Quantum models with spectrum generated by the flows of polynomial zeros

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Abstract
A class $\mathcal{R}$ of purely bosonic models is characterized having the following properties in a Hilbert space of analytic functions: (i) wave function $\psi(\epsilon, z) = \sum_{n=0}^{\infty} \phi_n(\epsilon) z^n$ is the generating function for orthogonal polynomials $\phi_n(\epsilon)$ of a discrete energy variable $\epsilon$, (ii) any Hamiltonian $\hat{H}_b \in \mathcal{R}$ has nondegenerate purely point spectrum that corresponds to infinite discrete support of measure $\nu(x)$ in the orthogonality relation of the polynomials $\phi_n$, (iii) the support is determined exclusively by the points of discontinuity of $\nu(x)$, (iv) the spectrum of $\hat{H}_b \in \mathcal{R}$ can be numerically determined as fixed points of monotonic flows of the zeros of orthogonal polynomials $\phi_n(\epsilon)$, (v) one can compute practically an unlimited number of energy levels (e.g. 253 in double precision). If a model of $\mathcal{R}$ is exactly solvable, its spectrum can only assume one of four qualitatively different types. The results are applied to spin-boson quantum models that are, at least partially, diagonalizable and have at least single one-dimensional irreducible component in the spin subspace. Examples include the Rabi model and its various generalizations.

Keywords: Rabi model, orthogonal polynomials, quasi-exact solvability, exact solvability

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1. Introduction
Our work concerns models for which one can formulate a formal quantization criterion in terms of infinite continued fraction

$$F(x) \equiv a_0 + \frac{-b_1}{a_1 + \frac{b_2}{a_2 + \frac{b_3}{a_3 + \cdots}}} = 0,$$ (1)
where the coefficients \( a_n \) and \( b_n \neq 0 \) are functions of an energy variable \( x \). A prototype of the criterion (1) is the Schweber quantization condition (see equation (A.16) of [1]) initially formulated for a displaced harmonic oscillator and the Rabi, or single boson, model [2]. The gist of the present work is to explore consequences of that the zeros of the function \( F(x) \) are equivalent to the poles of infinite continued fraction

\[
E(x) \equiv \frac{-b_0}{a_0 - \frac{b_1}{a_1 - \frac{b_2}{a_2 - \cdots}}} = -\frac{b_0}{F(x)}
\]

(2)

In particular, let us consider the Schrödinger equation

\[
\hat{H}\Psi(z) = E\Psi(z)
\]

induced by a model Hamiltonian \( \hat{H} \) in the product Hilbert space \( B = b \otimes \mathbb{C}^N \), where \( b \) is the Bargmann space of analytic functions [1, 3] and \( \mathbb{C}^N \) is \( N \)-dimensional spin subspace [4–9]. We assume that \( \hat{H} \) possesses a symmetry group \( G \) that has at least single one-dimensional irreducible representation in the spin subspace [4–11]. On many occasions (e.g. if \( \hat{H} \) is a linear combination of the bosonic operators \( a^*a, a \) and \( a^* \)) the purely bosonic Hamiltonian \( \hat{H}_b \) describing the irreducible component is intrinsically tridiagonal. Then the eigenvalue equation reduces to a three-term recurrence relation (TTRR) [1, 6–9]

\[
\phi_{n+1} + a_n\phi_n + b_n\phi_{n-1} = 0 \quad (n \geq 1),
\]

(4)

and a two-term condition on \( \phi_0 \) and \( \phi_1 \) [6]

\[
\phi_1 + a_0\phi_0 = 0.
\]

(5)

Here \( \{\phi_n\}_{n=0}^{\infty} \) are the sought expansion coefficients of an entire function in \( b \)

\[
\Psi(z) = \sum_{n=0}^{\infty} \phi_n z^n,
\]

(6)

corresponding to the one-dimensional irreducible component of \( \Psi \) described by \( \hat{H}_b \) (see section 5.2 below). In fact, there always exists an orthonormal basis \( \{e_n\}_{n=0}^{\infty} \) such that a given self-adjoint operator \( \hat{H} \) takes on a tridiagonal form

\[
\hat{H}e_n = \tilde{a}_n e_n + \tilde{b}_{n+1} e_{n+1} + \tilde{b}_n e_{n-1},
\]

(7)

with real recurrence coefficients, where \( \tilde{b}_n \geq 0, n \geq 0 \) [12, 13]. In such a basis, (i) the expansion coefficients \( \phi_n \) are polynomials of the \( n \)th order of an orthogonal polynomial sequence (OPS) of a discrete variable [7, 8, 12–15] and hence (ii) the wave function \( \psi(z) \) is the generating function for the polynomials [7, 8, 12, 13]. Here the discrete variable means that the distribution function \( \nu(x) \) in the orthogonality relations of the polynomials (see appendix) is an increasing step function.

The outline of the present work is as follows. In section 2 we define a recurrence class of purely bosonic models, \( R \), for which the quantization criterion (1) can be shown to follow from (4) [1, 6–9]. The class \( R \) is broad enough to encompass the Rabi model [7, 8] and its various generalizations. The Rabi model, which describes the simplest fully quantized interaction between light and matter (see equation (11) below), can be realized in a rich variety of different setups such as Josephson junctions, circuit quantum electrodynamics, trapped ions, superconductors, and semiconductors [16–19]. The model plays a fundamental role in various applications of quantum optics, in implementation of diverse protocols in contemporary quantum information, with potential applications to future quantum technologies [16–19]. In its semiclassical form, the model is the basis for understanding nuclear magnetic resonance.
In section 3 it is proven that \( E(x) \) is related to the measure \( d\nu(x) \) by the Stieltjes transform (equation (18) below), \( E(x) \) has only simple poles for \( \hat{H}_0 \in \mathcal{R} \), which coincide with the points of discontinuity of \( \nu(x) \). On labeling the poles of \( E(x) \) in increasing order, the \( n \)th pole can be alternatively recovered as a fixed point of the flow of the \( n \)th zeros of polynomials of the OPS. The transformation (2) from \( F(x) \) to \( E(x) \) enables one to translate the above results for the poles of \( E(x) \) to those for the zeros of \( F(x) \). In particular, \( \hat{H}_0 \in \mathcal{R} \) has nondegenerate purely point spectrum\(^1\) that corresponds to the points of discontinuity of \( \nu(x) \). As elaborated in section 4, a direct practical consequence of the result is an entirely new, efficient, and relatively general method in determining the spectrum. Contrary to searching for zeros of \( F(x) \), the spectrum coincides with the limit points of the flows of zeros of appropriate orthogonal polynomials of a discrete variable, which can be determined much more efficiently. For example, on using a very simple stepping algorithm, we were able to determine up to \( \text{ca} \, 1350 \) energy levels per parity subspace for the Rabi model (i.e. almost two orders of magnitude more than is possible to obtain from the Schwber quantization condition (1)) [8].

We sketch the basic features of an improved algorithm that allows to determine practically an unlimited number of energy levels within corresponding machine precision.

Section 5 is divided into a number of subsections where our results are extensively discussed from various angles: comparison of \( \mathcal{R} \) and quasi-exactly-solvable (QES) models (section 5.1), the concept of almost exactly solvable (AES) models (section 5.2), numerical issues (section 5.4), and relation with earlier work (section 5.5). We then conclude with section 6. Some additional technical remarks are relegated to appendices.

