Quasi-Exactly Solvable Systems and Orthogonal Polynomials

Carl M. Bender

Department of Physics, Washington University, St. Louis, MO 63130

Gerald V. Dunne

Department of Physics, University of Connecticut, Storrs, CT 06269

Abstract

This paper shows that there is a correspondence between quasi-exactly solvable models in quantum mechanics and sets of orthogonal polynomials \( \{P_n\} \). The quantum-mechanical wave function is the generating function for the \( P_n(E) \), which are polynomials in the energy \( E \). The condition of quasi-exact solvability is reflected in the vanishing of the norm of all polynomials whose index \( n \) exceeds a critical value \( J \). The zeros of the critical polynomial \( P_J(E) \) are the quasi-exact energy eigenvalues of the system.
In quantum mechanics there exist potentials for which it is possible to find a finite portion of the energy spectrum and associated eigenfunctions exactly and in closed form. These systems are said to be quasi-exactly solvable. In such systems the potential depends on a parameter \( J \); for positive integer values of \( J \) one can find \( J \) eigenvalues and eigenfunctions exactly. The usual approach to the analysis of quasi-exactly solvable systems is an algebraic one in which the Hamiltonian is expressed as a nonlinear combination of generators of a Lie algebra, not belonging to the center of the corresponding enveloping algebra. This technique is a modification of the dynamical symmetry approach to exactly solvable quantum-mechanical systems, in which one can find by algebraic means the entire spectrum in closed form.

In this paper we propose an alternative approach to quasi-exact solvability. We show that the solution \( \psi \) to the Schrödinger equation for a quasi-exactly solvable model,

\[
H \psi = E \psi, 
\]

is the generating function for a set of polynomials \( \{P_n(E)\} \) in the energy variable \( E \). These polynomials satisfy a three-term recursion relation and therefore form an orthogonal set with respect to some weight function \( w(E) \). For positive integer values of the parameter \( J \), corresponding to quasi-exact solvability, we find that the norm of \( P_n(E) \) vanishes for \( n \geq J \). Moreover, all polynomials \( P_n(E) \) beyond a critical polynomial \( P_J(E) \), factor into a product of two polynomials, one of which is \( P_J(E) \):

\[
P_{n+J}(E) = P_J(E)Q_n(E) \quad (n \geq 0). 
\]

The zeros of the critical polynomial \( P_J(E) \) are precisely the quasi-exact energy eigenvalues of the quantum-mechanical model.

We illustrate these features of quasi-exactly solvable models with the following infinite class of Hamiltonians first discussed by A. Turbiner

\[
H = -\frac{d^2}{dx^2} + \frac{(4s - 1)(4s - 3)}{4x^2} - (4s + 4J - 2)x^2 + x^6. 
\]
Here, $s$ is an arbitrary parameter. When $s$ lies between $\frac{1}{4}$ and $\frac{3}{4}$, there is an attractive centrifugal term; for $s$ outside this range the centrifugal term is repulsive. When $s = \frac{1}{4}$ or $s = \frac{3}{4}$, the centrifugal core term disappears leaving a nonsingular sextic oscillator Hamiltonian

$$H = -\frac{d^2}{dx^2} - (4s + 4J - 2)x^2 + x^6.$$  \hfill (4)

When the parameter $J$ in Eq. (3) is a nonnegative integer, the corresponding Schrödinger equation has $J$ exact, closed-form solutions for any value of $s$.

We seek a solution $\psi(x)$ to the Schrödinger equation for $H$ in Eq. (3) of the form

$$\psi(x) = \exp\left(-\frac{1}{4}x^4\right)x^{2s-1/2}\sum_{n=0}^{\infty} \left(-\frac{1}{4}\right)^n \frac{P_n(E)}{n!\Gamma(n + 2s)}x^{2n}. \hfill (5)$$

Observe that when $s = \frac{1}{4}$ this solution becomes an even-parity wave function of the oscillator Hamiltonian (4); when $s = \frac{3}{4}$, $\psi(x)$ becomes an odd-parity wave function of $H$ in (4).

