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NON-COMPACT GROUP $SU(1,1)$ OF A FREE PARTICLE IN THE SYMMETRIC DOUBLE-WELL POTENTIAL FIELD

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We analyze the equation of motion for a particle in the double-well potential. We find the symmetries through Lie's method of group analysis. In the corresponding quantum mechanical case, the method of spectrum-generating $su(1,1)$ algebra is used to find energy levels as solutions of the Schrödinger equation with double-well potential, without solving the equation explicitly. Finally, we discuss the symmetry version of the double-well potential with the vector-field formalism.

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1. Introduction

Many quantum systems of physics and chemistry are represented by a particle in the potential field in form of two wells with finite or infinite barrier and finite or infinite outside walls [1, 2]. The double-well potential has many of applications from the non-periodic to periodic quantum systems [3]. Also the symmetric version of this potential has been widely used in many area of physics. Since symmetries and breaking of symmetries play a crucial role in physics, the systematization of the symmetries is very helpful in understanding the role of such potentials [4]. The group analysis method of differential equations relevant to physics is an important way to analyse many physical potentials [5, 6]. The symmetry in the double-well potential allows to perform the group analysis of the Schrödinger equation with such a potential, which leads to the Lie symmetries. In this work we consider a double-well potential with infinitely high outside walls. For this potential in the external regions, an analytical solution of the energy spectrum is available by algebric method [7]. We applied $su(1,1)$ and $so(2,1)$ algebra to solve the $x^2 + 1/x^2$ potential using J_1, J_2, J_3 and Casimir operators as generators.

2. Double-well potential

Let us consider a quantum system representing a particle in the symmetric double-well potential field defined by

$$U(x) = \frac{m\omega^2}{2} \left\{ \begin{array}{lll} (x+x_0)^2 + \dfrac{\beta^2}{(x+x_0)^2} & \text{for} & x > a > 0\,, \\ F - Dx^2 & \text{for} & -a \leq x \leq a\,, \\ (x-x_0)^2 + \dfrac{\beta^2}{(x-x_0)^2} & \text{for} & x \leq -a \leq 0\,, \end{array} \right\} \tag{1}$$

where m and ω are mass and angular frequency of the particle, respectively, and β, F and D are positive constants. F determines the barrier height. The values of β, F and D are such that $U(x)$ is continuous at points $x = -a$ and $x = a$. The minima of the two potential wells are located at points $x_1 = (-\sqrt{\beta} + x_0)$ and $x_2 = (\sqrt{\beta} - x_0)$. The first part of the potential (1) is symmetric. Because of the sub-barrier tunnel effect and propagation at energies above the barrier, transitions of the particle between wells occur, i.e., it oscillates from one well to the other and back. To calculate the energy spectrum for the potential (1), the boundary conditions at $x \to \pm\infty$ play an important role.

The time independent Schrödinger equation in the external region (outsides of walls) can be written as

$$\frac{\partial^2 \psi}{\partial x^2} + \Big(\frac{A}{x^2} + Bx^2 + C'\Big)\psi(x) = 0\,, \tag{2}$$

with

$$x \leftarrow x - x_0 \qquad \text{for} \qquad x < -a\,,$$

$$x \leftarrow x + x_0 \qquad \text{for} \qquad x > a\,,$$

where the new parameters C',B and A are defined by the following relations

$$C' = \frac{2mE}{\hbar^2}, \qquad B = \frac{-m^2\omega^2}{\hbar^2}, \qquad A = \frac{-m^2\omega^2\beta^2}{\hbar^2}\,. \tag{3}$$

It is well established that algebric methods were found to be useful for solving the Schrödinger equation directly [6]. Therefore, we use this approach to obtain the Schrödinger equation's eigenvalues. The Lie algebra of non-compact groups

$SO(2,1)$ and $SU(1,1)$ can be realized in terms of a single variable. By expressing the generators according to the above equation, we define them by the following relations

$$\begin{aligned} J_1 &= \frac{\mathrm{d}^2}{\mathrm{d}x^2} + \frac{A}{x^2} + \frac{x^2}{16}\,, \\ J_2 &= \frac{-\mathrm{i}}{2}\Big(x\frac{\mathrm{d}}{\mathrm{d}x}\Big) + \frac{1}{4}\,, \\ J_3 &= \frac{\mathrm{d}^2}{\mathrm{d}x^2} + \frac{A}{x^2} - \frac{x^2}{16}\,. \end{aligned} \tag{4}$$

