ENERGY SPECTRUM DESIGN AND POTENTIAL FUNCTION ENGINEERING

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Starting with an orthogonal polynomial sequence \( \{p_n(s)\}_{n=0}^{\infty} \) that has a discrete spectrum, we design an energy spectrum formula \( E_k = f(s_k) \), where \( \{s_k\} \) is the finite or infinite discrete spectrum of the polynomial. Using a recent approach to quantum mechanics based not on potential functions but on orthogonal energy polynomials, we give a local numerical realization of the potential function associated with the chosen energy spectrum. We select the three-parameter continuous dual Hahn polynomial as an example. Exact analytic expressions are given for the corresponding bound-state energy spectrum, the phase shift of scattering states, and the wavefunctions. However, the potential function is obtained only numerically for a given set of physical parameters.

Keywords: energy spectrum design, potential function engineering, orthogonal polynomials, recursion relation, continuous dual Hahn polynomial, scattering phase shift, wavefunction

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1. Introduction

The structure of a quantum mechanical system is defined by its discrete bound states and resonances, whereas the dynamics is governed by its continuum scattering states. The discrete energy spectrum could be finite or countably infinite. If the system is modeled by a potential function, then there is a one-to-one correspondence between the complete energy spectrum (continuous and discrete) and the potential. The energy spectrum of a totally confined system consists only of discrete bound states (structure). On the other hand, dynamical information about a system interacting with its surroundings is found in the continuous part of the energy spectrum. Such information is contained in the scattering matrix (or scattering phase shift). All well-known quantum systems associated with exactly solvable potential functions (the harmonic oscillator, Coulomb, Morse, Pöschl–Teller, Eckart, Scarf, and other potentials) have simple discrete energy spectra \( \{E_k\} \) that behave as \( k, (k + \mu)^2, \) or \( (k + \mu)^{-2}, \) where \( \mu \) is a dimensionless parameter. It would be interesting and fruitful to design systems with a richer energy spectrum (for example, \( E_k \sim e^{-k^2}, E_k \sim \sinh(k), \) and \( E_k \sim \sin(k\pi/2N) \) with \( k \leq N, \) etc.) and to construct the corresponding potential function. In this paper, we propose a method to accomplish just that. If successful, it could be regarded as one of the solutions to the inverse problem, that is, constructing the potential function using knowledge of the energy spectrum data (see, e.g., [1]). As we show here, this solution is not unique due to an equivalence generated by similarity transformations of the corresponding Hamiltonian matrix. We now make an indispensable digression to address the notion of a potential function in quantum mechanics.

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The concept of a potential function originated long before the inception of quantum mechanics. It is rooted in our understanding of classical mechanics where the total energy of a particle (matter) moving in a field (nonmatter) is the sum of its kinetic and potential energies. The potential energy changes with the position of the particle, hence the concept of a potential function. For example, the potential function of a massive particle moving in the gravitational field of a point mass $M$ at the origin is $MG/r$ ($G$ being the gravitational constant and $r$ the radial distance from the point mass), whereas for a particle of charge $q$ moving in the electric field of a point charge $Z$ at the origin, it is $qZ/r$. Also, the potential function for a massive particle attached to a linear massless spring of constant $k$ is $kx^2/2$, etc. Subsequently, different types of potential functions where proposed to describe certain aspects of the system in complex surroundings. Examples include the Yukawa potential $Qe^{-\lambda r}/r$ to describe screening of the inverse square force, the oscillator potential $\omega^2 r^2$ to describe confined oscillatory motion, the Morse potential $D(e^{-2\lambda x} - 2\mu e^{-\lambda x})$ to describe vibrations in a diatomic molecule, etc.

The potential function concept was then carried over to quantum mechanics, via a particular construction of the system Hamiltonian, although none of the postulates of the theory requires it. In fact, the postulates of quantum mechanics involve only two fundamental objects: the space–time wavefunction $\Psi(t,\vec{r})$ and the Hamiltonian operator $H$. Other operators are developed to correspond to the desired physical property to be measured (e.g., position, linear momentum, angular momentum, spin, etc.). The wavefunction allows evaluating the expectation values (measurement results) of physical observables at a given time, and the Hamiltonian operator determines their time development. It is by an (arbitrary) choice that the Hamiltonian was split into the sum of a kinetic energy operator and a potential function as $H = T + V$; a suggestion that was inspired by, and carried over from, classical mechanics, which over many decades (of success) became the tradition.

An undergraduate student in quantum mechanics is taught to make a one-to-one correspondence between a given physical system and its classical potential function model. In fact, the present undergraduate physics curricula make classical mechanics a prerequisite to quantum mechanics courses. Hence, whatever one does or says to describe the quantum mechanical problem, the student would always ask about the potential function that he/she needs to incorporate into the wave equation to solve that problem. Imagine describing the oscillator problem by explaining in full detail how the particle moves and then ask the students “what is the energy spectrum?” Admittedly, this is not an easy task for the students because they would have to start by solving the inverse problem: finding the potential function from the given description, and then substituting that into the Schrödinger equation to solve for the energy spectrum. This is quite complicated. They were taught this way as the only way: they need the potential function to proceed. It is more than just a tradition, it is a religion.

