Group analysis of Schrödinger equation with generalised Kratzer type potential

Karmadeva Maharana
Physics Department, Utkal University, Bhubaneswar 751004, India
E-mail: karmadev@iopb.res.in

Abstract. Using the method of $su(1,1)$ spectrum generating algebra, we analyze one dimensional Schrödinger equation with potential in the form $\frac{C}{x^2} + \frac{D}{x}$ to obtain a class of potentials giving similar eigenvalues. By a group analysis of the differential equation it is found that the symmetry gets enhanced for particular values of $C$ and $D$. The generators of the Lie algebra do not close. The extension of the vector field gives rise to an interesting algebra.
1. Introduction

Kratzer’s type of molecular potential, \( V(x) = (\frac{a}{x} - \frac{1}{2} \frac{a^2}{x^2}) \), has been considered to obtain the molecular spectra since the early days of quantum mechanics[1]. Similar type of Schrödinger equation is also obtained for an electron moving in a model nonuniform magnetic field \( B_x = 0, B_y = 0 \) and \( B_z = \frac{1}{x^2} \) [2]. We analyse a generalisation of this potential, \( V(x) = \frac{C}{x^2} + \frac{D}{x} \), through the method of \( su(1,1) \) spectrum generating algebra. We have obtained the bound state spectrum for this case. Here we obtain a class of potentials that provide similar eigenvalues. This reminds us of the situation where reflectionless potentials are obtained through Bäcklund transforms for the scattering states.

Since symmetries and beaking of symmetries play such a crucial role in physics, the enumeration of the symmetries would be helpful in understanding the role of such potentials in spontaneous symmetry breaking, for example. The group analysis of differential equations relevant to physics has been quite fruitful in the context of finding solutions and constructing new solutions, gaining insight regarding asymptotic behaviour of the solutions, integrability conditions, conservation laws etc.. There is a vast literature on the application of this technique to mathematics and physics[3 4]. In this paper we also perform a group analysis of the above type of Schrödinger equation to obtain the Lie point symmetries. Some examples of this type of analysis for charged particles in the presence of specific magnetic fields have also been carried out in[9 2]. In the present case it is found that the symmetry gets enhanced for particular values of \( C \) and \( D \). The resulting generators of the Lie algebra do not close under the Lie product. For a special case we obtain an interesting looking extended infinite Lie algebra. This algebra has appearance similar to that of Kac - Moody - Virasoro type and the Dolan - Grady type which arose in the study of integrable models and symmetries of supersymmetric models in the presence of magnetic fields[10 11 12].

2. The quantum eigenvalues

We consider the Schrödinger equation of the form

\[
- \frac{\hbar^2}{2m} \left[ \frac{d^2 u}{dx^2} - \left( \frac{C}{x^2} + \frac{D}{x} \right) \right] u = Eu. \tag{1}
\]

where \( C \) and \( D \) are constants. The Schrödinger equation for Kratzer’s molecular potential is a special case of the above equation. The Kratzer molecular potential is of the form , in our notation,

\[
V(x) \propto (\frac{a}{x} - \frac{1}{2} \frac{a^2}{x^2}) \tag{2}
\]

and the eigenvalue equation had been solved by the usual series expansion method. The eigenfunctions turn out to be a general type of Kummer’s hypergeometric function \( _1F_1[1] \).
Group analysis of Schrödinger equation

But energy eigenvalues for this equation can also be obtained by mapping this problem to that of the spectrum generating algebra of $SU(1,1)$ by identifying the generators of the algebra with the (differential ) operator realization of the algebra, and calculating the Casimir invariant. Cordero and Ghirardi have calculated the energy eigenvalues for such cases using the spectrum generating algebra method [5]. Though in this method we directly get the eigenvalues, and not the eigenfunctions explicitly, it will be seen that it is easier to find a class of potentials which give similar eigenvalues. For completeness and also for familiarisation with the notation, we give below the details of the calculation.

