Gegenbauer-solvable quantum chain model

Miloslav Znojil*
Nuclear Physics Institute ASCR, 250 68 Řež, Czech Republic
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An N-level quantum model is proposed in which the energies are represented by an N-plet of zeros of a suitable classical orthogonal polynomial. The family of Gegenbauer polynomials $G(n,a,x)$ is selected for illustrative purposes. The main obstacle lies in the non-Hermiticity (aka crypto-Hermiticity) of Hamiltonians $H \neq H^\dagger$. We managed to (i) start from elementary secular equation $G(N,a,E_n)=0$, (ii) keep our H, in the nearest-neighbor-interaction spirit, tridiagonal, (iii) render it Hermitian in an *ad hoc*, nonunique Hilbert space endowed with metric $\Theta \neq I$, (iv) construct eligible metrics in closed forms ordered by increasing nondiagonality, and (v) interpret the model as a smeared N-site lattice.

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I. INTRODUCTION

In atomic, molecular, nuclear, and solid-state physics the simulation of quantum phenomena via *finite-dimensional* Schrödinger equations,

$$H^{(N)}\left|\psi_n^{(N)}\right\rangle = E_n^{(N)}\left|\psi_n^{(N)}\right\rangle, \tag{1}$$

is often motivated numerically. Indeed, whenever a realistic Hamiltonian gets approximated by its suitable N-by-N simplification $H = H^{(N)}$, the numerical solution of Eq. (1) becomes routine [1], especially when our finite-dimensional Hamiltonian is chosen to be tridiagonal,

$$H^{(N)} = \begin{bmatrix} a_0 & c_0 & 0 & 0 & \ldots & 0 & 0 \\ b_1 & a_1 & c_1 & 0 & \ddots & & 0 \\ 0 & b_2 & a_2 & c_2 & \ddots & \ddots & \vdots \\ 0 & 0 & \ddots & \ddots & \ddots & 0 & 0 \\ \vdots & \ddots & \ddots & b_{N-3} & a_{N-3} & c_{N-3} & 0 \\ 0 & & \ddots & 0 & b_{N-2} & a_{N-2} & c_{N-2} \\ 0 & 0 & \ldots & 0 & 0 & b_{N-1} & a_{N-1} \end{bmatrix}. \tag{2}$$

At a fixed N, various N-by-N matrix problems (1) + (2) are often used in ambitious phenomenological considerations since matrices $H^{(N)}$ (sometimes reinterpreted as the so-called chain-model Hamiltonians or lattice Hamiltonians with the nearest-neighbor interaction) may mimic, say, a solid-state spectrum of energies in condensed-matter physics. These concepts found new applications in the context of apparently non-Hermitian versions (we would rather call them "hiddenly Hermitian" or "crypto-Hermitian" [2] versions) of the XXZ spin chains [3], Bose-Hubbard models [4], Friedrichs-Fano-Anderson tight-binding lattice models [5], tightly bound lattices of electrons [6], optical lattices [7], etc. There exist many other articles which are also certainly worth mentioning. In their incomplete complementary sample we draw the attention of the reader to the close connections between non-Hermitian chain models and the so-called Reggeon field theory [8] or to Ising model and quantum spin chains [9].

The combined mathematical and physical appeal of the generic discrete and tridiagonal models (2) seems partially marred by the more or less purely numerical [10] or perturbative [11] nature of their solution. For this reason, analytically solvable models are often preferred in analysis [12]. Some authors simplified mathematics by paying attention to the effects connected with the restricted, one-parametric variation of the end-site-interaction matrix elements c_j and b_{j+1} with $j=0$ and $j=N-2$ in Eq. (2) [6,13].

Marginally, we could add that similar discrete solvable models with pairs of pointlike interactions played an important role in the recent extensive discussion of some conceptual problems of crypto-Hermitian quantum scattering [14,15]. In this context, a lot of misunderstandings emerged when people forgot to distinguish between the "formal coordinate" x [often chosen as playing the role of the argument in wave functions $\psi(x)$] and the "observable coordinate" (a position-operator eigenvalue denoted by another symbol, say, q). In a very well-written article [16], an interested reader may find a good explanation of this subtlety emerging as highly relevant even on the very elementary level of mathematics used in introductory textbooks on quantum mechanics.

Once one moves to the more sophisticated crypto-Hermitian models where the formal coordinate x itself ceases to be observable, the concept of "locality" must be reconsidered and used with enhanced care. For example, a very instructive comment given in Sec. 5 of Ref. [17] shows that the formal wave function of a physical *localized* state may look nonlocal as a function $\psi(x)$ of the formal coordinate x.

Alternatively, it has been noticed and emphasized by Jones [14] that in virtually any experimentally oriented setup we usually treat interaction V as if it were *prepared* as a specific function of the measurable coordinate q. In this sense, the crucial role of the specification of observables and of the difference between x and q gets even more important in a non-Hermitian setting [18].

In order to circumvent similar complications, a number of articles studied just bound-state problems and preferred their exactly solvable non-Hermitian models [19]. The

*znojil@ujf.cas.cz

solvability-guaranteeing simplifications may reduce the menu of interesting phenomena. Typically, the simplified models explain the emergence of fragile, unstable components in the spectra [20] but they can hardly compete with realistic models in offering sufficient variability of the parametric dependence of the energies [4]. The spectra obtained in the simplified solvable model of Ref. [6] admit, for example, just a very special form of the confluence of energy pairs, while a much richer menu of quantum catastrophes of this category may exist in general [21].

A remedy has been found in Ref. [22]. We revealed that there exist *non-numerical* chain models or quantum lattices (2) with a much less restricted qualitative variability of spectra. These models were characterized by a delocalized interaction exhibiting an up-down symmetry. The pairs of sites with indices m and $N-m$ were allocated the *same* strength of impurity or interaction. Although the productivity of such an artificial assumption was reconfirmed, say, in Refs. [6] and [23], its physical interpretation remained obscure. One would like to have some exactly solvable quantum-lattice models *without* such a symmetry. This motivated our present analysis during which we develop another class of solvable quantum-lattice models of form (2) without similar nonlocal, long-range auxiliary correlation.