So, J_1,J_2 and J_3 satisfy the well known standard algebra

$$[J_1, J_2] = -\mathrm{i}J_3\,,$$

$$[J_2, J_3] = \mathrm{i}J_1\,,$$

$$[J_3, J_1] = \mathrm{i}J_2\,,$$

and also the Casimir invariance condition related to $SU(1,1)$ group can be shown to be

$$\mathcal{C}^2 = J_3^2 - J_1^2 - J_2^2\,. \tag{5}$$

Therefore, we obtain the Casimir operator as follows,

$$\mathcal{C}^2 = \frac{-A}{4} + \Big(\frac{x}{4}\Big)\Big(\frac{\mathrm{d}}{\mathrm{dx}}\Big). + \frac{1}{16} \tag{6}$$

The second-order differential operator appearing in Eq. (3) in terms of the $SU(1,1)$ generators, given by

$$\frac{\partial^2}{\partial x^2} + \frac{A}{x^2} + Bx^2 + C' = \Big(\frac{1}{2} + 8B\Big)J_1 + \Big(\frac{1}{2} - 8B\Big)J_3 + C'\,, \tag{7}$$

can be rewriten as

$$\Big[\Big(\frac{1}{2} + 8B\Big)J_1 + \Big(\frac{1}{2} - 8B\Big)J_3 + C\Big]\psi(x) = 0\,.$$

It is also possible to perform a transformation of $\psi(x)$ and the J_1, J_2 and J_3 involving $\mathrm{e}^{(-\mathrm{i}\theta J_2)}$. In order to obtain the discrete energy eigenvalues, we must define θ such that the compact operator, J_3, will be diagonal. Therefore,

$$\tanh\theta = -\frac{\frac{1}{2} + 8B}{\frac{1}{2} - 8B}\,, \tag{8}$$

where

$$B = \frac{-m^2\omega^2}{\hbar^2}.$$

So we may get

$$4n + 2 + \sqrt{1-4A} = \frac{C'}{\sqrt{-B}}\,. \tag{9}$$

Finally, by substituting for parameters B, C' and A, we obtain

$$\begin{aligned} {E_n}^+ &= 2\hbar\omega\Big(n + \frac{1}{2} + \frac{\sqrt{1-4A}}{4}\Big)\,, \\ {E_n}^- &= 2\hbar\omega\Big(n + \frac{1}{2} - \frac{\sqrt{1-4A}}{4}\Big)\,. \end{aligned} \tag{10}$$

The results obtained here agree well with those of Ref. [9]. They contain two terms. The first term explains the periodicity of the potential and the second one describes its non-periodical property. So, the results show that there is no periodicity for the double-well potential in the given area. Because of the importance of the symmetrical version of this potential in physics, we will discuss vector fields and some aspects of symmetry. To do this, we rewrite the Schrödinger for the given potential,

$$\frac{\mathrm{d}^2\psi(x)}{\mathrm{d}x^2} + \Big(\frac{A}{x^2} + Bx^2 + C'\Big)\psi(x) = 0\,,$$

by changing the variable x to $y = \alpha x^2$ and by the definition of α and $\psi(y)$ as follows,

$$\alpha = \frac{m\omega}{\hbar} = \sqrt{-B}\,, \qquad \psi(y) = \Big(\frac{y}{\alpha}\Big)^{-1/4} w(y), \tag{11}$$

Then Eq. (3) transforms in to the standard Whittaker form [8],

$$\frac{\mathrm{d}^2 w}{\mathrm{d}y^2} + \Big[\frac{-1}{4} + \frac{C'}{4\sqrt{-B}}\frac{1}{y} + \Big(\frac{3}{16} + \frac{A}{4}\Big)\frac{1}{y^2}\Big] w(y) = 0. \tag{12}$$

Now we define the following parameters to rearrange Eq. (12),

$$G = \frac{-1}{4}\,, \qquad D = \frac{C'}{4\sqrt{-B}}\,, \qquad C = \Big(\frac{3}{16} + \frac{A}{4}\Big)\,.$$

Finally, we obtain

$$\frac{\mathrm{d}^2 w}{\mathrm{d}y^2} + \Big[\frac{C}{y^2} + \frac{D}{y} + G\Big] w(y) = 0\,. \tag{13}$$

It is well known that there are two symmetries in the double-well potential system, namely the spatial and the time translations generated by $\partial/\partial y$, $\partial/\partial u$, $\partial/\partial t$ and $y(\partial/\partial u) - u(\partial/\partial y)$, respectively. Other symmetries are given by the vector fields which generate the transformations $\omega \to \omega + k$ and $\omega \to \omega + q(u,y)$, where k is a constant and $q(u,y)$ is an arbitrary function.

