled units.

In this setting the mathematical questions emerge that concern not only the existence of similar models (this question will be answered here affirmatively and constructively) but also their further properties. In this sense, our present paper should be perceived as the first step toward a more extensive theory. Certainly, it will be non-Hermitian in  $\mathcal{H}^{(F)}$  (where the variable x is only a nonobservable auxiliary quantity) but safely Hermitian in  $\mathcal{H}^{(S)}$  (of course, only here the fully consistent concept of distance can be defined). In this context, Eq. (4) might acquire its proper meaning as mediator of coexistence between certain asymptotic locality and short-range nonlocality of certain less standard models of quantum dynamics.

#### III. TOY MODEL

The choice of the value of parameter  $\theta$  must stay compatible with our intuition and available experimental evidence. For example, even the extreme choice of a very large  $\theta$  may be tolerated in the context of bound states where the observable range of nonlocality will effectively be limited by the exponential decrease of wave functions [21]. In contrast, for a consistent description of scattering one must necessarily require that the bound  $\theta$  upon the nonlocality in Eq. (4) must at least asymptotically be very small [11]. In this sense it is rather encouraging that there exist several different solvable models of scattering where the smearing size  $\theta$  in Eq. (4) is strictly equal to zero [11,22]. The methodical importance of the latter family of illustrative examples is further underlined by the fact that for the vast majority of quantum models with nontrivial metrics the numerical value of  $\theta$  happened to remain infinite [21,23].

On this background one must be careful with predictions of the existence of Hamiltonians and metrics for which our upper estimate  $\theta$  of the built-in nonlocality proves nontrivial, i.e., nonvanishing and not too large. Thus, we have to offer an explicit, schematic, constructive example of such a Hamiltonian H and of its specific short-range-smearing metrics  $\Theta$ .

#### A. Runge-Kutta lattice of coordinates

Let us replace the differential form of a given Hamiltonian  $H = p^2 + V(x)$  by its discretized Runge-

Kutta approximation leading to the linear difference Schrödinger equation

$$-\frac{\psi(x_{k+1}) - 2\psi(x_k) + \psi(x_{k-1})}{h^2} + V(x_k)\psi(x_k)$$

$$= E\psi(x_k). \tag{5}$$

Using a suitable, finite or infinite cutoff L > 0 we set

$$x_{-K} = -L,$$
  $x_{-K+1} = -L + h, ..., x_0 = -\frac{h}{2},$  (6) 
$$x_1 = \frac{h}{2}, ..., x_{K+1} = L.$$

The lattice spacing h = 2L/(2K + 1) decreases with N = 2K in both the bound-state phenomenological regime (where L should be kept constant, cf. Ref. [24]) and the scattering regime (where L = L(N) should grow with N, see Ref. [11]).

On each level of precision  $\mathcal{O}(h)$  and for virtually any strictly local potential V(x) the latter recipe makes the practical numerical solution of non-Hermitian Schrödinger equations at a fixed lattice-point distance h decisively facilitated [25]. The discretization of the coordinates reduces also the above-mentioned double-integral orthonormalization rule (2) to its discrete analogue so that the integral kernels  $\Theta_{(x,y)}$  become replaced by matrices  $\Theta_{j,m}^{(N)}(\lambda)$ . Under suitable mathematical assumptions [19] these metric matrices define the inner product between any two elements  $\psi$  and  $\phi$  of our Runge-Kutta version of the physical Hilbert space of states  $\mathcal{H}^{(S)}$ ,

$$\sum_{n=-K+1}^{K} \sum_{n'=-K+1}^{K} \psi^{*}(x_{n}) \Theta_{n,n'}^{(2K)}(\lambda) \phi(x_{n'}) := \langle \langle \psi | \phi \rangle \quad (7)$$

(cf. [16] for more details).

#### B. Minimally nonlocal interactions of Ref. [11]

In our recent studies of scattering [11,22,26] we revealed that the finite-range constraint (4) can be satisfied (and that one can even easily reach its lower bound  $\theta = 0$ ) provided that a nonlocality is admitted in the potential. A "minimal" generalization of this type leads to the following Runge-Kutta Schrödinger equation

$$-\frac{\psi(x_{k+1}) - 2\psi(x_k) + \psi(x_{k-1})}{h^2} + V(x_k, x_{k+1})\psi(x_{k+1}) + V(x_k, x_k)\psi(x_k) + V(x_k, x_{k-1})\psi(x_{k-1}) = E\psi(x_k).$$
(8)

In principle, Eq. (8) must be complemented by asymptotic boundary conditions. Keeping in mind, nevertheless, that the analysis of the scattering scenario has already been performed in Ref. [11], we intend to deal with the bound-state option only,

$$\psi(x_{-K}) = 0, \qquad \psi(x_{K+1}) = 0.$$
 (9)

Let us pick up the most elementary nonlocal interaction as

recommended in Ref. [11] and return to the related Eq. (8) where just the two coupling constants will be different from zero,

$$V(x_0, x_1) = -\lambda, \qquad V(x_1, x_0) = +\lambda.$$
 (10)

At each finite  $K = 1, 2, 3, \ldots$  or  $N = 2, 4, 6, \ldots$  the resulting Schrödinger bound-state eigenvalue problem (8) + (9) + (10) will degenerate to the diagonalization of the respective *finite* matrix  $H^{(N)}(\lambda)$  with tridiagonal structure.

$$H^{(2)}(\lambda) = \begin{bmatrix} 2 & -1 - \lambda \\ -1 + \lambda & 2 \end{bmatrix}, \tag{11}$$

$$H^{(4)}(\lambda) = \begin{bmatrix} 2 & -1 & 0 & 0 \\ -1 & 2 & -1 - \lambda & 0 \\ 0 & -1 + \lambda & 2 & -1 \\ 0 & 0 & -1 & 2 \end{bmatrix}, (12)$$

$$H^{(6)}(\lambda) = \begin{bmatrix} 2 & -1 & 0 & 0 & 0 & 0 \\ -1 & 2 & -1 & 0 & 0 & 0 \\ 0 & -1 & 2 & -1 - \lambda & 0 & 0 \\ 0 & 0 & -1 + \lambda & 2 & -1 & 0 \\ 0 & 0 & 0 & -1 & 2 & -1 \\ 0 & 0 & 0 & 0 & -1 & 2 \end{bmatrix}, \dots$$

$$(13)$$

Qualitatively this family of Hamiltonians can be interpreted as a set of discrete analogues of the exactly solvable  $\mathcal{PT}$ -symmetric square well with a short-range non-Hermiticity [27].