Demanding that $\psi(x)$ in Eq. (5) obey the Schrödinger equation (1) leads to the following recursion relation for the expansion coefficients $P_n(E)$:

$$P_n(E) = EP_{n-1}(E) + 16(n - 1)(n - J - 1)(n + 2s - 2)P_{n-2}(E) \quad (n \geq 2), \hfill (6)$$

subject to the initial conditions

$$P_0(E) = 1 \quad \text{and} \quad P_1(E) = E. \hfill (7)$$

From these initial conditions the recursion relation (6) generates a set of monic polynomials, the next four of which are

$$P_2(E) = E^2 + (32 - 32J)s,$$

$$P_3(E) = E^3 + [(160 - 96J)s - 32J + 64]E,$$

$$P_4(E) = E^4 + [(448 - 192J)s - 128J + 352]E^2 + (3072J^2 - 12288J + 9216)s(s + 1),$$

$$P_5(E) = E^5 + [(960 - 320J)s - 320J + 1120]E^3 + [(15360J^2 - 81920J + 91136)s^2$$

$$+(25600J^2 - 141312J + 164864)s + 6144J^2 - 36864J + 49152]E. \hfill (8)$$

These polynomials have a number of noteworthy properties. First, for all values of the parameters $s$ and $J$ they form an orthogonal set. This follows from the fact that they
are generated by a second-order (three-term) recursion relation. For example, the corresponding recursion relation for an \( x^4 \) anharmonic oscillator potential, whose Hamiltonian is not quasi-exactly solvable, is a higher-order recurrence relation. The harmonic oscillator system leads to a two-term recursion relation; this system is exactly solvable rather than quasi-exactly solvable.

Second, from the expansion (5) we can see that the wave function \( \psi(x, E) \) is the generating function for the polynomials \( P_n(E) \).

The third and most significant property of the polynomials \( P_n(E) \) is that, when the parameter \( J \) takes positive integer values, the polynomials exhibit the factorization property in Eq. (3). This factorization occurs because the third term in the recursion relation (3) vanishes when \( n = J + 1 \), so that all subsequent polynomials have the common factor \( P_J(E) \). This factorization property holds for all values of the parameter \( s \). Furthermore, this factorization leads to the result that the zeros of the critical polynomial \( P_J(E) \) are just the quasi-exact energy eigenvalues. This is true because the expansion in (5) truncates when \( E \) is a zero of \( P_J(E) \); when this series truncates the wave function \( \psi(x) \) is automatically normalizable.

To illustrate this factorization we list in factored form the first six polynomials \( P_n(E) \) for the case \( J = 3 \):

\[
\begin{align*}
P_0(E) &= 1, \\
P_1(E) &= E, \\
P_2(E) &= E^2 - 64s, \\
P_3(E) &= E^3 - (128s + 32)E, \\
P_4(E) &= [E^3 - (128s + 32)E]E, \\
P_5(E) &= [E^3 - (128s + 32)E](E^2 + 128s + 192),
\end{align*}
\]

Observe that \( P_3(E) \) is a common factor of \( P_n(E) \) for \( n \geq 3 \). The zeros of \( P_3(E) \) are

\[
E = 0, \quad E = \pm \sqrt{128s + 32},
\]
which are the three exact energy eigenvalues for the quasi-exactly solvable Hamiltonian (3) when $J = 3$. The corresponding exact eigenfunctions are obtained by evaluating $\psi(x)$ in Eq. (5) at these values of $E$

\[
\psi_0(x) = \exp \left( -\frac{1}{4} x^4 \right) \frac{\Gamma^{2s-1/2}}{\Gamma(2s)} \left( 1 - \frac{x^4}{2s+1} \right),
\]

\[
\psi_+(x) = \exp \left( -\frac{1}{4} x^4 \right) \frac{\Gamma^{2s-1/2}}{\Gamma(2s)} \left( 1 - \frac{\sqrt{128s+32}}{8s} x^2 + \frac{x^4}{2s} \right),
\]

\[
\psi_-(x) = \exp \left( -\frac{1}{4} x^4 \right) \frac{\Gamma^{2s-1/2}}{\Gamma(2s)} \left( 1 + \frac{\sqrt{128s+32}}{8s} x^2 + \frac{x^4}{2s} \right).
\]  

(11)

Note that the energy levels may be ordered by the number of nodes of the corresponding wave function.

