

Formulation of Quantum Mechanics without Potential Function

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Abstract: We present an alternative formulation of quantum mechanics in which no reference is made to any potential function. In this formalism, the wavefunction is written as a bounded infinite sum in a complete and suitable basis with orthogonal polynomials in the energy as expansion coefficients. The asymptotics of these polynomials give the scattering phase shift, bound states and resonances for the corresponding physical system. In addition to the well-known quantum systems, this formulation enables one to obtain analytic realization of previously untreated problems.

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1 Introduction

In the standard formulation of quantum mechanics, one starts by proposing a potential function that models the physical system under study. The potential is then inserted into the Schrödinger equation, which is solved for the wavefunction, scattering phase shift, energy spectrum and/or resonances. Exact solvability of the equation limits the number of analytically realizable systems. These solutions are well known for a long time and have been arranged into a small number of classes (see, for example, [1] and references therein). Each one of these classes is associated with a potential function like the Coulomb, harmonic oscillator, Morse, Scarf, Eckart, etc. Nonetheless, we believe that the set of analytically realizable quantum systems is much larger than the set of exact solutions of the Schrödinger equation. Equivalently, we are affirming that the representation of the Hamiltonian operator in the wave equation $i\hbar \frac{\partial}{\partial t} \Psi = H\Psi$ as the sum of the kinetic energy operator and a potential function, $H = T + V$, is a particular choice that may limit the number of analytically realizable physical systems. In fact, the postulates of quantum mechanics have no reference at all to a potential function (see, for example, Ref. [2]). Only two elements of the physical system are specified in the postulates: the state function Ψ and the

Hamiltonian operator H . The former gives the expectation values (measurements) of physical observables and the latter determines the time development of the system. Accordingly, we are proposing here a formulation of quantum mechanics in which the potential function does not appear. The aim is to obtain a set of analytically realizable systems, which is larger than in the standard formulation. This implies that the potential functions corresponding to the newly found systems (if they exist) do not have analytic realizations or that the corresponding wave equation cannot be written in the conventional format (that is, it could become a differential equation of order higher than two or with nonlocal potential, etc.). Our recent work in [3], where we proposed a formulation of quantum mechanics for a finite level system whose potential function is not realizable, is a prelude to this one.

In the absence of a potential function, we propose a construction where the wavefunction is written as a bounded infinite sum in a suitable and complete basis, $\{\phi_n(x)\}_{n=0}^{\infty}$ with polynomial coefficients that are orthogonal on an appropriate domain in the energy space. That is, we write $\Psi(t, x) = e^{-iEt/\hbar} \psi(E, x)$ and $\psi(E, x) = \sum_n f_n^\mu(E) \phi_n(x)$ where E is the system's energy and μ stands for a set of physical parameters. Beside the requirements that the elements of the basis satisfy the

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boundary conditions and be compatible with the configuration space of the problem, there is very little information content beyond the kinematics (such as the angular momentum, etc.) which is common to all systems whose state functions are expanded as above. Structural and dynamical information about the specific system under study is contained only in the expansion coefficients $\{f_n^\mu(E)\}_{n=0}^\infty$. Using the completeness and orthogonality of the basis and writing $f_n^\mu(E) = f_0^\mu(E)P_n^\mu(\varepsilon)$ we obtain:

$$\int \rho^\mu(\varepsilon)P_n^\mu(\varepsilon)P_m^\mu(\varepsilon)d\varepsilon = \delta_{nm} \quad (1)$$

where ε is some proper function of the energy, $\varepsilon(\mu, E)$, and $\rho^\mu(\varepsilon) = [f_0^\mu(E)]^2$. Thus, $P_0^\mu(\varepsilon) = 1$ and $\{P_n^\mu(\varepsilon)\}_{n=0}^\infty$ becomes a complete set of orthogonal polynomials (see, for example [4]). Using earlier findings concerning the asymptotic property of the wavefunction expansion [5], we conclude that the orthogonal polynomials with physical relevance are only those with the following asymptotic $n \rightarrow \infty$ behavior:

$$P_n^\mu(\varepsilon) \approx A(\varepsilon) \cos \left[n^\xi \theta(\varepsilon) + \delta(\varepsilon) \right] \quad (2)$$