The time-dependent solution of the double-well potential was not included here. Therefore, apart from the above mentioned trivial symmetries, the double-well potential system admits only the following symmetries

$$X = A(y,u)\frac{\partial}{\partial y} + B(u,y)\frac{\partial}{\partial u}\,, \tag{14}$$

where A and B are (non constant) arbitrary differentiable functions. So, in order to find the Lie point symmetries of the corresponding quantum case, we write (13) using [4]

$$w'' = N(y,w,w')\,, \tag{15}$$

where

$$N(y,w,w') = -\Big[\frac{C}{y^2} + \frac{D}{y} + E\Big]w(y)\,. \tag{16}$$

The infinitesimal generator of the symmetry under which the differential equation remains unchanged is given by the following vector field [4]

$$Y = \xi(y,w)\frac{\partial}{\partial y} + \eta(y,w)\frac{\partial}{\partial w}\,, \tag{17}$$

and for a second-order differential equation, ξ and η can be obtained from the following relations

$$\begin{aligned} N\Big[\frac{\partial\eta}{\partial w} - 2\frac{\partial\xi}{\partial y} - 3w'\frac{\partial\xi}{\partial w}\Big] - \frac{\partial^2 N}{\partial y\partial\xi} - \frac{\partial^2 N}{\partial y\partial\eta} - \frac{\partial N}{\partial w'}\Big[\frac{\partial\eta}{\partial y} + w'\Big(\frac{\partial\eta}{\partial w} - \frac{\partial\xi}{\partial y}\Big) - w'^2\frac{\partial\xi}{\partial w}\Big] \\ + \frac{\partial^2\eta}{\partial y^2} + w'\Big(2\frac{\partial^2\eta}{\partial y\partial w} - \frac{\partial^2\xi}{\partial y^2}\Big) + w'^2\Big(\frac{\partial^2\eta}{\partial w^2} - 2\frac{\partial^2\xi}{\partial y\partial w}\Big) - w'^3\frac{\partial^2\xi}{\partial w^2} = 0\,. \end{aligned} \tag{18}$$

The symmetry condition (18) related to (15) can be given by

$$\begin{aligned} -\Big[\Big(\frac{C}{y^2} + \frac{D}{y} + G\Big)w(y)\Big]\Big(\frac{\partial\eta}{\partial w} - \frac{\partial\xi}{\partial y}\Big) + \Big[\frac{2C}{y^3} + \frac{D}{y^2}\Big](w\xi) + \Big[\frac{C}{y^2} + \frac{D}{y} + G\Big]\eta + \frac{\partial^2\eta}{\partial y^2} \\ -w'\Big[3\Big(\frac{C}{y^2} + \frac{D}{y} + G\Big)\frac{\partial\xi}{\partial w} + 2\frac{\partial^2\eta}{\partial y\partial w} - \frac{\partial^2\xi}{\partial y^2}\Big] + w'^2\Big[\frac{\partial^2\eta}{\partial w^2} - 2\frac{\partial^2\xi}{\partial y\partial w}\Big] - w'^3\frac{\partial^2\xi}{\partial w^2} = 0\,. \end{aligned} \tag{19}$$

By equating the coefficients of ${w'}^3$ and ${w'}^2$ to zero, one obtains

$$\begin{aligned} \frac{\partial^2 \xi}{\partial w^2} &= 0\,, \\ \frac{\partial^2 \eta}{\partial w^2} &= 2\frac{\partial^2 \xi}{\partial y \partial w}\,, \end{aligned} \tag{20}$$

where ξ and η satisfy the following equations,

$$\begin{aligned} \xi &= w\alpha(y) + \rho(y)\,, \\ \eta &= w^2\alpha'(y) + w\gamma(y) + \delta(y)\,. \end{aligned} \tag{21}$$

By equating the coefficients of w' in (21), we get

$$3\Big(\frac{C}{y^2} + \frac{D}{y} + G\Big)\frac{\partial \xi}{\partial w} + 2\frac{\partial^2 \eta}{\partial y \partial w} - \frac{\partial^2 \xi}{\partial y^2} = 0\,. \tag{22}$$

Substitution for ξ and η changes (22) into

$$3\Big[\frac{C}{y^2} + \frac{D}{y} + E\Big]\alpha(y) + 3w\alpha''(y) + 2\gamma'(y) - \rho''(y) = 0\,. \tag{23}$$

For $\alpha = 0$, we get

$$2\gamma'(y) = \rho''(y) \tag{24}$$

and

$$\gamma(y) = \frac{\rho'(y)}{2} + H\,, \tag{25}$$

where H is a constant.