Equation (1) can be written as

$$\frac{d^2 u}{dx^2} + \left( C \frac{x^2}{2} + D + \mathcal{E} \right) u = 0$$

(3)

where $\mathcal{E} = \frac{\mathbf{h}^2}{2m} E$.

The generation of the spectrum associated with a second order differential equation of the form

$$\frac{d^2 R}{ds^2} + f(s) R = 0$$

(4)

where

$$f(s) = \frac{a}{s^2} + bs^2 + c$$

(5)

has been analysed by several authors [6]. To bring equation (3) to the above form we set

$$x = s^2, \quad u(x) = s^{\frac{1}{2}} R(s)$$

(6)

to get

$$\frac{d^2 R}{ds^2} + \left( \frac{16C - 3}{4} \frac{1}{s^2} + 4\mathcal{E}s^2 + 4D \right) R = 0.$$  

(7)

We indicate in brief the procedure to obtain the 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

$$\Gamma_1 = \frac{\partial^2}{\partial s^2} + \frac{\alpha}{s^2} + \frac{s^2}{16}$$

(8)

$$\Gamma_2 = -\frac{i}{2} \left( s \frac{\partial}{\partial s} + \frac{1}{2} \right)$$

(9)

$$\Gamma_3 = \frac{\partial^2}{\partial s^2} + \frac{\alpha}{s^2} - \frac{s^2}{16}$$

(10)

so that the $\Gamma_i$’s satisfy the standard algebra

$$[\Gamma_1, \Gamma_2] = -i\Gamma_3, \quad [\Gamma_2, \Gamma_3] = i\Gamma_1, \quad [\Gamma_3, \Gamma_1] = i\Gamma_2.$$  

(11)

The existence of the Casimir invariant for $su(1,1)$

$$\Gamma^2 = \Gamma_3^2 - \Gamma_1^2 - \Gamma_2^2$$

(12)
Group analysis of Schrödinger equation

is exploited to obtain the explicit form of $\Gamma_i$'s. The second order differential operator in equation (11) in terms of the $su(1,1)$ generators is now given by

$$\frac{\partial^2}{\partial s^2} + \frac{a}{s^2} + bs^2 + c = \left(\frac{1}{2} + 8b\right)\Gamma_1 + \left(\frac{1}{2} - 8b\right)\Gamma_3 + c$$

and Eq.(11) becomes

$$\left[\left(\frac{1}{2} + 8b\right)\Gamma_1 + \left(\frac{1}{2} - 8b\right)\Gamma_3 + c\right]\mathcal{R} = 0.$$ (14)

Next a transformation involving $e^{-i\Gamma_2}$ can be performed on $\mathcal{R}$ and the $\Gamma_i$'s. A choice of $\theta$ such that

$$\tanh \theta = -\frac{1}{2} + \frac{8b}{2} - 8b$$

will diagonalize the compact operator $\Gamma_3$ and the discrete eigenvalues may be obtained.

The arguments of the standard representation theory then lead to the result,

$$4n + 2 + \sqrt{1 - 4a} = \frac{c}{\sqrt{-b}}; \quad n = 0, 1, 2, \ldots$$

Substitution of the corresponding values from equation (7)

$$a = \left(\frac{16C - 3}{4}\right), \quad b = 4\hat{E}, \quad c = 4D$$

gives

$$\hat{E} = -\frac{D^2}{\left[(2n + 1) + \sqrt{(1 - 4c)}\right]^2}.$$ (18)