The simplicity of our present family of toy Hamiltonians numbered by their finite matrix dimensions  $N=2K=2,4,\ldots$  can be perceived as the key benefit resulting from our preference of the nonperturbative Runge-Kutta discretization method. One can certainly expect that whenever needed, the present  $\theta>0$  techniques and constructions will remain applicable also to some other, less artificial and more phenomenologically oriented interaction models. Such a transition to more complicated models has already been shown feasible, in [22], at  $\theta=0$  and  $N=L=\infty$ . Similarly, some more-parametric models were shown tractable by the same method in Ref. [11]

### C. Two-parametric family of metrics $\Theta^{(N)}(\lambda)$ at N=2

At N=2 and  $\lambda=\cos\varphi$  closed formulae are available not only for the energies  $E=E_{\pm}^{(2)}=2\pm\sin\varphi$  but also for the norms of the eigenstates  $\psi_{\pm}$ . The Hamiltonian  $H^{(2)}(\cos\varphi)$  nicely illustrates the subtle difference between its right eigenvectors  $|\psi_{\pm}\rangle$  and their left-eigenstate partners  $\langle\langle\psi_{\pm}|$  at the same energy (the latter row vectors are denoted by doubled bras as in [16]),

$$|\psi_{\pm}\rangle \sim \begin{pmatrix} 1 + \cos\varphi \\ \mp \sin\varphi \end{pmatrix},$$

$$\mathcal{T}^{(F)}(\langle\langle \psi_{\pm}|\rangle) := |\psi_{\pm}\rangle\rangle \sim \begin{pmatrix} 1 - \cos\varphi \\ \mp \sin\varphi \end{pmatrix}.$$
(14)

A biorthogonal basis can be formed of these partner eigenvectors. Thus, the manifestly non-Hermitian matrix  $H^{(2)}(\cos\varphi)$  can be reinterpreted as a matrix that becomes Hermitian in the *ad hoc*, Hamiltonian-dependent Hilbert space of states  $\mathcal{H}^{(S)}$  endowed with a nontrivial Hermitian-conjugation operation  $\mathcal{T}^{(S)}$  of Eq. (3).

The key merit of our N = 2 example can be seen in the straightforward availability of *all* of its admissible metrics, which vary with two free parameters  $t_{\pm}$  [15,16],

$$\Theta = \Theta^{(2)}(\cos\varphi) = |\psi_{+}\rangle\rangle t_{+}\langle\langle\psi_{+}| + |\psi_{-}\rangle\rangle t_{-}\langle\langle\psi_{-}|.$$
(15)

The guarantee of the necessary positivity of these metrics reads  $t_{\pm} > 0$  and holds also, in the similar decoupled form, at all the higher dimensions N > 2. After the insertion of eigenvectors (14) in (15) we arrive at our first fully explicit matrix formula

$$\Theta \sim \begin{pmatrix} (1 - \cos\varphi)^2(t_+ + t_-) & (1 - \cos\varphi)\sin\varphi(-t_+ + t_-) \\ (1 - \cos\varphi)\sin\varphi(-t_+ + t_-) & \sin^2\varphi(t_+ + t_-) \end{pmatrix}.$$

$$\tag{16}$$

Its inspection reveals that up to an irrelevant overall factor it may be rewritten as a strictly equivalent superposition

$$\Theta^{(2)}(\lambda) = \alpha_1 M_1^{(2)}(\lambda) + \alpha_2 M_2^{(2)}(\lambda), \qquad \lambda = \cos \varphi, (17)$$

with the two new real free parameters  $\alpha_1 \propto t_+ + t_-$  and  $\alpha_2 \propto (-t_+ + t_-) \sin \varphi$  and with the following pair of manifestly  $\lambda$ -dependent sparse-matrix coefficients,

$$M_1^{(2)}(\lambda) = \begin{bmatrix} 1 - \lambda & 0 \\ 0 & 1 + \lambda \end{bmatrix}, \qquad M_2^{(2)}(\lambda) = \begin{bmatrix} 0 & 1 \\ 1 & 0 \end{bmatrix}.$$
(18)

Such a reparametrization modifies the overall multiplication factor in  $\Theta$  but it still leaves the positivity constraint very transparent,

$$\alpha_1 > 0, \qquad \alpha_1^2 (1 - \lambda^2) > \alpha_2^2, \qquad N = 2.$$
 (19)

We merely have to choose any  $\alpha_2$  from interval  $(-\alpha_1 \sin \varphi, \alpha_1 \sin \varphi)$ .

The mutual coupling between  $\alpha_1$  and  $\alpha_2$  is the price to be paid for the simplification of the  $\lambda$  dependence of the metric. At N=2, fortunately, the requirement of a bandmatrix form of  $\Theta$  implies that we have to set  $\alpha_2=0$  so that the positivity of the metric will be guaranteed by the

elementary inequality  $\alpha_1 > 0$ . At all the higher N = 2K > 2, similarly, the positivity of the metric will trivially be guaranteed by the set of requirements  $\alpha_1 > 0$  and  $\alpha_2 = \alpha_3 = \ldots = \alpha_N = 0$ . Although the domain of the positivity of the matrix  $\Theta^{(N)}(\lambda)$  will be perceivably larger at N > 2, its strict boundary can only be determined numerically in general (cf. also Ref. [28] for a very explicit sample study of the boundaries of the domain of positivity of the metric in the space of parameters).

# IV. COMPUTER-ASSISTED CONSTRUCTION OF ALL N METRICS $\Theta^{(N)}(\lambda)$ AT N=4 AND N=6

The mathematical study of the similarity relation

$$\Theta H = H^{\dagger} \Theta \tag{20}$$

between a Hamiltonian-type operator H and its adjoint  $H^{\dagger}$  dates back to early sixties [29]. In physics, the first use of such a feature of a sufficiently nontrivial and realistic Hamiltonian  $H \neq H^{\dagger}$  emerged much later [19]. In the so-called  $\mathcal{P}\mathcal{T}$ -symmetric quantum mechanics [10] an additional constraint has been accepted by which the metric  $\Theta$  is factorized into a product of parity  $\mathcal{P}$  and the so-called charge  $\mathcal{C}$  or quasiparity  $\mathcal{Q}$  [10,30].

In our present paper we shall simply use Eq. (20) as an (implicit) definition of all the eligible metrics  $\Theta = \Theta(H)$ . Our computer-assisted method of solving this linear set of algebraic equations for the matrix elements of  $\Theta$  will be straightforward, incorporating also all the standard requirements imposed upon the metric and listed, say, in [19]. A priori we shall not assume the existence of any other observable like charge or quasiparity. Hence, in our constructive considerations at finite dimensions only the necessary Hermiticity  $\Theta = \Theta^{\dagger}$  and positivity  $\Theta > 0$  of the metric must and will be required.