II. GEGENBAUER-POLYNOMIAL QUANTUM LATTICE

In connection with the definition of the concept of solvability, misunderstandings frequently emerge. The puzzle may find different resolutions. In a context-dependent way the property of being solvable is assigned, for example, to differential Hamiltonians $H=p^2+V(x)$ for which *all* of the wave functions $\langle x|\psi_n\rangle$ of bound states prove proportional to suitable classical orthogonal polynomials [24]. In our present article we transfer such a definition of exact solvability to the difference and finite-matrix equations. Thus, we *postulate* that the N-plet of our N-dimensional bound-state vectors $|\psi_n\rangle$ in Eq. (1) is given in advance.

Naturally, the most straightforward definition of these vectors would specify them directly in terms of some classical orthogonal polynomials. For the sake of brevity we pay attention solely to Gegenbauer polynomials $G(n,a,x)$ $(=C_n^a(x)$ in [25] or $C_n^{(a)}(x)$ in [26]; our notation is taken from MAPLE [27]). As long as these (sometimes called ultraspherical) polynomials degenerate to the different (viz., Chebyshev) polynomials at $a=0$, we assume that $a>0$. In this case they satisfy the well-known recurrence relations

$$nG(n,a,x)=2(n+a-1)xG(n-1,a,x)-(n+2a-2)G(n-2,a,x) \tag{3}$$

at $n=1,2,\ldots,$ with initial $G(0,a,x)=1$ and $G(1,a,x)=2ax$.

In the initial step of our constructive considerations, we guarantee the validity of our aforementioned matrix Schrödinger Eq. (1) by assuming its formal coincidence with the truncated version of recurrences (3). This means that we just use the following input form of the bound-state eigenvector,

$$|\psi_n^{(N)}\rangle=\begin{pmatrix}\langle 0|\psi_n^{(N)}\rangle=G(0,a,E_n)\\ \langle 1|\psi_n^{(N)}\rangle=G(1,a,E_n)\\ \vdots\\ \langle N-1|\psi_n^{(N)}\rangle=G(N-1,a,E_n)\end{pmatrix}, \tag{4}$$

and determine the nth energy level E_n as the value of coordinate x at which recurrences (3) terminate. Thus, every energy will coincide with one of the roots of the closed-form secular equation

$$G(N,a,E_n)=0. \tag{5}$$

Our Gegenbauerian Hamiltonian $H=H(a)$ just mimics recurrences (3). Its main diagonal vanishes [i.e., we set $a_0=a_1=\cdots=0$ in (2)] and the pair of nonvanishing neighboring diagonals are composed of elements numbered by $j=0,1,\ldots,N-2$,

$$\begin{aligned}c_j&=c_j(a)=1/(2a+2j),\\ b_{j+1}&=b_{j+1}(a)=(2a+j)/(2a+2j+2).\end{aligned} \tag{6}$$

This idea forms the starting point of our abstract message in its concrete Gegenbauer-polynomial realization. Within the more general class of quantum lattices and discrete models (2) exemplified by such a choice, the matrix elements are real but the matrix H itself is, generically, asymmetric, that is, non-Hermitian. Fortunately, its spectrum is real (i.e., potentially observable) so that we are allowed to treat this H as an *exactly solvable* effective Hamiltonian of a quantum system with the prescribed segment of spectrum fitted by an N-plet $E_n^{(N)}(a)$ of roots of Gegenbauer polynomial $G(N,a,E)$.

III. (HIDDEN) HERMITICITY

It is known that the manifest non-Hermiticity feature does not disqualify operator $H\neq H^\dagger$ from being used as a Hamiltonian of a quantum system. After all, not-too-dissimilar non-Hermitian phenomenological Hamiltonians (complex and acting in a finite-dimensional vector space) were used in Refs. [3–7]. An interested reader may find a compact introduction to quantum theory with similar crypto-Hermitian Hamiltonians either in our review [2] or in this section.

In essence, we must get rid of the over-restrictive and most elementary (often called "Dirac's" [28]) requirement of the current but very special Hermiticity defined via the mere vector or matrix transposition accompanied by complex conjugation. This defines dual vectors called, in the conventional textbook language, "Dirac's bra vectors,"

$$\mathcal{T}^{(\mathrm{Dirac})}:\ |\psi\rangle\ \to\ \langle\psi|. \tag{7}$$

The choice of $\mathcal{T}^{(\mathrm{Dirac})}$ (represented by appending superscript † when applied to operators) is *not* the only option. In models with Dirac non-Hermiticity $H\neq H^\dagger$ we must *necessarily* use another, less trivial definition of Hermitian conjugation. The point is that after such a change of definition our operator H must become self-adjoint and compatible with postulates of quantum mechanics.

The transition to general Hermitian conjugation requires a modification of conventional notation. First, the "new" dual vectors must be defined by the generalized formula

$$\mathcal{T}^{(\Theta)}: \ |\psi\rangle \ \to \ \langle\langle\psi| := \langle\psi|\Theta, \tag{8}$$

where matrix Θ is called "metric" [18] and where, whenever $\Theta \neq I$, the resulting dual vectors are marked as "brabras." Second, the same danger of misunderstanding threatens the application of the non-Dirac Hermitian conjugation to operators $\mathcal{A}$; therefore, we recommend that it be marked by a different (viz., doubled) superscript:

$$\mathcal{A} \ \to \ \mathcal{A}^{\ddagger} := \Theta^{-1}\mathcal{A}^{\dagger}\Theta. \tag{9}$$

In the spirit of any good textbook on linear algebra, functional analysis, or quantum mechanics, the metric must be invertible, Hermitian, and positive definite [18]. After two notation innovations [Eqs. (8) and (9)], the formalism of quantum theory remains unchanged. On the level of notation the symbol of double bras ($\langle\langle$) will replace all the Dirac's simple bras ($\langle$), especially whenever a mean value, physical probability, or measurements are concerned. Similarly, in formulas carrying physical meaning, the simple superscripts † must be all replaced by their doubled forms ‡. The "false" representation $\mathcal{H}^{(F)}$ of the Hilbert space with the Dirac's unacceptable $\Theta^{(F)} = I$ must *consequently* be replaced by the "standard" Hilbert space $\mathcal{H}^{(S)}$ of physical states ψ.

