Development of an approximation scheme for quasi-exactly solvable double-well potentials

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Abstract

We make use of a recently developed method to, not only obtain the exactly known eigenstates and eigenvalues of a number of quasi-exactly solvable Hamiltonians, but also construct a convergent approximation scheme for locating those levels, not amenable to analytical treatments. The fact that, the above method yields an expansion of the wave functions in terms of corresponding energies, enables one to treat energy as a variational parameter, which can be effectively used for the identification of the eigenstates. It is particularly useful for the quasi-exactly solvable systems, where the ground state is known and a number of eigenstates are bounded, both below and above. The efficacy of the procedure is illustrated by obtaining, the low-lying excited states of a prototypical double-well potential, where the conventional techniques are not very reliable. Our approach yields the approximate eigenfunctions and eigenvalues, whose accuracy can be improved to any desired level, in a controlled manner. Comparing the present results with those of an independent numerical method, it was found that, the first few terms in our approximate solutions are enough to yield the excited state eigenvalues, accurate upto the third place of the decimal.

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I. INTRODUCTION

Quasi-exactly solvable (QES) systems are intermediate to exactly solvable and non-solvable ones. These quantum systems are characterized by the fact that, only a finite number of the eigenstates can be analytically determined [1,2]. One dimensional examples include anharmonic potentials, some of which have a double-well structure. Interestingly, a QES potential with a centrifugal barrier appears in the treatment of ring lasers, where the Fokker-Planck equation is converted to an equivalent Schrödinger eigenvalue problem [3]. Other QES examples have been encountered in similar problems [4,5]. These type of Hamiltonians, amenable to partial algebraization, have also manifested in various other areas of physics [6] and have attracted considerable attention in the recent literature [7,8]. A number of independent methods, from group theoretical to algebraic ones, have been developed for studying the QES systems [2].

In the conventional approach to quasi-exactly solvable systems, one starts with an operator suitably constructed from the differential realizations of the generators of a given Lie algebra, acting in the finite dimensional space of monomials. A QES Hamiltonian is then arrived at by converting the above problem into a Schrödinger eigenvalue equation, through appropriate similarity transformations. Although much effort has gone into studying the structure of the analytically available part of the spectrum, there has not been any attempt in the literature, to the best of the authors' knowledge, to find the ones, not determined analytically. The fact that, some of the QES potentials exhibit a double-well structure, for which determining the approximate eigenvalues and eigenstates have been quite challenging, makes this problem worth investigating. Further, a number of these states are constrained to lie between certain range of energies; hence, apart from academic interest, developing an approximation scheme to locate these eigenvalues and eigenfunctions, provides an ideal ground for testing the proposed scheme. As mentioned earlier, a number of these type of potentials appear in the Schrödinger equation originating from the Fokker-Planck equation, governing the dynamics of non-equilibrium systems. Finding the low-lying states of these problems accurately have physical significance; for example the tunneling rate is related to the energy difference between the ground and first excited state [5,9,10].

The goal of this paper is to develop an accurate approximation scheme for finding the non-exactly determined eigenstates of the QES Hamiltonians. For this purpose, we employ a recently developed method for solving linear differential equations [11–13], used earlier for diagonalizing many-body interacting systems [12,14]. The analytically obtainable part of the spectra of a number of QES systems is first determined, in the following section, to demonstrate the working of the above method. We then proceed, in Sec.III, to compute approximately, those eigenvalues and eigenstates of a prototype QES system, which are not amenable to analytical treatment. The fact that our procedure yields a series solution for a differential equation in terms of energy, allows us to treat the same as a variational parameter. This can be effectively used for the identification of the eigenstates and corresponding eigenvalues, as will be shown in the text. It is particularly useful for the quasi-exactly solvable systems, where the ground state is known and a number of eigenstates are both bounded below and above.

The example of a double-well potential is taken deliberately, since the conventional techniques are not very reliable for the same. The usefulness of the present approach is shown
by computing a number of low-lying eigenstates. Our approach yields the approximate
eigenfunctions and eigenvalues, whose accuracy can be improved to any desired level, in a
controlled manner. We then compare our results, with another convergent numerical scheme
[15,16]; it is found that, the first few terms in our approximate solutions are enough to yield
the excited state eigenvalues, accurate upto the third place of the decimal. We conclude
in Sec.IV, after pointing out the advantages and limitations of the present approximation
scheme and directions for further investigations.

