Abstract

We present the analysis of mathematical structure of SU(2) group, specifically the commutation relation between raising and lowering operators of the Morse oscillator. The relationship between the commutator of operators and other parameters of Morse oscillator is investigated. We show that the mathematical structure of operators which depends on the parameters of Morse oscillator may change our conventional expectation. The parameter space of Morse oscillator is visualized to scrutinize the mathematical relations that are related to the Morse oscillator. This parameter space is the space of possible parameter values that depend on the depth of the Morse potential well and other parameters. The algorithm that we present is also applicable to other quantum systems with certain modifications.

Keywords: Morse potential, ladder operators, commutation relation, eigenvalue, parameter space.

1 Introduction

In the early development of quantum mechanics, the exactly solvable potentials attracted researchers’ attention. Different exactly solvable potentials were introduced such as Coulomb, Morse, Rosen-Morse, Pöschl-Teller and Eckart potentials. There are various studies that can be conducted regarding these potentials. For instance, the application of factorization method [1, 2] connected to raising and lowering operator method, supersymmetry and shape invariance [2, 3, 4]. Furthermore, the concept of ladder operators had been further extended to include its associated Lie algebras [5].

The Morse potential is important in the calculations in molecular spectroscopy and diatomic molecule’s modelling. It is often investigated analytically. A unified description of the position-space wave functions, the momentum-space wave functions, and the phase-space Wigner functions for the bound states of a Morse oscillator was presented [6]. The constructions of its ladder operators and its algebraic structure in terms of SU(2) were made in the previous studies [7].

The objective of this study is to analyse the commutation relation between the ladder operators for Morse potential. We show the relationship between the parameters in the ladder operators and commutator of ladder operators for the Morse oscillator. Besides, we also generate the plots of parameter space of Morse oscillator to examine some mathematical relations. This parameter space is the space of possible integer parameter values that depend on the depth of the Morse potential well and other parameters implicitly such as the mass of molecule and the “width” of the potential. This work is organized as follows. In the
following section, we provide the Morse potential and its solutions. We also introduce the lowering and raising operators of Morse oscillator that are constructed directly from its eigen-wave function. In Section 3, we analyse the commutation relation between the ladder operators. We also establish different mathematical forms of an operator deduced from the commutation relation. In Section 4, we present the implementation of an algorithm to investigate the operator that is established through the commutator of ladder operators. We display the plots of the parameter space of Morse potential in Section 5. We later discuss the equality of eigenvalues obtained through two different perspectives. These have not much been discussed in the literature previously. Our analysis expands the understanding of commutation relation for Morse quantum system. In the final section, we present our conclusions.

2 Ladder Operators for Morse Potential

The Morse potential has the following form [8]:

$$V(x) = V_0(e^{-2\beta x} - 2e^{-\beta x}),$$  \(1\)

where \(V_0 > 0\) corresponds to its depth, \(x\) is the relative displacement from the equilibrium position of the atoms and \(\beta\) is related to the “width” of the potential. The associated Schrödinger equation with different mathematical form of Eq. (1) is then given by [6],

$$-\hbar^2 \frac{d^2 \psi}{dx^2} + V_0(1 - e^{-\beta x})^2 \psi = E \psi, \quad (2)$$

where \(m\) is the mass of the molecule. The solutions of Eq. (2) have the form [6]

$$\psi_n^v(y) = N_n^v e^{-\frac{y^2}{2}} L_n^{2s}(y), \quad (3)$$

where \(L_n^{2s}(y)\) are the associated Laguerre functions. There is a coordinate transformation of argument \(x\) in which \(y = ve^{-\beta x}\). The normalization constant \(N_n^v\) is

$$N_n^v = \sqrt{\frac{\beta(v - 2n - 1)\Gamma(n + 1)}{\Gamma(v - n)}}, \quad (4)$$

where the parameters \(v\) and \(s\) are related to the depth of the potential well and energy eigenvalue respectively. The parameters \(v\) and \(s\) are