Moreover, exact solvability of the wave equation in the potential function picture limits the number of analytically realizable quantum systems. These systems are well known and arranged into a small number of classes. Each class is associated with a given potential function like the Coulomb, harmonic oscillator, Morse, Eckart, and other potentials.

Nevertheless, an alternative formulation of doing quantum mechanics was developed recently in [2]–[4] based on the premise that the set of analytically realizable quantum systems is much larger than the set of exact solutions of the Schrödinger equation in the potential function picture. Equivalently, the representation of the Hamiltonian operator in the wave equation, $i\hbar \frac{\partial}{\partial t} \Psi = H \Psi$, as the sum $H = T + V$ is a very restrictive choice that limits the number of analytically realizable physical systems. In this alternative formulation, the theory of orthogonal polynomials and special functions plays a major role. We believe that the potential function picture in quantum physics is a limitation. The objective of the alternative formulation is to obtain a set of analytically realizable systems that would be much larger than in the conventional potential formulation. Sometimes, this implies that the potential functions corresponding to
the newly found systems may not have analytic realizations or that the associated wave equation cannot be written in the conventional format (that is, it could become a differential equation of an order higher than two or with a nonlocal potential, etc.).

In the absence of a potential function, the new formulation gives the wavefunction as a pointwise convergent series of a complete set of square-integrable functions in configuration space. The expansion coefficients of the series are orthogonal polynomials in the energy and/or physical parameters. These energy polynomials carry all of the physical information about the system. Nonetheless, to establish a correspondence between the new formulation and the potential formulation, procedures were established to obtain sufficiently accurate numerical representations of the potential functions of the new quantum systems for a given set of physical parameters \([5]\). These procedures were used successfully in several studies \([5]–[8]\) to derive novel quantum systems and obtain their corresponding potential functions.

In this paper, we present a general scheme for obtaining a class of quantum systems associated with the three-parameter continuous dual Hahn orthogonal polynomials \(S^\mu_n(z^2; a, b)\) for a given choice of the energy spectrum formula \(E(z^2)\) and a given set of basis functions in configuration space, \(\{\phi_n(x)\}\). The energy spectrum, the scattering phase shift, and the wavefunction are obtained analytically. However, the corresponding potential function can only be derived numerically for a given set of physical parameters. By choosing the energy as a special function of the polynomial argument, \(E(z^2)\), we show in Sec. 2 how the energy spectrum, the scattering phase shift, and the wavefunction can be derived analytically. In Sec. 3, we show how to obtain the matrix elements of the potential function for a given choice of square-integrable basis functions \(\{\phi_n(x)\}\). Finally, in Sec. 4, we show local plots of the potential function as illustrative examples for a given set of physical parameters.

2. The quantum system

We start by giving a brief account of the formulation of quantum mechanics based on orthogonal energy polynomials but with no mention at all of any potential function. In the atomic units \(\hbar = M = 1\) and in one dimension, the total wavefunction in this formulation is written as the Fourier expansion in energy \([2]–[4]\),

\[
\Psi(x,t) = \int_X e^{-iEt} \psi(x,E) \, dE + \sum_{k=0}^N e^{-iE_k t} \psi_k(x),
\]

(1)

where \(X\) is the continuous energy interval(s) and \(\{E_k\}\) are the discrete bound state energies. The continuous and discrete Fourier components \(\psi(x,E)\) and \(\psi_k(x)\) are written as the pointwise convergent series

\[
\psi(x,E) = \sqrt{\rho(z)} \sum_{n=0}^{\infty} P_n(z^2) \phi_n(x),
\]

(2a)

\[
\psi_k(x) = \sqrt{\omega_k} \sum_{n=0}^{\infty} P_n(z_k^2) \phi_n(x),
\]

(2b)

where \(z^2 = z^2(E)\) is some proper function of energy (we assume that the function \(E(z^2)\) is invertible, giving \(z^2(E)\), and that \(z(E) > 0\) for \(E \in X\)), and \(\{\phi_n(x)\}\) is a complete set of square-integrable functions. Moreover, \(P_n(z^2)\) in (2a) and (2b) is a degree-\(n\) polynomial in \(z^2\) satisfying the general orthogonality and recursion relation \([2]–[4]\)

\[
\int_X \rho(z) P_n(z^2) P_m(z^2) \, dz + \sum_k \omega_k P_n(z_k^2) P_m(z_k^2) = \delta_{n,m},
\]

(3a)

\[
z^2 P_n(z^2) = A_n P_n(z^2) + B_{n-1} P_{n-1}(z^2) + B_n P_{n+1}(z^2),
\]

(3b)
where $A_n$ and $B_n$ are real numbers, which are independent of $z$ and such that $B_n \neq 0$ for all $n$. The three-term recursion relation (3b) gives all $\{P_n(z^2)\}$ starting with the two initial values $P_0(z^2) = 1$ and $P_1(z^2) = (z^2 - A_0)/B_0$.