A fourth property of the polynomials $P_n(E)$ concerns their norms. The norm (squared) $\gamma_n$ of $P_n(E)$ is defined as an integral:

\[
\gamma_n = \int dE w(E) |P_n(E)|^2.
\]  

(12)

It is possible to determine the norms of an orthogonal set of polynomials directly from the recursion relation; it is not necessary to know explicitly the weight function $w(E)$ with respect to which the polynomials are orthogonal. The procedure is simply to multiply the recursion relation (6) by $w(E)E^{n-2}$ and to integrate with respect to $E$. Using the fact that $P_n(E)$ is orthogonal to $E^k$, $k < n$, we obtain a simple, two-term recursion relation for $\gamma_n$:

\[
\gamma_n = 16n(J - n)(2s + n - 1)\gamma_{n-1}.
\]  

(13)

The solution to this equation with $\gamma_0 = 1$ is

\[
\gamma_n = \frac{16^n n! \Gamma(J) \Gamma(2s + n)}{\Gamma(J - n) \Gamma(2s)}.
\]  

(14)

This equation reveals that the space of orthogonal polynomials arising from a quasi-exactly solvable model is associated with a nonpositive definite norm. In particular, we can
see from Eq. (14) that $\gamma_n$ vanishes for $n \geq J$ if $J$ is a positive integer. The appearance of a vanishing norm coincides with the factorization mentioned above and is an alternative characterization of quasi-exact solvability.

It is interesting that while the polynomials $P_{n+J}(E)$ for $n \geq 0$ have vanishing norm when $J$ is a positive integer, the quotient polynomials $Q_n(E)$ in Eq. (2) form a new orthogonal set of polynomials for each value of $J$.

Having determined the norms $\gamma_n$ of the polynomials $P_n(E)$ it is natural to evaluate the integral of the square of the generating function (wave function) with respect to the weight function $w(E)$:

$$G(x) = \int dE \, w(E)[\psi(x, E)]^2,$$  \hspace{1cm} (15)

where $\psi(x, E)$ is given in Eq. (5). Using the orthogonality of the polynomials $P_n(E)$, we can express $G(x)$ as a confluent hypergeometric function:

$$G(x) = \frac{\Gamma(J)}{\Gamma(2s)} \exp \left( -\frac{1}{2} x^4 \right) \sum_{n=0}^{\infty} \frac{x^{4n+4s-1}}{n! \Gamma(n+2s)\Gamma(J-n)}.$$  \hspace{1cm} (16)

When $J$ is a positive integer, this sum truncates and we find that $G(x)$ can be expressed as a linear combination of the squares of the $J$ quasi-exact eigenfunctions of the Hamiltonian $H$ in Eq. (3). For example, when $J = 3$, we have

$$G(x) = \frac{1}{\Gamma(2s)} \exp \left( -\frac{1}{2} x^4 \right) x^{4s-1} \left[ 1 + \frac{x^4}{s} + \frac{x^8}{2s(2s+1)} \right]$$

$$= \frac{\Gamma(2s)}{\Gamma(2s)} \left( \frac{2s+1}{4s+1} [\psi_0(x)]^2 + \frac{s}{4s+1} [\psi_+(x)]^2 + \frac{s}{4s+1} [\psi_-(x)]^2 \right),$$  \hspace{1cm} (17)

where $\psi_0(x)$ and $\psi_{\pm}(x)$ are taken from Eq. (11). We emphasize that this result is highly nontrivial. Expressing $G(x)$ as a linear combination of the squares of the eigenfunctions requires that one solve an overdetermined system of $2J - 1$ equations for $J$ expansion coefficients.

Let us now investigate the properties of the weight function $w(E)$. From the polynomials $P_n(E)$ we can calculate the moments of $w(E)$. Let $a_n$ represent the $2n$th moment of $w(E)$:
\[ a_n = \int dE \, w(E) E^{2n}. \]  \hspace{1cm} \text{(18)}

(Because the polynomials have parity symmetry we know that the odd moments vanish.)

