Solution of the Schrödinger Equation with One and Two Timensional Double-well Potentials

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Abstract

The Schrödinger equation with one and two dimensional potentials are solved in the framework of the $sl_2(R)$ Lie algebra. Eigenfunctions of the Schrödinger equation for various asymmetric double-well potentials have been determined and the eigenstates are expressed in terms of the orthogonal polynomials. The solution of the double-well potential in two dimension have been analyzed.

Key Words: double-well potentials, exact solution, quantum formalism.

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1. Introduction

The importance of the double-well potentials in quantum mechanics, condensed matter physics, statistical physics or field theory can hardly be overestimated [1, 2]. The Schrödinger equation has no exact, analytical solution with double-well potentials. It can be solved by using approximate methods or numerical methods. On the other hand, in quantum mechanics there exist potentials for which it is possible to find a number of eigenvalues and associated eigenfunctions exactly and in a closed form. These systems are said to be quasi-exactly solvable (QES) and this property is ultimately connected with the existence of a hidden dynamical algebra [3].

In this article we present a quasi exact solution of the Schrödinger equation with one- and two dimensional double-well potentials. The Schrödinger equation with one dimensional double-well potential have been studied by a number of authors and it can be solved by using various methods [4]. Approximate QES and approximate analytical solutions of the double-well potential have been derived in [5].

There is not much attention for the solution of the two-dimensional double-well potential [6]. In this paper we develop a simple method to solve the Schrödinger equation which admits separation of variables with two-dimensional double-well potentials. We show the separated equations are still QES. The Schrödinger equation does not admit separation of variables in two dimensions, a topic of a future work.

The paper is organized as follows. Section 2 is devoted to a derivation of a QES one-dimensional double-well potential in the framework of the $sl_2(R)$ Lie algebra. Section 3 contains a solution of the two dimensional double-well potential which admits separation of variables. Finally, the results are discussed in section 4.

2. One dimensional double-well potential

The strategy we follow is described in [7]. One way to construct a quasi-exactly solvable differential equation is to express the Hamiltonian in terms of the generators of the Lie algebra. Let us consider the

$sl_2(R)$ algebra realized as follows:

$$J_+ = x^2 \frac{d}{dx} - jx, \qquad J_0 = x \frac{d}{dx} - \frac{j}{2}, \qquad J_- = \frac{d}{dx}. \tag{1}$$

The generators obey the commutation relation

$$[J_+,\, J_-] = -2J_0, \qquad [J_0,\, J_\pm] = \pm J_\pm, \tag{2}$$

and it may be verified that the eigensolutions of the generators are given explicitly by

$$J_- \,|\, m >= m \,|\, m - 1 >, \quad J_0 \,|\, m >= \left(m - \frac{j}{2} \right) |\, m>, \quad J_+ \,|\, m >= (m - j) \,|\, m + 1), \tag{3}$$

where the basis function is

$$|\, m >= R_{j+1}(x). \tag{4}$$

If j is a non-negative integer number, the algebra possesses a $(j+1)$-dimensional subspace

$$R_{j+1} = \left\langle\, x^0, x^2, \cdots, x^j \,\right\rangle. \tag{5}$$

The linear and bilinear combinations of the generators of the algebra form a second order differential equation possessing polynomial solutions. One possible way to get a QES Schrödinger operator is to transform the QES algebraic operators acting on the finite dimensional subspace of polynomials $R_{j+1}(x)$ into the Schrödinger-type equation. It can be done by a gauge transformation.

2.1. The model Potential I

Consider the double-well potential of the form

$$V(x) = \frac{A}{2}x^2 - \frac{B}{3}x^3 + \frac{C}{4}x^4, \tag{6}$$

where A, B and C are constants. If $2B^2 = 9AC$, the potential is a symmetric potential with two minima; otherwise the potential is an asymmetric potential with two minima. We are interested in the asymmetric double-well potential. The Schrödinger equation of this potential can be written as

$$\left(-\frac{d^2}{dx^2} + V(x) \right) \psi(x) = E\psi(x). \tag{7}$$

We can write the wavefunction $\psi(x)$ in the form

$$\psi(x) = \exp\left(-\frac{1}{2} \left(-3(j+1)\frac{Cx}{B} - \frac{Bx^2}{3\sqrt{C}} + \frac{\sqrt{C}x^3}{3} \right) \right) R(x). \tag{8}$$