Wavefunction (2a) associated with the continuous spectrum is characterized by bounded oscillations that do not vanish all the way to the boundaries of space. However, wavefunction (2b) associated with bound states is characterized by a finite number of patterns of oscillatory-like behavior (with the number of nodes equal to the bound state excitation level) that vanishes rapidly at the boundaries. Attempting to evaluate the wavefunction at an energy that does not belong to the continuous or discrete spectrum would only result in a diverging series (2a) and (2b). That is, the result is given by unstable endless oscillations that grow without bound all over space as the number of terms in sum (2a) and (2b) increases.

In addition to orthogonality property (3a) and recursion relation (3b), polynomials that are compatible with this alternative formulation of quantum mechanics must have an oscillatory asymptotics ($n \to \infty$) that takes the form

$$\lim_{n \to \infty} P_n(s) = \frac{1}{n^\tau \sqrt{\rho(s)}} \cos[n^\sigma \varphi(s) + \delta(s)],$$

(4)

where $\tau$ and $\sigma$ are positive real parameters, $\varphi(s)$ is an entire function, and $\delta(s)$ is the scattering phase shift. If $\sigma \to 0$, then $n^\sigma \to \ln n$. Almost all known hypergeometric orthogonal polynomials that populate the physics and engineering literature [9] have this asymptotic property. This includes the Wilson, continuous Hahn, Meixner–Pollaczek, Jacobi, Laguerre, Gegenbauer, Chebyshev, Hermite, and other polynomials. Bound states, if they exist, occur at a finite or countably infinite set $\{s_k\}$ that makes the scattering amplitude (the factor left of the sine in (4)) vanish: $\varrho(s)|_{s=s_k} \propto \delta(s-s_k)$. Some of the polynomials mentioned (e.g., the Hermite, Chebyshev, Laguerre, and Jacobi) do not have a discrete spectrum that could correspond to bound states. For a detailed discussion of the connection between the asymptotics of such polynomials and scattering, we refer the reader to [10]–[12] and the references therein.

For the current problem, we choose the orthogonal polynomial $P_n(z^2)$ to be a two-parameter special case of the continuous dual Hahn polynomial: $P_n(z^2) = S_n(z^2; a, a)$. The definition of the orthonormal version of the polynomial, $S_n(z^2; a, b)$, and its properties that are relevant to our study are given in Section IV.B and in the Appendix of [2]. Consequently, if $\mu < 0$, then in addition to the continuous spectrum, the system has a finite number of bound states with an energy spectrum that can be obtained by solving for $\{E_k\}$ in the energy spectrum formula [2]

$$z^2(E_k) = -(k + \mu)^2,$$

(5)

where $k = 0, 1, \ldots, N$ and $N$ is the largest integer less than $-\mu$. The scattering phase shift associated with the continuous spectrum is obtained from the asymptotics ($n \to \infty$) of $S_n(z^2; a, a)$ as [2]

$$\delta(E) = \arg \Gamma[2iz(E)] - \arg \Gamma[\mu + iz(E)] - 2 \arg \Gamma[a + iz(E)].$$

(6)

The corresponding total wavefunction (1) is determined once the continuous and discrete Fourier components are given as shown by Eq. (2a) and (2b). Therefore, having decided on the energy spectral function $E(z^2)$ with $P_n(z^2)$ chosen as $S_n(z^2; a, a)$, we only need the basis set $\{\phi_n(x)\}$ and the continuous and discrete weight functions $\rho(z)$ and $\omega_k$. These weight functions are given in Section IV.B of [2] in the form

$$\rho(z) = \left| \frac{\Gamma[\mu + iz(E)]^2 \Gamma[a + iz(E)] \Gamma[a - iz(E)]}{\Gamma[2iz(E)] \Gamma[2a] \Gamma(\mu + a)} \right|^{2 \pi \Gamma(2a) \Gamma(z) (\mu + a)},$$

$$\omega_k = \frac{(k + \mu) 2(-1)^{k+1}(2\mu)_k}{k! \Gamma(2a) \Gamma(1 - 2\mu) \Gamma(\mu + a + 1) \Gamma(\mu - a + 1)} \left[ \frac{\Gamma(a - \mu) (\mu + a)_k}{(\mu + a + 1)_k} \right]^2,$$

(7)

where $(a)_n = a(a+1)(a+2) \ldots (a+n-1) = \frac{\Gamma(n+a)}{\Gamma(a)}$ is the Pochhammer symbol (the shifted factorial).
Thus, for a given energy spectral function \( E(z^2) \) and basis \( \{\phi_n(x)\} \), we have obtained analytic expressions for the objects in Eqs. (2), (5)–(7). The analytically realizable components of the system are therefore given by the energy spectrum, the scattering phase shift, and the wavefunction. We do not ponder on these three items any more and instead seek the corresponding potential function; it can only be determined numerically given \( E(z^2) \), \( \{\phi_n(x)\} \), and a set of physical parameters.