IV. HILBERT-SPACE METRICS

From the pragmatic point of view, the theoretical imperatives of the preceding section may be softened, during practical calculations, by staying in the naive (and, by assumption, much friendlier) Hilbert space $\mathcal{H}^{(F)}$ and by the treatment of the obligatory doubled bras $\langle\langle$ of Eq. (8) and doubled superscripts ‡ of Eq. (9) as mere abbreviations. In Ref. [2] we summarized further reasons for a *parallel* use of spaces $\mathcal{H}^{(S)}$ together with their "friendly-false" partners $\mathcal{H}^{(F)}$. First, just the knowledge of the matrix Θ (which must be self-adjoint in $\mathcal{H}^{(F)}$ [18]) is fully sufficient for all purposes. Second, the key guarantee of unitarity of the evolution generated by H in $\mathcal{H}^{(S)}$ (where $H = H^{\ddagger}$ and $\Theta \neq I$) becomes more easily understandable in $\mathcal{H}^{(F)}$ via "translations" (8) and (9). In fact, a deeper explanation of this point deserves a separate paragraph, which follows.

A. Dieudonné equation

In Ref. [2] we explained the way in which the Hermiticity of H in $\mathcal{H}^{(S)}$ (based on the nontriviality of metric $\Theta^{(S)} \neq I$) may be understood as equivalent to the manifest Hermiticity of a suitable isospectral operator:

$$\mathfrak{h} = \Omega H \Omega^{-1} = \mathfrak{h}^{\dagger}. \tag{10}$$

The latter operator is defined, in principle, in another, third Hilbert space $\mathcal{H}^{(P)}$ with trivial metric $\Theta^{(P)} = I$ (the superscript stands for "paternal" or "physical"). It is assumed that spaces $\mathcal{H}^{(P)}$ and $\mathcal{H}^{(S)}$ are unitary equivalent so that we may recall Eq. (9), deduce

$$\mathfrak{h}^{\dagger} = (\Omega^{-1})^{\dagger} H^{\dagger} \Omega^{\dagger}, \tag{11}$$

abbreviate $\Omega^{\dagger}\Omega := \Theta$, and end up with the relation

$$H^{\dagger}\Theta = \Theta H, \tag{12}$$

dating back to the old article by Dieudonné [29]. That is why we call Eq. (12) "Dieudonné's equation" in what follows, keeping in mind that this is meant in a loose sense since Dieudonné himself admitted that Θ in (12) might not be invertible.

For our finite-dimensional real Hamiltonians $H = H^{(N)}$ which are given in advance, the latter equation forms the set of N^2 constraints imposed upon the $[N(N+1)/2]$-plet of the unknown real matrix elements of matrix $\Theta = \Theta^{\dagger}$. Our task may now be formulated as a non-numerical construction of complete solution of this linear algebraic system.

B. The method of solution

The constructive way of making Hamiltonian H and metric Θ compatible with Dieudonné's Eq. (12) is not too easy in general. The main result of our article is the non-numerical construction of the *general* metric Θ, which satisfies Eq. (12) for the Gegenbauerian input Hamiltonian $H^{(N)}(a)$. *Ipso facto*, this also makes our Hamiltonian self-adjoint in the respective physical Hilbert space $\mathcal{H}^{(S)}$.

In full detail, the construction of metrics are described in Sec. VI. In a preparatory phase, let us now just explain its key ideas. First, in the light of the linearity of Eq. (12), we assume that the metric may be sought in the form of superposition of certain simpler matrices $\mathcal{P}$ which satisfy the same equation,

$$\big(H^{(N)}(a)\big)^{\dagger}\mathcal{P} = \mathcal{P}H^{(N)}(a), \tag{13}$$

but which are not necessarily invertible or positive definite. Second, we assume that these "pseudometric" matrices form an N-plet of linearly independent solutions $\mathcal{P} = \mathcal{P}_k^{(N)}(a)$ with $k = 0, 1, \ldots, N-1$. This enables us to search for the metric in the form

$$\Theta = \Theta^{(N)}(\vec{\alpha}, a) = \alpha_0 \Theta_0^{(N)}(a) + \sum_{k=1}^{N-1} \alpha_k \mathcal{P}_k^{(N)}(a), \tag{14}$$

where the variability of the N-plet of real parameters $\vec{\alpha} = (\alpha_0, \alpha_1, \ldots, \alpha_{N-1})$ is only restricted by the requirement of the positivity of the matrix $\Theta^{(N)}(\vec{\alpha}, a)$.

The concrete implementation of the requirement of the simplicity of the individual auxiliary pseudometrics $\mathcal{P}_k$ is model-dependent. For our present model their explicit construction proved feasible when we assumed that every $\mathcal{P}_k$ is a $(2k+1)$-diagonal matrix. This assumption itself resulted from the experience which we gained during the similar constructions of metrics as performed in Ref. [30]. This experience also facilitated the organization of our concrete recurrent calculations.

The key idea of our present non-numerical algorithm of solution of Eq. (13) remained the same as in Ref. [30]. In concrete applications we see how this recipe employs the chess-board-like "coloring" of elements of relevant matrices. In this manner, each Hamiltonian H gets separated into its "white-field matrix elements" (say, all elements $H_{j,k}$ with $|j-k| =$ even) and "black-field matrix elements" (i.e., elements $H_{j,k}$ with $|j-k| =$ odd). Once the same coloring is applied

to the ansatz for the metric Θ [or rather to each indefinite and sparse pseudometric $\mathcal{P}_k^{(N)}(a)$], one is immediately able to decompose Eqs. (12) and (13) into their "same-color" subsystems and develop and employ some suitable ansatzs for their recurrent solution.

One should not forget that even before finishing the systematic construction of *all* of the components $\mathcal{P}_k^{(N)}(a)$ of the metric we may interrupt the process and turn attention to the truncated versions of series (14),

$$\Theta_k^{(N)}(\vec{\alpha}',a) = \Theta_0^{(N)}(a) + \sum_{j=1}^{k} \alpha_j \mathcal{P}_j^{(N)}(a). \tag{15}$$

Here the mere k free parameters α_j appear arranged in a shorter, primed array $\vec{\alpha}'$. One should also pay attention to the fact that in Ref. [30], as well as in our present model, the k-subscripted special metrics (15) still remain sparse, containing just $2k+1$ nonvanishing diagonals. The latter observation will certainly facilitate our ultimate task of imposing the positivity requirements upon expansions (14) or (15) of the metric.