It is interesting to note that by a substitution

$$s = y^3$$

the equation (11),

$$\frac{d^2\mathcal{R}}{ds^2} + \left(\frac{a}{s^2} + bs^2 + c\right)\mathcal{R} = 0$$

becomes

$$\frac{d^2\mathcal{R}}{dy^2} - 2 \frac{d}{dy} \frac{\partial}{\partial y} \mathcal{R} + 9\left(\frac{a}{y^2} + by^{10} + cy^4\right)\mathcal{R} = 0$$

and the corresponding $\Gamma_i$'s satisfying the commutation relations of Eq.(11) are

$$\hat{\Gamma}_1 = \frac{1}{9y^4} \frac{\partial^2}{\partial y^2} - 2 \frac{\partial}{9y^6} \frac{\partial}{\partial y} + \frac{\alpha}{y^6} + \frac{y^6}{16}$$

$$\hat{\Gamma}_2 = -\frac{i}{2} \left(\frac{y \partial}{3 \partial y} + \frac{1}{2}\right)$$

$$\hat{\Gamma}_3 = \frac{1}{9x^4} \frac{\partial^2}{\partial y^2} - 2 \frac{\partial}{9x^6} \frac{\partial}{\partial y} + \frac{\alpha}{y^6} - \frac{y^6}{16}.$$ (24)

These ultimately lead to a result similar to that of equation (16). Also if we let

$$\mathcal{R} = y\hat{\mathcal{R}}(y)$$

(25)
then we land up with the equation
\[
\frac{d^2 \hat{R}}{dy^2} - \frac{2}{y^2} \hat{R} + 9\left(\frac{a}{y^2} + by^4 + cy^4\right)\hat{R} = 0
\] (26)

Similarly, a substitution of the form
\[ s = y^\frac{2}{3} \] (27)

and
\[ \mathcal{R} = y^{-\frac{1}{3}}\hat{R} \] (28)

takes equation (20) to
\[
\frac{d^2 \hat{R}}{dy^2} + \left(\frac{a}{y^2} - \frac{5}{36y^2} + \frac{4}{9by^\frac{2}{3}} + \frac{c}{y^\frac{4}{3}}\right)\hat{R} = 0
\] (29)

and would have similar energy eigenvalues.

In fact we can go from equation (20) to a class of equations
\[
\frac{d^2 u}{dx^2} - \left(p^2 - 1\right)\left(\frac{1}{x^2}\right)
+ p^2\left(\frac{a}{x^2} + bx^{4p-2} + cx^{2p-2}\right)u = 0
\] (30)

with similar eigenvalues when
\[ \mathcal{R} = s^q u \] (31)

and \( s \) and \( x \) are related by
\[ s = x^p \] (32)

In the above, the diagonalisation of the compact operator \( \Gamma_3 \) gave rise to the discrete spectrum. If the noncompact operator \( \Gamma_1 \) is diagonalized instead of \( \Gamma_3 \), then continuous eigenvalue spectrum is obtained. For this the tilting angle for the transformation is to be put such that
\[ \tanh \theta = -\frac{1}{2} - \frac{8b}{\frac{1}{2} + 8b}. \] (33)

The eigenvalues are now characterized by a continuous spectrum \( \lambda \), where
\[ \lambda = \frac{-c}{4\sqrt{-b}} \] (34)

In the analysis of reflexionless potentials in quantum mechanics, for example, one comes across a whole two parameter family of potentials which are reflexionless. The related potentials are Bäcklund transforms of one another\[14\]. Though we suspect that in our treatment of the bound states a similar relation would exist, we have not yet found the explicit connexion.
3. Group Analysis

Since symmetries and symmetry breakings play such a fundamental role in physics, we are interested in finding the symmetry generators in the presence and in the absence of different type of potentials. We follow the method and notation of Stephani\[8\].

In order to find the Lie point symmetries of the corresponding quantum case we go back to the Schrödinger equation (3). We write this equation as

\[ u'' = \omega(x, u, u') \]  

where

\[ \omega(x, u, u') = -\left(\frac{C}{x^2} + \frac{D}{x} + \hat{E}\right)u(x). \]  

The infinitesimal generator of the symmetry under which the differential equation does not change is given by the vector field

\[ X = \xi(x, u) \frac{\partial}{\partial x} + \eta(x, u) \frac{\partial}{\partial u} \]  

and for a second order differential equation, \( \xi \) and \( \eta \) are to be determined from

\[ \omega(\eta, u - 2\xi_x - 3u'u, u_x) - \omega_x \xi - \omega_u \eta - \omega' u \left[ \eta_x + u' (\eta_u - \xi_x) - u'' \xi_u \right] + \eta_{xx} + u' \left[ 2\eta_{ux} - \xi_{xx} \right] + u'' \left( \eta_{uu} - 2\xi_{xu} \right) - u''' \xi_{uu} = 0 \]  

where a prime denotes differentiation with respect to \( x \), the partial derivative of a function by a comma followed by the variable with respect to which the derivation has been performed.