#### A. Ansatz at N=4

Hamiltonian  $H^{(4)}(\lambda)$  of Eq. (12) offers the first nontrivial simulation of the non-Hermitian dynamics, which is purely kinetic near its "distant" boundaries  $\pm L$  and which becomes dynamically nontrivial in the vicinity of the origin. The coupling  $\lambda$  merely connects two points in the middle of the lattice. The four eigenvalues of matrix  $H^{(4)}(\lambda)$  read

$$E_{\pm,\pm} = 2 \pm \frac{1}{2} \sqrt{6 - 2\lambda^2 \pm 2\sqrt{5 - 6\lambda^2 + \lambda^4}}$$
 (21)

and remain real in the *same* interval of couplings  $\lambda \in (-1, 1)$  as above. Symbolic manipulations on the computer enable us to find all the corresponding matrices of the metric

$$\Theta^{(4)}(\lambda) = \begin{bmatrix} \alpha_1(1-\lambda) & \alpha_2(1-\lambda) & \alpha_3 & \alpha_4 \\ \alpha_2(1-\lambda) & \alpha_1(1-\lambda) + \alpha_3(1-\lambda) & \alpha_4 + \alpha_2(1-\lambda^2) & \alpha_3 \\ \alpha_3 & \alpha_4 + \alpha_2(1-\lambda^2) & \alpha_1(1+\lambda) + \alpha_3(1+\lambda) & \alpha_2(1+\lambda) \\ \alpha_4 & \alpha_3 & \alpha_2(1+\lambda) & \alpha_1(1+\lambda) \end{bmatrix}.$$

They may be interpreted as the following sum with four variable real coefficients:

$$\Theta^{(4)}(\lambda) = \Theta^{(4)}_{[\alpha_1, \alpha_2, \alpha_3, \alpha_4]}(\lambda) 
= \alpha_1 M_1 + \alpha_2 M_2 + \alpha_3 M_3 + \alpha_4 M_4,$$
(22)

where each component is a sparse matrix carrying a specific  $\lambda$ -dependence,

$$M_{1} = \begin{bmatrix} 1 - \lambda & 0 & 0 & 0 & 0 \\ 0 & 1 - \lambda & 0 & 0 & 0 \\ 0 & 0 & 1 + \lambda & 0 & 0 \\ 0 & 0 & 0 & 1 + \lambda & 0 \end{bmatrix},$$

$$M_{2} = \begin{bmatrix} 0 & 1 - \lambda & 0 & 0 & 0 \\ 1 - \lambda & 0 & 1 - \lambda^{2} & 0 & 0 \\ 0 & 1 - \lambda^{2} & 0 & 1 + \lambda & 0 \end{bmatrix},$$

$$M_{3} = \begin{bmatrix} 0 & 0 & 1 & 0 & 0 \\ 0 & 1 - \lambda & 0 & 1 & 0 \\ 0 & 1 - \lambda & 0 & 1 & 1 \\ 1 & 0 & 1 + \lambda & 0 & 0 \end{bmatrix},$$

$$M_{4} = \begin{bmatrix} 0 & 0 & 0 & 1 & 0 \\ 0 & 1 & 0 & 0 & 0 \\ 1 & 0 & 0 & 0 & 0 \end{bmatrix}.$$

$$(23)$$

The first three items may also be treated as band matrices, i.e., as a diagonal, tridiagonal, and pentadiagonal matrix containing merely one, two, and three nonvanishing diagonals, respectively.

#### **B.** Positivity constraint

As we already indicated in Sec. III C the diagonal metric  $\Theta_{[1,0,0,0]}^{(4)}(\lambda) \equiv M_1^{(4)}(\lambda)$  remains safely positive definite inside the open interval of  $\lambda \in (-1,1)$ , with two plus two doubly degenerate eigenvalues  $\mu_{1,2}^{(-)} = 1 - \lambda$  and  $\mu_{1,2}^{(+)} = 1 + \lambda$ . The remaining three matrices in Eq. (23) are indefinite. Each of them possesses a pair of positive and a pair of negative eigenvalues, which are also easily obtainable in closed form.

Once we decide to fix  $\alpha_1=1$  and treat the remaining three parameters  $\alpha_2$ ,  $\alpha_3$ , and  $\alpha_4$  as small perturbations, we may also easily establish an allowed range of these perturbations for which the positivity of the metrics  $\Theta_{[1,\alpha_2,\alpha_3,\alpha_4]}^{(4)}(\lambda)$  remains robust and guaranteed.

Of course, starting from N=4 it is much less easy to describe the strict position of the  $\lambda$ -dependent boundary  $\partial \mathcal{D}$  of the *whole* (open) domain  $\mathcal{D}$  of our four real pa-

rameters  $\alpha_1(=1)$ ,  $\alpha_2$ ,  $\alpha_3$ , and  $\alpha_4$  in which the metric (22) is positive definite. At this boundary we may expect that the function  $F := \det\Theta^{(4)}_{[1,\alpha_2,\alpha_3,\alpha_4]}(\lambda)$  (which is equal to the product of the four eigenvalues of the metric in question) will vanish so that our specification of its zeros it needed. This task becomes particularly interesting in the maximally non-Hermitian dynamical regime, i.e., say, at the couplings  $\lambda = 1 - \varepsilon^2$  where the real variable  $\varepsilon$  remains very small and where the (real) energy levels of Eq. (21) get, pairwise, almost degenerate, with  $E_{0,1} = 1 \mp \varepsilon/\sqrt{2} + O(\varepsilon^2)$  while  $E_{2,3} = 3 \mp \varepsilon/\sqrt{2} + O(\varepsilon^2)$ .

In the zero-order approximation  $O(\varepsilon^0)$  we reveal, by direct computations, that the determinant F will vanish whenever  $\alpha_3 = \pm \alpha_4$ . For illustrative purposes, let us, therefore, accept this restriction to an exceptional subspace of parameters and choose the upper sign for the sake of definiteness. The same argument applied in the next-order approximation  $O(\varepsilon^2)$  leads to the specification of the next quantity  $\alpha_2 = 1 + \alpha_4/2$  and leaves just the single parameter in the metric unspecified,  $\alpha_4 := \gamma$ .