3. The potential matrix

The one-dimensional Schrödinger wave equation is \( i\frac{d}{dt}\Psi(x,t) = H\Psi(x,t) \), where \( H \) is the Hamiltonian operator. Substituting (1) and (2a), (2b), in this equation and then projecting from the left by \( \langle \phi_m(x) | \) and integrating over \( x \) gives two matrix wave equations

\[
\sum_n \mathcal{H}_{m,n} P_n(z^2) = E \sum_n \Omega_{m,n} P_n(z^2), \tag{8}
\]

\[
\sum_n \mathcal{H}_{m,n} P_n(z^2_k) = E_k \sum_n \Omega_{m,n} P_n(z^2_k), \tag{9}
\]

where \( \mathcal{H}_{m,n} = \langle \phi_m | H | \phi_n \rangle \) and \( \Omega_{m,n} = \langle \phi_m | \phi_n \rangle \). On the other hand, the three-term recursion relation (3b) can be rewritten as

\[
\sum_n R_{m,n} P_n(z^2) = z^2 \sum_n \delta_{m,n} P_n(z^2), \tag{9}
\]

where \( R \) is the tridiagonal symmetric matrix whose elements are

\[
R_{m,n} = A_m \delta_{m,n} + B_{m-1} \delta_{m,n+1} + B_m \delta_{m,n-1}.
\]

To simplify the analysis, we choose the basis \( \{\phi_n(x)\} \) as an orthonormal set, whence \( \Omega_{m,n} = \delta_{m,n} \). We can then write Eqs. (8) and (9) as \( \mathcal{H}|P\rangle = E|P\rangle \) and \( R|P\rangle = z^2|P\rangle \). In other words, \( |P\rangle \) is a common eigenvector for the two Hermitian matrices \( \mathcal{H} \) and \( R \) with the corresponding eigenvalues \( E \) and \( z^2 \).

Now, since \( E \) depends on \( z \) as \( E(z^2) \), we can write\(^1\)

\[
\mathcal{H} = \Lambda[E(R)]\Lambda^{-1}, \tag{10}
\]

where \( \Lambda \) is a similarity transformation (usually, an involutory matrix: \( \Lambda = \Lambda^{-1} = \Lambda^T \)). One such involutory matrix is the Householder transformation matrix that makes \( \mathcal{H} \) a tridiagonal symmetric matrix (see section 11.3 in [13]). Consequently, our solution is unique modulo a similarity transformation. In fact, noneuniqueness is a well-known feature of the solution of the inverse problem \cite{14}–\cite{16}. Since we have decided to choose the basis set \( \{\phi_n(x)\} \) as orthonormal, we can take \( \Lambda \) to be the identity matrix, yielding \( \mathcal{H} = E(R) \).\(^2\)

With the Hamiltonian matrix \( \mathcal{H} \) determined, we only need the matrix representation of the kinetic energy operator \( T \) in the basis \( \{\phi_n(x)\} \) to obtain the potential energy matrix as \( \mathcal{V} = \mathcal{H} - T \). Now, in one dimension, \( T \) is just \(-\frac{1}{2} \frac{d^2}{dx^2} \) and in two or three dimensions with cylindrical or spherical symmetry,

\[
T = -\frac{1}{2} \frac{d^2}{dx^2} + \frac{L^2 - 1/4}{2r^2}, \tag{11}
\]

\(^1\)According to a private communication from M. E. H. Ismail, the Jordan form can be used to show that Eq. (10) is valid for finite-size matrices if \( E(x) \) is a polynomial in \( x \). This can be extended to continuous functions \( E(x) \), which is sufficient for our present work because \( V(x) \) is approximated numerically using finite-size submatrices in \( \mathcal{V} = \mathcal{H} - T \).

\(^2\)Let \( \{\Sigma_{m,n}\}_{m=1}^{J-1} \) be the normalized eigenvector of a \( J \times J \) finite submatrix of \( R \) corresponding to the eigenvalue \( \lambda_n \). It can then be shown that \( E(R) = \Sigma W \Sigma^T \), where \( W \) is a diagonal matrix whose elements are \( W_{n,m} = \delta_{n,m} E(\lambda_n) \).
In the next section, we present several examples where we start by choosing the energy spectral function in section 3 in [5] to calculate the potential function. The potential function thus obtained is valid only locally. That is, the numerical plots obtained as a result of corresponding to an exactly solvable and well-known system, the Morse potential.

4. The potential function

In this section, we start by choosing an invertible spectral function $E(z^2)$ and then use the procedure outlined in Sec. 3 to obtain the matrix representation of the potential $V$ in a given basis $\{\phi_n(x)\}$. Next, we use one or more of the four methods in [5] to derive the potential function $V(x)$. We note that the potential function thus obtained is valid only locally. That is, the numerical plots obtained as a result of this procedure may not be valid globally over the whole configuration space.

The symmetric three-term recursion relation for $S_n^\mu(z^2; a, b)$ is given by Eq. (25) in [2]. Consequently, we obtain the following matrix elements of $R$:

$$
R_{n,n} = A_n = (n + \mu + a)^2 + n(n + 2a - 1) - \mu^2,
R_{n,n+1} = R_{n+1,n} = B_n = -(n + \mu + a)\sqrt{(n + 1)(n + 2a)}.
$$

(12)

To validate the accuracy of the procedure, we start with the exactly solvable system corresponding to the Morse potential.