$$v = \sqrt{\frac{8mV_0}{\beta^2\hbar^2}}, \quad s = \sqrt{\frac{-2mE}{\beta^2\hbar^2}}, \quad (5)$$

with the constraint condition on solutions of Eq. (2) such that

$$2s = v - 2n - 1. \quad (6)$$

The annihilation and creation operators for the Morse wave functions have been established with the relations related to the associated Laguerre polynomials [7]. The annihilation operator for the Morse oscillator has the form

$$\hat{K}_- = -\left[ \frac{d}{dy}(2s + 1) - \frac{1}{y}s(2s + 1) + \frac{v}{2} \right] \sqrt{\frac{s + 1}{s}}, \quad (7)$$

which it obeys the following equation:

$$\hat{K}_- \psi_n^v(y) = k_- \psi_n^{v-1}(y), \quad (8)$$

where

$$k_- = \sqrt{n(v - n)}. \quad (9)$$

The creation operator is defined by
\[
\hat{K} = \left[ \frac{d}{dy} (2s - 1) + \frac{1}{y} s(2s - 1) - \frac{v}{2} \right] \sqrt{\frac{s-1}{s}},
\]

in which it satisfies the equation

\[
\hat{K} \psi_n^v(y) = k_+ \psi_{n+1}^v(y),
\]

where

\[
k_+ = \sqrt{(n+1)(v-n-1)}.
\]

One can construct the commutator \([\hat{K}_+, \hat{K}_-]\) from the relations (8) and (11) that acts on the wave function of Morse oscillator

\[
[\hat{K}_+, \hat{K}_-] \psi_n^v(y) = 2k_0 \psi_n^v(y),
\]

where the eigenvalue is referred to as \(k'_0 = 2k_0\) with

\[
k_0 = n - \frac{v-1}{2}.
\]

Thus, we can define the operator \(\hat{K}_0\) using Eq. (14) as

\[
\hat{K}_0 = \hat{n} - \frac{v-1}{2}.
\]

It can also be rewritten in terms of differential operator with the help of the associated Schrödinger equation

\[
\left( y \frac{d^2}{dy^2} + \frac{d}{dy} - \frac{s^2}{y} - \frac{y}{4} + \frac{v}{2} \right) \psi_n^v(y) = 0,
\]

from which this operator \(\hat{K}_0\) is established as

\[
\hat{K}_0 = \left( y \frac{d^2}{dy^2} + \frac{d}{dy} - \frac{s^2}{y} - \frac{y}{4} + n + \frac{1}{2} \right).
\]

The operators \(\hat{K}_\pm\) and \(\hat{K}_0\) satisfy the following commutation relation

\[
[\hat{K}_+, \hat{K}_-] = 2\hat{K}_0 = \hat{K}'_0.
\]

It is important to point out that the operators \(\hat{K}_\pm\) and \(\hat{K}_0\) are dependent on two parameters, namely any combination of two elements from the set of \(\{s, n, v\}\). Equation (18) has been realized that it satisfies the algebra of SU(2).

### 3 Commutation relation between ladder operators \(\hat{K}_+\) and \(\hat{K}_-\)

There are two perspectives that we can look at from the commutation relation between ladder operators (18). The first perspective is that we consider the eigenstates of the Schrödinger equation that is given by Eq. (3) and the relations (8) and (11) of the ladder operators. This is exactly what Eq. (13) implies. The second perspective is that we consider any arbitrary test function and the differential form of the ladder operators. In the case without the consideration of the changes in parameter involved, we have
\[ \left[ \hat{K}_+, \hat{K}_- \right] f = \left[ \left( \frac{d}{dy} (2s - 1) + \frac{1}{y} s (2s - 1) - \frac{v}{2} \right) \sqrt{\frac{s - 1}{s}}, \right. \]
\[ \left. - \left( \frac{d}{dy} (2s + 1) - \frac{1}{y} s (2s + 1) + \frac{v}{2} \right) \sqrt{\frac{s + 1}{s}} \right] f \]
\[ = 2 \sqrt{1 - \frac{1}{s^2}} s (2s - 1)(2s + 1) \left[ \frac{d}{dy}, \frac{1}{y} \right] f \]
\[ = \frac{2 \sqrt{1 - \frac{1}{s^2}} s (2s - 1)(2s + 1)}{y^2} \cdot f \]
\[ = 2 \left( s^2 - 1 \right)^{\frac{1}{2}} (1 - 4s^2) \cdot f \]
\[ = 2 \hat{K}_0 \cdot f \]
\[ = \hat{K}'_0 \cdot f. \] (19)