Where $A(\varepsilon)$ is the scattering amplitude and ξ is a real positive constant that depends on the particular energy polynomial. The scattering phase shift $\delta(\varepsilon)$ which is defined modulo an integer multiple of $\pi/2$ depends on the energy and the set of physical parameters $\{\mu\}$. On the other hand, bound states (if they exist) occur at discrete real energies $\{\varepsilon_m\}$ at which $A(\varepsilon_m) = 0$. However, if $A(\varepsilon_m) = 0$ at complex energies $\{\varepsilon_m\}$ with negative imaginary parts, then these are the resonance energies and the imaginary part forces the wave function to vanish with time due to the factor $e^{-iE_m t/\hbar}$. In the following section, we give illustrative examples of two classes of problems where we obtain analytic representations for well-known quantum systems and for others that were not treated in the past.

2 Two Examples

As an illustration, we consider quantum systems on the positive real line with $\phi_n(x) = \sqrt{\frac{\Gamma(n+1)}{\Gamma(n+v+1)}}(\lambda x)^{\frac{v}{2}} e^{-\lambda x/2} L_n^v(\lambda x)$, where $L_n^v(z)$ is the Laguerre polynomial, $v > -1$ and λ is a real positive scale parameter. In addition to 1D systems, this basis is also suitable for the radial component of spherically symmetric 3D systems where x becomes the radial coordinate and v depends on the angular momentum quantum number ℓ . Thus, we construct wave functions of the form:

$$\psi(E, x) = \sum_{n=0}^{\infty} \sqrt{\rho^\mu(\varepsilon)} P_n^\mu(\varepsilon) \phi_n(x) \quad (3)$$

Below, we obtain analytic expressions for the phase shift, energy spectra and/or resonances for two classes of problems. The first one is associated with the Meixner-Pollaczek polynomial and the second with the continuous dual Hahn polynomial.

2.1 The Meixner-Pollaczek polynomial class

The energy polynomial considered here is a special case of the orthonormal version of the Meixner-Pollaczek polynomial, which we write as (see page 37 of [6])

$$P_n^\mu(y) = (i)^n \sqrt{\frac{\Gamma(n+2\mu)}{\Gamma(2\mu)\Gamma(n+1)}} {}_2F_1 \left(\begin{matrix} -n, \mu+iy \\ 2\mu \end{matrix} \middle| 2 \right) \quad (4)$$

Where, ${}_2F_1 \left(\begin{matrix} a, b \\ c \end{matrix} \middle| z \right)$ is the hypergeometric function, $y \in [-\infty, +\infty]$ and $\mu > 0$. These are polynomials of order n in y and satisfy the following symmetric three-term recursion relation:

$$2yP_n^\mu(y) = \sqrt{n(n+2\mu-1)}P_{n-1}^\mu(y) + \sqrt{(n+1)(n+2\mu)}P_{n+1}^\mu(y) \quad (5)$$

The associated normalized weight function is

$$\rho^\mu(y) = \frac{2^{2\mu-1}}{\pi\Gamma(2\mu)} |\Gamma(\mu+iy)|^2 \quad (6)$$

To derive the large n asymptotic formula we use Darboux's method (see Chapter 9 of [7]) which gives:

$$P_n^\mu(y) \approx \frac{1}{2^{\mu-1}\sqrt{n}|\Gamma(\mu+iy)|} \cos \left[n(\pi/2) + \arg \Gamma(\mu+iy) \right] \quad (7)$$

Comparing this with Eq. (2) gives the following scattering phase shift (modulo an integer multiple of $\frac{\pi}{2}$)

$$\delta(\varepsilon) = \arg \Gamma(\mu+iy) \quad (8)$$

The scattering amplitude is $A(\varepsilon) = [2^{\mu-1}\sqrt{n}|\Gamma(\mu+iy)|]^{-1}$. It vanishes if $iy = -(m+\mu)$ where $m = 0, 1, 2, \dots$ giving the energy spectrum formula $y^2 = -(m+\mu)^2$. If the solution of this formula, $\{\varepsilon_m\}$, is a real set then these provide the bound states energies. On the other hand, if it is a complex set with negative imaginary parts then those correspond to the resonance energies.