4.1. The Morse potential. For this system, $E(z^2) = \frac{1}{2}\lambda^2 z^2$, $\phi_n(x) = C_n y^{\nu} e^{-y/2} L^{2\nu-1}_n(y)$, where $\lambda$ is a positive scale parameter of inverse length dimension, $y = e^{-\lambda x}$, $L^{2\nu-1}_n(y)$ is the Laguerre polynomial with $\nu > 0$, and $C_n$ is a normalization constant chosen so as to make the basis set orthonormal (with respect to the integration measure $dx$): $C_n = \sqrt{\lambda^{\nu}\Gamma(n + 2\nu)}$.

The energy spectrum is $E_k = -\lambda^2 (k + \mu^2)/2$, where $k = 0, 1, \ldots, [\mu]$ and the scattering phase shift is obtained from Eq. (6) as

$$
\delta(E) = \arg \Gamma \left(2\frac{\kappa}{\lambda}\right) - \arg \Gamma \left(\mu + i\frac{\kappa}{\lambda}\right) - 2 \arg \Gamma \left(a + i\frac{\kappa}{\lambda}\right),
$$

(13)

where $\kappa = \sqrt{2E}$. It is well known that this energy spectrum and phase shift are associated with the 1D Morse potential [17]

$$
V(x) = \frac{\lambda^2}{8} [e^{-2\lambda x} + 2(2\mu - 1)e^{-\lambda x}].
$$

We now show that the potential function obtained numerically as outlined above does indeed reproduce this exact result if we choose $\nu = a$.

Using the differential equation, the recursion relation, and the orthogonality of the Laguerre polynomials, we obtain the matrix elements of the kinetic energy operator in the form

\[
-\frac{2}{\lambda^2} T_{n,m} = \frac{1}{\lambda^2} \langle \phi_n | \frac{d^2}{dx^2} | \phi_m \rangle = \frac{1}{4} (J^2)_{n,m} - [2(n + \nu)^2 + \nu(1 - \nu)] \delta_{n,m} + \\
+ \left(n + \nu - \frac{1}{2}\right) \sqrt{n(n + 2\nu - 1)} \delta_{n,m+1} + \left(n + \nu + \frac{1}{2}\right) \sqrt{(n + 1)(n + 2\nu)} \delta_{n,m-1},
\]

(14)
where
\[ J_{n,m} = 2(n + \nu)\delta_{n,m} - \sqrt{n(n + 2\nu - 1)}\delta_{n,m+1} - \sqrt{(n + 1)(n + 2\nu)}\delta_{n,m-1}. \]

The Hamiltonian matrix, on the other hand, is obtained simply as \( \mathcal{H} = E(R) = \lambda^2 R/2 \), giving the potential matrix in the basis \( \{ \phi_n(x) \} \) as \( \mathcal{V} = \mathcal{H} - \mathcal{T} \). Figure 1 is a plot of the potential function for a given set of physical parameters and with \( \nu = a \). The figure shows an excellent match with the exact result. All four methods in section 3 in [5] produced identical plots for the same parameters (however, see a relevant computational note in the last paragraph of Sec. 4).

### 4.2. First nonconventional system.

This system is in 3D with spherical symmetry, and we choose
\[ E(z^2) = \frac{1}{2} \lambda^2 (z^2 - \alpha^2 z^{-2}), \quad \phi_n(r) = \sqrt{\frac{2\lambda(n!)}{\Gamma(n + \ell + 3/2)}}(\lambda r)^{\ell+1}e^{-\lambda^2 r^2/2}E_{n+1/2}(\lambda^2 r^2), \]
where \( \ell \) is the angular momentum quantum number. In this case, the energy spectrum is
\[ E_k = -\frac{1}{2} \lambda^2 \left[ (k + \mu)^2 - \left( \frac{\alpha}{k + \mu} \right)^2 \right], \quad (15) \]
where \( k = 0, 1, \ldots, [-\mu] \) and \( \mu \) is not an integer. The scattering phase shift is obtained using Eq. (6) with
\[ z(E) = \frac{\sqrt{E}}{\lambda} \left[ 1 + \sqrt{1 + \left( \frac{\alpha \lambda^2}{E} \right)^2} \right]^{1/2}. \quad (16) \]