II. EXACT EIGENSTATES OF QUASI-EXACTLY SOLVABLE SYSTEMS: A
NOVEL APPROACH

In this section, we obtain the analytically solvable part of the eigenspectra, of a class
of QES systems, making use of a recently developed method for solving linear differential
equations [11]. In this procedure, the solution space of the differential equation is connected
with the space of monomials. We concentrate on the QES systems having polynomial
potentials, with or without a centrifugal barrier term, although the method can be applied
to other systems as well. As will become clear in the subsequent section, the same procedure
yields the approximate eigenfunctions and eigenvalues, for the analytically inaccessible states
of the QES systems, to the desired accuracy.

A single variable differential equation, after suitable manipulations (which will become
clear from the examples in the text), can be written as,

\[
[F(D) + P(x, d/dx)] y(x) = 0 ,
\]

where, \( D \equiv x \frac{d}{dx} \) is the Euler operator, \( F(D) \equiv \sum_{n=-\infty}^{\infty} a_nD^n \) and \( a_n \)'s are some parameters;
P\((x, d/dx)\) can be an arbitrary polynomial function of \( x, \frac{d}{dx} \) and other operators. It can be
straightforwardly shown by direct substitution that, the solution to Eq. (1) can be written
in the form,

\[
y(x) = C_{\lambda} \left\{ \sum_{m=0}^{\infty} \left( -1 \right)^m \frac{1}{F(D)} P(x, d/dx) \right\}^m x^{\lambda}
\]

provided, \( F(D)x^\lambda = 0 \) and the coefficient of \( x^\lambda \) in \( y(x) - C_{\lambda}x^\lambda \) is zero (no summation over \( \lambda \));
here, \( C_{\lambda} \) is a constant. This straightforward method, not only yields solutions to the familiar
differential equations [13], but also leads to the diagonalization of a number of correlated
many-body Hamiltonians [14].

For the QES case, we first consider the example of the sextic oscillator, whose Hamilton-
ian (in the units \( \hbar = 2m = 1 \)) is given by

\[
H = -\frac{d^2}{dx^2} + \alpha x^2 + \beta x^4 + \gamma x^6 .
\]

It is well-known that, this problem is QES, provided a certain relation exists between the
parameters \( \alpha, \beta \) and \( \gamma \). Instead of postulating the same, we first illustrate how this condition
emerges naturally. Asymptotic analysis indicates a measure of the form \( \psi_0 \equiv e^{-(ax^2+bx^4)} \),
with the unknown parameters, \( a \) and \( b \) to be determined from the Hamiltonian parameters
\( \alpha, \beta \) and \( \gamma \). A similarity transformation \( \hat{H} = \hat{\psi}_0^{-1} H \hat{\psi}_0 , \) yields;
\[
\hat{H} = -\frac{d^2}{dx^2} + 8bx^3 \frac{d}{dx} + 4ax \frac{d}{dx} + (\alpha - 4a^2 + 12b)x^2 \\
+ (\beta - 16ab)x^4 + (\gamma - 16b^2)x^6 + 2a .
\]  

(4)

Setting the coefficients of \(x^4\) and \(x^6\) equal to zero, one obtains,

\[
a = \frac{\beta}{4\sqrt{\gamma}} \quad \text{and} \quad b = \frac{\sqrt{\gamma}}{4} .
\]  

(5)

Assuming that the solution of the eigenvalue equation \(\hat{H}P_n(x) = EP_n(x)\) is a polynomial, of degree \(n\), one observes that, the operators, \(2\sqrt{\gamma}x^3 \frac{d}{dx}\) and \((\alpha - \frac{\beta^2}{4\gamma} + 3\sqrt{\gamma})x^2\) increase the degree of \(P_n(x)\) by two. Preserving the degree of the polynomial leads to the above mentioned relationship between the coupling parameters of the sextic oscillator [7]:

\[
\frac{1}{\sqrt{\gamma}} \left( \frac{\beta^2}{4\gamma} - \alpha \right) = 2n + 3 .
\]  

(6)

It is worth mentioning that, in exactly solvable problems, the differential operators do not increase the degree of the polynomial and hence no additional condition is required there.