### 2. Recurrence class \( \mathcal{R} \) of purely bosonic models

The coefficients \( \{\hat{q}_n\}_{n=0}^\infty \) define an entire function in \( \mathfrak{b} \) whenever the sum \( \sum_{n=0}^\infty |\hat{q}_n|^2 n! \) converges (see equation (1.4) of [3]). (Note in passing that the Bargmann condition, which corresponds to the Hilbert space of entire functions of growth \( \frac{1}{2}, 2 \), presumes the standard measure \( (1/\pi)e^{-|z|^2} \, dz \, dz \in \mathbb{C} \). In the Hilbert spaces of entire functions of different growth another measure and convergence criterion apply [20].) The quantization criterion (1) is rigorous consequence of the eigenvalue equation (3) provided that the TTRR (4) [unless otherwise stated, considered in the absence of the two-term condition (5)] has a minimal solution \( \{m_n\}_{n=0}^\infty \) with \( m_0 \neq 0 \) (see theorem 1.1 due to Pincherle in [21]). The minimal solution exists if for any other linearly independent solution \( \{d_n\}_{n=0}^\infty \) of the TTRR (4) one has \( \lim_{n \to \infty} \frac{m_n}{d_n} = 0 \) [21]. In the latter case all other linearly independent solutions are called dominant [21]. The latter are not unique as any linear combination of \( m_n \) and \( d_n \) yields another dominant solution. (Note that there might be TTRR which do not have any minimal solution; for instance, for the Chebyshev polynomials see [22].)

In what follows, we limit ourselves further to the case when:

(A) the coefficients \( a_n \)'s are linear functions of an energy variable \( x \), i.e., \( a_n = -(a_n x - c_n) \), where the coefficients \( a_n \) and \( c_n \) are real and independent of \( x \) and \( a_n \neq 0 \) for \( n \geq 1 \).

The condition (A) is not a serious constraint, because it is always met in Haydock’s basis [12]. The TTRR (4) then becomes a defining equation for orthogonal polynomials. Indeed, according to the Favard–Shohat–Natanson theorems (given as theorems I-4.1 and I-4.4 of [23]), the necessary and sufficient condition for a family of polynomials \( \{\hat{p}_n\} \) (with degree

\(^1\) Such a spectrum, and as in case (c) below, is typical for any regular Sturm–Liouville problem comprising among other potential wells in one dimension with infinitely high walls and a continuous bottom \( V(x) \).
\( p_n = n \) to form a positive definite OPS is that \( p_n \)’s satisfy a TTRR (4) and (5) with the coefficients as specified above, together with the initial condition \( p_{-1} = 0 \) and \( p_0 = \text{const.} \). Without any loss of generality, a suitable rescaling of \( \phi_n \) \([7, 8]\) enables one to recast (4) as the TTRR of a monic OPS

\[
p_n(x) = (x - c_{n-1})p_{n-1}(x) - \lambda_{n-1}p_{n-2}(x), \quad (8)
\]

\[
p_{-1}(x) = 0, \quad p_0(x) = 1, \quad (9)
\]

where \( \lambda_n \neq 0, n \geq 1 \) and we keep the notation \( c_n \) also for the rescaled coefficients. Because neither the TTRR (4) nor the two-term condition (5) contains \( b_0 \), one can in virtue of \( p_{-1} \equiv 0 \) always set the rescaled \( b_0 \) as \( \lambda_0 = 1 \) \([7, 8]\).

Because the present work is concerned with the part of spectrum corresponding to a one-dimensional irreducible component of \( \Psi \) described by purely bosonic \( \hat{H}_b \in \mathcal{R} \), it is obvious to focus on the discrete spectrum. The spectrum can be discrete only if (i) dominant solutions of the TTRR (4) do not generate an element of \( b \) and, simultaneously, (ii) the minimal solution of the TTRR (4) with (5) as an initial condition has always a unique solution \([21]\). The unique solution is in general a linear combination of the minimal and dominant solutions. However, the unique solution is in \( b \) only in the special case if it reduces to the minimal solution \([6]\). Under all other circumstances either both minimal and dominant solutions generate functions from \( b \), or none does so. In the latter case the spectrum is obviously empty, whereas in the former case the spectrum is necessarily continuous. Indeed, for any energy there would exist a unique solution of the TTRR (4) with (5) \([21]\). Irrespective if the solution is a dominant or minimal one, it would be in \( b \), and hence in the spectrum.

Let the recurrence coefficients assume an asymptotic powerlike dependence as a function of \( n \) \([6]\)

\[
a_n \sim an^\alpha, \quad b_n \sim bn^\beta \quad (n \to \infty), \quad (10)
\]

where \( a \) and \( b \) are proportionality constants. The Perron–Kreuser theorem (theorem 2.3 in \([21]\)) implies that (i) a minimal solution exists and (ii) discrete spectrum is possible provided that any of the following alternatives is satisfied:

- (a) \( \alpha > -1/2, \beta < \alpha - (1/2) \),
- (b) \( \alpha > -1/2, \beta = \alpha - (1/2), |b| < |a| \),
- (c) \( \alpha = -1/2, |a| \geq 1, \beta < -1 \),
- (d) \( \alpha = -1/2, \beta = -1, |b| \geq 1, |t_1| < 1 \).

Here the first three alternatives follow from case (a) of the Perron–Kreuser theorem, whereas the last one is a consequence of the theorem case (b). The conditions (a)–(d) define a ‘recurrence’ class \( \mathcal{R} \) of quantum models. The class is here defined broader than in our earlier work \([6]\) by including also cases (c) and (d), in order to accommodate more general Hilbert spaces of entire functions \([20]\).

\( \quad \)

\( \quad 2 \) The reason for a different nomenclature regarding TTRR’s (4) and (8) is that the TTRR of the form (4) is common in general theory of recurrences \([21]\), whereas the TTRR of the form (8) are employed in the theory of orthogonal polynomials \([23]\). We maintained the respective notations in order to facilitate comparison with relevant results of \([21, 23]\).
2.1. Examples

After a rather formal and abstract introduction of $\mathcal{R}$, we argue that the conditions for $\mathcal{R}$ are, in broad sense, natural. For example, the condition (A) is automatically satisfied if $\hat{H}$ is a linear combination of $a^*a$, $a$ and $a^*$. Indeed, upon the action of $a^*a$, $a = (d/dz)$ and $a^* = z$ on $\psi(z)$ in equation (6), the coefficient of the resulting $z^n$ monomial will become $n\phi_n$, $(n + 1)\phi_{n+1}$, and $\phi_{n-1}$, respectively. Therefore, if $\hat{H}$ is a linear combination of $a^*a$, $a$ and $a^*$, the eigenvalue equation for any $\mathcal{R} \in \mathcal{E}$ describing the one-dimensional irreducible component of $\Psi$ inevitably reduces to a TTRR of the type (A) with $\alpha = 0$ and $\beta = -1$, i.e., corresponding to case (a). Even if the condition (A) is not automatically satisfied, it is only a question of finding an appropriate orthonormal basis $\{e_n\}_{n=0}^\infty$ to bring a given Hamiltonian to a tridiagonal form (7)\[12, 13].