Using the differential equation, the recursion relation, and the orthogonality of the Laguerre polynomials, we obtain the matrix elements of the kinetic energy operator in the form
\[ \frac{2}{\lambda^2} T_{n,m} = \frac{2}{\lambda^2} \left\{ \phi_n \right\} \left[ -\frac{1}{2} \frac{d^2}{dr^2} + \frac{\ell(\ell + 1)}{2r^2} \right] \left\{ \phi_m \right\} = \left( 2n + \ell + \frac{3}{2} \right) \delta_{n,m} + \sqrt{n \left( n + \ell + \frac{1}{2} \right)} \delta_{n,m+1} + \sqrt{(n + 1) \left( n + \ell + \frac{3}{2} \right)} \delta_{n,m-1}. \]
The Hamiltonian matrix, on the other hand, is obtained as $\mathcal{H} = E(R) = \lambda^2 (R - \alpha^2 R^{-1})/2$. To compute an $N \times N$ finite version of this matrix, we can use the results in [18], [19] to obtain the inverse of the tridiagonal symmetric submatrix of $R$ as

$$(R^{-1})_{j,j} = \frac{C_{j+1} C_{j+2} \cdots C_{N-1}}{D_j D_{j+1} \cdots D_{N-1}}, \quad j = 0, 1, \ldots, N - 1,$$

$$(R^{-1})_{n,m} = (-1)^{n+m} \frac{C_{m+1} C_{m+2} \cdots C_{N-1}}{D_n D_{n+1} \cdots D_{N-1}} B_n B_{n+1} \cdots B_{m-1},$$

where $n = 0, 1, \ldots, N - 2$ and $m = n + 1, n + 2, \ldots, N - 1$. The numbers $C_n$ and $D_n$ are obtained recursively as

$$C_{N-1} = A_{N-1}, \quad C_n = A_n - \frac{B_n^2}{C_{n+1}}, \quad n = N - 2, N - 3, \ldots, 0,$$

$$D_0 = A_0, \quad D_n = A_n - \frac{B_n^2}{D_{n-1}}, \quad n = 1, 2, \ldots, N - 1.$$  \hspace{1cm} (18)

Finally, the $N \times N$ potential matrix is obtained as $V = \mathcal{H} - \mathcal{T}$. The potential function $V(r)$ is obtained using these matrix elements and the basis \{\phi_n(r)\}. Figure 2 shows this potential function (in units of $\lambda^2$) computed using the method explained in the Appendix for a given set of physical parameters \{\ell, \mu, a\} and with $\alpha = \ell/2$.

![Figure 2](image)

**Fig. 2.** The potential function given in Sec. 4.2 (bold line) calculated using its matrix representation in the basis given therein. The energy spectrum is shown with horizontal lines. The energy and potential are measured in units of $\lambda^2$. The physical parameter values are \{\mu, a, \ell, \alpha\} = \{-7.7, -\mu, 1, \ell/2\}.

### 4.3. Second nonconventional system.

For this system, we choose

$$E(z^2) = \frac{1}{2} \lambda^2 (e^{\alpha z^2} - 1), \quad \alpha > 0, \quad \phi_n(x) = \frac{\sqrt{\lambda}}{\sqrt{2^n n! \sqrt{\pi}}} e^{-\lambda^2 x^2/2} H_n(\lambda x).$$

In this case, the energy spectrum is given by the remarkable formula

$$E_k = \frac{1}{2} \lambda^2 [e^{-\alpha(k+\mu)^2} - 1],$$

where $k = 0, 1, \ldots, [-\mu]$. The scattering phase shift is obtained using Eq. (6) with

$$z(E) = \sqrt{\alpha^{-1} \ln \left( 1 + \frac{2E}{\lambda^2} \right)}.$$
Using the differential equation, the recursion relation, and the orthogonality of the Hermite polynomials, we obtain the matrix elements of the kinetic energy operator in the form

\[ T_{n,m} = -\frac{1}{2} \langle \phi_n \mid \frac{d^2}{dx^2} \mid \phi_m \rangle = \frac{\lambda^2}{4} \left( (2n+1)\delta_{n,m} - \sqrt{n(n-1)}\delta_{n,m+2} - \sqrt{(n+1)(n+2)}\delta_{n,m-2} \right). \]  

(20)

The Hamiltonian matrix, on the other hand, is obtained as \( \mathcal{H} = E(R) = \lambda^2 (e^{\alpha R} - 1)/2 \), giving the potential matrix in the basis \( \{ \phi_n(x) \} \) as \( \mathcal{V} = \mathcal{H} - \mathcal{T} \). Figure 3 shows the potential function \( V(x) \) in units of \( \lambda^2 \) computed using the method explained in the Appendix for a given set of physical parameters \( \{ \alpha, \mu, a \} \).

Fig. 3. The potential function given in Sec. 4.3 (bold line) calculated using its matrix representation in the basis given therein. The energy spectrum is shown with horizontal lines. The energy and potential are measured in units of \( \lambda^2 \). The physical parameter values are \( \{ \mu, a, \alpha \} = \{-0.3, -\mu, 0.2\} \).