We have derived an operator \( \hat{K}'_0 \). There is an additional constraint that should be placed on this derived operator. The constraint that we want to look at is that the derived operator \( \hat{K}'_0 \) satisfies the eigenvalue equation in the form
\[ \hat{K}'_0 \psi_n(y) = k'_0 \psi_n(y). \] (20)

Since this derived operator does not satisfy the eigenvalue equation, we consider another possible condition. In the case with the consideration of the changes in parameter involved, we have
\[ \left[ \hat{K}_+, \hat{K}_- \right] f = \left[ \hat{K}^{n-1,v}_+, \hat{K}^{n,v}_- - \hat{K}^{n+1,v}_- \hat{K}^{n,v}_+ \right] f \]
\[ = \left[ \hat{K}^{s+1,v}_+ \hat{K}^{s,v}_- - \hat{K}^{s-1,v}_- \hat{K}^{s,v}_+ \right] f \]
\[ = s \left( - \frac{8}{y} \frac{d}{dy} \frac{d^2}{dy^2} + \frac{8s^2}{y^2} - \frac{4v}{y} \right) f \]
\[ = \hat{K}'_0 \cdot f. \] (21)

This derived operator from Eqs. (21) is examined through an algorithm by computing its eigenvalues. One should keep in mind that there are three definitions for operator \( \hat{K}'_0 \) or \( \hat{K}_0 \), as shown in Eqs. (15), (17) and (21). Hence, the eigenvalues \( k'_0 \) can be obtained in three different ways. However, the eigenvalues \( k'_0 \) calculated using the definitions in Eqs. (15) and (17) are always equal due to their mathematical constructions.

4 Implementation in Mathematica

The Mathematica code is divided into six different blocks for an implementation of the algorithm to compute and compare the eigenvalues \( k'_0 \) in the two different perspectives. Figure 1 shows the first block of Mathematica code of an algorithm. In the first block, we define the differential operator \( \frac{d}{dy} \) to construct the operators \( \hat{K}_\pm, \hat{K}_0 \) and \( \hat{K}'_0 \) later. Besides, we define the constraint condition, normalization constant and the wave function of Morse potential according to Eqs. (6), (4) and (3) respectively. The value of the parameter \( \beta \) is set to 1, in which its value will not affect the result of our analysis. Lastly, we define some empty sets for graphics later.

After executing the first block, we continue to execute the second and third blocks of the code as shown in figure 2. Second block defines the operators \( \hat{K}_\pm, \hat{K}_0 \) and \( \hat{K}'_0 \) in terms of differential operator. The next block is to determine the parameter values which lead to undefined or zero operators.
Figure 1: The first block of Mathematica code to implement an algorithm to compute and compare the eigenvalues in the two different perspectives.

```
<<Initializations

diff[f_] := D[f];

s[n_, v_] := (- (2 n) + v - 1);

normalizationconst[n_, v_, beta_] := \[\sqrt{\frac{\beta (- (2 n) + v - 1) \text{Gamma}[n + 1]}{\text{Gamma}[v - n]}}\];

f[y_] := \[\frac{\text{normalizationconst}[n, v] y^{(n, v)}}{y^{1/2}}\];

beta = 1;
listtt = {};
listf = {};
listundefined = {};
listzero = {};
listf0ther = {};
listtother = {};
listwithps = {};
listwithins = {};
listst = {};
listsf = {};
listkdagger = {};
listkminus = {};
listk = {};
listk0prime = {};