Not surprisingly, the class $\mathcal{R}$ is broad enough to encompass the Rabi model [7, 8] and its various generalizations. The Rabi model [2] describes the simplest interaction between a cavity mode with a frequency $\omega$ and a two-level system with a resonance frequency $\omega_0$. The model is characterized by the Hamiltonian [1, 2]

$$\hat{H}_R = \hbar \omega \hat{a}^\dagger \hat{a} + \hbar g \sigma_1 (\hat{a}^\dagger + \hat{a}) + \mu \sigma_3$$

acting in the Hilbert space $\mathcal{H} = \mathbb{C}^2 \otimes \mathbb{C}^2$, where $\mu = \hbar \omega_0/2$, $\hat{a}$ and $\hat{a}^\dagger$ are the conventional boson annihilation and creation operators satisfying commutation relation $[\hat{a}, \hat{a}^\dagger] = 1$, and $g$ is a coupling constant [1, 3]. In what follows, $1$ is the unit matrix, $\sigma_j$ are the Pauli matrices in their standard representation, and we set the reduced Planck constant $\hbar = 1$. $\hat{H}_R$ is invariant under the parity $\hat{\Pi} = \sigma_3 \hat{\pi}$, where $\hat{\pi}^\dagger = -\pi$ and $\hat{\pi} \hat{\pi}^\dagger = -1$. $\mathcal{B}$ can be thus written as a direct sum $\mathcal{B} = B_+ \oplus B_-$ of the parity eigenspaces, or of invariant subspaces $\mathcal{B}_\pm$. In each of them the Rabi model is characterized by a corresponding three-term recurrence (see equation (37) of [6])

$$\phi_{n+1}^\pm + \frac{1}{\kappa(n + 1)} [n - \kappa \pm (-1)^n \Delta] \phi_n^\pm + \frac{1}{n + 1} \phi_{n-1}^\pm = 0,$$  \hspace{1cm} (12)$$

where energy variable $x = \kappa \equiv E^2/\omega$, $\kappa = g/\omega$ reflects the coupling strength, and $\Delta = \mu/\omega$ [6]. Upon comparing with (10), one has $\alpha = 0$, $\beta = -1 < -1/2$, which corresponds to case (a) [6–8]. The substitution $\phi_n \rightarrow P_n/n!$ transforms the initial recurrence (12) into TTRR (8) of a positive definite monic OPS [7]. The case of a displaced harmonic oscillator is the exactly solvable limit of $\hat{H}_R$ for $\mu = 0$ that corresponds to $\Delta = 0$, whereby the recurrences (12) reduce to equation (A.17) of [1].

It is useful to remind here that the Rabi model with a ‘wrong’ negative sign of its parameters $g$ and $\mu$ (see equation (12) of [11]) was used to describe an excitation hopping between two sites and the interaction of a dipolar impurity (paraelectric or paraelastic) with a crystal lattice [11]. The sign change induces sign reversal of $\kappa$ and $\Delta$ in the TTRR (12), but otherwise does not change any its essential features.

Further models can be obtained by changing or introducing different interaction terms to the Rabi model. Following appendix of [24], the Rabi Hamiltonian (11) supplemented with a momentum dependent interaction term

$$V = i\sigma_2 g_0 (a - a^*)$$

remains invariant with regard to the parity operator $\hat{\Pi}$, and thus amenable to the Fulton–Gouterman transformation (FGT) [4, 25], resulting in a pair of TTRR.
Several groups [26, 27] studied the generalized Rabi model
\[ \hat{H}_{gk} = \omega \hat{a}^\dagger \hat{a} + \mu \sigma_3 + g_1 \left( \hat{a}^\dagger \sigma_+ + a \sigma_- \right) + g_2 \left( \hat{a}^\dagger \sigma_+ + a \sigma_- \right), \]
which interpolates between the Jaynes and Cummings model (for \( g_2 = 0 \)) and the original Rabi model \( g_1 = g_2 \). The model, which is again invariant with regard to the parity operator \( \hat{\Pi} \), and thus amenable to the FGT [25], can be mapped onto the model describing a two-dimensional electron gas with Rashba \( (g_R \sim g_1) \) and Dresselhaus \( (g_D \sim g_2) \) spin–orbit couplings subject to a perpendicular magnetic field.

There is an outside chance that a driven Rabi model having an extra driving term \( \lambda \sigma_1 \) [9, 28, 29] could also be treated within our framework. Although the driven Rabi model is not invariant with regard to \( \hat{\Pi} \), Gardas and Dajka [28] argued that it possesses a nonlocal parity. However explicit form of the nonlocal parity operator has not been provided and it is unclear if it could be useful for a FGT.

Another option is to consider models in the spin space \( \mathbb{C}^N \) with \( N > 2 \). The so-called Rabi model for \( N \)-state atoms which can be diagonalized in the spin subspace has been recently studied by Albert [5]. A \( \mathbb{Z}_N \) symmetric chiral Rabi model has been recently introduced by Zhang [10].

Nonlinear single-mode terms (such as \( \hat{a}^k \) and \( (\hat{a}^\dagger)^k \) with \( k \geq 2 \)) and multi-mode terms (e.g. \( \hat{a}_1 \hat{a}_2 \) and \( \hat{a}^\dagger_1 \hat{a}^\dagger_2 \)) would naively lead to higher-order recurrences than the fundamental TTRR (4). Nonetheless, through judicious application of the representation theory for higher order polynomial deformations of the \( su(1, 1) \) Lie algebra via a Jordan–Schwinger like construction method [9, 30, 31], and ensuing algebraization of the spin-boson systems, such nonlinear models are not excluded from the scope of the present work. Indeed, as shown by Zhang [9], a TTRR also arises in the case of the two-photon and two-mode Rabi models, which both enjoy a parity symmetry and which can be described by \( \hat{H}_b \in R \) [32].

### 3. Spectrum generated by the flows of polynomial zeros

For \( \hat{H}_b \in R \), the infinite continued fraction in equation (1) can be expressed as the limit [7]
\[ n_0 = \lim_{n \to \infty} \frac{P^{(2)}_n(x)}{P^{(1)}_n(x)}, \quad (13) \]
where, given TTRR (8), the polynomials \( P^{(\nu)}_n \), \( \nu = 0, 1, 2 \) are defined by
\[ P^{(\nu)}_n(x) = (x - c_{n-1+\nu})P^{(\nu)}_{n-1}(x) - \lambda_{n-1+\nu}P^{(\nu)}_{n-2}(x), \quad (n \geq 1). \quad (14) \]
The initial condition is the same as in equation (9). For the sake of notation, the polynomials of the OPS for \( \nu = 0 \) will be denoted simply as \( P_n \). Thus the \( p_n \)'s, defined earlier by the TTRR (8) that follows directly from the initial TTRR (4), has become \( P_n \). The respective monic OPS with \( \nu = 1, 2 \) are called associated to \( \{P_n\} \) (see section III-4 of [23]). The need of three different OPS is obvious: whereas \( \{P_n\} \) determines the expansion coefficients of the physical state, the pair \( \{P^{(1)}_n\} \) and \( \{P^{(2)}_n\} \) defines the infinite continued fraction in equation (1).

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3 Here we depart from the notation of our earlier publications [7, 8] where the respective OPS for \( \nu = 0, 1, 2 \) corresponded to \( \nu = -1, 0, 1 \) and where we called the respective monic OPS with \( \nu = 0 \) associated to \( \{P^{-1}_n\} \) (see section III-4 of [23]).
Analogously to the infinite continued fraction in equation (1)

\[ E(x) = \lim_{n \to \infty} \frac{p_n^{(1)}(x)}{p_n(x)} \]  

(see equation (13)). Indeed, the infinite continued fraction (2) is obtained from that in equation (1) by a substitution \((a_n, b_n) \to (a_{n-1}, b_{n-1})\). The latter corresponds to the substitution \(\nu \to \nu - 1\) in equation (14).

Let \(x_{nl}, l = 1, 2, \ldots, n\), denote the zeros of \(P_n(x)\) arranged in increasing order\(^4\). For any \(n\) and \(l = 1, 2, \ldots, n - 1\) one has

\[ x_{nl} < x_{n-1,l} < x_{n,l+1} \]  

(see theorem I-5.3 of [23]). Because \(x_{nl} < x_{n,l+1}\), the zeros of any \(P_n(x)\) are all simple (see theorem I-5.2 of [23]). The first inequality in (16) implies that the sequence \(\{x_{nl}\}_{n=l}^{\infty}\) is strictly decreasing for any fixed \(l\). Therefore, the respective limits

\[ \lim_{n \to \infty} x_{nl} = \xi_l \]  

exist. The above properties are intrinsic signatures of any OPS [23]. In what follows, we denote the set of all the limit points by \(\Xi = \{\xi_l | l = 1, 2, 3, \ldots\}\).