The eigenvalue problem can be cast in a form as given in Eq. (1):

\[
\left[ D(D - 1) - 2\sqrt{\gamma}x^5 \frac{d}{dx} - \frac{\beta}{\sqrt{\gamma}} x^3 \frac{d}{dx} + 2n\sqrt{\gamma}x^4 + \left( E - \frac{\beta}{2\sqrt{\gamma}} \right) x^2 \right] P_n(x) = 0 .
\]  

(7)

The condition \(F(D)x^\lambda = 0\), yields \(\lambda = 0\) and \(1\). It is easy to see that the two values of \(\lambda\) separate the Hilbert space into even and odd sectors. The solution, corresponding to the root \(\lambda = 0\), can be expanded as,

\[
P_n^0(x) = C_0 \sum_{m=0}^{\infty} (-1)^m \left[ \frac{1}{D(D - 1)} \left( \tilde{E}x^2 - \frac{\beta}{\sqrt{\gamma}} x^3 \frac{d}{dx} + 2n\sqrt{\gamma}x^4 - 2\sqrt{\gamma}x^5 \frac{d}{dx} \right) \right]^m x^0 \\
= \sum_{k=0}^{\infty} Q_k(\tilde{E}) \frac{x^{2k}}{2^k k!} ,
\]  

(8)

where \(\tilde{E} = E - \beta/2\sqrt{\gamma}\) and \(Q_k(\tilde{E})\) is an appropriate polynomial in energy.

Since the degree of the polynomial has been already fixed at \(n\), an even integer in this case, we impose the condition that the series terminates at the desired point by putting the coefficient of the subsequent term to zero. As will be explicitly seen, the same coefficient appears as a factor in rest of the terms of the series, thereby ensuring that the degree of the polynomial is maintained. Writing \(n = 4j\), where \(j\) can take semi-integer values, one needs to put \(Q_{2j+1}(\tilde{E}) = 0\) to obtain the above result. This condition leads to \(2j + 1\) independent solutions for energy and the corresponding eigenfunctions. We would like to emphasize that, so far we have not assumed any additional property of the spectral problem, for arriving at these results.

In similar fashion, one can easily incorporate the centrifugal barrier into QES problems. The Hamiltonian of the sextic oscillator for \(\beta = 0\), with a centrifugal barrier is given by,

\[
\hat{H} = -\frac{d^2}{dx^2} + \frac{\sigma}{x^2} + \alpha x^2 + \gamma x^6 ;
\]  

(9)
the corresponding measure is of the form \( \psi_0 = x^{2l} \exp(-ax^4/4) \). Performing an appropriate similarity transformation and setting the coefficients of \( x^6 \) and \( 1/x^2 \) to zero, we obtain,

\[
\left[ -\frac{d^2}{dx^2} + \frac{-4l}{x} \frac{d}{dx} + 2\sqrt{\gamma}x^3 \frac{d}{dx} + (\alpha + 3\sqrt{\gamma} + 4l\sqrt{\gamma}) x^2 \right] P_n(x) = EP_n(x) \ ,
\]

with \( a = \sqrt{\gamma} \) and \( l = \frac{1}{4} + \frac{1}{2}\sqrt{\frac{1}{4} + \sigma} \).

The condition that \( P_n(x) \) is a polynomial of degree \( n \), leads to,

\[
-\frac{\alpha}{4\sqrt{\gamma}} + \frac{1}{2}\sqrt{\frac{1}{4} + \sigma} = n/2 + 1 \ .
\]

Multiplication of Eq. (10) with \(-x^2\) yields,

\[
\left[ D(D + 4l - 1) + Ex^2 + 2n\sqrt{\gamma}x^4 - 2\sqrt{\gamma}x^5 \frac{d}{dx} \right] P_n(x) = 0 \ ,
\]

which \( \lambda = 0 \) and \( 1 - 4l \), as the solutions of \( F(D)x^\lambda = 0 \). A suitable parameterization in the form of

\[
\alpha = -4a\left(s + \frac{1}{2} + \mu\right) \text{and} \quad \sigma = 4\left(s - \frac{1}{4}\right)\left(s - \frac{3}{4}\right)
\]

makes the result amenable for comparison with the existing literature [7]. Analogous to the earlier example, one can now find solutions corresponding to various values of \( n \). For \( n = 2 \) one finds,

\[
E_{2\pm} = \pm\sqrt{32as} \quad \text{and} \quad P_{2\pm}(x) = \left[ax^2 - \frac{E_{2\pm}}{4\gamma}\right] .
\]

Even states for other values of \( n \) can also be similarly obtained.