Along the boundary  $\partial \mathcal{D}$  we must have  $F = F(\gamma, \varepsilon) = 0$ . This is an equation that establishes an implicit polynomial relationship between  $\gamma$  and  $\varepsilon$ , i.e., between the "admissibility boundary" specifying the span of the positive-definite metrics inside their selected extremal subset and the strength of the interaction, respectively. Although the resulting particular curve  $\gamma = \gamma(\varepsilon)$  may be specified by a quadruplet of explicit formulae for the segments of its boundary,

$$\gamma = \gamma_{\pm}^{(\pm)} = -2 \pm \sqrt{4 \pm 2\epsilon \sqrt{8 - 4\epsilon^4 + \epsilon^6} + 4\epsilon^2 - 2\epsilon^4}.$$

Figure 1 offers a better display of all of its relevant features. We should emphasize that our considerations are now nonperturbative so that the independent variable  $\varepsilon \in (-\sqrt{2},\sqrt{2})$  need not stay small. The picture covers its full range. We may conclude that the interior of all of the four closed loops in Fig. 1 represents the prohibited area in which the determinant F is negative so that the requirement of the positivity of the metric matrix is manifestly violated there.

#### C. Verification of the ansatz at N=6

The  $\lambda$  dependence of all of the six eigenvalues of matrix  $H^{(6)}(\lambda)$  may be expressed in closed form as well. They all prove real [so that the metric  $\Theta^{(6)}(\lambda)$  exists] for all  $\lambda \in (-1,1)$ . The metric is obtainable either via its spectral representation [15,16] or, more easily, from Eq. (20), via its computer-assisted solution. The resulting matrices

 $\Theta^{(6)}(\lambda)$  form a six-parametric family

orm a six-parametric family 
$$\begin{bmatrix} \alpha_1(1-\lambda) & \alpha_2(1-\lambda) & \alpha_3(1-\lambda) & \dots \\ \alpha_2(1-\lambda) & \alpha_1(1-\lambda) + \alpha_3(1-\lambda) & \alpha_2(1-\lambda) + \alpha_4(1-\lambda) & \dots \\ \alpha_3(1-\lambda) & \alpha_2(1-\lambda) + \alpha_4(1-\lambda) & \alpha_1(1-\lambda) + \alpha_3(1-\lambda)(1-\lambda^2) + \alpha_5(1-\lambda) & \dots \\ \alpha_4 & \alpha_3(1-\lambda^2) + \alpha_5 & \alpha_2(1-\lambda^2) + \alpha_4(1-\lambda^2) + \alpha_6 & \dots \\ \alpha_5 & \alpha_4 + \alpha_6 & \alpha_3(1-\lambda^2) + \alpha_5 & \dots \\ \alpha_6 & \alpha_5 & \alpha_4 & \alpha_4 & \dots \end{bmatrix}$$

$$= \begin{bmatrix} \dots & \alpha_4 & \alpha_5 & \alpha_6 \\ \dots & \alpha_3(1-\lambda^2) + \alpha_5 & \alpha_4 + \alpha_6 & \alpha_5 \\ \dots & \alpha_2(1-\lambda^2) + \alpha_4(1-\lambda^2) + \alpha_6 & \alpha_3(1-\lambda^2) + \alpha_5 & \alpha_4 \\ \dots & \alpha_1(1+\lambda) + \alpha_3(1+\lambda)(1-\lambda^2) + \alpha_5(1+\lambda) & \alpha_2(1+\lambda) + \alpha_4(1+\lambda) & \alpha_3(1+\lambda) \\ \dots & \alpha_2(1+\lambda) + \alpha_4(1+\lambda) & \alpha_1(1+\lambda) + \alpha_3(1+\lambda) & \alpha_2(1+\lambda) \\ \dots & \alpha_3(1+\lambda) & \alpha_3(1+\lambda) & \alpha_2(1+\lambda) & \alpha_1(1+\lambda) \end{bmatrix}.$$

This formula can be read as a confirmation that in our model an optimal representation of the general metric will be based on the use of the general ansatz

$$\Theta^{(N)}(\lambda) = \sum_{j=1}^{N} \alpha_j M_j^{(N)}(\lambda). \tag{24}$$

Its  $\lambda$  dependence is solely carried by its N-dimensional sparse-matrix coefficients. The matrix elements  $(1 \pm \lambda)$  containing the minus sign always sit in the left upper

triangle (i.e., above the second diagonal) and *vice versa*. This antisymmetry of the sign of  $\lambda$  with respect to the reflection of the matrix  $\Theta^{(2K)}(\lambda)$  by its second diagonal simplifies the notation and will hold, incidentally, at all the integers  $K = 1, 2, \ldots$ 

The individual  $\lambda$ -dependent coefficients  $M_j^{(N)}(\lambda)$  are sparse matrices at all the dimensions N=2K. For illustration, the real and symmetric matrix  $M_K^{(2K)}(\lambda)$  may be recalled at K=4,

$$\begin{bmatrix} 1 - \lambda & 1 - \lambda^2 & 1 -$$

This expression exhibits a seven-diagonal band-matrix structure. The similar band-matrix structure will be exhib-

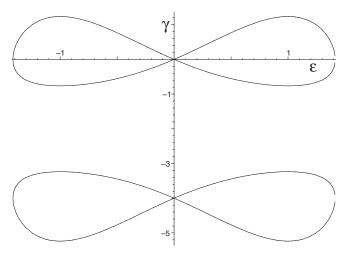


FIG. 1. The boundary curve  $\gamma = \gamma(\varepsilon)$ .

ited by all the matrices  $M_j^{(N)}(\lambda)$  at any N=2K and at all the subscripts j with the exception of the last one, j=N. Precisely this property of the matrix components of the metric (24) is responsible for the possibility of the introduction of a nontrivial fundamental length  $\theta$ .

#### V. EXTRAPOLATION TOWARD ANY N = 2K

Starting from N = 8, matrices  $M_j^{(N)}(\lambda)$  get large and cease to be printable easily. Still, the computer-supported symbolic manipulations with these matrices remain routine and straightforward. Moreover, their structure acquires certain features which enable us to extrapolate their low-N forms to all the even dimensions N = 2K and test the validity of our extrapolations, with much less effort, afterward.

One of the most important extrapolation tricks involves the observation that all of the matrix elements of metric components  $M_k^{(N)}(\lambda)$  form just the collection of the following sequence of polynomials:

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$$P_0 = 1,$$
  $P_1^{(\pm)} = 1 \pm \lambda,$   $P_2 = 1 - \lambda^2,$   $P_3^{(\pm)} = (1 \pm \lambda)(1 - \lambda^2),$   $P_4 = (1 - \lambda^2)^2,$  (25)  $P_5^{(\pm)} = (1 \pm \lambda)(1 - \lambda^2)^2,$   $P_6 = (1 - \lambda^2)^3, \dots$ 

Their allocation is also not too difficult.