Corresponding to the OPS \(\{P_n\}\), there is a positive-definite moment functional \(\mathcal{L}\) (see A.1). According to the representation theorem (theorem II-3.1 of [23]), \(\mathcal{L}\) can be characterized by a right continuous distribution function \(\nu\) that is determined through a suitable limit process (see appendix A.1). The set of all the points \(x\) where \(\nu(x)\) has either a finite jump or increases continuously

\[ \delta(\nu) = \{x \mid \nu(x + \delta) - \nu(x - \delta) > 0 \text{ for all } \delta > 0\} \]

is called the spectrum of \(\nu\), or alternatively the support of \(\mathcal{L}\) (see p 51 of [23]), or the support of the Stieltjes integral measure \(d\nu\) induced by \(\nu\). For any positive-definite moment functional the set is infinite [23].

On recalling the arguments of [7], \(E(z)\) can be defined as a regular analytic function of a complex variable \(z \in \mathbb{C}\)

\[ E(z) = \int_{-\infty}^{\infty} \frac{d\nu(x)}{z - x} \]  

(18)

\(E(z)\) is thus the Stieltjes function [33–35]. The distribution function \(\nu\) in the Stieltjes transform representation (18) is, assuming the normalization \(\nu(-\infty) = 0\), unique (see footnote 30 on p 268 of [36]). The determinacy of the Stieltjes measure \(d\nu\) follows also independently from Carleman’s criterion (see equation (VI-1.14) of [23]; p 59 of [37]) which says that the moment problem is determined if \(\sum_{l=1}^{\infty} \lambda_l^{-1/2} = \infty\). The latter is obviously satisfied in our case. Note that the polynomials on the rhs of equation (15) are monic and all their zeros are on the real axis. Then if \(\lim_{l \to \infty} E(z)\) exists and if the limit is finite (e.g. equals to one) in any sector \(\varepsilon \leq \arg z \leq \pi - \varepsilon \), \(0 < \varepsilon < \pi/2\), the Stieltjes transform representation (18) holds with a bounded and non-decreasing \(\nu(x)\) (see lemma 2.2 of [37]).

Hamburger’s theorem XII’ [36] guarantees the Stieltjes transform representation (18) in any closed finite region \(\Omega\) of the complex plane \(\mathbb{C}\) which does not contain any part of the real axis. An important result of [7] was that the representation (18) can be extended to any closed interval on real axis located within the open intervals where \(\nu = \text{const}\). In other words, one

\(^4\) The zeros of \(P_n(x)\) are the eigenvalues of a corresponding Jacobi matrix, which are special case of Hermitian tridiagonal matrices (see exercise I-5.7 of [23] or appendix of [7]).
can employ the representation (18) within any closed interval of the real axis which does not have any common point with \( \Sigma(\nu) \). The result can be regarded as an extension of the Markov theorem (theorem 2.6.2 of Ismail book [38] or p 90 of [23]).

Denote
\[
\sigma \equiv \lim_{j \to \infty} \xi_j.
\]

There are only the following possibilities regarding the behavior of the \( \xi_j \) (pp 62–63 of [23]):

- (a') \( \xi_1 = \sigma = -\infty \) \((l \geq 1)\)
- (b') \( -\infty < \xi_1 < \xi_2 < \ldots < \xi_l = \sigma \) for some \( l \geq 1 \)
- (c') \( -\infty < \xi_1 < \xi_2 < \ldots < \xi_l < \ldots < \sigma = \infty \).

In the first two cases the set \( \Xi \) is finite and thus cannot coincide with the infinite \( \Sigma(\nu) \).

The latter comprises infinitely many points in addition to the elements of \( \Xi \). The first two cases are also unphysical. The first one already from the very fact that physical models have their energy spectrum bounded from below, whereas all energy levels would be at \(-\infty\) in case (a'). In case (b') the corresponding physical model would have, following the analysis of [7], a finite number of energy levels, with \emph{infinitely degenerate} highest energy level. We recall that energy levels corresponds to the zeros of \( F(z) \), which are bracketed by the poles of \( F(z) \) [7]. According to equation (13), the poles of \( F(z) \) correspond to the limit points \( \xi_l^{(i)} \) of sequences \( x_{nl}^{(i)} \) [7]. Now for any associated OPS' (see section 3.4 of [23]), the zeros of \( P_n^{(\sigma)}(x) \) and \( P_{n-1}^{(\sigma)}(x) \) are \emph{interlaced} (theorem III-4.1 of [23]). Specifically
\[
\xi_{nl}^{(0)} < \xi_{nl}^{(0+1)} < \xi_{nl}^{(0)} + 1, \quad \nu = 0, 1.
\]

The latter implies \( \xi_l \leq \xi_l^{(i)} \leq \xi_{l+1} \) and thereby justifies the above conclusions for energy levels in cases (a') and (b').

In case (c'), the infinite spectrum \( \Sigma(\nu) \) is formed exclusively by the points of \( \Xi \) (see the summary of section II-4 on pp 62–63 of [23]). In other words, \( \Sigma(\nu) \) reduces to a one-dimensional discrete lattice \( A \equiv \Xi \) representing the infinite discrete support of \( d\nu(x) \) (see footnote 1). Indeed, \( \nu \) experiences a \emph{finite jump} at any point \( \xi_k \in \Xi \)
\[
0 < \nu(\xi_k) - \nu(\xi_k - 0) = M_k = \left[ \sum_{j=0}^{\infty} \frac{P_j^2(\xi_k)}{n_l} \right]^{-1},
\]

where
\[
n_l = L[1] \lambda_1 \ldots \lambda_l = \| P(x) \|^2
\]
is the squared norm of \( P_k(x) \), and the positive numbers \( M_k \) satisfy the condition
\[
\sum_{k=0}^{\infty} M_k = 1 \quad [7, 23].
\]

The determinacy of the Stieltjes measure \( d\nu \) implies that at all other points of the real axis the sum in the square bracket is \emph{divergent} (see theorem 2.9 and corollary 2.8 of [37]; theorem 2.5.3 and corollary 2.5.3 of [39]). The divergence is a hallmark of that the TTRR (4), with the two-term condition (5) taken as an initial condition, can only be satisfied by a \emph{dominant} solution of the TTRR [6, 21]. Case (c') implies that for any \emph{physical} model of \( R \), the OPS defined by the TTRR (8) are to be formed by the polynomials of a \emph{discrete} variable with an unbounded spectrum \( \Sigma(\nu) \). Furthermore, in any irreducible subspace the model spectrum is, as expected, \emph{nondegenerate} [7] (see section 5.1 for discussion of this point). There are no level crossings allowing the unique labeling of each state.

On physical grounds we assume \( R \) be limited to case (c') in what follows. Although there is a number of sufficient conditions on recurrence coefficients that ensure \( \sigma = \infty \) (see equation (IV-3.7) of [23] that was employed for the Rabi model in [7]), they are expected to
be satisfied for physical models and there is no need to discuss them here. Similarly to $F(z)$ studied in [7], $E(z)$ can be then represented as a Mittag–Leffler partial fraction decomposition

$$E(z) = \sum_{k=1}^{\infty} \frac{M_k}{z - \xi_k},$$

defining a meromorphic function in the complex plane $\mathbb{C}$ with real simple poles and positive residues. The series is absolutely and uniformly convergent in any finite domain having a finite distance from the simple poles $\xi_j$, and it defines there a holomorphic function of $z$. The corresponding $\hat{H}_b \in \mathcal{R}$ (in general any one-dimensional irreducible component of $\mathcal{V}$ in a spin subspace—see section 5.2 below) has infinite number of nondegenerate energy levels without (apart from $+\infty$) any accumulation point. This concludes the proof of the main result of the present work.