Then the Schrödinger equation takes the form

$$-\frac{d^2 R(x)}{dx^2} + \left(-3(j+1)\frac{C}{B} - \frac{2B}{3\sqrt{C}}x + \sqrt{C}x^2 \right) \frac{dR(x)}{dx} -$$
$$\left(\varepsilon + j \left(-\frac{B}{3\sqrt{C}} + \sqrt{C}x \right) \right) R(x) = 0 \tag{9}$$

with the constraint

$$A = \frac{\left(2B^3 - 27(j+1)C^{5/2} \right)}{9BC}$$
$$E = \varepsilon - \frac{(j+1)B}{3\sqrt{C}} - \left(\frac{3(j+1)C}{2B} \right)^2. \tag{10}$$

The potential (6) is asymmetric for all values of j when $B > 0$ and $C > 0$, and the location of minimum points depends on the values of j. In order to solve (9), we introduce the linear and bilinear combination of the algebraic operators

$$T = -J_-^2 - 3(j+1)\frac{C}{B}J_- - \frac{2B}{3\sqrt{C}}J_0 + \sqrt{C}J_+ \tag{11}$$

for which one can define the spectral problem

$$\mathrm{TR}(x) = \varepsilon R(x), \tag{12}$$

where ε is a spectral parameter. The algebraic structure (11) is quasi-exactly solvable and the insertion of (1) into (11) leads to the differential equation (9). The basis function (5) can be written as

$$R(x) = \sum_{m=0}^{\infty} a_m P_m(\varepsilon)x^m, \tag{13}$$

where $P_m(\varepsilon)$ is polynomial in ε and it can be given by the recurrence relation

$$-m(m-1)P_{m-2}(\varepsilon) - 3m(j+1)\frac{C}{B}P_{m-1}(\varepsilon) + \sqrt{C}\,(m-j)\,P_{m+1}(\varepsilon) -$$
$$\left(\frac{2B}{3\sqrt{C}}(m-\frac{j}{2}) + \varepsilon\right)P_m(\varepsilon) = 0, \tag{14}$$

with the initial condition $P_0 = 1$. The spectral parameter ε can be determined from the recurrence relation (14). If ε_j is a root of the polynomial $P_{m+1}(\varepsilon)$, the series (13) truncates at $m \geqslant (j+1)$ and ε_j belongs to the spectrum of the double-well potential. The first four of these polynomials are given by

$$
\begin{aligned}
P_1(\varepsilon) &= \varepsilon \\
P_2(\varepsilon) &= 9BC\varepsilon^2 - B^3 - 54C^{5/2} \\
P_3(\varepsilon) &= 9BC\varepsilon^3 - 4\left(B^3 + 81C^{5/2}\right)\varepsilon + 36BC^2 \\
P_4(\varepsilon) &= 9B^2C^2\varepsilon^4 - \left(10B^4C + 1080BC^{7/2}\right)\varepsilon^2 + \\
&\quad 216B^2C^3\varepsilon + \left(B^6 + 216B^3C^{5/2} + 11664C^5\right)
\end{aligned} \tag{15}
$$

for $j = 0, 1, 2$ and 3, respectively. Analytical solutions of the recurrence relation (14) are available only for the first few values of j. For $j > 2$ the solutions become numerical.

2.2. The Model Potential II

We consider the following potential treated by Burrows [5]:

$$V(x) = V_0 - Ax + \frac{x^2}{2}(B + Cx)^2. \tag{16}$$

The potential is symmetric when $A = 0$, with double minima at $x = -\frac{B}{C}$ and $x = -\frac{B}{2C}$. The Schrödinger equation with the potential (16) is given by

$$\left(-\frac{d^2}{dx^2} + V(x)\right)\psi(x) = E\psi(x). \tag{17}$$

In order to transform the Schrödinger equation to the form of an algebraic equation, we introduce the transformation

$$\psi(x) = \exp\left(-\frac{Bx^2}{2\sqrt{2}} - \frac{Cx^3}{3\sqrt{2}}\right)R(x). \tag{18}$$

Then the Schrödinger equation takes the form

$$-\frac{d^2R(x)}{dx^2} - \sqrt{2}x(B + Cx)\frac{dR(x)}{dx} + \tag{19}$$

$$\left(V_0 - E - Ax + \sqrt{2}Cx - \frac{B}{\sqrt{2}}\right)R(x) = 0.$$

The linear and bilinear combinations of the operators of the Lie algebra

$$T = -J_-^2 - \sqrt{2}BJ_0 - \sqrt{2}CJ_+; \quad TR(x) = \varepsilon R(x) \tag{20}$$

is equivalent to the situation in (19) when the parameters of the Schrödinger equation is constrained to

$$\begin{aligned} A &= -\sqrt{2}C(j+1) \\ E &= \varepsilon - \frac{(j+1)B}{\sqrt{2}}. \end{aligned} \tag{21}$$