#### A. Indexing arrays

Let us consider the mapping  $M_k^{(N)}(\lambda) \Leftrightarrow S_k^{(N)}$  between our matrix expansion coefficients and certain arrays of the same size. This specifies, uniquely, each  $\lambda$ -dependent matrix coefficient in series (24) using an auxiliary array. At the simplest choice of N=2 we have

$$M_1^{(2)}(\lambda) = \begin{bmatrix} P_1^{(-)} & 0\\ 0 & P_1^{(+)} \end{bmatrix} \Leftrightarrow S_1^{(2)} = \begin{bmatrix} 1\\ & 1 \end{bmatrix}, \quad (26)$$

$$M_2^{(2)}(\lambda) = \begin{bmatrix} 0 & P_0 \\ P_0 & 0 \end{bmatrix} \Leftrightarrow S_2^{(2)} = \begin{bmatrix} 0 \\ 0 \end{bmatrix}. \tag{27}$$

At N=4 this offers a method of an easy coding or reconstruction of the four matrices (23), proceeding via the following four indexing arrays  $S_j^{(4)}$  at j=1, 2, 3, 4, respectively:

The same observations can be formulated at N = 6 where the indexing arrays form the following sextuplet  $S_j^{(6)}$  at j = 1, 2, ..., 6, respectively:

Once we summarize these N=4 and N=6 computergenerated results as well as their N=8 and N=10descendants we reveal the existence of the following universal rules:

- (i) For any polynomial  $P_n^{(\pm)}$  entering any matrix element  $[M_j^{(N)}(\lambda)]_{ik}$  the superscripted  $\pm$  sign must be chosen as + when i > k or as when i < k or as absent when i = k.
- (ii) The indexing symbols  $S_k^{(N)}$  as defined by Eqs. (26) and (27) at k = 1, 2 and N = 2 get generalized to any dimension N = 2K. They always contain either empty entries or non-negative integer entries "n."
- (iii) The numerical value of each entry "n" must coincide with the value of the subscript n of the related matrix element  $P_n^{(\pm)}$  in the corresponding matrix  $M_{\nu}^{(N)}(\lambda)$ .

In light of these rules the complete determination of the functions  $M_j^{(N)}(\lambda)$  [needed in formula (24)] requires just the knowledge of the related indexing arrays  $S_j^{(N)}$ . The decoding  $S \to M$  using the above three rules would enable us to reconstruct all the metric matrices  $\Theta^{(2K)}(\lambda)$  via formulae (24) and (25). At any K the indexing arrays  $S_j^{(2K)}$  with arbitrary subscript  $j=1,2,\ldots,2K$  can be computed in recurrent manner. The description of the details of such a recipe will be provided in the rest of this section.

# B. Recurrences for off-central indexing arrays $S_i^{(2K)}, j \neq K$

The inspection of the symbols  $S_j^{(2K)}$  evaluated by the direct methods at the first few integers  $K=1,2,\ldots$  reveals that at any given N=2K the explicit form of the first K-1 matrices  $S_j^{(2K)}$  with  $j=1,2,\ldots,K-1$  may immediately be deduced from their predecessors  $S_j^{(2K-2)}$ . The core of such a recurrent construction consists in an enlargement of the dimension followed by a symmetric attachment of the two j plets of units "1" in the empty parts of the left upper corner and of the right lower corner.

The last K matrices  $S_{2K+1-j}^{(2K)}$  with  $j=1,2,\ldots,K$  become formed in similar manner. Their K predecessors  $S_{2K-1-j}^{(2K-2)}$  must be modified by attaching j zeros "0" in the right upper corner and in the left lower corner.

In both these "leftmost-subsequence" and "rightmost-subsequence" scenarios, the results displayed in Sec. VA offer a sufficiently instructive illustration of the recipe. They also indicate that at the "central" subscript j = K the construction of the most complicated missing member  $S_K^{(2K)}$  of the family must be discussed separately. Although it naturally belongs to the "leftmost" subsequence, its (2K-2)-dimensional predecessor (to be denoted as  $\mathcal{L}^{(2K-2)}$ ) proves different from the naively expected matrix  $S_K^{(2K-2)}$ .

## C. Recurrences for central indexing arrays $S_K^{(2K)}$

The sequence of the "middle" or central matrices  $S_K^{(2K)}$  should be treated as exceptional though still generated by a recurrent recipe. Its idea will rely on the use of specific predecessor matrices  $\mathcal{L}^{(2K-2)}$ . Of course, we shall proceed in the "leftmost-subsequence" manner enlarging the dimension of  $\mathcal{L}$  and filling K units 1 in the left upper corner and in the right lower corner.

In order to define the suitable predecessors  $\mathcal{L}^{(2K-2)}$  let us start from the old middle matrix  $S_{K-1}^{(2K-2)}$  and apply a specific two-step recipe. Firstly, we replace each "old" numerical element in  $S_{K-1}^{(2K-2)}$  by its successor, i.e., we replace old "0" by "1," old "1" by "2," etc. In the second step, we form a left-right reflection of the resulting matrix and arrive at the final form of the necessary predecessor  $\mathcal{L}^{(2K-2)}$  as a result. Thus, at N=4 we have the sequence

$$S_1^{(2)} = \begin{bmatrix} 1 & \\ & 1 \end{bmatrix} \rightarrow \begin{bmatrix} 2 & \\ & 2 \end{bmatrix} \rightarrow \mathcal{L}^{(2)} = \begin{bmatrix} & 2 \\ 2 & \end{bmatrix} \rightarrow S_2^{(4)}.$$