V. DIAGONAL METRICS

A. The construction of $\Theta_0(a)$

All the details of the implementation of our preceding recipe depend on the form of the input Hamiltonian H. For its Gegenbauerian choice given by Eq. (6), this Hamiltonian is an extremely elementary, purely black-field matrix, rendering the recurrent solution of Eq. (12) particularly straightforward. For illustration purposes, let us now consider the diagonal (i.e., $k=0$) ansatz

$$\Theta_0(a) = \begin{bmatrix} \theta_0 & 0 & \ldots & 0 & 0 \\ 0 & \theta_1 & 0 & \ldots & 0 \\ \vdots & \ddots & \ddots & \ddots & \vdots \\ 0 & \ldots & 0 & \theta_{N-2} & 0 \\ 0 & 0 & \ldots & 0 & \theta_{N-1} \end{bmatrix}. \tag{16}$$

As long as the individual matrix elements do *not* vary with the growth of dimension N, we may leave the value of N unspecified. The inspection of recurrences (12) then reveals that they connect just equal-color elements. This means that, *a priori*, ansatz (16) may lead to nontrivial solutions. We may start their recurrent construction from any nonvanishing element, say, from $\theta_0 = 2a^2$. After a comparatively tedious algebra, this choice of normalization leads to the compact and transparent final result with $\theta_1 = a+1$ and with

$$\theta_j = \frac{a+j}{(1+2a)(2+2a)\cdots(j-1+2a)} \tag{17}$$

at all the remaining $j = 2,3,\ldots,N-1$.

B. A comment on matrices $\mathfrak{h}$

An important feature of the previously constructed metric $\Theta_0(a)$ is that it is easily invertible and manifestly positive definite at any $a > 0$ and any $N \geqslant 1$. The existence of such a metric is an important merit of the model because we may now recall relation (10), define the matrix elements of the simplest auxiliary matrix $\Omega = \Omega_0$,

$$(\Omega_0)_{mn} = \delta_{mn}\sqrt{\theta_n}, \tag{18}$$

and obtain finally the simplest explicit partner Hamiltonian,

$$\mathfrak{h}_0^{(N)}(a) = \begin{bmatrix} 0 & \mu_0 & 0 & 0 & \ldots & 0 \\ \mu_0 & 0 & \mu_1 & 0 & \ddots & \vdots \\ 0 & \mu_1 & 0 & \mu_2 & \ddots & 0 \\ \vdots & \ddots & \ddots & \ddots & \ddots & 0 \\ 0 & \ldots & 0 & \mu_{N-3} & 0 & \mu_{N-2} \\ 0 & \ldots & 0 & 0 & \mu_{N-2} & 0 \end{bmatrix}, \tag{19}$$

acting in space $\mathcal{H}^{(P)} = \mathcal{H}_0^{(P)}$, isospectral with our original non-Hermitian matrix $H^{(N)}(a)$ and possessing matrix elements easily derived in closed form,

$$\mu_k = \frac{1}{2}\sqrt{\frac{2a+k}{(a+k)(a+k+1)}}, \quad k = 0,1,\ldots,N-2. \tag{20}$$

Due to the unitary equivalence between Hilbert spaces $\mathcal{H}_0^{(P)}$ and $\mathcal{H}^{(S)} = \mathcal{H}_0^{(S)}$, we may conclude that Eq. (16) represents the simplest possible Hermitization of our Gegenbauer-oscillator Hamiltonian $H^{(N)}$.

The existence of the partner Hamiltonian (19) trivially reconfirms the well-known fact that the spectra of energies $E_n^{(N)}(a)$ defined by Eq. (5) are all real [26]. Moreover, the manifest positivity and diagonality of $\Theta_0(a)$ makes the explicit construction of matrix Ω_0 virtually trivial. The latter observation is not easily transferred to other models. For example, interested readers may consult Ref. [17] showing that and in which way a very simple Hamiltonian H may be assigned extremely complicated isospectral partners $\mathfrak{h}$.

Exceptions to the latter generic rule exist. In the present context of models on lattices a typical one has been found in Ref. [31]. A nondiagonal, band-matrix metric Θ has been shown there to admit a transparent, sparse-matrix structure of factors in $\Theta = \Omega^\dagger\Omega$, as well as of the corresponding isospectral Hamiltonian $\mathfrak{h}$. Of course, this type of result must be considered exceptional. Formally, the reason is that the use of formula (10) which defines the partner Hamiltonian $\mathfrak{h}$ requires the explicit knowledge of the inverse matrix Ω^{-1}, which is usually not a sparse matrix even if Ω itself is.

This being said, it is necessary to admit that one cannot exclude that our present Gegenbauerian example will prove exceptional and that it will also admit the existence of compact formulas for $\mathfrak{h}$, for example, at some coordinate-smearing choice of $k = k_{(\text{exceptional})} \geqslant 1$. With the notable exception of our knowledge of tridiagonal $k_{(\text{exceptional})} = 0$ matrix (19), the existence and possible structure of such formulas constitute an open problem at present. In fact, the lack of our explicit knowledge of all of the manifestly Hermitian Hamiltonians $\mathfrak{h}$ hinders, first of all, the most common strategy of interpretation of the system in question illustrated, for example, in Ref. [32] and based on the correspondence principle applied directly inside $\mathcal{H}^{(P)}$.

A positive aspect of the existence of missing parts of the puzzle is that if any relevant matrix $\mathfrak{h}$ really remained sufficiently simple and defined in closed and compact form, all the reasons for working with its equivalent representation H in $\mathcal{H}^{(S)}$ would, in fact, be lost. The situation is similar to the preference of H in nuclear physics [18] where the more complicated partner $\mathfrak{h}$ is even well known in advance. The same preference of the maximally simple representation of the Hamiltonian remains recommended for concrete calculations even though we proceed here in the opposite direction, viz., from the choice of H to the construction of its Hermitizations mediated by Θs in alternative Hilbert spaces $\mathcal{H}^{(S)}$.

