Analysis of Parameter Space of Morse Oscillator

M.Y. Tan\(^{a,b}\), M.S. Nurisya\(^{a,b}\) and H. Zainuddin\(^{a,b}\)

\(^{a}\)Laboratory of Computational Sciences and Mathematical Physics, Institute for Mathematical Research (INSPEM), Universiti Putra Malaysia, 43400 UPM Serdang, Selangor, Malaysia.

\(^{b}\)Department of Physics, Faculty of Science, Universiti Putra Malaysia, 43400 UPM Serdang, Selangor, Malaysia.

Abstract

We present the analysis of the parameter space of the Morse oscillator. By scrutinizing the mathematical relations that are related to Morse oscillator, the parameter space of Morse oscillator is visualized. This parameter space is the space of possible parameter values that are depended on the depth of the Morse’s potential well and other variables. The relationship between an eigenvalue and other parameters of Morse oscillator is investigated. We show the mathematical structures of operators which are dependent on the values of the parameters of Morse oscillator may change our conventional expectations. The algorithm that we present is also applicable for other quantum systems with certain modifications.

**Keywords:** Morse potential, parameter space, eigenvalue, ladder operators.

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 construction of its ladder operators and its algebraic structure in terms of SU(2) was made in the previous studies \([7]\).

The objective of this study is to generate the parameter space for the bound states of Morse oscillator. This parameter space is the space of possible integer parameter values that are depended on the depth of the Morse’s potential well and other variables implicitly such as the mass of molecule and the curve of the Morse’s potential at the energy minimum point. Besides, we show the relationship between parameters in the ladder operators of Morse oscillator and eigenvalue of a particular commutation relation. This work is organized as follows. In the following section, we show the Morse potential and its solution. We also establish the lowering and raising operators of Morse oscillator that are constructed directly from its eigen-wave function. In Section

\(\ast\)gs58392@upm.edu.my

\(\dagger\)risya@upm.edu.my
3. We present the implementation of the algorithm to investigate the parameter space of Morse oscillator. We display the plots of the parameter space of Morse potential. These have not much been discussed in the literature previously. Then, we discuss how the parameters in the ladder operators of Morse oscillator are related to eigenvalue of a particular commutation relation. Our analysis expands the understanding of parameter space of Morse quantum system. In the final section, we present our conclusions.

2 Ladder Operators for Morse Potential

The Morse potential has the following form \[8\]:

\[ V(x) = V_0(e^{-2\beta x} - 2e^{-\beta x}), \]

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 curve of the potential at the energy minimum point. The associated Schrödinger equation with different mathematical form of Eq. (1) is then given by,

\[ -\frac{\hbar^2}{2m} \frac{d^2\psi}{dx^2} + V_0(1 - e^{-\beta x})^2\psi = E\psi. \]

The solution of Eq. (2) have the form \[6\]

\[ \psi_v^m(y) = N_v^m e^{-\frac{y}{2}} y^s L_n^{2s}(y), \]

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 \( N_v^m \) is defined as

\[ N_v^m = \sqrt{\frac{\beta(v - 2n - 1)\Gamma(n + 1)}{\Gamma(v - n)}}, \]

and the parameters \( v \) and \( s \) are related to the depth of the potential well and eigenenergy value respectively. The parameters \( v \) and \( s \) are

\[ v = \sqrt{\frac{8mV_0}{\beta^2\hbar^2}}, \quad s = \sqrt{-\frac{2mE}{\beta^2\hbar^2}}, \]

where \( m \) is the mass of the molecule with the constraint condition of solution of Eq. (2) such that

\[ 2s = v - 2n - 1. \]

The annihilation and creation operators for the Morse wave functions are established with the relations among the associated Laguerre polynomials \[7\]. The annihilation operator for the Morse oscillator has the form

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

which it obeys the following equation:

\[ \hat{K}_-\psi_v^m(y) = k_-\psi_v^{m-1}(y), \]

where

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

The creation operator is defined as

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

in which it satisfies the equation

\[ \hat{K}_+\psi_v^m(y) = k_+\psi_v^{m+1}(y), \]

in which it satisfies the equation
\[
\hat{K}^+ \psi_n^v(y) = k_+ \psi_{n+1}^v(y),
\]
where
\[
k_+ = \sqrt{(n+1)(v-n-1)}.
\]