### 4.4. Third nonconventional system

For this system, we choose

\[ E(z^2) = \frac{1}{2} \lambda^2 \sinh(\alpha z^2), \quad \alpha > 0, \]

\[ \phi_n(x) = 2^n \Gamma(n+\nu) \sqrt{\frac{\lambda(n+\nu)n!}{2\pi(n+2\nu)}} (1 - y^2)^{\frac{\nu}{2} + \frac{1}{4}} C_n^\nu(y), \quad y = \tanh(\lambda x), \]

and \( C_n^\nu(y) \) is the Gegenbauer (ultra-spherical) polynomial with \( \nu > -1/2 \). In this case, the energy spectrum becomes

\[ E_k = -\frac{1}{2} \lambda^2 \sinh[\alpha(k + \mu)^2], \]  

where \( k = 0, 1, \ldots, [-\mu] \). The scattering phase shift is obtained using Eq. (6) with

\[ z(E) = \sqrt{\frac{\alpha^{-1} \sinh^{-1} \frac{2E}{\lambda^2}}{2E}}. \]

Using the differential equation, the recursion relation, and the orthogonality of the Gegenbauer polynomials, we obtain the matrix elements of the kinetic energy operator in the form

\[
\frac{2}{\lambda^2} T_{m,n} = -\frac{1}{\lambda^2} \langle \phi_n \mid \frac{d^2}{dx^2} \mid \phi_m \rangle = \\
= \left[ n^2 + (2n+1)\nu + \frac{1}{2} \right] \delta_{m,n} - 2nG_n K_{m,n+1} + 2(n+2\nu)G_{n-1} K_{m,n-1} - \\
- \left[ (n+\nu)^2 + 2\nu + \frac{3}{4} \right] (K^2)_{m,n},
\]

(22)
where
\[ K_{n,m} = G_{n-1} \delta_{n,m+1} + G_n \delta_{n,m-1}, \quad G_n = \frac{1}{2} \sqrt{\frac{(n+1)(n+2\nu)}{(n+\nu)(n+\nu+1)}}, \]
and we have used the differential property
\[ (1 - y^2) \frac{d}{dy} C^\nu_n(y) = \frac{1}{2} \frac{1}{n + \nu} [(n + 2\nu)(n + 2\nu - 1)C^\nu_{n-1}(y) - n(n + 1)C^\nu_{n+1}(y)]. \quad (23) \]

The Hamiltonian matrix, on the other hand, is obtained as
\[ H = E(R) = \frac{\lambda^2}{2} \sinh(\alpha R)/2, \]
giving the potential matrix in the basis \( \{ \phi_n(x) \} \) as
\[ V = H - T. \]
Figure 4 shows the potential function \( V(x) \) in units of \( \lambda^2 \) computed using the method explained in the Appendix for a given set of physical parameters \( \{\alpha, \nu, \mu, a\} \).

**Fig. 4.** The potential function given in Sec. 4.4 (bold line) calculated using its matrix representation in the basis given therein. The energy spectrum is shown with horizontal lines. The energy and potential are measured in units of \( \lambda^2 \). The physical parameter values are \( \{\mu, a, \alpha\} = \{-3.2, -\mu, 0.3\} \), and the basis parameter is \( \nu = a \).

Finally, we would like to reiterate and ascertain that the potential functions that were obtained numerically and shown in various plots in this paper are valid only locally. Our method does not give a global representation of the potential that could be valid over the entire configuration space. For example, had the plot in Fig. 3 been assumed valid for all \( x \in (-\infty, +\infty) \), that would have resulted in the one-dimensional oscillator potential with its well-known linear energy spectrum of an infinite size, rather than the exponential spectrum given by Eq. (19) with a finite size. Nevertheless, the plot is valid only locally. We cannot determine its behavior for larger \( |x| \) that causes the spectrum to become finite (of size 5) and exponential in nature. In fact, if the energy spectrum in this problem becomes large in size (i.e., \( \mu \) is a large negative number), then the lowest energy levels (i.e., for small \( k \)) become linear in \( k \):
\[ E_k \approx -E_0 + \frac{\lambda^2}{2}, \quad E_0 = -\frac{\alpha \mu \lambda^2 e^{-\alpha \mu^2}}{2}. \]

The same argument holds for the other examples except the first one in Sec. 4.1, where the problem is exactly solvable.

**Appendix**

In this appendix, we detail one of the methods to calculate the potential function using its matrix representation in a given basis set. Let \( V \) denote a quantum mechanical Hermitian operator that stands
for the real potential energy and let \( V \) be its matrix representation in a given square-integrable basis set \( \{ \phi_n(x) \}_{n=0}^{\infty} \):

\[
V_{n,m} = \langle \phi_n | V | \phi_m \rangle = \int \phi_n(x) V(x) \phi_m(x) \, dx.
\]

Using the Dirac notation, we can write

\[
\langle x | V | x' \rangle = V(x) \delta(x - x'),
\]

where \( \delta(x - x') = \langle x | x' \rangle \) and \( x \) stands for the configuration space coordinate. Moreover, \( \langle x | \phi_n \rangle = \phi_n(x) \) and \( \langle x | \bar{\phi}_n \rangle = \bar{\phi}_n(x) \), where \( \langle \phi_n | \bar{\phi}_m \rangle = \langle \bar{\phi}_n | \phi_m \rangle = \delta_{n,m} \). Using the completeness of configuration space, \( \int |x\rangle\langle x| \, dx = 1 \), we can write the expression \( \langle x | V | \phi_n \rangle \) as