VI. BAND-MATRIX METRICS

It has been explained in Refs. [15] and [30] that tridiagonal metrics, that is, in our case, the one-parametric family of matrices,

$$\Theta_1^{(N)}(\alpha_1,a) = \Theta_0^{(N)}(a) + \alpha_1 \mathcal{P}_1^{(N)}(a), \tag{21}$$

simulate a nearest-neighbor smearing of coordinates while the pentadiagonal metrics,

$$\Theta_2^{(N)}(\alpha_1,\alpha_2,a) = \Theta_0^{(N)}(a) + \alpha_1 \mathcal{P}_1^{(N)}(a) + \alpha_2 \mathcal{P}_2^{(N)}(a), \tag{22}$$

may mimic a next-to-nearest neighborhood smearing, etc. In this manner the index k in Eq. (15) is tractable as a certain measure of a *dynamical*, Hilbert-space-related "nonlocality" of the quantized lattices in question.

A. Tridiagonal metrics $\Theta_1^{(N)}(\alpha_1,a)$

In Gegenbauer example (6) all the generalized $k = 1,2,\ldots$ metrics (14) may be constructed in closed form, non-numerically, by the recurrent solution of Eq. (12). After some trial-and-error experimenting, the first nontrivial, tridiagonal metric $\Theta_1^{(N)}(\alpha_1,a)$ (containing just the single item in the primed array of parameters $\vec{\alpha}' \equiv \alpha_1$) may be found via the tridiagonal (or, more strictly speaking, bidiagonal) $k = 1$ ansatz for its only nontrivial sparse-matrix component:

$$\mathcal{P}_1^{(N)}(a) = \begin{bmatrix} 0 & \kappa_1 & 0 & \ldots & 0 & 0 \\ \kappa_1 & 0 & \kappa_2 & 0 & \ldots & 0 \\ 0 & \kappa_2 & 0 & \kappa_3 & \ddots & \vdots \\ \vdots & \ddots & \ddots & \ddots & \ddots & 0 \\ 0 & \ldots & 0 & \kappa_{N-2} & 0 & \kappa_{N-1} \\ 0 & 0 & \ldots & 0 & \kappa_{N-1} & 0 \end{bmatrix}. \tag{23}$$

The combined use of the experience and computer algebra leads to the truncation-independent result. Using the convenient initial $\kappa_1 = 2a$ and $\kappa_2 = 1$, one obtains the closed formula

$$\kappa_j = \frac{1}{(1+2a)(2+2a)\cdots(j-2+2a)} \tag{24}$$

for the solution (23) of Eq. (12) valid at all $j = 3,4,\ldots,N-1$. Let us re-emphasize that these matrix elements exhibit the remarkable property of not changing their form with the matrix dimension N.

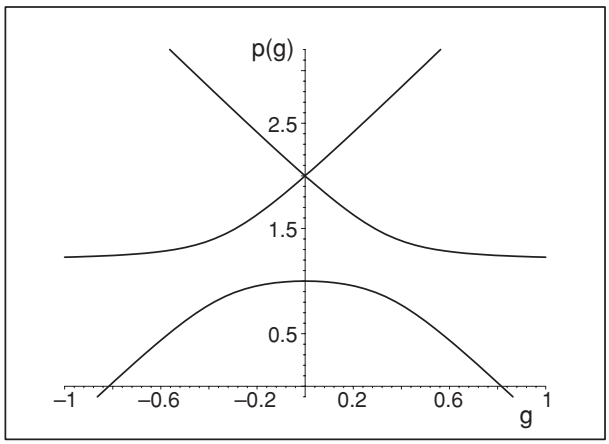

FIG. 1. Three eigenvalues $p = p(g)$ of metric $\Theta_1^{(3)}(g,1)$.

B. The domains of positivity of metrics $\Theta_1^{(N)}(\alpha_1,a)$

It is worth noticing that the positive definiteness of the tridiagonal metrics (21) would be lost for larger $\alpha_1 > \alpha_{\text{critical}}^{(N)}(a)$. Using an analytic method, this expectation may be illustrated via a slightly renormalized two-dimensional metric,

$$\Theta_1^{(2)}(b/2,a) = \begin{bmatrix} 2a^2 & ab \\ ab & a+1 \end{bmatrix},$$

possessing two real eigenvalues:

$$1/2a + 1/2 + a^2 \pm 1/2\sqrt{-3a^2 + 2a - 4a^3 + 1 + 4a^4 + 4(ab)^2}.$$

It is easy to deduce that the domain D of positivity of this metric coincides with the interval of

$$b \in (-\sqrt{2a+2}, \sqrt{2a+2}).$$

At $N > 2$ a graphical determination of the domains $D^{(N)}$ may be used. For illustration, let us consider $N = 3$ and metric

$$\Theta_1^{(3)}(\alpha_1,a) = \begin{bmatrix} 2a^2 & 2\alpha_1 a & 0 \\ 2ga & a+1 & \alpha_1 \\ 0 & \alpha_1 & \frac{a+2}{2a+1} \end{bmatrix},$$

with the α_1 dependence of its three eigenvalues illustrated by Fig. 1 at $a = 1$.

The pattern of the graphical localization of the eigenvalues of our tridiagonal metrics $\Theta_1^{(N)}(\alpha_1,a)$ remains qualitatively very similar in a broad range of parameters N, α_1, and a. In particular, we may be sure that the matrix $\Theta_1^{(N)}(\alpha_1,a)$ remains positively definite at all the sufficiently small nondiagonalities, that is, in a nonempty subdomain of $D^{(N)}$ where $|\alpha_1| \ll a$.

Several interesting as well as practically highly relevant questions arise when one tries to extend the graphical analysis to higher dimensions N. First of all, the growth of the necessary numerical precision makes the analysis a bit costly. Indeed, one must be careful with the numerical localization of the eigenvalues of the metric because even our fully explicit formula (17) leads to a perceivable numerical contrast between the maximal eigenvalues $\theta_0 = \theta_1 = 1$ and the unexpectedly quickly decreasing roots $\theta_7 \sim 0.000\,396\,8$ or $\theta_8 \sim 0.000\,049\,6$ (etc.) of the corresponding secular equation.

TABLE I. The N dependence of boundaries $\pm G$ of the domain $D_1^{(N)}$ at $a = 1$.

