# QUANTUM ANHARMONIC POTENTIALS WITH OPERATOR AND FACTORIZATION METHODS

By

**TAN MIN YANG**

**Thesis Submitted to the School of Graduate Studies, Universiti Putra Malaysia,**
**in Fulfilment of the Requirements for the Degree of Master of Science**

**March 2023**

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# DEDICATIONS

*I dedicate my thesis work to my family and friends. A special feeling of gratitude to my parents, who always trust their little son's decision.*

*I also dedicate this thesis to my supervisor, Dr. Nurisya Mohd Shah, who have supported me throughout the process.*

*And also I would like to give special thanks to QuEST group members, who always share their knowledge with me.*

Abstract of thesis presented to the Senate of Universiti Putra Malaysia in fulfilment
of the requirement for the degree of Master of Science

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**Chair : Nurisya Mohd Shah, PhD**
**Faculty : Science**

Anharmonic potential is one of the main focuses of this research. This research is also carried out to deepen our understanding of the mathematical tools in non-relativistic quantum mechanics. Specifically, the mathematical tools, namely factorization method and supersymmetry are interesting. Factorization method is effective in determining the energy spectra of one-dimensional exactly solvable potentials. On the other hand, given any potential, supersymmetry allows us to build a partner potential with an identical energy spectrum except for the ground state. This research can be divided into two distinct parts.

In the first part of this research, the mathematical structure of SU(2) group, that is, the commutation relation of ladder operators of the Morse oscillator, which is anharmonic, is examined. The concept of ladder operator often appears in the context of factorization method. It is realized that the mathematical structure of the ladder operators of the Morse oscillator depends on some Morse oscillator's parameters. The commutation relation is analysed analytically by considering the effect of parameters on the operators. The parameter space of Morse oscillator is visualised to scrutinise the mathematical relations that are related to Morse oscillator. This parameter space is the space of all possible parameter values depending on the depth of Morse potential well and other molecular constants. The equality of eigenvalues calculated in two different perspectives is investigated. It is possible for the algorithm in this work to be also applicable to other one-dimensional quantum systems with certain modifications.

The second part of this research is more focusing on the connection between deductive method and supersymmetric quantum mechanics. The traditional factorization method and supersymmetric quantum mechanics are immensely explored in the literature. However, the so-called deductive method proposed by Green in 1965 is less being considered by researchers. This deductive method can be reinterpreted as a different formulation of factorization method. It is shown to be related to the supersymmetric quantum mechanics. An alternative way to obtain the superpotential in terms of supersymmetric quantum mechanics is deduced. Finally, our reasoning is successfully demonstrated with two anharmonic systems, namely Deng-Fan and generalized Mobius square potentials.

Abstrak tesis yang dikemukakan kepada Senat Universiti Putra Malaysia sebagai memenuhi keperluan untuk ijazah Master Sains

# KEUPAYAAN ANHARMONIK KUANTUM DENGAN KAEDAH PENGOPERASI DAN PEMFAKTORAN

Oleh

**TAN MIN YANG**

**Mac 2023**

**Pengerusi : Nurisya Mohd Shah, PhD**
**Fakulti : Sains**

Keupayaan anharmonik adalah salah satu fokus utama penyelidikan ini. Penyelidikan ini juga dijalankan untuk memperdalamkan pemahaman kita mengenai alat matematik dalam mekanik kuantum bukan relativistik. Khususnya, alat matematik, iaitu kaedah pemfaktoran dan supersimetri menarik. Kaedah pemfaktoran adalah berkesan dalam menentukan spektrum tenaga keupayaan satu dimensi yang boleh diselesaikan dengan tepat. Selain daripada itu, sebarang keupayaan, supersimetri membolehkan kita membina pasangan keupayaan dengan spektrum tenaga yang sama kecuali pada keadaan dasar. Penyelidikan ini boleh dibahagikan kepada dua bahagian yang berbeza.

