Shi-Hai Dong

Factorization Method in Quantum Mechanics

Dong

This work introduces the factorization method in quantum mechanics at an advanced level with an aim to put mathematical and physical concepts and techniques like the factorization method, Lie algebras, matrix elements and quantum control at the reader's disposal. For this purpose a comprehensive description is provided of the factorization method and its wide applications in quantum mechanics which complements the traditional coverage found in the existing quantum mechanics textbooks. Related to this classic method are the supersymmetric quantum mechanics, shape invariant potentials and group theoretical approaches. It is no exaggeration to say that this method has become the milestone of these approaches. In fact the author's driving force has been his desire to provide a comprehensive review volume that includes some new and significant results about the factorization method in quantum mechanics since the literature is inundated with scattered articles in this field, and to pave the reader's way into territory as rapidly as possible. The results clear and understandable discussions with the necessary mathematical steps included so that the intelligent reader should be able to follow the text with relative ease, in particular when mathematically difficult material is presented.

Audience:
Researchers and students of physics, mathematics, chemistry and electrical engineering.

Springer

Factorization Method in Quantum Mechanics

Fundamental Theories of Physics

An International Book Series on The Fundamental Theories of Physics:
Their Clarification, Development and Application

Volume 150

Factorization Method in Quantum Mechanics

by

Shi-Hai Dong

Instituto Politécnico Nacional,
Escuela Superior de Física y Matemáticas, México

This book is dedicated to my wife Guo-Hua Sun, my lovely children Bo Dong and Jazmin Yue Dong Sun.

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Preface

This work introduces the factorization method in quantum mechanics at an advanced level addressing students of physics, mathematics, chemistry and electrical engineering. The aim is to put the mathematical and physical concepts and techniques like the factorization method, Lie algebras, matrix elements and quantum control at the reader's disposal. For this purpose, we attempt to provide a comprehensive description of the factorization method and its wide applications in quantum mechanics which complements the traditional coverage found in the existing quantum mechanics textbooks. Related to this classic method are the supersymmetric quantum mechanics, shape invariant potentials and group theoretical approaches. It is no exaggeration to say that this method has become the milestone of these approaches. In fact, the author's driving force has been his desire to provide a comprehensive review volume that includes some new and significant results about the factorization method in quantum mechanics since the literature is inundated with scattered articles in this field and to pave the reader's way into this territory as rapidly as possible. We have made the effort to present the clear and understandable derivations and include the necessary mathematical steps so that the intelligent and diligent reader should be able to follow the text with relative ease, in particular, when mathematically difficult material is presented. The author also embraces enthusiastically the potential of the LaTeX typesetting language to enrich the presentation of the formulas as to make the logical pattern behind the mathematics more transparent. Additionally, any suggestions and criticism to improve the text are most welcome since this is the first version. It should be addressed that the main effort to follow the text and master the material is left to the reader even though this book makes an effort to serve the reader as much as was possible for the author.

This book starts out in Chapter 1 with a comprehensive review for the traditional factorization method and builds on this to introduce in Chapter 2 a new approach to this method and to review in Chapter 3 the basic properties of the Lie

algebras su(2) and su(1, 1) to be used in the successive Chapters. As important applications in non-relativistic quantum mechanics, from Chapter 4 to Chapter 13, we shall apply our new approach to the factorization method to study some important quantum systems such as the harmonic oscillator, infinitely deep square well, Morse, Pöschl-Teller, pseudoharmonic oscillator, noncentral ring-shaped potential quantum systems and others. One of the advantages of this new approach is to easily obtain the matrix elements for some related physical functions except for constructing a suitable Lie algebra from the ladder operators. In Chapter 14 we are going to study the position-dependent mass Schrödinger equation for a singular oscillator based on the algebraic approach. We shall carry out the applications of the factorization method in relativistic Dirac and Klein-Gordon equations with the Coulomb and hyperbolic potentials from Chapter 15 to Chapter 18. As an important generalized application of this method related to the group theory in control theory, we shall study the quantum control in Chapters 19 and 20, in which we briefly introduce the development of the quantum control and some well known theorems on control theory and then apply the knowledge of the Lie algebra generated by the system's quantum Hamiltonian to investigate the controllabilities of the quantum systems for the Morse, Pöschl-Teller (PT) and PT-like potentials. Some conclusions and outlooks are given in Chapter 21.

This book is in a stage of continuing development, various chapters, e.g., on the group theory, on the supersymmetric quantum mechanics, on the shape invariance, on the higher order factorization method will be added to the extent that the respective topics expand. At the present stage, however, the work presented for such topics should be complete enough to serve the reader.