Now, if we choose the parameters as $\mu = \ell + 1$ and $y = Z/k$ where $k = \sqrt{2E}$ then we obtain the following phase shift $\delta(E) = \arg \Gamma(\ell + 1 + iZ/k)$ and the energy spectrum formula $E_m = -Z^2/2(m + \ell + 1)^2$. Obviously, these results agree with the well-known Coulomb problem. However, taking $y = (\alpha/k)^{2\ell+1}$, where α is a

real parameter, then we obtain the following phase shift and energy spectrum

$$\delta(E) = \arg \Gamma \left[\mu + i(\alpha/k)^{2\ell+1} \right] \quad (9a)$$

$$E_m = -\alpha^2 / 2(m + \mu)^{1/(\ell+1/2)} \quad (9b)$$

These results are not associated with any of the known exactly solvable problems in the standard formulation of quantum mechanics. A final example in this class, which is designed with a resonance structure, corresponds to the parameters assignment $\mu = \alpha / \sqrt{2E}$ and $y = \beta / \alpha$ where $\alpha > \beta > 0$. The energy spectrum formula $y^2 = -(m + \mu)^2$ gives the following discrete energies

$$E_m = \frac{\frac{1}{2}(m^2\alpha^2 - \beta^2) - im\alpha\beta}{(m^2 + \beta^2/\alpha^2)^2} \quad (10)$$

The result is a single bound state at $E_0 = -\frac{1}{2}(\alpha^2/\beta)^2$ and an infinite number of resonances at $E = E_1, E_2, \dots$ that tend to $E = 0$ as $m \rightarrow \infty$.

2.2 The continuous dual Hahn polynomial class

Here, the energy polynomial is the orthonormal version of the continuous dual Hahn polynomial, which we write as (see page 29 of [6])

$$S_n^\mu(y^2; a, b) = \sqrt{\frac{(\mu+a)_n(\mu+b)_n}{n!(a+b)_n}} {}_3F_2 \left(\begin{matrix} -n, \mu+iy, \mu-iy \\ \mu+a, \mu+b \end{matrix} \middle| 1 \right) \quad (11)$$

where, $(z)_n = z(z+1)(z+2)\dots(z+n-1)$, $y > 0$ and $\{\mu, a, b\}$ are positive parameters except for a pair of complex conjugates with positive real parts. These are polynomials of order n in y^2 and the corresponding normalized weight function reads as follows:

$$\rho^\mu(y; a, b) = \frac{1}{2\pi} \frac{|\Gamma(\mu+iy)\Gamma(a+iy)\Gamma(b+iy)/\Gamma(2iy)|^2}{\Gamma(\mu+a)\Gamma(\mu+b)\Gamma(a+b)} \quad (12)$$

Again, we use the Darboux's method to obtain the following asymptotic ($n \rightarrow \infty$) formula:

$$S_n^\mu(y^2; a, b) \approx \frac{2\sqrt{\Gamma(\mu+a)\Gamma(\mu+b)\Gamma(a+b)}|\Gamma(2iy)|}{|\Gamma(a+iy)\Gamma(b+iy)\Gamma(\mu+iy)|\sqrt{n}} \times \cos(y \ln n + \gamma) \quad (13)$$

Where, $\gamma = \arg \{ \Gamma(2iy) / \Gamma(\mu+iy)\Gamma(a+iy)\Gamma(b+iy) \}$ Now, since $\ln n \approx o(n^\xi)$ for any $\xi > 0$, then we extract the following phase shift

$$\delta(\varepsilon) = \arg \{ \Gamma(2iy) / \Gamma(\mu+iy)\Gamma(a+iy)\Gamma(b+iy) \} \quad (14)$$