```

Figure 2: The second and third blocks of Mathematica code to implement an algorithm to compute and compare the eigenvalues in the two different perspectives.

```
<<Define operators

Kdagger[f_, n_, v_, beta_] := \[\frac{s[n, v] - 1}{s[n, v]} \left(\text{diff}[f] \left(2 s[n, v] - 1\right) + \frac{f (2 s[n, v] - 1) s[n, v]}{y} - \frac{f y}{2}\right)\];

Kminus[f_, n_, v_, beta_] := \[\frac{s[n, v] + 1}{s[n, v]} \left(-\left(\text{diff}[f] \left(2 s[n, v] + 1\right) - \frac{f s[n, v] (2 s[n, v] + 1)}{y} + \frac{f y}{2}\right)\right)\];

K0[f_, n_, v_, beta_] := \[\frac{f s[n, v]^2}{y} + y \text{diff}[\text{diff}[f]] + \text{diff}[f] + f n - \frac{f y}{2}\];

K0prime[g_, n_, v_, beta_] := \[\text{Evaluate}[\text{PowerExpand}[\text{Apart}[\text{Kdagger}[\text{Kminus}[g[y], n, v], n - 1, v] - \text{Kminus}[\text{Kdagger}[g[y], n, v], n + 1, v]]]]\];

<<Check operators and know the values of parameters that they are undefined or zero

For[n = 0, n <= 10, n++,
  checkpairkdagger = \{[s[n, v], n, v], Kdagger[\text{testf}[y], n, v]\};
  checkpairkminus = \{[s[n, v], n, v], Kminus[\text{testf}[y], n, v]\};
  checkpairk0 = \{[s[n, v], n, v], K0[\text{testf}[y]]\};
  checkpairk0prime = \{[s[n, v], n, v], K0prime[\text{testf}[y]]\};
  If[Kdagger[\text{testf}[y], n, v] === \text{Indeterminate} || Kdagger[\text{testf}[y], n, v] === \text{ComplexInfinity} || Kdagger[\text{testf}[y], n, v] === \text{\()
    AppendTo[listkdagger, checkpairkdagger];
  If[Kminus[\text{testf}[y], n, v] === \text{Indeterminate} || Kminus[\text{testf}[y], n, v] === \text{ComplexInfinity} || Kminus[\text{testf}[y], n, v] === \text{\()
    AppendTo[listkminus, checkpairkminus];
  If[K0[\text{testf}[y]] === \text{Indeterminate} || K0[\text{testf}[y]] === \text{ComplexInfinity} || K0[\text{testf}[y]] === \text{\()
    AppendTo[listk0, checkpairk0];
  If[K0prime[\text{testf}[y]] === \text{Indeterminate} || K0prime[\text{testf}[y]] === \text{ComplexInfinity} || K0prime[\text{testf}[y]] === \text{\()
    AppendTo[listk0prime, checkpairk0prime];
  Clear[checkpairkdagger, checkpairkminus, checkpairk0, checkpairk0prime];
];

Clear[n, v];
```
Figure 3: The fourth, fifth and sixth blocks of Mathematica code to implement an algorithm to compute and compare the eigenvalues in the two different perspectives.