Dalam bahagian pertama penyelidikan ini, struktur matematik kumpulan SU(2), iaitu hubungan kanonik bertukar-tertib antara pengoperasi tangga pengayun Morse yang anharmonik diperiksa. Konsep pengoperasi tangga ini sering muncul dalam konteks kaedah pemfaktoran. Adalah disedari bahawa struktur matematik pengoperasi tangga pengayun Morse bergantung pada beberapa parameter pengayun. Hubungan kanonik bertukar-tertib dianalisis secara analitikal dengan mempertimbangkan kesan parameter pada pengoperasi. Ruang parameter pengayun Morse digambarkan untuk meneliti hubungan matematik yang berkaitan dengan pengayun Morse. Ruang parameter ini ialah ruang bagi semua nilai parameter yang mungkin bergantung pada kedalaman perigi keupayaan Morse dan pemalar molekul lain. Kesamaan nilai eigen yang dikira dalam dua perspektif berbeza disiasat. Adalah mungkin untuk algoritma dalam kerja ini juga boleh digunakan untuk sistem kuantum satu dimensi lain dengan pengubahsuaian tertentu.

Bahagian kedua penyelidikan ini lebih memberi tumpuan kepada hubungan antara kaedah deduktif dan mekanik kuantum supersimetri. Kaedah pemfaktoran tradisional dan mekanik kuantum supersimetri banyak diterokai dalam penerbitan ilmiah. Walau bagaimanapun, kaedah deduktif yang dicadangkan oleh Green pada tahun 1965 kurang dipertimbangkan oleh penyelidik. Kaedah deduktif ini boleh ditafsirkan semula sebagai formulasi kaedah pemfaktoran yang berbeza. Ia terbukti berkaitan dengan mekanik kuantum supersimetri. Satu cara alternatif untuk mendapatkan keupayaan super dari segi mekanik kuantum supersimetri disimpulkan. Akhirnya, penaakulan kami berjaya ditunjukkan dengan dua sistem anharmonik, iaitu keupayaan Deng-Fan dan keupayaan segi empat Mobius teritlak.

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This thesis was submitted to the Senate of Universiti Putra Malaysia and has been accepted as fulfilment of the requirement for the degree of Master of Science. The members of the Supervisory Committee were as follows:

**Nurisya Mohd Shah, PhD**
Senior Lecturer
Faculty of Science & Institute for Mathematical Research
Universiti Putra Malaysia
(Chairman)

**Hishamuddin Zainuddin, PhD**
Associate Professor
Faculty of Science & Institute for Mathematical Research
Universiti Putra Malaysia
(Member)

**ZALILAH MOHD SHARIFF, PhD**
Professor and Dean
School of Graduate Studies
Universiti Putra Malaysia

Date: 08 June 2023

**Declaration by the graduate student**

I hereby confirm that:

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This is to confirm that:

- the research conducted and the writing of this thesis was under our supervision;
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Signature: ______________________________
Name of
Chairman of
Supervisory
Committee: Nurisya Mohd Shah, PhD

Signature: ______________________________
Name of
Member of
Supervisory
Committee: Hishamuddin Zainuddin, PhD

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| | |
|---|---|
| GMP | Generalized Morse Potential |
| GMS | Generalized Mobius Square |
| H-SUSY QM | Higher-Order Supersymmetric Quantum Mechanics |
| ML | Mathews-Lakshmanan |
| PDM | Position-Dependent Mass |
| PDMSE | Position-Dependent Mass Schrödinger Equation |
| QM | Quantum Mechanics |
| RKR | Rydberg-Klein-Rees |
| SUSY | Supersymmetry |
| SUSY QM | Supersymmetric Quantum Mechanics |
| SIP | Shape-Invariant Potential |

# CHAPTER 1

# INTRODUCTION

Quantum mechanics (QM) is one of the most significant physical theories that was developed in the 20th century. It allows us to describe the physical properties of nature at the scale of subatomic particles and atoms. This fundamental theory has been verified by experiments again and again. The development of quantum mechanics drives the discoveries of other physical theories, including quantum field theory (QFT). In the latter half of the 20th century, Standard Model of particle physics in the context of quantum field theory was developed through the efforts of many scientists throughout the world. The Standard Model has become the most successful scientific theory at describing many aspects of nature that we can observe in particle physics experiments.