Substituting from equations (24), (25) and (21) into (19), one obtains

$$\begin{aligned} -\Big[\frac{C}{y^2} + \frac{D}{y} + G\Big]w(y)\frac{\partial \eta}{\partial w} + \Big[\frac{C}{y^2} + \frac{D}{y} + G\Big]w(y)\frac{\partial \xi}{\partial y} + \Big[\frac{2C}{y^3} + \frac{D}{y^2}\Big]w\xi \\ + \Big[\frac{C}{y^2} + \frac{D}{y} + G\Big]\eta + \frac{\partial^2 \eta}{\partial y^2} = 0\,. \end{aligned} \tag{26}$$

After straightforward calculations to obtain $\partial\eta/\partial w$, $\partial\xi/\partial y$, and $\partial^2\eta/\partial y^2$, and using $\rho(y)$ instead of $\gamma(y)$ from (25), we have

$$\begin{aligned} \rho'''(y) + 4\Big[\frac{C}{y^2} + \frac{D}{y} + G\Big]\rho'(y) + \Big[\frac{4C}{y^3} + \frac{2D}{y^2}\Big]\rho(y) + \Big[\frac{2C}{y^2} + \frac{2D}{y} + G\Big]\delta(y) \\ + \Big[\frac{4C}{y^3} + \frac{2D}{y^2}\Big]w^2\alpha(y) + 2w^2\alpha'''(y) + 2\delta''(y) = 0\,. \end{aligned} \tag{27}$$

The last four terms of equation (27) and parameters $\alpha(y)$ and $\alpha'(y)$ are equal to zero. Therefore, the reminding terms are also zero, what leads to the Schrödinger-like equation

$$\rho'''(y) + 4\Big[\frac{C}{y^2} + \frac{D}{y} + G\Big]\rho'(y) - \Big[\frac{4C}{y^3} + \frac{2D}{y^2}\Big]\rho(y) = 0\,. \tag{28}$$

The solution is

$$\rho(y) = \frac{p}{y} + q\,. \tag{29}$$

This equation leads to the following conditions,

$$\begin{aligned} q &= 2pD\,, \\ C &= \frac{-3}{4}\,, \\ D^2 &= -G\,, \end{aligned} \tag{30}$$

and

$$D = \frac{C'}{4\sqrt{-B}}, \qquad C = \Big(\frac{3}{16} + \frac{A}{4}\Big)\,,$$

where $A = -15/4$. From Eq. (2), we obtain β and C' as follow,

$$\beta = \frac{\hbar}{m\omega}\sqrt{\frac{15}{4}}\,,$$

$$C' = 2\sqrt{-B}\,. \tag{31}$$

By using relations (17) and (21), we get

$$Y = [w\alpha(y) + \beta(y)]\frac{\partial}{\partial y} + [w^2\alpha'(y) + w\gamma(y) + \delta(y)]\frac{\partial}{\partial w} \tag{32}$$

which is a type of symmetry for the double-well potential.

3. Conclusion

The approach of group analysis of the double-well potential on the basis of energy spectrum is presented in this work. By using the generators of $SU(1,1)$ non-compact group of a particle in the symmetric double-well potential field, we obtain the energy spectrum for n_+ and n_- cases. Finally, we present the symmetry part of this potential with the help of a vector field.

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NEKOMPAKTNA GRUPA $SU(1,1)$ SLOBODNE ČESTICE U SIMETRIČNOM DVOJAMNOM POTENCIJALNOM POLJU

Analiziramo jednadžbu gibanja čestice u dvojamnom potencijalu. Lieovom metodom grupne analize nalazimo simetrije. U odgovarajućem kvantno-mehaničkom slučaju primjenjujemo algebru $SU(1,1)$ kojom se izvode spektri, radi dobivanja energija stanja za Schrödingerovu jednadžbu s dvojamnim potencijalom, bez njenog izravnog rješavanja. Na kraju raspravljamo simetričnu inačicu dvojamnog potencijala u okviru formalizma vektorskog polja.