Since $j \geqslant 0$, the potential is an asymmetric double-well potential. The Spectral parameter ε can be calculated from the recurrence relation

$$-m(m-1)P_{m-2}(\varepsilon) - \left(\sqrt{2}B\left(m - \frac{j}{2}\right) + \varepsilon\right)P_m(\varepsilon) - \tag{22}$$

$$\sqrt{2}C(m-j)P_{m+1}(\varepsilon) = 0,$$

with the initial condition $P_0(\varepsilon) = 1$. The first four values of the $P_m(\varepsilon)$ are given as follows:

$$\begin{aligned} P_1(\varepsilon) &= \varepsilon \\ P_2(\varepsilon) &= 2\varepsilon^2 - B^2 \\ P_3(\varepsilon) &= \sqrt{2}\left(\varepsilon^3 - 2\varepsilon B^2 - 4BC\right) + 4\varepsilon C \\ P_4(\varepsilon) &= 4\varepsilon^4 - 20\left(B^2 - 2\sqrt{2}C\right)\varepsilon^2 + 96\varepsilon BC + 9B^2\left(B^2 - 4\sqrt{2}C\right), \end{aligned} \tag{23}$$

for $j = 0, 1, 2, 3$, respectively.

3. Two-Dimensional double-well potential

In this section the quasi exact solution of the Schrödinger equation with two dimensional double-well potential is treated. We develop a systematic procedure for constructing a QES of a double-well potential and we illustrate our method in the situation where the Schrödinger equation admits separation of variables. The Schrödinger equation in two dimensions is given by

$$\left(-\frac{\partial^2}{\partial x^2} - \frac{\partial^2}{\partial y^2} + V(x,y)\right)\psi(x,y) = E\psi(x,y), \tag{24}$$

and can be solved exactly for a few potentials. The ground state wave function of the Schrödinger equation can be written in the form

$$\psi_0(x,y) = \exp(-W(x) - F(y) - f(xy)), \tag{25}$$

where $W(x)$ and $F(y)$ are functions of x and y, respectively, while $f(xy)$ is function of the product of x and y. The potential and ground state energy of the system with the given ground state wave function takes the form

$$V_0(x,y) - E_0 = \frac{d^2W}{dx^2} + \frac{d^2F}{dy^2} + \frac{\partial^2 f}{\partial x^2} + \frac{\partial^2 f}{\partial y^2} - \left(\frac{dW}{dx} + \frac{\partial f}{\partial x}\right)^2 - \left(\frac{dF}{dy} + \frac{\partial f}{\partial y}\right)^2. \tag{26}$$

When $f(xy)$ is zero, then the equation is separable and the general solution of the system can be obtained by solving two one dimensional differential equation. The wave function of the excited states can be written as

$$\psi(x, y) = \phi(x, y)\psi_0(x, y), \tag{27}$$

where the function $\phi(x, y)$ is polynomial in x and y. Substituting (27) into Schrödinger equation (24) we obtain the differential equation

$$-\frac{\partial^2 \phi}{\partial x^2} - \frac{\partial^2 \phi}{\partial y^2} - 2\left(\frac{dW}{dx} + \frac{\partial f}{\partial x}\right)\frac{\partial \phi}{\partial x} - 2\left(\frac{dF}{dy} + \frac{\partial f}{\partial y}\right)\frac{\partial \phi}{\partial y} + \tag{28}$$
$$(V - V_0 + E_0 - E)\phi = 0.$$

In the exactly solvable case, the potentials V and V_0 are same. In the quasi exactly solvable case, the functional form of the potential remain same for all states, but a parameter changes from state to state. Let us illustrate our method on the separable systems. In the case $f = 0$ the potentials can be written as

$$V - V_0 = g(x) + h(y), \tag{29}$$

then substituting $\phi = R(x)Q(y)$ we obtain

$$-\frac{d^2 R}{dx^2} - 2\frac{dW}{dx}\frac{dR}{dx} + (g(x) + E_0 - E + c_1)R = 0$$
$$-\frac{d^2 Q}{dy^2} - 2\frac{dF}{dx}\frac{dQ}{dy} + (h(y) - c_1)Q = 0. \tag{30}$$

In the following we illustrate our method on two examples.