The recurrent reconstruction of the matrix  $S_{N/2}^{(N)}$  at N=6 will now result from adding six units 1 to the auxiliary predecessor matrix  $\mathcal{L}^{(4)}$  in the formula

$$S_{2}^{(4)} = \begin{bmatrix} 1 & & & & \\ 1 & & 2 & & \\ & 2 & & 1 \end{bmatrix} \rightarrow \begin{bmatrix} 2 & & & \\ 2 & & 3 & \\ & 3 & & 2 \end{bmatrix} \rightarrow \mathcal{L}^{(4)}$$

$$= \begin{bmatrix} & & 2 & \\ & 3 & & 2 \\ 2 & & 3 & \\ & 2 & & \end{bmatrix} \rightarrow S_{3}^{(6)},$$

etc. We may conclude that the central matrices  $S_K^{(2K)}$  at the respective K = 1, 2, 3, 4 (etc) form the sequence

$$\begin{bmatrix} 1 & 1 \\ & 1 \end{bmatrix}, \quad \begin{bmatrix} 1 & 2 \\ & 2 & 1 \end{bmatrix}, \\ \begin{bmatrix} 1 & 2 \\ & 2 & 1 \end{bmatrix}, \\ \begin{bmatrix} 1 & 3 & 2 \\ & 2 & 3 & 1 \\ & & 1 & \end{bmatrix}, \\ \begin{bmatrix} 1 & 3 & 2 \\ & 1 & 3 & 2 \\ & 1 & 3 & 2 \\ & 2 & 4 & 3 & 1 \\ & & 2 & 3 & 1 \\ & & & 2 & 1 \\ & & & & 1 & \end{bmatrix}$$

(etc). The general pattern of their recurrent production is obvious and our mathematical construction is complete.

#### VI. DISCUSSION

Our main mathematical result (24) represents the general metric matrix as its expansion in terms of its sparsematrix components  $M_j^{(N)}(\lambda)$ . The latter set has unambiguously been determined by certain elementary indexing arrays  $S_j^{(N)}$ . Let us now turn attention to some consequences of such a result in the context of physics.

#### A. Fundamental length $\theta$ at large N

Once we pick up the virtually trivial special case where  $\lambda \to 0$  our present toy-model Hamiltonians  $H^{(N)}(0)$  become Hermitian, i.e., tractable as operators of an observable quantity also in  $\mathcal{H}^{(F)}$ . Then the elements  $|\psi\rangle$  of this friendly Hilbert space may also be reinterpreted as acquiring an entirely standard probabilistic interpretation. This leads to a rather exotic arrangement (published in [18]) where the strict free-motion analogue of our present  $\lambda=0$  Hamiltonian has been assigned the family of nonstandard metric operators at  $N=\infty$ ,

$$\Theta^{\text{(Mostafazadeh)}} \sim I \cdot \cosh \kappa - \mathcal{P} \cdot \sinh \kappa.$$
 (28)

Here, symbol I represents the identity operator, while  $\mathcal{P}$  denotes parity and  $\kappa$  is an arbitrary real constant [cf. Eq. (64) in Ref. [18]]. The absence of any fundamental length has been postulated during the derivation of Eq. (28) in [18]. Thus, in our present Runge-Kutta discretization scenario the latter result may simply be interpreted, via identifications  $I \to M_1^{(N)}(0)$  and  $\mathcal{P} \to M_N^{(N)}(0)$ , as a particular choice of parameters with vanishing  $\alpha_2 = \alpha_3 = \ldots = \alpha_{N-1} = 0$  and nonvanishing  $\alpha_1 \neq 0$  and  $\alpha_N \neq 0$ . Thus, in our present terminology one has the vanishing elementary length  $\theta = 0$  at  $\kappa = 0$  and its unbounded alternative  $\theta = \infty$  at  $\kappa \neq 0$ .

Let us now assume, in contrast, the existence of a finite fundamental length in our schematic square-well-type example where the total width 2L of the well need not vary but where the dimension N=2K itself must always grow to infinity in continuous limit. In a preparatory step let us assume that N is fixed and that our toy-model metric  $\Theta^{(N)}(\lambda)$  is a (2R+1)-diagonal band matrix. In such a case the natural elementary-length candidate is  $\theta=2Rh=4LR/(N+1)\sim R$ .

In the next step where N starts growing the situation becomes more complicated because the elementary-length candidate  $\theta > 0$  should be kept N independent at large N. We arrive at the conclusion that whenever we try to fix  $\theta \neq 0$  and perform the limiting transition  $h \rightarrow 0$  (i.e.,  $N \rightarrow \infty$ ), we must let the number  $\sim 2R + 1$  of nonvanishing diagonals *grow* with the dimension. This is the reason why *all* the metrics must be available.

This observation enhances the relevance of our present solvable model where all the necessary constructions were exact. In some purely phenomenological applications of the theory with nontrivially nonlocal metric we may just search for some approximate results and keep the lattice spacing h fixed. Then we are allowed to fix the value of R and to select and construct just the particular subset of metrics with 2R+1 diagonals. Even in such an entirely pragmatic setting our present oversimplified example (which admitted the changes of both N and R) might still prove useful as a methodical guide.

Alternatively, we might pick up a nontrivial R > 0 and keep this integer (i.e., the number of diagonals in  $\Theta^{(N)}$ ) fixed even during the limiting transition  $N \to \infty$  (yielding, formally,  $\theta = 0$  of course). Then we still obtain the sequence of metrics, which may converge, typically, to a nontrivial operator  $\Theta^{(\infty)}$  represented by a generalized, momentum-dependent kernel entering an appropriate operator generalization of our present, smooth normalization integral (2), etc. Naturally, this is a promising but mathematically difficult possibility, which we could not address here.

#### B. The reality of the energies at large N

From our most elementary toy Hamiltonian  $H^{(2)}(\lambda)$  we deduced the energies most easily,  $E = E_{\pm}^{(2)} = 2 \pm \sqrt{1 - \lambda^2}$ . They remain real in the closed interval of  $\lambda \in (-1, 1)$ . The purely numerical analysis of a few further members  $H^{(N)}(\lambda)$  of the family reveals that the related energy spectra remain real in the same interval of the couplings  $\lambda \in (-1, 1)$ .

Empirically, the validity of this observation is illustrated here by Figs. 2 and 3. Sometimes, it may prove useful to reparametrize  $\lambda = \cos \varphi \in (-1, 1)$  with  $\varphi \in (0, \pi)$ , therefore (cf., e.g., Sec. III C above).

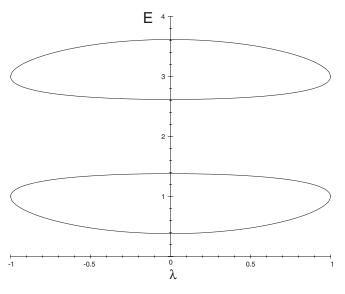


FIG. 2. Spectrum of  $H^{(4)}(\lambda)$ .

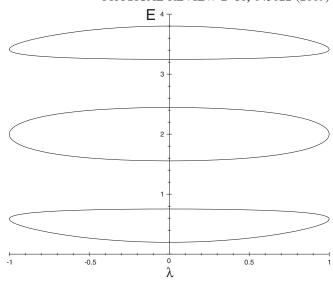


FIG. 3. Spectrum of  $H^{(6)}(\lambda)$ .

