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MORSE POTENTIAL IN NONCOMMUTATIVE QUANTUM MECHANICS FRAMEWORK

A.H. NADHIRA, M.S. NURISYA¹, AND K.T. CHAN

ABSTRACT. Morse potential is one of the well-known exact solvable potentials which attracts many applications in quantum mechanics especially in quantum chemistry. Unlike harmonic potential, Morse potential describes more accurate results on the interaction of diatomic molecules. This work proposes noncommutative quantum mechanics framework of Morse potential in two-dimensional system. A set up of the Morse potential in terms of its Hamiltonian, generalized commutation relations, deformed ladder operators and their associated energy eigenvalues in noncommutative phase space are highlighted. Discussion on the relation to the case of noncommutative harmonic case is also presented.

1. INTRODUCTION

Other than well-known quantum systems like the hydrogen atom and harmonic oscillator, the exactly solvable physical problems are not that numerous. Therefore, harmonic oscillator models are commonly used for describing interaction force of diatomic molecules. Nevertheless, it is known that the actual diatomic molecular behaviour possesses anharmonicity. Thus, many quantum system models describing this extensively have been introduced since, including Morse potential. Notably, Morse potential (oscillator) has been in the spotlight for it is a more

¹corresponding author

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realistic potential to describe diatomic molecular behaviour as opposed to the classic harmonic potential. Like harmonic potential, solutions to Morse potential are exactly solvable (bound states), which describe the vibrational states of molecules with discrete energy. Interestingly, one can also study the unbound states due to the dissociation energy involved. In addition, this model also explains a better analysis in terms of the molecular spectroscopy. Therefore, studies on this type of model may be found valuable in the area of quantum chemistry. The concern is mainly focused on the physical potential behaviour of molecules namely the interaction energy of two atoms.

Algebraic formulation is a very popular method used to determine the solution that is stationary from the Schrödinger equation with Morse potential which mostly deals with one-dimensional case. Using this method, ladder operators are introduced accordingly, to extract both mathematical and physical interpretation of the complete results in terms of the energy spectrum and their associated quantum states. This method is powerful such that it reduces the problems either in 1D or higher dimensions of oscillator in the form of linear algebra for which most properties are well-defined.

In the case of noncommutative quantum mechanics (NCQM), it is safe to say that the idea of having noncommutative (NC) configuration space traces back to the field of NC geometry first established by Connes in the 1990s. Mathematical physicists extend the idea of NCQM particularly to the phenomena involving small particles and thus looking at the quantum theory in noncommutative phase space (NCPS). The formulation of some physical systems in NCQM and their pivotal roles were contributed by [1] and the references therein which emphasise on the harmonic potential. For example, results for the harmonic potential in NCQM in a physical realisation model can be seen in the discussion of Landau level problem [2].

The idea of introducing NC phase space relates closely with the uncertainty principle, which in addition illustrates some physical effects arising from the NC nature of the phase space [3]. Extensively, NC space is a space that accommodates points that are very close to each other and cannot be exactly distinguished. The coordinates do not commute in the same manner as the momentum and the coordinate operators do not commute in ordinary quantum mechanics [4].

The key feature of NCQM usually involves different kinds of the so-called NC transformation [5]. It is possible to represent a quantum system governed by the

Hilbert space of the NCQM in the form of standard quantum mechanics which is portrayed by the well-known canonical commutation relations (CCR) [6]

(1.1)
$$[x_i, x_j] = 0, \quad [p_i, p_j] = 0, \quad [x_i, p_j] = i\hbar\delta_{ij}.$$

In this paper, we deal with coordinate transformation from commutative to NC configuration space such that the CCR in equation (1.1) are deformed to