3.1. The model potential I

Consider the following model potential with the parameter α:

$$V(x, y; \alpha) = A^2 x^4 + ABx^2 + C^2 y^2 + 2A\alpha x. \tag{31}$$

The Schrödinger equation with this potential is separable and can be solved by reduction to two one-dimensional systems. The parameter α is depends on the state of the wave function. Let us call it the "state parameter". The wave function of the ground state with the energy E_0 can be written in the form

$$\psi_0(x, y) = \exp\left(-\frac{Ax^3}{3} - \frac{Cy^2}{2} - Bx\right)$$
$$E_0 = C - B^2. \tag{32}$$

The wave functions of the excited states with the energy E we write as

$$\psi(x, y) = R(x)Q(y)\psi_0(x, y). \tag{33}$$

Substituting (30) in (24) with the potential (31), then after a straightforward calculation we obtain two one-dimensional differential equations:

$$-\frac{d^2 Q}{dy^2} + 2By\frac{dQ}{dy} - c_1 Q = 0 \tag{34}$$

$$-\frac{d^2 R}{dx^2} + 2(C + Ax^2)\frac{dR}{dx} + (E - E_0 + c_1 + 2Ax(1 - \alpha))R = 0, \tag{35}$$

where c_1 is a constant. The first equation is exactly solvable and its solution is given by

$$Q(y) = N_1 {}_1F_1\left(\frac{1}{2} - \frac{c_1}{4B}, \frac{3}{2}, By^2\right) + N_2 {}_1F_1\left(-\frac{c_1}{4B}, \frac{1}{2}, By^2\right), \tag{36}$$

where N_1 and N_2 are normalization constants and $_1F_1(\cdots)$ is a confluent hypergeometric function. The second equation is a quasi-exactly solvable differential equation. The following combinations of the operators of the Lie algebra

$$T = -J_-^2 + 2BJ_- + 2AJ_+ \quad TR = (E_0 - E - c_1)R \tag{37}$$

is equivalent with (35) if $\alpha = j + 1$. Following the procedure given in section 2, the spectrum of the system can be obtained by using the following recurrence relation:

$$-m(m-1)P_{m-2}(E) + 2BmP_{m-1}(E) + \tag{38}$$
$$2A(m-j)P_{m+1}(E) - (E_0 - E - c_1)P_m(E) = 0.$$

Some of the polynomial is given by

$$\begin{aligned}
P_1(E) &= (c_1 - E_0 + E) \\
P_2(E) &= (c_1 - E_0 + E)^2 + 4AB \\
P_3(E) &= (c_1 - E_0 + E)^3 + 16AB(c_1 - E_0 + E) - 16A^2 \\
P_4(E) &= (c_1 - E_0 + E)^4 + 40AB(c_1 - E_0 + E)^2 - \\
&\quad 96A^2(c_1 - E_0 + E) + 144A^2B^2,
\end{aligned} \tag{39}$$

for $j = 0, 1, 2, 3$, respectively. The roots of the polynomials $P_j(E)$ produce the spectrum of the system.

3.2. The model potential II

The last example is the following double-well potential:

$$V(x, y; \alpha; \beta) = A_1^2 x^4 + A_2^2 y^4 + 2A_1 B_1 x^2 + 2A_2 B_2 y^2 - 2A_1 \alpha x - 2A_2 \beta y. \tag{40}$$

As we mentioned before, α and β are state parameters. The ground state wave function is given by

$$\begin{aligned}
\psi_0(x, y) &= \exp\left(-\frac{A_1 x^3}{3} - \frac{A_2 y^3}{3} - B_1 x - B_2 y\right); \\
E_0 &= B_1^2 + B_2^2.
\end{aligned} \tag{41}$$

Since the Schrödinger equation is separable with the given potential, the wave function can be written as

$$\psi(x, y) = R(x) Q(y) \psi_0. \tag{42}$$

Insertion of (42) into (24) with the potential (40) leads to the following two differential equations:

$$-\frac{d^2R}{dx^2} + 2\left(B_1 + A_1 x^2\right)\frac{dR}{dx} + (E - E_0 + c_1 + 2A_1(1-\alpha)x) = 0 \tag{43}$$

$$-\frac{d^2Q}{dy^2} + 2\left(B_2 + A_2 y^2\right)\frac{dQ}{dy} - (c_1 - 2A_2(1-\beta)y) = 0. \tag{44}$$

These equations are QES.

4. Conclusion

The QES of the double-well potential in one and two dimensions have been discussed. The solution of Schrödinger equations which does not admit separation of variables are left for treatment in future work.

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