The symmetry condition (38) for our equation (35) is

\[ \omega(\eta_{,u} - 2\xi_{,x} - 3u'u, u_x) - \omega_x \xi - \omega_u \eta - \omega' u \left[ \eta_x + u' (\eta_u - \xi_x) - u'' \xi_u \right] + \eta_{xx} + u' \left[ 2\eta_{ux} - \xi_{xx} \right] + u'' \left( \eta_{uu} - 2\xi_{xu} \right) - u''' \xi_{uu} = 0 \]  

Equating to zero the coefficients of \( u''' \) and \( u'' \) we get

\[ \xi_{,uu} = 0, \quad \eta_{,uu} = 2\xi_{,xu} \]  

which are satisfied for

\[ \xi = u\alpha(x) + \beta(x), \quad \eta = u^2 \alpha'(x) + u\gamma(x) + \delta(x). \]  

Using these and equating the coefficient of \( u' \) to zero one obtains

\[ 3u \left[ \alpha''(x) + \left(\frac{C}{x^2} + \frac{D}{x} + \hat{E}\right)\alpha(x) \right] + 2\gamma'(x) - 2\beta''(x) = 0. \]  

This shows that either

\[ \alpha = 0 \]  

or \( \alpha(x) \) satisfies the same equation as \( u(x) \) does and

\[ 2\gamma'(x) = \beta''(x). \]
This integrates to

$$\gamma(x) = \frac{\beta'(x)}{2} + \kappa$$

(45)

where \( \kappa \) is a constant. The rest of the equation, after using the fact that \( \alpha(x) \) satisfies the same equation as \( u(x) \) does, becomes

$$\beta''(x) + 4\left(\frac{C}{x^2} + \frac{D}{x} + \hat{E}\right)\beta'(x) - \left(\frac{4C}{x^3} + \frac{2D}{x^2}\right)\beta(x) = 0$$

(46)

with \( \delta(x) \) also obeying the same equation as \( u(x) \) does. The simplest nontrivial solution to this equation is

$$\beta(x) = \frac{p}{x} + q$$

(47)

where \( p \) and \( q \) are constants and \( C, D \), and \( \hat{E} \) must satisfy

$$q = 2pD, \quad C = -\frac{3}{4}, \quad D^2 = -\hat{E}.$$  

(48)

It is now observed that the condition \( D^2 = -\hat{E} \) is satisfied for \( C = -\frac{3}{4} \) if we take the square root to be only negative while evaluating \( \sqrt{1 - 4a} \) and for \( n = 1 \). Also note that the symmetry is present for a particular value of the energy. It may be recalled that \( n \) must be zero or a positive integer for our analysis if any meaningful eigenvalue is to be obtained. The above result indicates that only for \( n = 1 \) there is the symmetry corresponding to \( \beta = \frac{p}{x} + q \). So the original equation (35) has the symmetry represented by the vector field

$$X = \left[u\alpha(x) + \frac{p}{x} + 2pD\right] \frac{\partial}{\partial x} + \left[u^2\alpha'(x) - u\frac{p}{x^2} + u\kappa + \delta(x)\right] \frac{\partial}{\partial u}.$$  

(49)

Here \( u, \alpha, \) and \( \delta \) are related to the hypergeometric functions \( _1F_1 \) which are solutions to generalised Kummer type of equations mentioned in section 2. A consequence of this is that the generators do not close under the Lie product. We also note that, if, further, \( D = \frac{1}{2} \) then

$$u = \alpha = e^{\frac{3}{2}x}x^{-\frac{1}{2}}.$$  

(50)