In the absence of a centrifugal barrier, for the anharmonic oscillator of Eq.(7), under similar condition \( (n = 2) \), the energy eigenvalues can be derived from,

\[
Q_2(\tilde{E}) = \tilde{E}^2 - \frac{2\beta\tilde{E}}{\sqrt{\gamma}} - 4n\sqrt{\gamma} = 0 \quad .
\]

The corresponding two solutions,

\[
E_{\pm} = \frac{3\beta}{2\sqrt{\gamma}} \pm \left(\frac{\beta^2}{\gamma} + 8\sqrt{\gamma}\right)^{1/2} \ ,
\]

yield,

\[
\psi_{2\pm}(x) = \exp\left(-\frac{\beta x^2}{4\sqrt{\gamma}} - \frac{\sqrt{\gamma}x^4}{4}\right)P_{2\pm}(x) \ ;
\]

\[
\text{here} \quad P_{2\pm}(x) = 1 + \left[\frac{\beta}{\sqrt{\gamma}} \pm \left(\frac{\beta^2}{\gamma} + 8\sqrt{\gamma}\right)^{1/2}\right] x^2 .
\]
The case of $n = 4$, with $\beta = 0$ and for negative values of $\alpha$, is a double-well potential. For specificity, we take $\gamma = 1$, which yields $\alpha = -11$ and hence

$$\hat{H} = -\frac{d^2}{dx^2} - 11x^2 + x^6.$$  

The energy eigenvalues for this Hamiltonian are obtained from, $Q_3(E) = E(E^2 - 64) = 0$, which gives $E = -8, 0$ and $+8$. The respective polynomial parts of the wave functions are,

- $P_{4-}(x) = 1 + 4x^2 + 2x^4$ \,(18)
- $P_{40}(x) = 1 - (2/3)x^4$ \,(19)
- $P_{4+}(x) = 1 - 4x^2 + 2x^4$ \,(20)

It is clear that, the ground state has no nodes on the real line and the subsequent two states have, respectively two and four nodes on the real line, as desired. The above procedure straightforwardly extends to higher values of $n$. We note that, polynomial potentials, with the highest degree $4m + 2$, with $m$ integer can also be solved in an analogous manner, provided appropriate conditions are imposed on the couplings. It should also be pointed out that, the solutions obtained so far, correspond to the root $\lambda = 0$. The other root $\lambda = 1$, does not lead to a closed form expression for the solution. Hence, the odd states are not amenable to an analytical treatment. This is a manifestation of the QES nature of these quantal problems.

III. APPROXIMATION SCHEME FOR THE ANALYTICALLY INACCESSIBLE STATES

As is clear from the previous example, it is not possible to analytically determine the states, other than the ones allowed by the condition given in Eq.(6). In this section, we present an approximation scheme for finding these analytically inaccessible states, taking the first excited state of the above mentioned double-well potential, as the example. Assuming that, the measure is same for all the states, the residual part, which will be suitably approximated to a finite degree polynomial in the following, should have one zero on the real line. The rest of the zeros, if present, should lie on the complex plane. In developing an approximation scheme, one also needs to take care of the convergence of the series. The above two criteria are utilized for finding out the approximate eigenvalue and eigenfunction of the first excited state, which can then be extended to other states.

Expanding Eq. (7) for $\lambda = 1$, one obtains,

$$P_{4}^{1}(x) = x - E\frac{x^3}{3!} + (E^2 - 36)\frac{x^5}{5!} + (76E - E^3)\frac{x^7}{7!} + (E^4 + 8E^2 - 3024)\frac{x^9}{9!} + \cdots \quad (21)$$

This series does not terminate at any finite order. In developing an approximation scheme, one possible way is to equate the coefficient of an appropriate term in the series to zero, in order to approximate it as a polynomial. This determines the energy eigenvalue and eigenfunction; one also has to show that higher order terms attain sufficiently small values to ensure convergence.
The other possible way is a variational approach. The fact that our procedure of solving the differential equation yields a series solution in terms of energy, allows us to treat the same as a variational parameter. This can be effectively used for the identification of the eigenstates and corresponding eigenvalues, as will be shown below. Since the ground state is known and we want to approximate the excited state as a product of the ground state measure and a finite degree polynomial, we are left to identify only the polynomial part of the excited state. This can be carried out in a convergent manner to the desired degree of accuracy. We first terminate the series given by Eq.(21) at some finite order. Now we check that this approximate polynomial solution \( u(x) \) has one zero on the real line, this gives us a range of energy values satisfying the above mentioned condition. Since, we know that \( u(x) \) is an approximate solution, substitution of the same in the eigenvalue equation \( \hat{H}u(x) = Eu(x) \) will leave a residual term. To get the best approximate value for the energy at this order, we minimize \( \Delta \) defined as,

\[
\Delta = \left| \int_{-\infty}^{\infty} e^{-\frac{x^4}{2}} u^*(x)(\hat{H} - E)u(x)dx \right| ,
\]

using \( E \), as a variational parameter. For a better appreciation of the above points, we give below a plot of \( \Delta \) versus \( E \) for a given approximate solution. Minimum of the plot indicates the best approximate excited state for a given degree of the polynomial. The approximate energy eigenvalue obtained by a higher degree polynomial gives better result, as can be easily seen by comparison with the numerically calculated value, given in Table I. This can also be noticed from Fig.1, which clearly shows that, the minimum of \( \Delta \) of the higher degree polynomial occurs for a value of \( E \) closer to the correct result. It should also be noticed that the value of the residual term \( \Delta \) is much smaller for the higher order polynomial. Incorporation of higher order terms makes the convergence better in the present scheme. It is found that, the first few terms in our approximate solutions are enough to yield the excited state eigenvalues, accurate upto the third place of the decimal, as shown in Table I.