The concept of operator is essential in the mathematical formulation of QM. Any observable that can be measured in an experiment should be connected with a self-adjoint operator. This operator must produce real eigenvalues because it represents the values of experimental measurement outcomes. The common operators are the position and momentum operators. For a pair of operators $\hat{A}$ and $\hat{B}$, there is a meaningful quantity called commutator, also known as commutation relation. It is given by

$$\left[\hat{A},\hat{B}\right] = \hat{A}\hat{B} - \hat{B}\hat{A}. \tag{1.0.1}$$

In matrix mechanics, the mathematical formulation of QM, any pair of non-commuting self-adjoint operators are subject to an uncertainty limit, which is the fundamental limit to the accuracy of the values for certain pairs of observables of a particle, like momentum, $p$, and position, $x$, can be determined from initial conditions. This can be understood in terms of the common general form of an uncertainty principle called the Robertson uncertainty relation, which is defined by

$$\sigma_{\hat{A}}\sigma_{\hat{B}} \geq \frac{1}{2}\left|\left\langle\left[\hat{A},\hat{B}\right]\right\rangle\right|. \tag{1.0.2}$$

In quantum mechanics, we can model a physical system with a chosen quantum potential. This quantum potential is a term that describes the interaction in a quantum mechanical physical system. There are various types of potentials, such as the harmonic oscillator, Coulomb and anharmonic potentials. The anharmonic oscillator potentials (Kazakov, 2012) can be approximated to a harmonic oscillator potential.

They can represent the potential energy of a diatomic molecule as a function of atomic spacing in quantum chemistry.

In order to obtain the wave functions and energy eigenvalues of a Schrödinger equation that describe the quantum system, different methods have been proposed. The time-independent Schrödinger equation is an instance of an eigenvalue equation. The most common method to solve it is the method of factorization. In the context of factorization method, we can construct the ladder operators, which are the powerful tools in raising or lowering the state of a quantum system. These operators can be considered as the generators of a Lie algebra or a Lie group. Although the method of factorization sounds simple and effective, we should notice that there are different mathematical formulations of this method. For example, the so-called deductive method was proposed by Green in 1965, which we named it Green factorization method.

There are other derived or related mathematical tools that have been proposed with the development of the traditional factorization method. One of them is supersymmetric quantum mechanics (SUSY QM). It is a useful tool for producing new potentials with known energy spectra departing from an initial exact solvable one. Few examples are the harmonic oscillator, Morse, Coulomb and Pöschl-Teller potentials (Dutt et al., 1988). With the help of the concept of shape invariance introduced by Gendenshteïn (1983) and supersymmetry (SUSY), the operator method can be generalized. This setup allows us to determine the eigenfunctions and energy eigenvalues of all known exactly solvable potentials in an elegant way.

## 1.1 Problem Statement

Factorization method is widely used in quantum mechanics. It is often introduced in terms of operators. One can easily construct a commutation relation between operators. However, the interpretation of this commutation relation may be unclear especially when the operators depend on some parameters. Therefore, we are motivated to analyse the mathematical structure in terms of operators, specifically the commutation relation between the ladder operators for the Morse potential.

Secondly, we look at the mathematical tools, i.e., Green factorization method and supersymmetric quantum mechanics. In the literature, there is no well-established connection between Green factorization method and supersymmetric quantum mechanics. We are interested in their connection that seems to be crucial. This may offer an alternative perspective on the superpotential in terms of the supersymmetric quantum mechanics.