This is to be put in (19) to get the generators. Defining

$$X = 2D \frac{\partial}{\partial x}, \quad Y_{-n} = \frac{1}{x^n} \frac{\partial}{\partial x}, \quad Z_{-n} = \frac{e^x}{x^n} \frac{\partial}{\partial x}$$

(51)

the extended Lie algebra has the commutation relations

$$[Y_{-n}, X] = nY_{-n-1}$$

$$[Z_{-n}, X] = -Z_{-n} + nZ_{-n-1}$$

$$[Y_{-n}, Y_{-m}] = (n - m)Y_{-(n+m+1)}$$

$$[Z_{-m}, Y_{-n}] = (m - n)Z_{-(n+m+1)} - Z_{-(m+n)}$$

$$[Z_{-m}, Z_{-n}] = (m - n)e^xZ_{-(n+m+1)}$$

(52)

We also find that

$$\beta(x) = \frac{g_2}{x^2} + \frac{g_1}{x} + g_0$$

(53)
Group analysis of Schrödinger equation

will satisfy the equation \[ g_0 = -\frac{2\hat{E}}{D} g_1, \quad g_1 = 2Dg_2, \quad C = -2. \] (54)

This would imply

\[ \hat{E} = -\frac{d^2}{4}. \] (55)

This can only be obtained if we again take the negative root of \( \sqrt{1 - 4a} \) and \( n = 2 \). Hence there is again an enhancement of symmetry at another possible eigenvalue and for another value of \( n \). The vector-field for this case is

\[
X = \left[ u\alpha(x) + \left( \frac{1}{4\hat{E}x^2} - \frac{2\hat{E}}{Dx} \right)g_0 \right] \frac{\partial}{\partial x}
+ \left[ u^2\alpha'(x) - u\left\{ \frac{1}{2\hat{E}x^3} + \frac{2\hat{E}}{Dx^2} \right\}g_0 - \kappa \right] \frac{\partial}{\partial u}
\] (56)

and again all Lie products do not close.

Taking

\[ \beta(x) = \frac{g_3}{x^3} + \frac{g_2}{x^2} + \frac{g_1}{x} + g_0 \] (57)

the relation between \( g_i \)'s with \( l = 0, 1, 2, \) and \( 3 \), becomes

\[
g_3 = \frac{3}{2D}g_2, \quad g_2 = \frac{12D}{9\hat{E} + 5D^2}g_1, \quad g_1 = \frac{5}{\frac{32DE}{9E + 5D^2} + 2D}g_0, \quad C = -\frac{15}{4}.
\] (58)

All the previous considerations apply in this case with \( n = 3 \). The vector field can be easily determined.

Hence, in all above cases, we find that the symmetry gets enhanced at particular eigenvalues.

We expect that similar analysis can be performed by including the higher negative powers of \( x \), such as,

\[ \beta(x) = \sum g_n x^{-n}, \quad n = 0, 1, 2, \ldots. \] (59)

as a solution of (46).

In the absence of any potential, equation (55) reduces to

\[ u'' + u = 0 \] (60)

where we have scaled \( u \) so that \( \hat{E} \) becomes equal to unity. For comparison, the vector field in this case is

\[
X = \left[ a_1u\sin(x + a_2) + a_7\sin(2x + a_8) + a_6 \right] \frac{\partial}{\partial x}
+ \left[ a_1u^2\cos(x + a_2) + u\left\{ a_7\sin(2x + a_8) + a_5 \right\} + a_3\sin(x + a_4) \right] \frac{\partial}{\partial u}.
\] (61)