(1.2)
$$[\hat{x}_i, \hat{x}_j] = \theta_{ij}, \quad [\hat{p}_i, \hat{p}_j] = i\zeta_{ij}, \quad [\hat{x}_i, \hat{p}_j] = i\hbar\delta_{ij}$$

with i, j = 1, 2 suggesting that the dimension is two. θ_{ij} and ζ_{ij} are both antisymmetric tensors that represent the NC parameters which measure the noncommutativity between either position or momentum coordinates. Physical interpretation from equation (1.2) is, one could not measure simultaneously the pair (\hat{x}_i, \hat{x}_j) , (\hat{p}_i, \hat{p}_j) and (\hat{x}_i, \hat{p}_i) in great precision. There is an ample discussion in [7] on quantum mechanics in NC space considering both coordinate and momentum operators. The justification of introducing NC parameters is to express the set of NC operators as a linear combination of the canonical variables [5]. Although from another point of view, the parameters are to indicate the intrinsic property of the phase space, whereby the formulation is justifiable to appraise the noncommutativity of other physical systems. Such formulation is said to give better insight of noninteracting systems, hence, one is expected to express the parameters to be consistent with the approximation [8].

To our knowledge, representation of Morse potential in NCPS has not been discussed and constructed properly. This might be due to the fact that for Morse potential in higher dimension (in NC case, dimension should at least two), solutions can be non-exact. The aim of this paper is thus to show that such a construction can be closely related to the case of the harmonic potential in NCPS.

This paper is organised as follows: in section 2 we review relevant results on exact solution of the time-independent Schrödinger equation with Morse potential that relates to the quantum system with infinite potential, specifically its total energy equation in one dimension which later can be derived to two-dimensional. In section 3, we give a mathematical representation of Morse potential, which includes the commutation relations and their associated ladder operators in the NCPS. In section 4, we present the shifted energy levels of Morse potential in terms of the NC parameter and how this relates very closely to the solution of harmonic potential in NCPS. We end this paper with conclusions in section 5.

2. EIGEN-ENERGY EQUATION OF MORSE POTENTIAL

The one-dimensional Morse potential is given by

 $V_M(x) = V_0(e^{-2\alpha x} - 2e^{-\alpha x}),$

where the space variable x represents the displacement of the two atoms from their equilibrium positions, V_0 is a scaling energy constant representing the depth of the potential well at equilibrium, x = 0 and α is the parameter of the model (related to the characteristics of the well, such as its depth and width) [9]. The eigen-energy equation then takes the form

(2.1)
$$H_M \psi(x) = \left(\frac{\hat{p}^2}{2\mu} + V_M(x)\right) \psi(x) = E \psi(x),$$

such that μ is reduced mass of the oscillating system composed of two atoms of masses m_1 and m_1 , \hat{p} is the differential form of momentum operator namely $\hat{p} = -i\hbar \frac{d}{dx}$. If taking a change of variable such that $y(x) = \nu e^{-\alpha x}$ [10] where

(2.2)
$$\nu = \sqrt{\frac{8\mu V_0}{\alpha^2 \hbar^2}}, \qquad s = \sqrt{\frac{-2\mu E}{\alpha^2 \hbar^2}},$$

one can rewrite the equation (2.1) from the time-independent Schrödinger equation (SE) in terms of variable y parameterised by ν and s respectively [10]:

(2.3)
$$\left[\frac{d^2}{dy^2} + \frac{1}{y}\frac{d}{dy} + \left(\frac{\nu}{2y} - \frac{s^2}{y^2} - \frac{1}{4}\right)\right]\psi(y) = 0.$$

Equation (2.3) is a second order differential equation with solutions such that $\psi(y)$ is represented by the associated Laguerre polynomials. Next, it is easy to see that the equation (2.1) of Morse potential in 2D takes the form [9]

$$H_M(x_i) = \frac{\hat{p_i}^2}{2\mu} + V_0(e^{-2\alpha x_i} - 2e^{-\alpha x_i}),$$

for i = 1, 2. It is necessary to check the commutation relation between the position and the momentum that is given by

$$[y(x), p_x] = -i\hbar\alpha e^{\alpha x}.$$

This is important since in the later part, we will need to check this condition once we proceed with the algebraic method to solve the SE. To note, equation (2.4) is analogous to CCR in equation (1.1).