We have just shown that the distribution function $\nu(x)$ in the orthogonality relations of the polynomials of discrete variable is an increasing step function. The spectrum of $\hat{H}_b \in \mathcal{R}$ corresponds to $\Sigma$, which is given by the set $\Sigma$ of points of discontinuity of $\nu(x)$. Borrowing renormalization group language, the discrete flows generated by the polynomials zeros flow toward the spectral points. If $\Sigma$ denotes the spectrum of $\hat{H}_b \in \mathcal{R}$, $\Sigma$ coincides with the corresponding discrete lattice $\Lambda \equiv \Sigma = \mathcal{S}(\nu)$.

4. Numerical implications

Obviously, if one knows $\nu(x)$ in equation (18) explicitly, one also knows $\mathcal{S}(\nu)$, and the corresponding model can be solved exactly. Unfortunately, a general procedure of recovering $\nu(x)$ from an initial TTRR is not known. The task can only be performed for the so-called classical OPS [14, 15, 23, 38]. In all other cases, apart from some special cases [38], the spectrum have to be determined numerically. However, one can identify numerically only a small number of the very first eigenvalues from the functional dependence of $\Phi(x)$ (see figures 1, 2 of [6]; figure 1 of [7, 40]). Soon afterwards, $\Phi(x)$ displays a featureless monotonically decreasing behavior [8]—see data files [42]. In spite of the sharp inequalities

$$x_{n-1, l-1}^{(2)} < x_{n}^{(1)} < x_{n+1, l+1},$$

which follow from the second of the rigorous sharp inequalities in equation (19), one soon finds that after a first few of initial zeros (for instance for the Rabi model beginning with $l \geq 2$ for $(\kappa, \Delta) = (0.2, 0.4)$) [8]

$$x_{n-1, l-1}^{(2)} \approx x_{n}^{(1)} \approx x_{n+1, l+1}. \quad (21)$$

For $l \geq 4$ and the Rabi model with $(\kappa, \Delta) = (0.2, 0.4)$ the zeros coincide up to more than five decimal places (provided that $n$ is sufficiently large)—see data files [42]. Because of the coagulation of zeros (21), the respective higher order poles and zeros of $\Phi(x)$ turn out soon to be closer to each other than machine precision. Thus any singularity and any zero of $\Phi(x)$, and most probably also that of $E(x)$, become numerically invisible [8]. The latter implies that any practical implementation of the Schweber method that consists in locating zeros of $\Phi(x)$ fails for higher order eigenvalues [8]. Depending on model parameters, one can determine merely up to 10–20 eigenvalues, and that already in the exactly solvable limit of the displaced harmonic oscillator [8]—see F77 code made available online [41].
Our recipe for determining the first $N_0$ energy levels of $\hat{H}_b \in \mathcal{R}$ does not involve either searching for zeros of $F(x)$ or for the poles of $E(x)$ from the functional dependence of neither of the two functions. Instead our analytic results enable one to get rid of both $F(x)$ and $E(x)$ and to focus exclusively on the flows of polynomial zeros $x_{nl}$. The recipe is as follows:

- choose $N_c \geq N_0$ and determine the first $N_0$ zeros $x_{N_0l}$, $1 \leq N_0$, of $P_N(x)$. Usually a good starting point is to take $N_c \approx N_0 + 20$. Because $P_N(x)$ has $N_c$ simple zeros, any omission of a zero could be easily identified.
- Gradually increase the cut-off value of $N_c$. The latter is what drives the incessant flows of polynomial zeros $x_{N_0l}$ (see the first sharp inequality in equation (16)), wherein each flow is characterized by the parameter $l$.
- Monitor convergence of the respective flows induced by the very first $n$ zeros of $P_N(x)$. Each flow is a monotonically decreasing sequence having necessary a fixed limit point (17). Terminate your calculations when the $N_0$th zero of $P_N(x)$ converged to $\xi_{N_0}$ within predetermined accuracy. Then as a rule all other flows $x_{N_0l}$ with $l < N_0$ have converged, too.

The examples of [8] show that the convergence of the zeros to the spectrum is very fast. The numerical limits in calculating zeros were set by over- and under-flows. Typically, with increasing $N_c$, the respective recurrences yielded first increasing and then decreasing $P_N(x)$. Here we sketch the basic features of an improved algorithm that allows to determine practically an unlimited number of energy levels within corresponding machine precision. Our procedure to avoid the over- and under-flows is rather straightforward. Taking as an example the recurrences (12) and common double precision, one monitors the magnitudes of the current three recurrence terms $\phi_{n+1}, \phi_n$, and $\phi_{n-1}$ as $n$ increases toward $N_c$. If the magnitude approaches $10^{308}$ ($10^{-308}$), the last three recurrence terms $\phi_{n+1}, \phi_n$, and $\phi_{n-1}$ are rescaled by $10^{-308}$ ($10^{308}$). Because the recurrence coefficients are well behaving (they are fairly monotonic with exponents $\alpha = 0$ and $\beta = -1$), such a rescaling will move all three recurrence terms away from over- or under-flows. The TTRR (12) is then restarted anew with the rescaled $\phi_{n+1}, \phi_n$, and $\phi_{n-1}$. Such a rescaling by a constant factor obviously does not alter the position of zeros of the final $\phi_{N_c}$. Also no loss of valid digits is involved, because the change only involves exponent. Thus by the above rescaling one can stitch the recurrence pieces together, thereby avoiding potential over- and under-flows. The stitching can be continued up to the cut-off $N_c$ as large as the largest integer that can be stored within a given precision (e.g. 2^{2^{53}} in double precision [43]). Further numerical details are relegated to forthcoming publication [44].

5. Discussion

5.1. $\mathcal{R}$ versus QES models

We have established the following properties of the models described by $\hat{H}_b \in \mathcal{R}$: (i) the solution $\psi$ to the Schrödinger equation (3) is the generating function for a set of polynomials $\{P_n(E)\}$ in the energy variable $E$, and (ii) the spectral points of $\hat{H}_b \in \mathcal{R}$ can be determined as fixed points of the flows generated by the polynomials zeros. The properties resemble those of a subset of QES problems of quantum mechanics [45–47]. The QES models are distinguished by the fact that a finite (and only a finite) part of their spectrum can be solved algebraically. The corresponding energy eigenvalues are called the quasi-exact energy eigenvalues [45, 46], and are commonly referred to as an exceptional spectrum [4]. The solution to the Schrödinger
equation (3) is the generating function for a set of polynomials in the energy variable $E$ [47] and the quasi-exact energy eigenvalues can be determined as the zeros of a critical Bender–Dunne polynomial $P_J(E)$ [12, 13, 47]. The condition of quasi-exact solvability is reflected in the vanishing of the norm of all polynomials whose degree $n$ exceeds a critical value $J$ [12, 13, 47]. The corresponding moment functional $\mathcal{L}$ of such a polynomial system is necessarily degenerate (see appendix A.1). Thus the Bender–Dunne polynomials do not form a conventional OPS. Importantly, one speaks about the quasi-exact solvability already if the above properties apply for a discrete subset of model parameters. There are in general infinitely many parameters for which need not exist any polynomial solution, yet a model is still called QES.