However, the algebra we obtain, (141), looks more interesting.
It is also observed that for a harmonic oscillator potential, the equation corresponding to Eq. (35) does not admit the term containing $\beta$ in the vector field. For the harmonic oscillator,

$$u'' = \omega(x, u, u')$$

with

$$\omega(x, u, u') = (x^2 + \hat{E})u(x)$$

where $\hat{E}$ is proportional to the energy eigenvalue. Using the same notation as in Eq. (38) with the obvious changes, we arrive at the differential equation for $\beta$ as

$$\beta'''(x) - 2(x^2 + \hat{E}\beta' - 2x\beta) = 0$$

which do not have solutions like (47). $\alpha$ obeys the same equation as $u$ does and the vector field is

$$X = u\alpha(x) \frac{\partial}{\partial x} + \left[ u^2 \alpha'(x) + \delta(x) \right] \frac{\partial}{\partial u}.$$ 

with

$$u \propto e^{-\frac{x^2}{2}} H_n(x)$$

where $H_n$ is the Hermite polynomial. $\alpha$ and $\delta$ are constant multiples of $u$.

4. Conclusion

In the present case, a simple group theoretic calculation gives the eigenvalues for the quantum mechanical problem. We also obtain a class of potentials which give rise to similar eigenvalues. In some sense, this is analogous to the Bäcklund transform for continuum states.

Further, the group analysis of the differential equation shows how the symmetries are enhanced at certain values of energy and correspondingly terms get added to the vector field characterising the symmetry. For the lowest values of $n$ we also obtain vector fields that do not close under Lie product. The structure of the extended vector field appear similar to that of the algebras of Kac - Moody - Virasoro type \[10\] which arise in the case of integrable models. In the context of some solvable models, and supersymmetric theories in the presence of magnetic fields, this type of analysis has resulted in Dolan-Grady and related algebras\[11, 12\]. So it would be interesting to look for the unifying feature of all these algebras.

Symmetry generators and the breaking of particular ones play crucial role in phase transitions and setting up of models in particle physics. Though the above analysis is not for spontaneous symmetry breaking, but for the symmetries of the solutions, it is expected that this analysis and also the considerations of the symmetry breaking in going from linear to nonlinear systems\[13\] would be helpful in having a better understanding of spontaneous symmetry breaking.
References

[1] Flügge S 1994 Practical Quantum Mechanics ( Berlin: Springer Verlag )
[2] Maharana K 2003 math-ph/0306069
[3] Olver P J 1993 Application of groups to differential equations ( Berlin: Springer)
    Ovsiannikov L V 1982 Group analysis of differential equations ( Academic: New York)
    Ibragimov N H 1994 (ed.) CRC handbook of Lie group analysis of differential equations (Boca
    Raton: CRC Press)
    Hill J M 1982, Solution of differential equations by means of one parameter groups (Boston:
    Pitman Advanced Publishing Program)
[4] Gaeta G 1994 Nonlinear symmetries and nonlinear equations ( Dodrecht: Kluwer Academic
    Publishers)
[5] Cordero P and Ghirardi G C 1971 Nuovo Cimento 2A 217
[6] Wybourne B G 1974 Classical Groups for Physicists ( New York: John Wiley )
    Bohm A Neeman Y and Barut A O 1988 Dynamical Groups and Spectrum Generating Algebras
    ( Singapore: World Scientific )
[7] Lanik J 1967 Nucl. Phys. B5 263
[8] Stephani H 1989 Differential equations, their solution using symmetries( Cambridge: Cambridge
    University Press )
[9] Maharana K 2001 hep-th/0106198
[10] Goddard P and Olive D 1988 Kac - Moody and Virasoro algebras ( Singapore: World Scientific )
[11] Dolan L and Grady M 1982 Phys. Rev. D 25 1587
[12] Klishchevich S M and Plyushchay M S 2001 Nucl.Phys. B616 403
    2002 Nucl.Phys. B628 217
[13] Maharana K 2000 Phys. Rev. E 62 1683
[14] Dodd R K Eilbeck J C Gibbon J D and Morris H C 1982 Solitons and Nonlinear Wave Equations
    ( London: Academic Press London )