We are free to normalize \( w(E) \) so that its zeroth moment is unity:

\[ a_0 = 1. \]  \hspace{1cm} \text{(19)}

The remaining moments can then be determined algebraically:

\[ a_1 = 32(J - 1)s, \]
\[ a_2 = 32^2(J - 1)s(3Js - 5s + J - 2), \]
\[ a_3 = 32^3(J - 1)s(15J^2s^2 - 60Js^2 + 61s^2 + 15J^2s - 67Js + 74s + 4J^2 - 19J + 22), \]
\[ a_4 = 32^4(J - 1)s(105J^3s^3 - 735J^2s^3 + 1743Js^3 - 1385s^3 + 210J^3s^2 - 1596J^2s^2 + 4038Js^2 - 3372s^2 + 147J^3s - 1179J^2s + 3114Js - 2688s + 34J^3 - 282J^2 + 765J - 674), \]
\[ a_5 = 32^5(J - 1)s(945J^4s^4 - 10080J^3s^4 + 40950J^2s^4 - 74400Js^4 + 50521s^4 + 3150J^4s^3 - 35910J^3s^3 - 153990J^2s^3 + 292154Js^3 + 205228s^3 + 4095J^4s^2 - 48960J^3s^2 + 218337J^2s^2 - 427524Js^2 + 307860s^2 + 2370J^4s - 29306J^3s + 134373J^2s - 269085Js + 197206s + 496J^4 - 6272J^3 + 29292J^2 - 59531J + 44134). \]  \hspace{1cm} \text{(20)}

These moments have some interesting mathematical properties. For example, all the moments \( a_n, n \geq 1, \) have a factor of \( (J - 1)s. \) Furthermore, in the residual factor the coefficient of \( (Js)^{n-1} \) is \( (2n - 1)!! \) and the coefficient of \( s^{n-1} \) is the \( n \)th Euler number \( E_n. \) \[ 1 \]

The outstanding property of the moments \( a_n \) concerns their rapid rate of growth. This rate of growth can be determined using the fact that there is a simple relationship between the moments \( a_n \) and the coefficients \( b_{n-1} \) of \( P_{n-2}(E) \) in the recursion relation \( (3). \) Specifically, the Taylor series

\[ f(z) = \sum_{n=0}^{\infty} a_n z^n, \]  \hspace{1cm} \text{(21)}

whose coefficients are the moments in Eq. (18), is equivalent to a continued fraction.
\[ f(z) = \frac{1}{(1 - b_1 z / (1 - b_2 z / (1 - b_3 z / (1 - \ldots))))}, \] (22)

whose coefficients are \( b_n \). Since \( b_n \) is a cubic polynomial in \( n \) we deduce that the moments \( a_n \) grow like \((3n)!\). [11]

It is unusual to find orthogonal polynomials whose weight functions have moments that grow so rapidly. The classical orthogonal polynomials, such as the Hermite polynomials, typically have moments that grow like \( n! \). This is also true of discrete versions of the classical orthogonal polynomials, such as the Hahn polynomials. [12] The Euler and Bernoulli polynomials are distinctive [13] in that their moments grow like \((2n)!\). However, the polynomials \( P_n(E) \) associated with quasi-exactly solvability are of an entirely new type due to the rapid rate of growth of their moments. Carleman’s condition states that when the moments grow faster than \((2n)!\), the moment problem is not guaranteed to have a unique solution. [15]

Almost certainly, the weight function \( w(E) \) is not unique! This nonuniqueness corresponds to a kind of gauge invariance that underlies these quasi-exactly solvable systems. Indeed one may conjecture that the nonuniqueness of the weight function is related to the Lie algebraic symmetry of quasi-exactly solvability.

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[7] Here, monic means that the coefficient of the highest power of $E$ is one.

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[9] Note that the actual domain of integration over $E$ in (12) is from $-\infty$ to $+\infty$, but depending on the weight function this domain may be further truncated. Knowing the domain corresponds to knowing the explicit weight function, which is in general a difficult problem. However, knowledge of the domain is unnecessary for our algebraic approach.

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