One should add that several other features of bound states (e.g., the evaluation of matrix elements of some operators of observables) remain transparent and well illustrated by our discrete short-range model  $H^{(N)}(\lambda)$  and, in particular, by its most elementary special cases (11)–(13).

## C. The role of $\mathcal{PT}$ and $\mathcal{CPT}$ symmetry

On the background of the existence and undeniable physical appeal of the so-called  $\mathcal{PT}$ -symmetric differential-equation models as reviewed by Bender [10] one reveals that also all the elements of our sequence of the Runge-Kutta discretized models can be incorporated in the same context. Indeed, our Hamiltonian matrices (11)–(13), etc. may be identified as  $\mathcal{PT}$  symmetric, provided only that we treat the operator  $\mathcal{T}$  as mediating transposition and that the parity  $\mathcal{P}$  is represented by the matrix with units along its second diagonal,

$$\mathcal{P}_{1,N} = \mathcal{P}_{2,N-1} = \ldots = \mathcal{P}_{N,1} = 1.$$

The specific merits of our discrete model involve, furthermore, the simplicity of mathematical analysis since we avoided the Rayleigh-Schrödinger-type perturbation expansions reported, in Refs. [18,21], as fairly difficult and complicated. In this context the Runge-Kutta discretization opened a way toward our straightforward and efficient application of linear-algebraic techniques.

The post-multiplication or premultiplication of any matrix H by the parity matrix  $\mathcal{P}$  mediates the left-right or updown reflection, respectively. We immediately see that our toy Hamiltonians are not only  $\mathcal{PT}$  symmetric but also, in the standard terminology of linear algebra,  $\mathcal{P}$ -pseudo-Hermitian [15] and  $\Theta$ -quasi-Hermitian [19]. In this spirit we may recollect Ref. [10] and try to factorize the metric  $\Theta = \mathcal{CP}$ . Without the usual additional constraint  $\mathcal{C}^2 = I$  this merely defines certain additional, "protocharge" operators  $\mathcal{C}$ . Vice versa, the incorporation of the constraint

 $C^2 = I$  converts the protocharge factors into the popular "charges" [10,31]. In principle, their existence imposes a fairly severe constraint upon our freedom in the choice of the parameters in the metric [32]. At the same time, these constraints may still be expected to leave some residual freedom in the domain  $\mathcal{D}$  of admissible parameters  $\alpha_j$  [18,33].

#### VII. SUMMARY AND OUTLOOK

In the mathematical part of our paper we presented an exact construction of the most general metric operator  $\Theta^{(N)}(\lambda)$  (i.e., of the most general positive-definite inner product) for one-parametric non-Hermitian matrix Hamiltonians  $H^{(N)}(\lambda)$  introduced in Ref. [11]. The construction proceeded in two steps. Firstly, the brute force use of a computer enabled us to generate an exhaustive list of all the admissible matrices  $\Theta^{(N)}(\lambda)$  at the first few (even) matrix dimensions N = 2K. In the second step, we revealed a clear pattern of the dependence of these lowdimensional matrices on their dimension N and on the coupling constant  $\lambda$ . This enabled us to arrange each  $\Theta^{(N)}(\lambda)$  as a linear superposition of its N elementary sparse-matrix components  $M_i^{(N)}(\lambda)$  with band-matrix structure. In the third step, an ansatz for the latter components has been found, and its validity has been confirmed by extrapolation and its subsequent facilitated verification. In the final, fourth step, the determination of the matrix elements in  $M_j^{(N)}(\lambda)$  was reduced to their indexing via arrays  $S_j^{(N)}$  with integer or empty entries defined via an elementary recurrent recipe.

Beyond the horizon given by our particular illustrative example we paid our main attention to the rather serious problem of the constructive approach to the models with fundamental length  $\theta$  and, in particular, to the practical feasibility of the necessary construction of the related, "fine-tuned" metric operators  $\Theta$ . We tried to overcome the well-known difficulties encountered, in the literature, during perturbation constructions of the metrics. We found a way how to get rid of at least some of the current methodical obstructions resulting from the immanent weakness of perturbation techniques. In this context, the so-called Runge-Kutta approximation techniques were found very productive and strongly recommendable.

In the parallel physics-motivated discussion of the relevance of our results in the abstract quantum theory as well as in its various applications we remind the readers, first of all, that our toy Hamiltonians  $H^{(N)}(\lambda)$  with  $N=\infty$  and  $\lambda \neq 0$  did already serve as a guide during the recent discussion and clarification of some conceptual problems concerning the quantum scattering by non-Hermitian point interactions [11]. In the present continuation of their study we succeeded in reconfirming the relevance of the similar schematic interaction models also in the theory of bound states.

Our main attention has been paid to conceptual questions again. We opposed, e.g., the frequently postulated absence of fundamental length in PT-symmetric and non-Hermitian models. The resolution of some concrete technical problems has been found. In particular we revealed that the extreme simplicity of our model opens an interesting nonperturbative way toward an innovative and fully constructive understanding of the emergence of an elementary length in the quantum system in question. We were also able to add a few new ideas to the lasting discussions concerning the interpretation of the presence of a fixed scale  $\theta > 0$  in quantum theory. We proposed that in the language using the concept of metric operators many theoretical considerations may remain feasible even when a nontrivial constant  $\theta$  is introduced. Last but not least we offered a few arguments supporting the possibility of using alternatives to the popular and widespread strategy that connects the "coordinate-smearing" quantity  $\theta > 0$ , indirectly and exclusively, to a hypothetical noncommutativity of classical coordinates.

#### **ACKNOWLEDGMENTS**

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#### APPENDIX A: SPARSE MATRICES $M^{(N)}(\lambda)$ AT $\lambda = 0$

The formal structure of the complete sets of metrics  $\Theta^{(N)}(\lambda)$  collected at the smallest dimensions  $N \leq 6$  gets fully transparent in the vanishing-potential limit  $\lambda \to 0$  when all the Hamiltonians become Hermitian in the N-dimensional Hilbert spaces  $\mathcal{H}^{(F)}$ . The textbook choice of the metric looks unique because people tacitly assume that there exists no nontrivial fundamental length in the theory (cf., e.g., Ref. [18]). In our present notation such an option coincides with the special case where  $\theta = 0$ ,  $\alpha_1 > 0$  (i.e., say,  $\alpha_1 = 1$ ) and  $\alpha_2 = \alpha_3 = \ldots = \alpha_N = 0$ .