N	Boundary value G	Neighboring G'	Next G''
1	∞		
2	1		
3	0.816 496 580 9		
4	0.783 580 923 5	2.210 430 034	
5	0.777 215 245 3	1.528 761 895	
6	0.776 173 893 3	1.347 821 298	3.702 152 325
7	0.776 036 784 2	1.284 679 682	2.333 798 009
8	0.776 022 003 8	1.261 982 266	1.922 171 587
9	0.776 020 659 2	1.254 396 565	1.747 726 425

Fortunately, the extremely elementary form of the matrix elements of our Gegenbauerian tridiagonal metrics (21) still supports the practical feasibility of the direct numerical localization of the boundaries of the related two-dimensional domains $D_1^{(N)}$ of admissible parameters α_1 and a up to the fairly large dimensions. Moreover, there exists an encouraging numerical evidence that these boundaries $\partial D_1^{(N)}$ stabilize and remain only very weakly dependent on the dimension at large $N \gg 1$.

A persuasive sample of such an evidence is provided by Table I, where we choose $a = 1$ and tabulate the values of G [our metric $\Theta_1^{(N)}(g,1)$ is positive definite for $g \in (-G,G)$] together with auxiliary values G' and G'' [our metric $\Theta_1^{(N)}(g,1)$ has at most one or at most two negative eigenvalues in the larger intervals $g \in (-G',G')$ and $g \in (-G'',G'')$, respectively].

Table I strongly and very persuasively supports the N independence of $G \approx 0.776$ in the limit $N \to \infty$ (i.e., the existence and stability of a nonempty domain $D_1^{(N)}$, where the metric is positive). Indeed, the left column of the table indicates that the Nth value of G only differs from its predecessor in the $(N-3)$rd decimal digit.

C. Pentadiagonal metrics

At $k = 2$ and variable N we may try to solve Eq. (12) by pentadiagonal ansatz,

$$\mathcal{P}_2^{(N)}(a) = \begin{bmatrix} 0 & 0 & \gamma_1 & 0 & 0 & 0 & \dots & 0 \\ 0 & \delta_1 & 0 & \gamma_2 & 0 & 0 & \dots & 0 \\ \gamma_1 & 0 & \delta_2 & 0 & \gamma_3 & 0 & \ddots & \vdots \\ 0 & \gamma_2 & 0 & \delta_3 & 0 & \gamma_4 & \ddots & 0 \\ 0 & 0 & \ddots & \ddots & \ddots & \ddots & \ddots & 0 \\ \vdots & \ddots & \ddots & \gamma_{N-4} & 0 & \delta_{N-3} & 0 & \gamma_{N-2} \\ 0 & \dots & 0 & 0 & \gamma_{N-3} & 0 & \delta_{N-2} & 0 \\ 0 & 0 & \dots & 0 & 0 & \gamma_{N-2} & 0 & \omega^{(N)} \end{bmatrix}, \tag{25}$$

using the same recurrent method as earlier. The selection of $\gamma_1 = a$ and the consistent specification of $\gamma_2 = (1+a)/(4+2a)$ initiate now the combined recurrences for two unknown sequences in (25). These recurrences may be extracted, from linear algebraic Eq. (12), as a subset of all of its linearly independent items. The result of their solution (which was, naturally, computer-assisted and rather lengthy) can be written down in closed form, with $j = 3,4,\dots,N-1$ in

$$\gamma_j = \frac{1+a}{(2j+2a)\Gamma_{j-2}}, \quad \Gamma_n = (1+2a)(2+2a)\cdots(n+2a) \tag{26}$$

and with $\Gamma_0 = 1$ and $j = 1,2,\dots,N-1$ in

$$\delta_j = \frac{2[2a^3+3a^2-(4j-5)ja-(2j^2-1)(j-1)]}{(2j+2+2a)(2j-2+2a)\Gamma_{j-1}}. \tag{27}$$

At the smallest subscripts j there occur incidental factorizations which simplify slightly the numerators,

$$\delta_1 = \frac{2(2a^3+3a^2+a)}{2a(4+2a)} = \frac{(a+1)(2a+1)}{2(a+2)}$$

and

$$\delta_2 = \frac{2(2a^3+3a^2-6a-7)}{(6+2a)(2+2a)(1+2a)} = \frac{2a^2+a-7}{2(2a+1)(a+3)}.$$

The last missing element $\omega^{(N)} = \omega^{(N)}(a)$ in formula (25) is exceptional. Due to its manifest truncation dependence, its value must be computed, at each $N \geqslant 3$, by direct insertion in Eq. (12). At the first few dimensions, this is an easy calculation which gives the (incidentally, negative though comparatively simple) series of formulas

$$\omega^{(3)} = -\frac{3}{2(1+2a)}, \qquad \omega^{(4)} = -\frac{5+3a}{2(1+2a)(1+a)(2+a)} \quad \dots. \tag{28}$$

Their extrapolation inspires the general ansatz,

$$\omega^{(N)} = -\frac{(u_N + v_N a)}{(2N-4+2a)\Gamma_{N-2}}, \tag{29}$$

and its subsequent confirmation, giving

$$u_N = (2N-3)(N-2), \quad v_N = 3N-6. \tag{30}$$

This completes our closed-form construction of pentadiagonal solutions (25) of Dieudonné's Eq. (12) at any matrix dimension $N = 3,4,\dots$.

VII. DISCUSSION

In contrast to the recent theoretical experiments with discrete models possessing pointlike impurities [6] or boundary terms [13], the interaction in our one-parametric solvable toy model is a smooth function of position. This is an innovation which may be considered natural. In various limits and dynamical regimes we may then specify energies E_n and wave functions $|\psi_n\rangle$ using the broad menu of formulas available for orthogonal polynomials in question. In our article the eigenstates of H were selected, for the sake of definiteness, in the closed form of Gegenbauer polynomials.

In the context of mathematics, the main obstacle of calling the related solvable matrices H Hamiltonians appeared in their asymmetry (i.e., non-Hermiticity). This seemed to disqualify these matrices from playing the role of operators of observables. Fortunately, such a conclusion would be erroneous. The clarification of the paradox dates back to Scholtz *et al.* [18] and Bender *et al.* [33]. We just recalled and used their argumentation in a concrete application.

Our method of the reconstruction of the metric based on the use of discrete Hamiltonians and mediated by the computer-assisted solution of Dieudonné's Eq. (12) proved very efficient. It led to compact analytic formulas for a family of metrics. A different discrete-lattice quantum model has been found as described by the pair of matrices (H,Θ). The first component of this pair is the N-dimensional Gegenbauerian Hamiltonian H which has been chosen tridiagonal. The second component Θ of this pair is the reconstructed (and nonunique) metric.