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3. Morse potential in noncommutative quantum mechanics

In the case of Morse potential in NC configuration space, checking the commutator of two coordinates gives

(3.1)
$$[\hat{y}_1, \hat{y}_2] = [\nu e^{-\alpha \hat{x}_1}, \nu e^{-\alpha \hat{x}_2}] = \frac{\nu^2}{2i} e^{-\alpha (\hat{x}_1 + \hat{x}_2)} \sin\left(\frac{\alpha^2 \theta}{2}\right)$$

Equation (3.1) is obtained by using Baker-Campbell-Housdorff (BCH) formula (exponential product of operator X, Y, Z), such that

$$e^{X}e^{Y} = e^{Z} = -\alpha X - \alpha Y + \frac{1}{2}\alpha^{2}[X, Y],$$

which also includes commutators of equation (1.2). We denote \hat{y}_i with a "hat" to distinguish the NC coordinates from the commutative ones. It is easy to see that for the case of standard Morse potential, commutator (3.1) is equal to zero. Relation (3.1) however gives no physical insight of having noncommutativity of positions between two molecules. Therefore at this point, we seek the advantage of the property of harmonic limit of Morse potential. According to [10], by approximating ν which later influences the potential V from equation (2.2), one obtains the ladder operators:

$$\lim_{\nu \to \infty} b^{\dagger} = \frac{\alpha \sqrt{\nu}}{2} x - \frac{1}{\alpha \sqrt{\nu}} \frac{d}{dy} = \sqrt{\frac{m\omega}{2\hbar}} x - \sqrt{\frac{\hbar}{2m\omega}} \frac{d}{dx} = a^{\dagger},$$
$$\lim_{\nu \to \infty} b = \frac{\alpha \sqrt{\nu}}{2} x + \frac{1}{\alpha \sqrt{\nu}} \frac{d}{dy} = \sqrt{\frac{m\omega}{2\hbar}} x + \sqrt{\frac{\hbar}{2m\omega}} \frac{d}{dx} = a.$$

 a, a^{\dagger} are the ladder operators for harmonic potentials with their commutators $[a_i^{\dagger}, a_j] = \delta_{ij}$, and $[b_i^{\dagger}, b_j] = \delta_{ij}$ with i, j = 1, 2 corresponding to the two dimensional case. Since this is true, we are able to treat the Morse potential in NCQM as a similar problem to the case of Landau problem of an electron in a constant magnetic field.

We then introduce deformed operators for two-dimensional Morse potential such that

(3.2)
$$Q_1 = \frac{\alpha\sqrt{\nu}}{2}x - \frac{\theta}{\alpha\sqrt{\nu}}p_y; \quad Q_2 = \frac{\alpha\sqrt{\nu}}{2}y + \frac{\theta}{\alpha\sqrt{\nu}}p_x; \quad P_1 = p_x; \quad P_2 = p_y,$$

and check their commutation relations for which we obtain

(3.3)
$$[Q_i, P_j] = i \frac{\alpha \sqrt{\nu}}{2} \delta_{ij}; \qquad [Q_i, Q_j] = i \theta_{ij}$$

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The first equation above is closely related to the commutator that we found in equation (2.4), where the second commutator reveals the property of noncommutativity in position coordinates. The deformed coordinates (3.2) in this case represent the Morse potential in NC space since the momentum coordinates commute with each other. In another way, $[Q_i, P_j]$ in equation (3.3) signifies the CCR. Such coordinate transform is called Bopp's shift [5]. Having this form of coordinates, it is deduced to the case of Landau level problem which also involves the interaction force between two molecules and therefore one seeks particularly on the vibration energy spectrum. We have thus the following Landau Hamiltonian on Morse potential in NC space, H_M^{ncs} (in some conveniently chosen units) [2]

(3.4)
$$H_M^{ncs} = \frac{1}{2} \left(P_1 + \frac{Q_2}{2} \right)^2 + \frac{1}{2} \left(P_2 + \frac{Q_1}{2} \right)^2.$$