5.2. AES models

The case when $\Psi \in \mathbb{C}^N$ can be fully diagonalized in the spin subspace (e.g. the Rabi model) deserves a special attention. A sufficient condition for the full diagonalization is that the Hamiltonian $\hat{H}$ possesses an Abelian (e.g. cyclic) symmetry $G$ of the order $N$. Then $G$ has precisely $N$ one-dimensional irreducible representations (IR) $\Gamma_\gamma$, $\gamma = 1, 2, \ldots, N$. Let $g_j \in G$ are represented by $N \times N$ matrices $R_j$ in $\mathbb{C}^N$ (e.g. realized in terms of the Sylvester generator $S$ [5, 48]). The corresponding one-dimensional orthogonal projectors into particular IR $\Gamma_\gamma$ of $G$ are given by [49, 50]

$$P_j = \frac{1}{N} \sum_{\gamma = 1}^{N} \chi_\gamma^*(g_j) R_j,$$

where $\chi_\gamma(g_j)$ are the characters of $g_j \in G$ in the given IR $\Gamma_\gamma$. The total wave function $\Psi \in \mathbb{C}^N$ can be thus projected out into one-dimensional irreducible components, each satisfying its own eigenvalue equation (3). The FGT [25] employed for $N = 2$ [4] can be considered as a special case of the more general projection method of explicitly determining IR of a finite group [49, 50]. The property (c') of section 3 of energy levels of the respective $\hat{H}_b \in \mathcal{R}$ describing the one-dimensional irreducible components of $\Psi$ does not exclude degeneracies in the whole spectrum. Any degeneracy corresponds to a nonzero overlap of the nondegenerate discrete spectra in the respective irreducible (e.g. parity invariant) subspaces governed by different $\hat{H}_b \in \mathcal{R}$ [7]. In most cases the special points of the overlap correspond to the QES part of the spectrum [7, 27].

The fully diagonalizable models in the spin subspace could be thought of as AES models. Indeed, had the flows of zeros terminated for some finite $N$, any such model would be considered as exactly, i.e. algebraically, solvable. In contrast to the QES models, the almost exact solvability applies (i) to the entire spectrum and (ii) for all model parameters. As exemplified by the QES Rabi model, the AES models comprise some of the QES models. Additionally, the example of a displaced harmonic oscillator shows that the AES models may comprise exactly solvable models.

5.3. Exactly solvable models

Let $D_\alpha$ be a suitable divided-difference operator (discrete derivative) [33–35] that maps $\Pi_n[x]$, the linear space of polynomials in $x$ over $\mathbb{C}$ with degree at most $n \in \mathbb{Z}_{\geq 0}$, into $\Pi_{n-1}[x]$ [14, 15, 33–35, 51]. Being a polynomial of degree $n - 1$, one can represent $D_\alpha P_n(x)$ in general only as (see theorem I-2.2 of [23, 33, 35])
\[ D_{n} P_{n}(x) = \sum_{r=0}^{n-1} c_{n,r} P_{r}(x), \]

with some constant coefficients \( c_{n,r} \). The hallmark of exactly solvable models is existence of a structure relation satisfied by the corresponding OPS \( \{ B_{n}(x) \}_{n=0}^{\infty} \)

\[ D_{n} P_{n}(x) = -B_{n}(x)P_{n}(x) + A_{n}(x)P_{n-1}(x), \quad (22) \]

where the coefficients \( A_{n}(x) \) and \( B_{n}(x) \) are in general nonpolynomial functions \([14, 15, 33–35, 51]\). Obviously, if there is one structure relation \( (22) \), there is another one. The other one results by expressing \( P_{n-1} \) from the fundamental TTRR \( (8) \) and substituting it back into the original structure relation \( (22) \). The resulting pair of structure relations (i) leads directly to a pair of mutually adjoint raising and lowering ladder operators \([51]\), (ii) implies that orthogonal polynomials satisfy in general a second-order difference equation (see section 4 of \([51]\)), and (iii) allows one to introduce a discrete analogue of the Bethe ansatz equations (see section 5 of \([51]\)). The structure relation \( (22) \) can be established for any classical OPS \( (p\ 783 \ of \ [52];\ section\ 6 \ of \ [53];\ proposition\ 2.6 \ of \ [54]), \) semi-classical OPS \( (theorem\ 1 \ of \ [34];\ proposition\ 4.4 \ of \ [35]), \) and any OPS orthogonal with respect to a discrete measure supported on equidistant points \( (theorem\ 1.1 \ of \ [51]). \) (In the semi-classical case, the function \( E(x) \) itself satisfies a first order difference equation with polynomial coefficients \( (theorem\ 1 \ of \ [34];\ proposition\ 4.1 \ of \ [35]).\) In brief one finds a structure relation essentially only for the OPS which belong to the Askey scheme \( (p\ 183 \ of \ [55]) \) or to the \( q \)-analogue of the Askey scheme \( (p\ 413 \ of \ [55]). \) In each of the above cases, \( \Lambda \equiv \Xi \) representing the infinite discrete support of \( dr(x) \) is necessarily one of four primary classes of special non-uniform lattices \([33–35]; \) the linear lattice, the linear \( q \)-lattice, the quadratic lattice, and the \( q \)-quadratic lattice (for their properties see table 2 of \([35]\)). The \( q \)-quadratic lattice, in its general non-symmetrical form, is the most general case and the other lattices can be found from this by limiting processes \([35]\).

More specifically, either

\[ \Lambda = \{ x \mid x = u_{2}n^{2} + u_{1}n + u_{0}, \quad n \in \mathbb{N} \}, \quad (23) \]

or

\[ \Lambda = \{ x \mid x = u_{2}q^{-n} + u_{1}q^{n} + u_{0}, \quad n \in \mathbb{N} \}, \quad (24) \]

where \( u_{j} \) are real constants and \( 0 < q < 1 \). Thus the spectrum \( \Sigma \) of an exactly solvable \( H_{p} \in \mathcal{R} \) can only assume one of the above forms of \( \Lambda \). Thereby we have independently arrived at essentially the same type of exactly solvable spectra as did Odake and Sasaki \([56]\) within the framework of their exactly solvable discrete quantum mechanics (dQM) with real shifts \( (rdQM) \) (see equations \( (4.7–11) \) of \([56]\)). Conversely, it appears that if \( \Sigma \neq \Lambda \), where \( \Lambda \) is one of the above types \( (23) \) and \( (24) \), then the model cannot be exactly solvable.

An example is provided by exactly solvable displaced harmonic oscillator having equidistant spectrum \( \Sigma \). The corresponding OPS is that of the Charlier polynomials \([23, 59]\) and \( \Lambda \equiv \Xi \) is an equidistant lattice which coincides with \( \Sigma \) \([8]\). \( \Delta \neq 0 \) in the Rabi Hamiltonian \( (11) \) induces a deformation of the Charlier polynomials to non-classical discrete orthogonal polynomials and, at the same time, a deformation of the underlying equidistant lattice \( \Lambda \). The deformed lattice does not correspond to any of the primary lattice classes implying that the Rabi model is not exactly solvable. Although neither the weight function nor the deformed lattice are analytically known, the above deformation is a norm preserving deformation of the underlying OPS \([8]\).

Algorithmic complexity theory \([57]\) has been used, although without much success, to discuss the degree of randomness of the sequence of energy eigenvalues of conservative
quantum systems [58]. In the present case, an alignment of the physical spectrum $\Sigma$ with one of the primary classes (23) and (24) of lattices $\Lambda \equiv \Xi$ can identify a model as exactly solvable. The degree of randomness of the sequence of energy eigenvalues could be then defined as a minimal distance from the four primary classes of special non-uniform lattices. Further details will be discussed elsewhere [44].