In a historical detour, let us remind the readers that nuclear physicists began studying the problematic question of $\Theta \neq I$ about 20 years ago [18] when considering fermionic Hamiltonians $\mathfrak{h}$ (acting in complicated Fock's space $\mathcal{H}^{(P)}$ of "physical" states $|\psi^{(P)}\rangle$) as transformed into isospectral operators H (acting in another "friendly" space $\mathcal{H}^{(F)}$). The net gain was that the bound-state energies became obtainable by the diagonalization of the simplified bosonic Hamiltonian $H \neq H^\dagger$. The price to be paid was that the latter operator proved *manifestly non-Hermitian* in the usual, "friendly" Hilbert space $\mathcal{H}^{(F)}$ with trivial $\Theta^{(F)} = I$.

In other branches of physics the recipe has been revitalized in connection with the emergence of $\mathcal{PT}$-symmetric quantum systems [34–36]. This opened new horizons in particle physics [37] and in relativistic quantum field theory [38]. The key theoretical idea of the formalism (viz., the nontriviality of the product $\Omega^\dagger\Omega := \Theta \neq I$) remained the same but the philosophy has been changed. In place of starting from the knowledge of the physical, self-adjoint $\mathfrak{h} = \mathfrak{h}^\dagger$ and from the subsequent *clever choice* of a simplifying map Ω, the updated model-building strategy (cf. [28,39]) takes a manifestly non-Hermitian "friendly" candidate for the Hamiltonian $H = H^{(F)} \neq (H^{(F)})^\dagger$ and tries to reconstruct the "physical" Hamiltonian $\mathfrak{h} = H^{(P)}$ via Eq. (10).

Our present proposal of a new solvable model was inspired by the main weakness of the latter scenario, which lies in a huge uncertainty and ambiguity of the assignment $H \to \mathfrak{h}$ marked, say, by an N-component multi-index λ attached to $\Omega = \Omega(\lambda)$. This ambiguity was inessential during the nuclear-physics mappings $\mathfrak{h} \to H(\lambda)$. In $\mathcal{PT}$-symmetric context and in its pseudo-Hermitian generalizations [40] it is more serious. It implies the *nonuniqueness of physics* represented by the λ-dependent operator $\mathfrak{h}(\lambda)$. The *same* initial operator H admits *many* experimentally nonequivalent physical interpretations. The variations of λ generate nonequivalent self-adjoint Hamiltonians $\mathfrak{h}(\lambda)$. This means that the *same* spectrum of energies may coexist with *different* observable characteristics (e.g., coordinates [30,32]).

The suppression of the ambiguity of the multi-indexed mappings $\Omega(\lambda)$ *and* of Hamiltonians $\mathfrak{h}(\lambda)$ may be performed, according to Scholtz *et al.* [18], via an explicit specification of some other observables $\mathcal{C}$, $\mathcal{D}$, etc. They have to obey the same Dieudonné's conditions of crypto-Hermiticity. In practice, this goal may be achieved by requiring that one of the observables used for this purpose is a charge with involutivity property $\mathcal{C}^2 = I$ [28]. In our present considerations we used another strategy proposed in Ref. [30] and based on the hypothesis of existence of a nontrivial, fundamental "smearing" length.

We showed in [30] that the smearing length does not vanish and does not diverge in models where some of the the metrics possess the $(2k+1)$-diagonal band-matrix form $\Theta = \Theta_k$. The subscript $k = 0,1,\ldots$ has been interpreted there as the measure of the size of the smearing.

The simplest physical scenario of this form certainly emerges when one decides to use just the diagonal metrics $\Theta_0 \neq I$. In Ref. [30], as well as in our present concrete model, this "no-smearing" option proved allowed. The related diagonal-matrix operator of the coordinate remained merely scaling-noninvariant. Our quantum Hamiltonians then became tractable as living on *deformed* but still local one-dimensional discrete N-site lattices.

Once we turn attention to our present model and to its generic band-matrix metrics $\Theta_k(a)$ with $1 \leqslant k \ll N$, the picture is changed and the coordinates prove smeared [41]. This feature could make our elementary solvable model tractable, for example, as a weakly and controllably nonlocal alternative to a deformed local $k = 0$ lattice [30,42].

On the *experimental* level, one expects that such a weakly nonlocal scenario and its consequences (including, e.g., phase transitions) might find simulations in classical systems. A decisive theoretical as well as experimental progress in this direction has already been reported in optics [43,44]. The practical implementation of the parallel experimenting in quantum world is hindered by several mutually interrelated obstacles. The most serious one may be identified with a certain conflict between the simplicity of the matrix H and the complicated guarantee of its Hermiticity via metric Θ. Our resolution of this conflict has been based on the *simultaneous* simplicity of *both* the operators H and Θ.

The main *theoretical* profit provided by the fully nonnumerical tractability of our model may be seen in its manifest compatibility with postulates of quantum mechanics in which one works, simultaneously [2], with a *triplet* of Hilbert-space representations $\mathcal{H}^{(P,F,S)}$ of the quantum system in question. The Hermiticity status of operators depends on the space but they only stay non-Hermitian in the "naive" and "false" space $\mathcal{H}^{(F)}$. Thus, in our model, the knowledge of the friendly input matrix $H \neq H^\dagger$ is complemented by the equally friendly nature of the *ad hoc* metric $\Theta = \Theta^{(S)} \neq I$ and, *ipso facto*, of the reconstructed standard Hilbert space $\mathcal{H}^{(S)}$.

In practical terms our Gegenbauerian example exhibits several specific friendly features. First of all, it is nontrivial that our metrics are banded. This property only followed from the explicit solution of the Dieudonné's equation. Second, the matrix elements of the pseudometrics (i.e., of the sparse-matrix components $\mathcal{P}_j$ of the metrics) emerged as elementary functions of the free real parameter a. Last but not least, the matrix elements of the diagonal, tridiagonal, and pentadiagonal metrics exhibited even an almost complete independence of the truncation N.