\[
\langle x | V | \phi_n \rangle = \int \langle x | V | x' \rangle \langle x' | \phi_n \rangle \, dx' = V(x) \phi_n(x),
\]

where we used (A.1) in the last step. The completeness of the basis takes the form

\[
\sum_m |\bar{\phi}_m\rangle \langle \phi_m| = \sum_m |\phi_m\rangle \langle \bar{\phi}_m| = I,
\]

where \( I \) is the identity. Using this completeness allows writing the left-hand side of Eq. (A.2) as

\[
\langle x | V | \phi_n \rangle = \sum_{m=0}^{\infty} \langle x | \bar{\phi}_m \rangle \langle \phi_m | V | \phi_n \rangle = \sum_{m=0}^{\infty} \bar{\phi}_m(x) \mathcal{V}_{m,n}.
\]

Equations (A.2) and (A.3) give the potential function as

\[
V(x) = \frac{1}{\phi_n(x)} \sum_{m=0}^{\infty} \bar{\phi}_m(x) \mathcal{V}_{m,n}.
\]

For a finite \( N \times N \) matrix calculation, we obtain the approximation

\[
V(x) \approx \frac{1}{\phi_n(x)} \sum_{m=0}^{N-1} \bar{\phi}_m(x) \mathcal{V}_{m,n}, \quad n = 0, 1, \ldots, N - 1.
\]

Equations (A.2) and (A.3) give the potential function as

\[
\langle x | V | \phi_n \rangle = \sum_{m=0}^{N-1} \bar{\phi}_m(x) \mathcal{V}_{m,n,0}.
\]

Conflicts of interest. The authors declare no conflicts of interest.
REFERENCES

1. V. P. Krainov, Selected Mathematical Methods in Theoretical Physics, Taylor and Francis, London (2002).
2. A. D. Alhaidari and M. E. H. Ismail, “Quantum mechanics without potential function,” J. Math. Phys., 56, 072107, 19 pp. (2015).
3. A. D. Alhaidari, “Formulation of quantum mechanics without potential function,” Quant. Phys. Lett., 4, 51–55 (2015).
4. A. D. Alhaidari, “Representation of the quantum mechanical wavefunction by orthogonal polynomials in the energy and physical parameters,” Commun. Theor. Phys. (Beijing), 72, 015104, 15 pp. (2020).
5. A. D. Alhaidari, “Reconstructing the potential function in a formulation of quantum mechanics based on orthogonal polynomials,” Commun. Theor. Phys. (Beijing), 68, 711–728 (2017).
6. A. D. Alhaidari, “Construction of potential functions associated with a given energy spectrum – An inverse problem,” Internat. J. Modern Phys. A, 35, 2050104, 17 pp. (2020).
7. A. D. Alhaidari and H. Aounallah, “Construction of potential functions associated with a given energy spectrum – An inverse problem II,” Internat. J. Modern Phys. A, 35, 2050159, 24 pp. (2020).
8. A. D. Alhaidari and T. J. Taiwo, “Confined systems with a linear energy spectrum,” Modern Phys. Lett. A, 36, 2150064, 12 pp. (2021).
9. R. Koekoek, P. A. Lesky, and R. F. Swarttouw, Hypergeometric Orthogonal Polynomials and Their q-Analogues, Springer, Berlin (2010).
10. K. M. Case, “Orthogonal polynomials from the viewpoint of scattering theory,” J. Math. Phys., 15, 2166–2174 (1974).
11. J. S. Geronimo and K. M. Case, “Scattering theory and polynomials orthogonal on the real line,” Trans. Amer. Math. Soc., 258, 467–494 (1980).
12. J. S. Geronimo, “A relation between the coefficients in the recurrence formula and the spectral function for orthogonal polynomials,” Trans. Amer. Math. Soc., 260, 65–82 (1980).
13. W. H. Press, S. A. Teukolsky, W. T. Vetterling, and B. P. Flannery, Numerical Recipes: The Art of Scientific Computing, Cambridge Univ. Press, Cambridge (2007).
14. A. Kh. Ostromogil’skii, “The uniqueness of the solution of the inverse problem in potential theory,” USSR Comput. Math. Math. Phys., 9, 283–287 (1969).
15. T. Aktosun and R. G. Newton, “Non-uniqueness in the one-dimensional inverse scattering problem,” Inverse Problems, 1, 291–300 (1985).
16. A. Neamaty, S. Mosazadeh, and M. Bagherzadeh, “A uniqueness theorem of the solution of an inverse spectral problem,” Casp. J. Math. Sci., 1, 80–87 (2012).
17. P. C. Ojha, “SO(2, 1) Lie algebra, the Jacobi matrix and the scattering states of the Morse oscillator,” J. Phys. A: Math. Gen., 21, 875–883 (1988).
18. G. A. Meurant, “A review on inverse of symmetric tridiagonal and block tridiagonal matrices,” SIAM J. Matrix Anal. Appl., 13, 707–728 (1992).
19. R. A. Usmani, “Inversion of a tridiagonal Jacobi matrix,” Linear Algebra Appl., 212–213, 413–414 (1994).