5.4. Comparison with other numerical methods

Our method of determining energy levels differs from any of the known methods that involve (i) a brute force numerical diagonalization, (ii) computation of a correlation function $\langle \psi(r, 0) \psi(r, 1) \rangle$ from a numerical solution $\psi(r, t)$ as in a spectral method by Feit et al [60], (iii) searching for zeros of analytic functions having infinite number of poles and zeros on the real axis (e.g. determined by infinite continued fractions as in the Schweber method (see equation (A.16) of [1]) or as in Braak’s approach [4]), and (iv) numerical diagonalization using Hill’s determinant approach [61].

A brute force numerical diagonalization allows one to determine around 2000 energy levels in double precision (ca 16 digits) for the Rabi model. This is much less than is possible by our approach. Also any deeper analytic insight is missing. Searching for zeros of analytic functions yields only ca. 20 levels. Employing further tricks one can hardly overcome the range of $\approx$100 levels. Using Hill’s determinant approach one can determine $\approx$500 levels, which is still merely half of what was possible to obtain by the simple stepping algorithm employed in [8].

5.5. Relation with earlier work

A proof of our main result in the special case of a displaced harmonic oscillator has been provided in our earlier work [8]. Yet the proof was not general. It was made possible thanks to a largely fortuitous coincidence that the orthogonal polynomials of discrete variable relevant for the displaced harmonic oscillator are the well-known (monic) Charlier polynomials [59] (see equations VI-1.4–5 of [23]) [8]. For the case of the Rabi model [1, 2], the relevant orthogonal polynomials of discrete variable are not classical one and have not been studied in detail so far [8]. As a consequence, only a partial proof of the above statement could have been provided that was limited to the case when a dimensionless interaction constant $\kappa < 1$ [8]. On using the identity (2), the latter has now been proven rigorously, thereby confirming earlier numerical evidence that the statement remains to be valid also for $\kappa \geq 1$ [8].

On adopting the notation $\psi(n) = p_n(x)$, our TTRR (8) can be interpreted as a finite difference Schrödinger equation [56, 62]

$$\psi(n + 1) + c_n \psi(n) + \lambda_n \psi(n - 1) = \chi \psi(n), \quad (25)$$

with $x$ playing the role of an eigenvalue. Thus our recurrence class of purely bosonic models with polynomial coefficients, $R$, provides a realization of $\hat{H}$ of Odake and Sasaki in the so-called dQM with rdQM (see section III of [56]). Equation (25) has been earlier studied by Spiridonov et al [62].

6. Conclusions

A class $R$ of purely bosonic models has been characterized having the following properties in the Bargmann Hilbert space of analytic functions: (i) wave function $\psi(\epsilon, z) = \sum_{n=0}^{\infty} \phi_n(\epsilon) z^n$ is the generating function for orthogonal polynomials $\phi_n(\epsilon)$ of a discrete energy variable $\epsilon$,
(ii) any Hamiltonian $\hat{H}_b \in \mathcal{R}$ has nondegenerate purely point spectrum that corresponds to infinite discrete support of measure $d\nu(x)$ in the orthogonality relation of the polynomials $\phi_n$, (iii) the support is determined exclusively by the points of discontinuity of $\nu(x)$, (iv) the spectrum of $\hat{H}_b \in \mathcal{R}$ can be numerically determined as fixed points of monotonic flows of the zeros of orthogonal polynomials $\phi_n(x)$, (v) one can compute practically an unlimited number of energy levels (e.g. $2^{33}$ in double precision). If a model of $\mathcal{R}$ is exactly solvable, its spectrum can only assume one of four qualitatively different types. Our results were shown to apply to a class of spin-boson quantum models that are, at least partially, diagonalizable in a spin subspace. The class is broad enough to encompass the Rabi model and its various generalizations.

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Appendix. Mathematical remarks

A.1. Moment functional $\mathcal{L}$

Satisfying the TTRR such as (8) is the necessary and sufficient condition that there exists a unique positive definite moment functional $\mathcal{L}$, such that for the family of polynomials $\{p_n\}$ holds

$$\mathcal{L}[1] = \lambda_0, \quad \mathcal{L}\left[p_n(x)p_m(x)\right] = \lambda_0\lambda_1\ldots\lambda_p\delta_{mn},$$

(A.1)

where $m, n = 0, 1, 2, \ldots$ and $\delta_{mn}$ is the Kronecker symbol. Thereby the polynomials $\{p_n\}$ form an OPS. Because $\lambda_n > 0$, the norm of the polynomials $p_n$ is positive definite, $\mathcal{L}[p_n^2(x)] > 0$, and $\mathcal{L}$ is a positive definite nondegenerate moment functional (p 16 of [23]). It is reminded here that the QES models have degenerate $\mathcal{L}$, i.e., $\lambda_{J+1} = 0$ for some $J > 0$ [12, 13, 47].

According to the representation theorem (theorem II-3.1 of [23]), the distribution function $\nu$ of the positive moment functional $\mathcal{L}$

$$\mathcal{L}\left[x^n\right] = \int_{-\infty}^{\infty} x^n \, d\nu(x) = \mu_n \quad (n = 0, 1, \ldots),$$

(A.2)

is the limit of a sequence of bounded, right continuous, nondecreasing step functions $\nu_n(x)$’s

$$\nu_0(x) = 0 \quad (-\infty \leq x < x_{n1}),$$

$$\nu_n(x) = M_{n1} + \ldots + M_{np} \quad (x_{np} \leq x < x_{n,p+1}),$$

$$\nu_n(x) = \mu_0 \quad (x \geq x_{n}),$$

(A.3)

where $x_{nl}, l = 1, 2, \ldots, n$, are the zeros of $p_n(x)$. Consequently

- $\nu_0(x)$ has exactly $n$ points of increase, $x_{nl}$,
- the discontinuity of $\nu_n(x)$ at each $x_{nk}$ equals $M_{nk}$ ($k = 1, 2, \ldots, n$),
at least the first \((2n - 1)\) moments of \(\nu_\alpha(x)\) are identical with those of \(\nu(x)\), i.e.
\[
\int_{-\infty}^{\infty} x^l \, d\nu_\alpha(x) = \mu_l \quad (l = 0, 1, 2, \ldots, 2n - 1).
\] (A.4)

### A.2. The ratio in equation (15) for a finite \(n\)

An indication of that the poles of \(E(x)\) could correspond to the set \(\Xi\) is provided by considering the ratio in (15) for a finite \(n\). Then the ratio in (15) enables the partial fraction decomposition (theorem III-4.3 of [23])
\[
\frac{P_{n-1}(z)}{P_n(z)} = \int_{-\infty}^{\infty} \frac{d\nu_\alpha(x)}{z - x} = \sum_{k=1}^{n} \frac{M_{nk}}{z - x_{nk}},
\] (A.5)
where the numbers \(M_{nk}\) are all positive (see appendix A.1) and satisfy the condition
\[
\sum_{k=1}^{n} M_{nk} = 1 \quad [7, 23].
\]

### A.3. Further consequences of the Perron–Kreuser theorem

The Perron–Kreuser theorem (theorem 2.3 in [21]) implies that the dominant solutions of the TTRR (4) do not generate an element of \(b\) if

- (a") \(2\alpha > \beta\) and either (i) \(\alpha > -1/2\) or (ii) \(\alpha = -1/2\) and \(|\alpha| \geq 1\),
- (b") \(2\alpha = \beta\) and either (i) \(\alpha > -1/2\) or (ii) \(\alpha = -1/2\) and the larger root \(|\alpha| \leq |\alpha|\) of \(t^2 + \alpha t + \beta = 0\) satisfies \(|\alpha| \geq 1\).