**Table I. Comparison of approximate eigenvalues \( E_1 \) and \( E_2 \) for the solutions of degrees five and nine respectively, with corresponding numerically calculated values \( E_{Num} \)**

| Energy State | \( E_{Num} \) | \( E_1 \) | Deviation | \( E_2 \) | Deviation |
|--------------|----------------|---------|-----------|---------|-----------|
| 1            | -7.917350      | -7.913704 | 0.04%     | -7.916400 | 0.011%    |
| 3            | 2.520359       | 2.419229 | 4.01%     | 2.549348 | 1.15%     |
| 5*           | 14.112964      | 13.403590 | 5.02%     | --       | --        |

* This eigenvalue corresponds to an approximate solution of degree thirteen.
FIG. 1. Plots depicting the minima of $\Delta$ near the numerically evaluated eigenvalue, for the first excited state of the double-well potential. The solid and dashed curves show the variations of $\Delta$, when the approximate polynomial parts of the wave function are of degrees nine and five, respectively.

Apart from finding the states in between the known ones, as has been done above, one can also approximate the even and odd states lying above the analytically determinable part of the spectrum. For this purpose, we plot $\Delta$ for odd and even states in a range of energy values, in Figs. 2 and 3 respectively. This is computed taking approximate solution of degree nine for the odd states; and twelve for the even ones.

FIG. 2. Variations of $\Delta$ with respect to $E$, in the odd-parity sector. Here the polynomial part of the wave function has degree nine and the energy range is much bigger, as compared to Fig.1. One clearly notices that several minimum values of $\Delta$ occur closer to the numerically determined eigenvalues.
FIG. 3. Plot of $\Delta$ versus $E$, for the even states, when the approximate polynomial solution is of degree twelve. Like the odd sector in Fig.2, here also some of the minima are located close to the corresponding numerical values.

It is extremely interesting to observe that, various minima of the plot show the expected locations of the states in the energy space, with reasonable accuracy, as seen from Table II, containing the numerically calculated eigenvalues of higher excited states. It is worth pointing out that, all the minima of the plot do not correspond to physically acceptable states. One needs to take those values, which fulfill the required conditions on the wave functions. At this stage of approximation, the computed eigenvalues for the higher excited states agree with the numerically obtained ones upto 5% accuracy. As has been done earlier, in order to improve the result further, one needs to take still higher degree polynomials.

Below, we give another table containing numerically calculated energy eigenvalues of higher excited states of the double-well potential. It is clear from the spectrum, that higher excited states are approximately equispaced as expected.

Table II. Numerically calculated energy eigenvalues of a number of excited states of the double-well potential

| Energy State | $E_{\text{Num}}$ | Energy State | $E_{\text{Num}}$ |
|--------------|------------------|--------------|------------------|
| 6            | 21.1575028       | 13           | 89.0540515       |
| 7            | 28.9747742       | 14           | 100.9447956      |
| 8            | 37.4938424       | 15           | 113.3093212      |
| 9            | 46.6606249       | 16           | 126.1303320      |
| 10           | 56.4324169       | 17           | 139.3922937      |
| 11           | 66.7742029       | 18           | 153.0811528      |
| 12           | 77.6565110       | 19           | 167.1841151      |

IV. CONCLUSIONS

In conclusion, we have applied a recently developed scheme for solving linear differential equations, to find the exact eigenstates of a wide class of quasi-exactly solvable Hamiltonians and also to develop a convergent approximation scheme to determine the states not obtainable by analytical treatments. The fact that the method used provided an expansion of the wave functions in terms of the corresponding energies, allowed us to treat energy as a variational parameter, in the approximation scheme. An independent numerical scheme was used to check that the low-lying eigenvalues are accurate up to third place of decimal, with only a few terms from the series expansion. The higher excited states need more number of
terms, since these have 5% accuracy, under similar conditions. It also needs to be pointed out that, the QES systems treated here are equipped with a ground state measure, which facilitates the working of the approximation scheme. It will be interesting to extend the present scheme to other anharmonic potentials.

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