The fourth block of code defines the functions to calculate the eigenvalues. The first function is constructed with the algebraic manipulation of Eq. (20). The second function in this block evaluates the eigenvalues, \(k'_0\) through the operator \(\hat{K}_0\) as given by Eq. (17). The “PowerExpand”, “Apart” and “FullSimplify” commands simplify the calculation, including the cancellation of normalization constant. The execution of loops takes place in the fifth block of code as depicted in figure 3. The integer parameters \(n\) and \(v\) are set to be in the range from 0 to 100. In the loop body, we define the associated Laguerre polynomial with the Mathematica command “LaguerreL”. We obtain the eigenvalues for each pair of parameters \((n,v)\) and denote them in the Mathematica code by “eigenvalue1”, “eigenvalue2” and “eigenvalue3”. Since the “eigenvalue2” and “eigenvalue3” are always equal, hence the comparison between the “eigenvalue1” and “eigenvalue2” becomes our interest. There are a lot of if statements in the loop for the extractions of values into the sets for the visualization purpose. The sixth block as shown in figure 3 creates our visualization scheme. Two plots on the parameter space of \(n\) and \(v\) of the Morse oscillator will be displayed.

5 Results and Discussion

With the algorithm, we calculate the eigenvalues with different mathematical formulas and then compare them. We want to verify that the derived operator \(\hat{K}'_0\) satisfies the eigenvalue equation (20). The parameter space of \(n\) and \(v\) of the Morse oscillator is plotted to visualise our analysis as shown in figure 3. We check the equality of eigenvalues 10201 times in total for pairs of \((n,v)\). Since we do not determine the mathematical expression of the eigenvalues \(k'_0\) of the derived operator \(\hat{K}'_0\) explicitly, we can only claim that we are highly confident that the derived operator \(\hat{K}'_0\) satisfies the eigenvalue equation (20). Two perspectives on the commutation relation are consistent, because the equality of eigenvalues obtained through two different perspectives seems to hold. However, the conclusion is not definite. There is a caveat which concerns the computation. The derived operator \(\hat{K}'_0\) is zero at parameter \(s\) equals 0, which is ambiguous. Coincidentally, we compute its eigenvalues to be also zero at \(s = 0\), which is a trivial solution.

Figure 4 shows the plot of parameter space of \(n\) and \(v\) with green, and yellow dots. According to the definition of the parameter \(s\) in Eqs. (5), the values of the parameter \(s\) can only take non-negative real
Figure 4: (color online) The parameter space of $n$ and $v$ of the Morse oscillator. Blue dot represents the equality of eigenvalue.

Figure 5: (color online) The parameter space of $n$ and $v$ of the Morse oscillator. Green dot represents the eigenvalue with the parameter $s$ that is greater than or equal to zero while yellow dot represents the eigenvalue with the parameter $s$ that is less than zero.
numbers, $\mathbb{R}_{\geq 0} = \{ x \in \mathbb{R} \mid x \geq 0 \}$. Besides that, the parameter $s$ is further constrained by Eq. (6) which it leads to the inequality $v \geq 2n + 1$. This is clearly indicated in the plot, see figure 5.

6 Conclusions

The present paper provides, for the first time, a detailed analysis on a particular commutation relation of the dynamic group SU(2) for the Morse oscillator. There is no evidence of detailed discussion on a specific commutation relation between the generators of the dynamic group SU(2) for the Morse potential before. The question may be raised regarding the interpretation of commutation relation between operators that depend on some parameters. The consideration for some changes in the parameter of the operators in a commutation relation is needed. We speculate that the derived operator may be related to the adjoint of operator $\hat{K}_0$ in Eq. (17). This may be the reason that this derived operator satisfies the eigenvalue equation (20). An operator can be undefined or zero at some parameter values if it relies on the parameters explicitly. The mathematical structure of the differential form of operators and commutator that depends on parameters may restrict the region in the parameter space. The regions in the parameter space can be bounded by different conditions. For example, the parameter $s$ forms a boundary in the parameter space at zero due to the inequality $s \geq 0$ imposed by its definition. We have paid attention to the interpretation of commutation relation that involves operators with parameters. We choose the Morse oscillator to illustrate our point of view. The algorithm that is written in Mathematica code may also be applied to other quantum systems after some modifications. The modern-day computing power allows us to scrutinize the mathematical relations with the help of computer. We believe that our analysis will provide better understanding of the loophole that may occur in a mathematical relation, for instance, the commutation relation between the ladder operators for the Morse potential.

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