These ladder operators with the relations (10) and (11) can construct the commutator \( [\hat{K}^+, \hat{K}^-] \) 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 \( \hat{K}_0 \) operator using Eq. (14) as
\[
\hat{K}_0 = \hat{n} - \frac{v - 1}{2}.
\]

It can also be rewritten in terms of differential operators 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 the \( \hat{K}_0 \) operator 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
\[
[\hat{K}^+, \hat{K}^-] = 2\hat{K}_0 = \hat{K}'_0.
\]

The eigenvalue \( k'_0 \) can be obtained in three different ways, since there are a few different mathematical forms of \( \hat{K}_0 \) operator. The first way to calculate \( k'_0 \) is through the Eq. (13). With the algebraic manipulation of Eq. (13), \( k'_0 \) can be easily arranged to one side of equation. Besides, this eigenvalue can be obtained with the relations (14) and (17). The eigenvalue \( k'_0 \) that is calculated with these relations is always equal due to the way of its mathematical construction. However, the equality of \( k'_0 \) does not always hold if we make the comparison with the eigenvalue that is calculated through the Eq. (13).

3 Implementation in Mathematica

The Mathematica code is divided into five different blocks for an implementation of the algorithm to compute the eigenvalue, \( k'_0 \) and study the parameter space of Morse oscillator. Figure 1 shows the first block of Mathematica code of an algorithm. In the first block, we define the differential operator with respect to \( y \) to construct the \( \hat{K}_\pm \) and \( \hat{K}_0 \) operators later. Besides, we define the constraint condition, normalization constant and the wave function of Morse system according to Eqs. (6), (4) and (3) respectively. The value of variable \( \beta \) is set to be equal to 1, in which its value will not affect the results of our analysis. Lastly, we define some empty sets for graphics later on.

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 \( \hat{K}_\pm \) and \( \hat{K}_0 \) operators in terms of differential operators. The next block of code defines the functions to calculate the eigenvalue. The first function is constructed with the algebraic manipulation of commutation relation of Eq. (13). The second function in this block evaluates the eigenvalue, \( k'_0 \) through the operator \( \hat{K}_0 \) as in Eq. (17). The “FullSimplify” command simplifies the calculation with the cancellation of normalization constant.
Figure 1: The first block of Mathematica code to implement the algorithm to study the parameter space of Morse oscillator.

\begin{verbatim}
• Initializations
diff[f_] := D[y, f];
1
s[n_, v_] := \frac{-((2n) + v - 1)}{2};

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

f[y_] := \frac{\sqrt{\beta((-2n) + v - 1) \Gamma(n + 1)}}{\Gamma(v - n)} \cdot e^{y^2};

\beta = 1;
listt = {};
listf = {};
listsubset = {};
linstsubset = {};
lisstwithps = {};
lisstwithns = {};
lisstst = {};
lisstf = {};
lisstwithindeterminate = {};
lisstwithnoindeterminate = {};
lisstfdifferent = {};
lisstindeterminate = {};
lisstdifferent = {};
\end{verbatim}

Figure 2: The second and third blocks of Mathematica code to implement the algorithm to study the parameter space of Morse oscillator.

\begin{verbatim}
• Define operators
Kdagger[f_, n_, v_] := \sqrt{\frac{s(n, v) - 1}{s[n, v]}} \left( \frac{diff[f] (2s[n, v] - 1) s[n, v] f v}{y} - \frac{f v}{2} \right);

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

K0[f_] := \frac{fs[n, v]^2}{y} + y\text{diff}[diff[f]] + \text{diff[f]} + fn - \frac{fy}{4} + \frac{f t}{2};

• Algebraic manipulation and simplification to determine eigenvalue
K0valueRemoveNormalizationconst[n_, v_, y_] :=
Evaluate[FullSimplify[Kdagger[Kminus[f[y], n, v], n - 1, v] - Kminus[Kdagger[f[y], n, v], n + 1, v]]];

k0withoutnormalconstant[n_, v_] := Evaluate[FullSimplify[2 K0[f[y]]/f[y]]];
\end{verbatim}
Figure 3: The fourth and fifth blocks of Mathematica code to implement the algorithm to study the parameter space of Morse oscillator.