Moreover, the discrete bound/resonance states correspond to the zeros of the scattering amplitude that occur for $iy = -(m+c)$ where c stands for any one of the three parameters $\{\mu, a, b\}$. However, in this case c must be negative and the energy spectrum is finite corresponding to $m = 0, 1, 2, \dots, N$ where N is the largest integer less than or equal to $-c$. Now, if we choose $y = \sqrt{2E}/\alpha$, $a = \mu$ and $b = \frac{1}{2} - \alpha^{-1}\beta\sqrt{2V_0}$, where $\{\alpha, \beta, V_0\}$ are real positive parameters such that $b < 0$ then the scattering phase shift and energy spectrum become:

$$\delta(E) = \arg \Gamma \left(2i\alpha^{-1}\sqrt{2E} \right) - 2 \arg \Gamma \left(\mu + i\alpha^{-1}\sqrt{2E} \right) - \arg \Gamma \left[\frac{1}{2} + \alpha^{-1} \left(i\sqrt{2E} - \beta\sqrt{2V_0} \right) \right] \quad (15a)$$

$$E_m = -\frac{\alpha^2}{2} \left(m + \frac{1}{2} - \alpha^{-1}\beta\sqrt{2V_0} \right)^2 \quad (15b)$$

and $m = 0, 1, \dots, N$ where N is the largest integer less than or equal to $-b$. These results are associated with the 1D Morse potential $V(x) = V_0(e^{-2\alpha x} - 2\beta e^{-\alpha x})$ where $b = -N - \mu$ and $1 > \mu \geq 0$. If, on the other hand, we choose the physical parameters as: $y = \sqrt{\beta^{-1} \ln(1 + 2E/\alpha^2)}$ where $\beta > 0$ and $\mu < 0$ then the associated energy spectrum is obtained as:

$$E_m = \frac{\alpha^2}{2} [e^{-\beta(m+\mu)^2} - 1] \quad (16)$$

where $m = 0, 1, \dots, N$ and N is the largest integer less than or equal to $-\mu$. This energy spectrum does not belong to any of the known classes of exactly solvable problems.

3 Discussion on Physical Applications

In the standard formulation of quantum mechanics, a physical application typically starts by engineering the potential function, which is believed to model the physical system under study. Such engineering is built on the experience of working with various potential configurations and on the physical insight one develops in dealing with these settings such as the connection between potential functions and the properties of bound states and resonances, tunnelling effects, location of stable points, phase transitions, classical turning points etc. Subsequently, the equation of motion is solved and the properties of the system are calculated. Fine-tuning of the potential is performed to arrive at the desired or sought-after system characteristics. Now, in our formulation the same process is maintained except that "potential engineering" is replaced by "polynomial engineering". For that, one needs to develop an insight into the relationship between the physical features of a given system and the properties of the associated orthogonal polynomials. Such properties include, but not limited to, the shape of the weight functions, nature of the

generating functions, distribution and density of the zeros, recursion relations, asymptotics, differential or difference equations, etc. Fine-tuning is done by slightly altering one or more of these polynomial properties such as adjusting the polynomial parameters, deforming the recursion relation, perturbing the differential equation, etc. The asymptotics of the modified polynomials are then calculated as shown above and the physical properties (such as the energy spectrum and phase shift) are extracted. The process is repeated until the desired physical features are obtained. As an example of such application, we investigate the density of states of a given physical system associated with an orthogonal energy polynomial that satisfies the following three-term recursion relation

$$\varepsilon P_n^\mu(\varepsilon) = a_n P_n^\mu(\varepsilon) + b_{n-1} P_{n-1}^\mu(\varepsilon) + b_n P_{n+1}^\mu(\varepsilon) \quad (17)$$