### A.4. Stieltjes transform

One can, in principle, find \(\nu\) and determine its infinite discrete support \(\Lambda \equiv \Xi\) by inverting the Stieltjes transform (18). Indeed if the representation (18) holds for \(z \not\in \mathbb{R}\), then \([37, 39]\)
\[
\frac{1}{2} \left[ \nu(x_2) + \nu(x_2 - 0) \right] - \frac{1}{2} \left[ \nu(x_1) + \nu(x_1 - 0) \right] = -\frac{1}{2\pi i} \lim_{\epsilon \to 0} \int_{x_1}^{x_2} [E(t + i\epsilon) - E(t - i\epsilon)] \, dt.
\] (A.6)

Recovering \(\nu\) from \(E\) constitutes the famous problem of moments \([37, 39]\). Every isolated pole \(z = u\) of \(E(z)\) contributes a discrete mass of \(\nu\) at \(x = u\) and the mass equals the residue of \(E(z)\) at \(z = u\), which is given by equation (20). At all other points the limit in our case vanishes. The orthogonality measures of several important systems of orthogonal polynomials were found by (i) computing the large \(n\) asymptotic of \(P_n(x)\) and \(P_n^{(1)}(x)\) in the representation (18) followed by (ii) the inversion of the Stieltjes transform \([38]\).

### References

[1] Schweber S 1967 Ann. Phys., NY 41 205–29
[2] Rabi I I 1936 Phys. Rev. 49 324–8
[3] Bargmann V 1961 Commun. Pure Appl. Math. 14 187–214
[4] Braak D 2011 Phys. Rev. Lett. 107 100401
[5] Albert V V 2012 Phys. Rev. Lett. 108 180401
[6] Moroz A 2012 Europhys. Lett. 100 60010
[7] Moroz A 2013 Ann. Phys., NY 338 319–40
[8] Moroz A 2014 Ann. Phys., NY 340 252–66
[9] Zhang Y-Z 2013 arXiv:1304.7827[quant-ph]
[10] Zhang Y-Z 2014 Ann. Phys., NY 347 122–9
[11] Shore H B and Sander L M 1973 Phys. Rev. B 7 4537–46
[12] Haydock R 1980 The recursive solution of the Schrödinger equation (Solid State Physics vol 35) ed H Ehrenreich, F Seitz and D Turnbull (New York: Academic) pp 215–94
[13] Moroz A Haydock’s recursive solution of self-adjoint problems discrete spectrum Ann. Phys., NY at press doi:10.1016/j.aop.2014.09.022
[14] Nikiforov A F, Suslov S K and Uvarov V B 1991 Classical Orthogonal Polynomials of a Discrete Variable (Berlin: Springer)
[15] Shore H B and Sander L M 1973 Phys. Rev. B 7 4537–46
[16] Haydock R 1980 The recursive solution of the Schrödinger equation (Solid State Physics vol 35) ed H Ehrenreich, F Seitz and D Turnbull (New York: Academic) pp 215–94
[17] Bourassa J, Gambetta J M, Abdumalikov A A Jr, Astafiev O, Nakamura Y and Blais A 2009 Phys. Rev. A 80 032109
[18] Form-Díaz P, Lisenfeld J, Marcos D, García-Ripoll J J, Solano E, Harmans C J P M and Mooij J E 2010 Phys. Rev. Lett. 105 237001
[19] Niemczyk T et al 2010 Nat. Phys. 6 772–6
[20] Barut A O and Girardello L 1971 Commun. Math. Phys. 21 41–55
[21] Gauthschi W 1967 SIAM Rev. 9 24–82
[22] Gauthschi W 2013 private communication
[23] Chihara T S 1978 An Introduction to Orthogonal Polynomials (New York: Gordon and Breach)
[24] Wagner M 1984 J. Phys. A: Math. Gen. 17 2319–33
[25] Fulton R L and Gouterman M 1961 J. Chem. Phys. 35 1059–71
[26] Schiró M, Bordyuh M, Öztöür B and Türeci H E 2012 Phys. Rev. Lett. 109 053601
[27] Tomka M, El Araby O, Pletyukhov M and Gritsev V 2013 arXiv:1307.7876[quant-ph]
[28] Gardas B and Dajka J 2013 J. Phys. A: Math. Theor. 46 265302
[29] Larson J 2013 J. Phys. B: At. Mol. Opt. Phys. 46 224016
[30] Lee Y-H, Yang W-L and Zhang Y-Z 2011 Nonlinearity 24 1975–86
[31] Zhang Y-Z and Moroz A in preparation
[32] Magnus A P 1988 Associated Askey–Wilson polynomials as Laguerre–Hahn orthogonal polynomials Orthogonal Polynomials and their Applications, Proc. Springer Lecture Notes in Mathematics (Segovia, 1986) ed M Alfaro et al vol 1329 (Berlin: Springer) pp 261–78
[33] A P Magnus 1995 J. Comput. Appl. Math. 65 253–65
[34] Witte N S 2012 arXiv:1204.2328[math.CA]
[35] Hamburger H 1920 Math. Ann. 81 234–319 (can be freely accessed through the European digital mathematical library at http://eudml.org)
[36] Shohat J A and Tamarkin J D 1970 The Problem of Moments (Providence, RI: American Mathematical Society)
[37] Ismail M E H 2005 Classical and Quantum Orthogonal Polynomials in One Variable (Cambridge: Cambridge University Press)
[38] Akhiezer N I 1965 The Classical Moment Problem and Some Related Questions in Analysis (Edinburgh: Oliver and Boyd)
[39] Moroz A 2012 arXiv:1205.3139[quant-ph]
[40] The source code can be freely downloaded from http://www.wave-scattering.com/rabi.html
[41] Data files *gp2dp4n300.dat obtained for $\kappa\Delta$ = (0.2, 0.4) and $n = 300$ are available from http://www.wave-scattering.com/rabi.html
[42] IEEE 2008 standard for floating-point arithmetic (IEEE 754–2008)
[43] Moroz A in preparation
[44] Turbiner A V and Ushveridze A G 1987 Phys. Lett. A 126 181–3
[45] Turbiner A V and Ushveridze A G 1988 Commun. Math. Phys. 118 467–74
[46] Bender C M and Dunne G V 1996 J. Math. Phys. 37 6–11
[47] Sachse C 2006 Theor. Math. Phys. 149 1299–311
[48] Meijer P H E 1954 Phys. Rev. 95 1443–9
[49] Finkelstein R J and Moe M 1955 Phys. Rev. 100 1775–9
[50] Ismail M E H, Nikolova I and Simeonov P 2005 Ramanujan J. 8 475–502
[52] Abramowitz M and Stegun I A 1973 Handbook of Mathematical Functions (New York: Dover)
(http://people.math.sfu.ca/~cbm/aands/page_783.htm)
[53] Al-Salam W A 1990 Characterization theorems for orthogonal polynomials In Orthogonal
Polynomials: Theory and Practice (NATO ASI series C vol 294) ed P Nevai (Dordrecht: Kluwer) pp 1–24
[54] García A G, Marcellán F and Salto L 1995 J. Comput. Appl. Math. 57 147–62
[55] Koekoek R, Lesky P A and Swarttouw R F 2010 Hypergeometric Orthogonal Polynomials and
their q-Analogues 1st edn (Berlin: Springer)
[56] Odake S and Sasaki R 2008 J. Math. Phys. 49 053503
[57] Martin-Löf P 1966 Inform. Control 9 602–19
[58] Casati G, Guarneri I and Valz-Gris F 1984 Phys. Rev. A 30 1586–8
[59] Charlier C V L 1905–06 Ark. Mat. Astron. Fys. 2 1–9
[60] Feit M D, Fleck J A Jr and Steiger A 1982 J. Comput. Phys. 47 412–33
[61] Wang Q-W and Liu Y-L 2013 J. Phys. A: Math. Theor. 46 435303
[62] Spiridonov V, Vinet L and Zhedanov A 1993 Lett. Math. Phys. 29 63–73