The execution of loops takes place in the fourth block of code is depicted in figure 3. The integer parameters \( n \) and \( v \) are set to be in the range from 0 to 100. In the loops body, we define the associated Laguerre polynomial with the Mathematica command “LaguerreL”. We obtained the eigenvalues that are denoted in the Mathematica code by “eigenvalue1”, “eigenvalue2” and “eigenvalue3” with the pairs of parameters \((n, v)\). Since the “eigenvalue2” and “eigenvalue3” are always equal to each other, hence the comparison of 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 fifth block as shown in figure 3 creates our visualization scheme. Three plots on parameter space of \( n \) and \( v \) of Morse oscillator will be displayed.

4 Results and Discussion

With the algorithm, we calculated the eigenvalues that are computed with different mathematical formulas. Since the ways of obtaining the eigenvalues are different, this allows us to make comparison for the eigenvalues. The parameter space of \( n \) and \( v \) for the Morse oscillator is plotted to make some analyses. Figure 4 shows the plot of parameter space of \( n \) and \( v \) with blue and red dots. The “eigenvalue1” is obtained by using Eq. (13). The commutation relation in Eq. (13) can only be satisfied with the wave functions of Morse oscillator which is different from the cases in quantum harmonic oscillator and others that we can use any test function. The operators \( \hat{K}_- \) and \( \hat{K}_+ \) as given in Eq. (7) and Eq. (10) respectively are dependent on the parameters \( s \) and \( v \) which are constrained by condition Eq. (6). These complicated relations may make the eigenvalue, “eigenvalue1” as indeterminate as an output in the Mathematica instead of a numerical value. The indeterminate is output when there are zeros in the numerator and the denominator, \( k_0' = \frac{0}{0} \). There are a few possibilities for this to occur. The most common scenario is that it occurred after the direct substitution of parameters \( n \) and \( v \) into the operators \( \hat{K}_- \) and \( \hat{K}_+ \). The “eigenvalue2” is calculated with the relation in Eq. (14) which it is always a numerical value. The inequality between “eigenvalue1” and “eigenvalue2” happens when the “eigenvalue1” is an indeterminate or a numerical value different from the numerical value of “eigenvalue2”.

Figure 5 shows the plot of parameter space of \( n \) and \( v \) with green and black dots. According to Eq. (5), the value of variable \( s \) can only take non-negative real numbers, \( \mathbb{R}_{\geq 0} = \{ x \in \mathbb{R} \mid x \geq 0 \} \). Besides that, the variable \( s \) is further constrained by the Eq. (6) which it leads to the inequality \( v > 2n + 1 \). This is clearly indicated in the plot, see figure 5.
Figure 4: (color online) The parameter space of $n$ and $v$ for the Morse oscillator. Blue dot represents the equality between “eigenvalue1” and “eigenvalue2”, while red dot represents the inequality between “eigenvalue1” and “eigenvalue2”.

Figure 5: (color online) The parameter space of $n$ and $v$ for the Morse oscillator. Green dot represents the equality between “eigenvalue1” and “eigenvalue2” with the parameter $s$ greater than or equal to zero while black dot represents the equality between “eigenvalue1” and “eigenvalue2” with the parameter $s$ less than zero.
As we discussed before, there are two scenarios where the “eigenvalue1” is different from “eigenvalue2” as shown in figure 6. We realize that when the value of variable $s$ is an element in the set \{0, 1, $-1$\}, the eigenvalue that is calculated through the commutation relation as in Eq. 13, “eigenvalue1” is an indeterminate which is different from “eigenvalue2”. When the value of variable $s$ is an element in the set \{-1/2, 1/2\}, the numerical value of “eigenvalue1” is different from the eigenvalue that is calculated through the relationship in the Eq. [8], i.e. “eigenvalue2”. One of the possible explanations for this realization is that this is due to analysis artifact.

5 Conclusions

The present paper provides, for the first time, the detailed analysis on the parameter space of $n$ and $v$ for the Morse oscillator which the regions in the parameter space are bounded by different conditions. There is no evidence of detailed discussion on the parameter space of the Morse oscillator before. The commutation relation of a quantum system doesn’t always hold for any test function. The test function for the commutation relation of operators has to be chosen carefully, especially when the operators are depended on other parameters. The cancellations of mathematical terms in the commutation relation don’t always occur to give us a desired result. The mathematical structures of the differential forms of operators and commutator of a Morse oscillator restrict the regions in the parameter space. We have paid attention to the problem of the equality of eigenvalues in connection with the parameter space of a Morse oscillator. The algorithm that is written in Mathematica code may also be applied for 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 the mathematical relations.

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