where ε is the system's energy scaled by some characteristic frequency and $P_0^\mu(\varepsilon) = 1$. The recursion coefficients are taken as $a_n = 0$, $b_{2n} = \mu$, and $b_{2n+1} = 1 - \mu$ where μ is a real parameter in the range $0 < \mu < \frac{1}{2}$. The energy density of states could be calculated using $\rho(\varepsilon) = \frac{1}{\pi} \text{Im}G(\varepsilon + i0)$ where $G(z)$ is the Green's function associated with these polynomials which has the following continued fraction representation

$$G(z) = \frac{-1}{z - a_0 - \frac{b_0^2}{z - a_1 - \frac{b_1^2}{z - a_2 - \dots}}} \quad (18)$$

The resulting density of states for $\mu = 0.4$ is shown as the solid curve in the figure. It is a symmetric two-band density in the range $-1 \leq \varepsilon \leq 1$ with a forbidden energy gap, $|\varepsilon| \leq 1 - 2\mu$ centered about the origin. Now, we modify the system by adjusting only the first diagonal recursion coefficient as $a_0 = \gamma$ where γ is a deformation parameter.

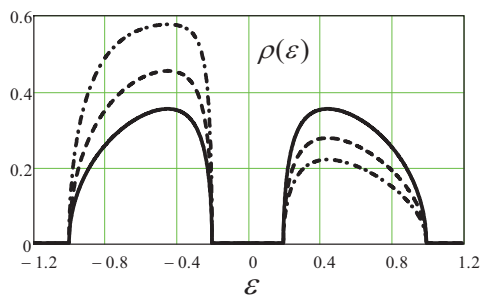


Fig. 1: The density of states for the physical system associated with the energy polynomials (17) for $\mu = 0.4$ (solid curve) and for two values of the deformation parameters: $\gamma = -0.1$ (dashed) and $\gamma = -0.2$ (dashed-dotted).

The figure shows the result of this modification on the density of states for several values of the parameter γ . The

dashed and dashed-dotted curves in the figure correspond to $\gamma = -0.1$ and $\gamma = -0.2$, respectively.

4 Conclusion

In this Letter, we introduced an alternative formulation of quantum mechanics in which the potential function does not appear. Our aim is to find analytically realizable quantum systems despite the lack of knowledge of the potential. Using the postulate of quantum mechanics, we proposed the existence of a wavefunction that contains all structural and dynamical information about the system. We wrote this state function as a bounded infinite sum in a discrete and complete basis functions with polynomial coefficients that are orthogonal in the energy space. The asymptotic properties of these polynomials give exact analytic expressions for the phase shift of the continuum scattering states and for the spectrum formula of the discrete bound states and/or resonances. In addition to the well-known quantum systems, this formulation enabled us to present exact realizations of previously untreated problems. The examples presented above constitute a testimony to our claim. Thus, instead of giving the potential function as is done in the standard formulation, we propose orthogonal polynomials in the energy as the expansion coefficients of the wavefunction in a suitable complete basis. The physical properties of the system are contained in these polynomials and their corresponding weight functions.

Finally, we make the following remarks: (1) our recent work on the Dirac-Coulomb problem [8] suggests that a relativistic extension of this formulation is feasible. (2) One can also show that the wave equation in this formulation becomes equivalent to the three-term recursion relation satisfied by the energy polynomials (as illustration, see Ref. [9]). (3) One can also formulate perturbative and non-perturbative calculation in this formalism by altering the recursion relation associated with the energy polynomials (see, for example, Ref. [3] where we also make use of the J-matrix method of scattering). (4) In the two examples of Sec. 2, we made a seemingly arbitrary choice of polynomials and only by a specific choice of parameters and polynomial arguments that we were able to obtain the physical properties of the corresponding system. However, with time and after working with many such examples together with a careful analysis of the properties of these polynomials, one can develop an insight into a solid relationship between properties of the polynomials and the features of the corresponding physical systems. Such properties include the weight function, recursion relation, asymptotics, distribution of the zeros, etc.

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