Whenever we intend to build the theory where the choice of  $\theta > 0$  sets a nontrivial length scale, Hamiltonian H need not be non-Hermitian in  $\mathcal{H}^{(F)}$ . In our toy model at  $\lambda = 0$ , in particular, we may still define a non-Dirac metric using formula (24) with some nonvanishing values of parameters  $\alpha_2$  and  $\alpha_3$ , etc. It is only necessary to guarantee that the metric matrix itself remains positive (for illustration, recollect inequality (19), which specifies the full allowed range of parameters at N = 2).

Although our models  $H^{(N)}(\lambda)$  admit a nontrivial fundamental length  $\theta > 0$  even in their square-well limit  $\lambda = 0$  of Ref. [24], possible physics represented by such an extreme example looks rather artificial. Still, its methodical merits are remarkable. Firstly, the coefficient matrices  $M = M_j^{(N)}(0)$  become solely filled by the matrix elements

0 or 1. Secondly, their knowledge may prove useful for coding the indexing arrays in computer-assisted manipulations. Thirdly, the simplicity of the model implies that the j-th member of the sequence  $M_j^{(N)}(0)$  can be defined by the following closed formula:

$$(M_j^{(N)})_{ik}(0) = 1$$
 iff  $i - k = m$ ,  
 $N + 1 - i - k = n$ ,  
 $m = j - 1, j - 3, \dots, 1 - j$ ,  
 $n = N - j, N - j - 2, \dots, j - N$ , (A1)

and the verification of validity of this formula by its direct insertion in Eq. (20) is very quick. Fourthly, the existence of this and related formulae may prove useful for perturbation constructions in weakly non-Hermitian dynamical regime where  $|\lambda| \ll 1$ .

# APPENDIX B: OUR TOY HAMILTONIANS AT LARGE N

At a sufficiently large N our particular one-parametric Hamiltonians  $H^{(N)}(\lambda)$  may be interpreted as discrete versions of a differential operator with a point interaction localized in the origin. For a deeper understanding of such a correspondence let us abbreviate  $2-h^2E=\cos\epsilon$  as usual [24]. We may then treat  $\epsilon\in(0,\pi)$  as a new energy variable and visualize the wave functions  $\psi(x)$  with  $x\neq 0$  as satisfying a free-motion equation complemented by the respective left and right initial conditions  $\psi(-L)=\psi(L)=0$ . At a fixed L and in the  $N=2K\gg 1$  approximation these free-motion-like solutions must be further restricted by the pair of  $\lambda$ -dependent constraints near the origin

$$(1+\lambda)\psi(x_1) - 2\cos\epsilon\psi(x_0) + \psi(x_{-1}) = 0, \quad (B1)$$

$$\psi(x_2) - 2\cos\epsilon\psi(x_1) + (1 - \lambda)\psi(x_0) = 0.$$
 (B2)

In the limit  $h \to 0$  we may expect the emergence of a discontinuity in  $\psi(x)$  at x = 0. Even at all the finite  $N \sim 1/h \gg 1$  the wave functions remain well represented by their respective one-sided Taylor series near x = 0 so that Eqs. (B1) and (B2) may be interpreted as a matching condition. Once we return to the original energy variable  $h^2E = 2 - 2\cos\epsilon \equiv F$  and insert the truncated expansions

$$\psi(x_{-1}) = \psi_L(0) - \frac{3}{2}h\psi'_L(0) + \mathcal{O}(h^2),$$

$$\psi(x_0) = \psi_L(0) - \frac{1}{2}h\psi'_L(0) + \mathcal{O}(h^2),$$

$$\psi(x_1) = \psi_R(0) + \frac{1}{2}h\psi'_R(0) + \mathcal{O}(h^2),$$

$$\psi(x_2) = \psi_R(0) + \frac{3}{2}h\psi'_R(0) + \mathcal{O}(h^2)$$

in Eqs. (B1) and (B2), a straightforward algebra leads to the following elementary condition:

$$\frac{h}{2} \begin{pmatrix} -(1+\lambda) & F+1 \\ -(F+1) & 1-\lambda \end{pmatrix} \begin{pmatrix} \psi_R'(0) \\ \psi_L'(0) \end{pmatrix}$$

$$= \begin{pmatrix} 1+\lambda & F-1 \\ F-1 & 1-\lambda \end{pmatrix} \begin{pmatrix} \psi_R(0) \\ \psi_L(0) \end{pmatrix}, \tag{B3}$$

which matches the wave functions and their derivatives in the origin.

In the domain of sufficiently small h > 0 the latter relation is equivalent to the original constraints (B1) and (B2). We may conclude that at all the nonvanishing small h > 0 our conditions (B3) leave our interaction in the origin translucent and manifestly energy dependent.

Various special cases of our  $N \gg 1$  bound-state model may be studied noticing, for example, that the energy dependence disappears in the low-excitation regime where the quantity  $F = h^2 E$  remains negligible. At a generic energy F > 0 the above set of h > 0 solutions must be complemented by the two additional, anomalous bound states emerging at the two exceptional energies  $F = F_{+} =$  $1 \pm \sqrt{1 - \lambda^2}$ , which make the coefficient matrix singular. At these energies, both the values of  $\psi_{RL}(0)$  are, in general, nonvanishing and firmly determined by our choice of the two derivatives  $\psi'_L(-L)$  and  $\psi'_R(L)$  at  $x = \pm L$ , respectively. Thus, both the left and right branches of our two exceptional bound states are obtained by the same matching in the origin as above. Their specific feature is that at both our exceptional energies  $F_{\pm}$  the two lines of Eq. (B3) degenerate, at all the sufficiently small  $h \approx 0$ , to the single  $\psi_R(0)\sqrt{1+\lambda} \pm \psi_L(0)\sqrt{1-\lambda} = 0.$ constraint manifestly asymmetric wave functions are obtained.

In the continuum limit  $N \to \infty$  our sequence of the matrix Hamiltonians  $H^{(N)}(\lambda)$  can be reinterpreted as a series of dynamical models that converge to a specific differential equation with a point interaction potential in the origin. It is easily seen that at a generic energy E the  $h \to 0$  limit of Eq. (B3) leads to the vanishing  $F = \mathcal{O}(h^2)$  so that the above-mentioned "exceptional" solutions disappear from the spectrum. At any  $\lambda \neq 0$ , only the elementary opaque-wall constraint  $\psi_R(0) = \psi_L(0) = 0$  survives and leads, say, to the two independent series of bound-state solutions, which live solely on the left or right half-interval of x, respectively.

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