Substituting equation (3.2) into equation (3.4), one arrives at

(3.5)
$$H_M^{ncs} = \frac{1}{2} \left[\left(1 + \frac{\theta}{\alpha\sqrt{\nu}} \right) p_x + \frac{\alpha\sqrt{\nu}}{4} y \right]^2 + \frac{1}{2} \left[\left(1 + \frac{\theta}{\alpha\sqrt{\nu}} \right) p_y - \frac{\alpha\sqrt{\nu}}{4} x \right]^2 \right]^2$$

We further simplify by letting $\gamma = \left(1 + \frac{\theta}{\alpha\sqrt{\nu}}\right)$ and introduce the following operators

$$\hat{Q}_1 = \sqrt{\gamma}p_x + \frac{1}{\sqrt{\gamma}}\frac{\alpha\sqrt{\nu}}{4}y; \qquad \hat{P}_1 = \sqrt{\gamma}p_y - \frac{1}{\sqrt{\gamma}}\frac{\alpha\sqrt{\nu}}{4}x,$$

and note that $[Q_1, P_1] = i \frac{\alpha \sqrt{\nu}}{2}$ which satisfies equation (3.3). Finally one can rewrite equation (3.5) such that

(3.6)
$$H_M^{ncps} = \frac{1}{2}\gamma \Big[\Big(1 + \frac{\theta}{\alpha\sqrt{\nu}} \Big) p_x + \frac{\alpha\sqrt{\nu}}{4} y \Big]^2 + \frac{1}{2} \Big[\Big(1 + \frac{\theta}{\alpha\sqrt{\nu}} \Big) p_y - \frac{\alpha\sqrt{\nu}}{4} x \Big]^2,$$

which denotes the Hamiltonian form of the Morse potential in NCPS denoted by H_M^{ncps} . This final form is simply a *generalised* Hamiltonian for Morse potential in harmonic limit.

4. Shifted energy levels for Morse potential in NCPS

From equation (3.6) we may also obtain the following

(4.1)
$$H_M^{ncps} = \frac{1}{2} \left(1 + \frac{\theta}{\alpha \sqrt{\nu}} \right) \left(\hat{P}_1^2 + \hat{Q}_1^2 \right),$$

where we denote this as the Morse potential in NCPS, for which both position and momentum operators are noncommute. Since equation (4.1) is Hamiltonian of harmonic potential with additional factor, we can see the effect of the noncommutativity is to shift all energy levels of the Morse potential by the amount

$$\Delta E = \frac{\theta}{2\alpha\sqrt{\nu}}$$

5. CONCLUSION

In this work, we propose a framework to solve time-independent Schrödinger equation with Morse potential in NCQM model. We construct deformed operators of Morse taking the harmonic limit property. We then show that the shifted energy levels for Morse potential take a value of $\frac{\theta}{2\alpha\sqrt{\nu}}$ for which we consider both position and momentum coordinates being noncommute.

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LABORATORY OF COMPUTATIONAL SCIENCES AND MATHEMATICAL PHYSICS, INSPEM UNIVERSITI PUTRA MALAYSIA, 43300 SERDANG, SELANGOR, MALAYSIA. *Email address*: nharis27@gmail.com

LABORATORY OF COMPUTATIONAL SCIENCES AND MATHEMATICAL PHYSICS, INSPEM & DEPARTMENT OF PHYSICS, FACULTY OF SCIENCE, UNIVERSITI PUTRA MALAYSIA 43300 SERDANG, SELANGOR, MALAYSIA. *Email address*: risya@upm.edu.my

LABORATORY OF COMPUTATIONAL SCIENCES AND MATHEMATICAL PHYSICS, INSPEM & DEPARTMENT OF PHYSICS, FACULTY OF SCIENCE, UNIVERSITI PUTRA MALAYSIA 43300 SERDANG, SELANGOR, MALAYSIA. *Email address*: chankt@upm.edu.my