Since there is no well-established connection between the Green factorization method and the supersymmetric quantum mechanics, we want to show their connection with some specific examples of anharmonic oscillators. The Green factorization method for solving the anharmonic oscillators is less considered in the literature. Researchers seem to have overlooked this method, which is elegant and simple.

## 1.2 Research Objectives

The direction of this thesis pivots on a few main objectives that aim to be achieved by the end of this research. The research objectives are as follows:

1. To analyse the mathematical structure of dynamic group for Morse potential that realises in the operator language formalism
2. To establish a connection between the Green factorization method and the supersymmetric quantum mechanics in terms of operators
3. To demonstrate the connection between the Green factorization method and the supersymmetric quantum mechanics with Deng-Fan and generalized Mobius square potentials

## 1.3 Research Scope

In this research, the mathematical tools used in non-relativistic quantum mechanics, namely the factorization method and supersymmetric quantum mechanics, are investigated by looking at their mathematical objects. Such mathematical objects are operators and commutation relation between two operators. The analysis of the commutation relation between operators that depend on parameters is one of the highlights to be expected in this research. For that purpose, the mathematical software used is Wolfram Mathematica 11.3. This research mainly focuses on the anharmonic quantum potentials, such as Morse, Deng-Fan and generalized Mobius square potentials.

## 1.4 Research Methodology

Most of the calculations used in this research involve the concepts of linear algebra. These include solving eigenvalue equation.

In the first part of this work, the Morse oscillator was considered. We looked at two perspectives on the commutation relation between the ladder operators for Morse oscillator. This commutation relation was examined under two different conditions. The changes in the parameter were not taken into consideration in the first condition. On the other hand, the changes in the parameter were taken into consideration in the second condition. Consequently, the operators were derived from both conditions. The validity of these derived operators was checked by taking a look at their eigenvalues. Most of the computations for this analysis were performed by the Mathematica. The results of calculations were visualised using some plots of parameter space. The first part of this research was discussed in detail in Chapter 3.

In the second part of this work, a connection between the Green factorization method and supersymmetric quantum mechanics was worked out with some relations. In order to illustrate our argument, two tables with some known exactly solvable potentials were drawn. In the first table, shifted oscillator, Coulomb, Scarf, and Morse potentials were included. On the other hand, harmonic oscillator, Morse oscillator, atom of hydrogen type, and Pöschl-Teller potentials were contained in the second table. A connection between the Green factorization method and supersymmetric quantum mechanics could be realised, although this connection is not obvious at first glance. This connection was exemplified by the anharmonic potentials, such as Deng-Fan, and generalized Mobius square potentials. The second part of this research was discussed in detail in Chapter 4.

## 1.5 Thesis Organisation

This thesis follows certain order of research where it is divided into two distinct divisions. First, we deepen our understanding of commutation relation between operators that depend on some parameters. Second, we find the connection between two mathematical tools, namely the Green factorization method and the supersymmetric quantum mechanics.

This thesis is structured into five chapters. In Chapter 1, we prepare an introductory write-up on the contents of this research as a whole.

In Chapter 2, we review the literature related to our studies. The summary of the relevant publications on anharmonic potentials, including Morse, Deng-Fan, four-parameter and generalized Mobius square potentials is provided. Besides, we synthesize, and summarize the arguments and ideas of some mathematical tools, such as the factorization method and supersymmetry.

Then, in Chapter 3, a discussion on the first part of this research is made. We introduce the ladder operators for the Morse potential. We analyse the commutation relation between the ladder operators. The results of our computations are visualised using the plots of parameter space of Morse oscillator.

Next, the topics of the Green factorization method and supersymmetric quantum mechanics are focused in Chapter 4. We begin with a proper introduction of Green factorization method and supersymmetric quantum mechanics for the second part of our research. Then we work out the connection between the Green factorization method and supersymmetric quantum mechanics. We illustrate our point of view with some examples of anharmonic potentials, that is, Deng-Fan and generalized Mobius square potentials.

In the final chapter, we conclude this research in two parts. The future works and projects are also recommended in this chapter.

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