All of these features of our Gegenbauerian model reconfirm the feasibility of our original intention of finding a new

model-building recipe. Certainly, this (and similar) solvable models would guarantee a viability of fitting many *measured* (and not just equidistant) N-plets of levels $E_n^{(\text{experimental})}$ by the suitable N-plets $E_n^{(\text{theoretical})}$ of the well-known zeros of an appropriate (i.e., in our exemplification, Gegenbauer) classical orthogonal polynomial.

APPENDIX: LONG-RANGE METRICS WITH $k = N - 1$

Equations (25) and (28) with $N = 3$ offer the simplest nontrivial example of the metric $\Theta_k^{(N)}$ with maximal $k = N - 1$ in which some of the matrix elements become truncation-dependent. We found that this form of manifest N-dependence characterizes all the Gegenbauer metrics with $k \geqslant 2$. In this sense, the diagonal and tridiagonal metrics appear exceptional. In principle, one could hope that a similar exceptionality could characterize the antidiagonal-like metrics which were found in some other models [30] and which could tentatively be characterized by the triangularity property

$$\left[\mathcal{P}_{N-1}^{(N)}(a)\right]_{jk} = 0 \quad \text{for} \quad j < k. \tag{A1}$$

The failure of these expectations can already be detected at the next dimension $N = 4$ because the explicit violation of antidiagonality already characterizes the heptadiagonal pseudometric

$$\mathcal{P}_3^{(4)}(a) = \begin{bmatrix} 0 & 0 & 0 & a \\ 0 & 0 & \frac{a^2+2a+1}{a+3} & 0 \\ 0 & \frac{a^2+2a+1}{a+3} & 0 & -\frac{3a+5}{(a+3)(2a+1)} \\ a & 0 & -\frac{3a+5}{(a+3)(2a+1)} & 0 \end{bmatrix}. \tag{A2}$$

We see that the loss of the up-down symmetry is transferred from the Hamiltonian H to the metric. Thus, one can only expect that at a given N, the most elementary longest-range component $\mathcal{P}_{N-1}^{(N)}(a)$ of the Gegenbauer metrics will possess the following triangular equal-color form:

$$\mathcal{P}_{N-1}^{(N)}(a) = \begin{bmatrix} 0 & 0 & 0 & \dots & 0 & 0 & p_{11} \\ 0 & 0 & \dots & 0 & 0 & p_{12} & 0 \\ \vdots & \vdots & \iddots & \iddots & \iddots & 0 & p_{21} \\ \vdots & 0 & 0 & p_{14} & \iddots & \iddots & 0 \\ 0 & 0 & p_{13} & 0 & p_{23} & \iddots & \iddots \\ 0 & p_{12} & 0 & p_{22} & 0 & p_{32} & \dots \\ p_{11} & 0 & p_{21} & 0 & p_{31} & 0 & \dots \end{bmatrix}. \tag{A3}$$

The quick growth of complexity of the, presumably, closed but much less compact formulas for the matrix elements in (A3) may be illustrated for intermediate $N = 8$ for which the maximal-range 15-diagonal (pseudo)metric matrix may be constructed by solving Eq. (12) via ansatz (A3). In the normalization where $[\mathcal{P}_{N-1}^{(N)}(a)]_{1N} = a$, our calculations yielded the elements

$$p_{11} = a = \frac{2a^2 + a}{2a + 1},$$

$$p_{12} = \frac{(a+1)(a+3)}{a+7} = \frac{2a^3 + 9a^2 + 10a + 3}{(2a+1)(a+7)},$$

$$p_{13} = \frac{2a^4 + 17a^3 + 52a^2 + 67a + 30}{(2a+1)(a+7)(a+6)} = \frac{(a+1)(a+3)(2a+5)(a+2)}{(2a+1)(a+7)(a+6)},$$

$$p_{14} = \frac{2a^5 + 25a^4 + 124a^3 + 305a^2 + 372a + 180}{(2a+1)(a+7)(a+6)(a+5)} = \frac{(2a+5)(a+3)^2(a+2)^2}{(2a+1)(a+7)(a+6)(a+5)},$$

plus perceivably less compact

$$p_{21} = -3\frac{3a^2 + 19a + 26}{(2a+1)(a+7)(a+6)} = -3\frac{(3a+13)(a+2)}{(2a+1)(a+7)(a+6)},$$

$$p_{22} = -5\frac{3a^5 + 52a^4 + 342a^3 + 1064a^2 + 1551a + 828}{(2a+1)(a+6)(a+5)(a+1)(a+7)^2} = -5\frac{(a+4)(3a^2 + 22a + 23)(a+3)^2}{(2a+1)(a+6)(a+5)(a+1)(a+7)^2},$$

$$p_{23} = -6\frac{6a^7 + 143a^6 + \cdots + 40218a^2 + 37901a + 14640}{(a+5)(2a+3)(2a+1)(a+1)(a+7)^2(a+6)^2} = -6\frac{(2a+5)(a+3)(3a^5 + 55a^4 + 380a^3 + 1223a^2 + 1811a + 976)}{(a+5)(2a+3)(2a+1)(a+1)(a+7)^2(a+6)^2},$$

where the higher-degree polynomials in numerators have noninteger roots which are all real, and

$$p_{31} = -2\frac{(a+4)(3a^5 + 25a^4 - 78a^3 - \cdots - 2025)}{(a+5)(2a+3)(2a+1)(a+1)(a+7)^2(a+6)^2},$$

where the fifth-degree polynomial in numerator has solely three real noninteger roots,

$$p_{32} = -3\frac{(a+3)(6a^7 + 95a^6 + 176a^5 - 5106a^4 - \cdots - 82\,280)}{2(a+5)(2a+3)(2a+1)(a+2)(a+1)(a+6)^2(a+7)^3},$$

where the seventh-degree polynomial in numerator has solely five real noninteger roots, and, finally,

$$p_{41} = -\frac{6a^8 + 59a^7 - 621a^6 - \cdots - 60\,120}{2(2a+5)(2a+3)(2a+1)(a+5)(a+2)(a+1)(a+6)^2(a+7)^3},$$

with just four real and four complex roots of the eighth-degree polynomial in the numerator. Summarizing, these results demonstrate not only the efficiency of our computer-assisted algorithms but also, in parallel, the quick decrease of the *practical* appeal of working with more-than-pentadiagonal metrics $\Theta_k^{(N)}(a)$ with $k \gg 2$.

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