This book shall give the theoretical physicists and chemists a fresh outlook and new ways of handling the important quantum systems for some potentials of interest in all branches of physics and chemistry and of studying quantum control. The primary audience of this book shall be the graduate students and young researchers in physics, theoretical chemistry and electric engineering.

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SHI-HAI DONG

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Acknowledgments

First, I would like to thank Prof. Zhong-Qi Ma for encouragement and continuous support in preparing this work. Prof. Ma was always there to give me some positive and helpful suggestions. I am also very grateful to Prof. Lozada-Cassou for hospitality given to me at the Instituto Mexicano del Petróleo, where some of works were carried out.

Second, I shall give special thanks to Profs. Ley-Koo, Cruz and García-Ravelo, who have offered me unselfish help both in my job and in life. In particular, I would like to thank Prof. Ley-Koo for reading the manuscript of this book carefully and for many positive and invaluable suggestions. The mild and bracing climate in Mexico city has kept me in a good spirit.

Third, I am very indebted to my collaborators Drs. Lemus, Frank, Tang, Lara-Rosano, Peña, Profs. Popov, Chen, Qiang, Ms. Guo-Hua Sun and others. Also, I really appreciate the support from Dr. Mares and Maestro Escamilla, who are the successive Directors of the Escuela Superior de Física y Matemáticas, Instituto Politécnico Nacional. In particular, this work was supported in part by project 20062088-SIP-IPN in the course of this book.

Fourth, I thank my previous advisor Prof. Feng Pan for getting me interested in group theory and Lie algebras.

Last, but not least, I would like to thank my family: my wife, Guo-Hua Sun, for giving me continuous encouragement and for devoting herself to the whole family; my lovely son and daughter, Bo Dong and Jazmin Yue Dong Sun for giving me encouragement; my parents, Ji-Tang Dong and Gui-Rong Wang, for giving me life, for unconditional support and encouragement to pursue my interests, even when the interests went beyond boundaries of language and geography; my older brother and sister Shi-Shan Dong and Xiu-Fen Dong for looking after our parents meticulously in China.

PART I

INTRODUCTION

Chapter 1

INTRODUCTION

1. Basic review

The factorization method is a kind of basic technique that reduces the dynamic equation of a given system into a simple one that is easier to handle. Its underlying idea is to consider a pair of first order differential equations which can be obtained from a given second-order differential equation with boundary conditions. The factorization method is an operational procedure that enables us to answer questions about the given quantum system eigenvalue problems which are of importance for physicists. Generally speaking, we are able to apply this method to treat the most important eigenvalue problems in quantum mechanics. For example, the solutions can be obtained immediately once the second-order differential equations are factorized by means of the linear ladder operators. The complete set of normalized eigenfunctions can be generated by the successive action of the ladder operators on the key eigenfunctions, which are the exact solutions of the first order differential equation.

The interest and advantage of the factorization method can be summarized as follows. First, this method applies only to the discrete energy spectra since the continuous energy levels are countless. Second, the main advantage of this method is that we can write down immediately the desired eigenvalues and the normalized eigenfunctions from the given Hamiltonian and we need not use the traditional quantum mechanical treatment methods such as the power series method or by solving the second-order differential equations to obtain the exact solutions of the studied quantum system. Third, it is possible to avoid deriving the normalization constant, which is sometimes difficult to obtain. Fourth, we may discover the hidden symmetry of the quantum system through constructing a suitable Lie algebra, which can be realized by the ladder operators.

Up to now, this method has become a very powerful tool for solving second-order differential equations and attracted much attention of many authors. For example, more than two hundreds contributions to this topic have been appearing in the literature during only the last five years. Nevertheless, the literature on this topic is inundated with scattered articles. For this purpose, we attempt to provide a comprehensive description of this method and its wide applications in various fields of physics. Undoubtedly, this will complement the traditional coverage found in the existing quantum mechanics textbooks and also makes the reader be familiar with this key method as rapidly as possible. On the other hand, some of new ideas to be addressed in this work, e. g., the quantum control will give added attraction not only to physicist but also to some engineering students.

Let us first give a basic review of the factorization method before starting our new approach to the factorization method. Among almost all of contributions to this topic, it seems that most people have accepted such a fact that the factorization method owes its existence primarily to the pioneering works by Schrödinger [1–3], whose ideas were analyzed in depth by many authors like Infeld, Hull and others and generalized to different fields [4–9]. For example, Lin has used the Infeld's form to obtain the normalization of the Dirac functions [9]. Actually, there were earlier indications of this idea in Weyl's treatment of spherical harmonics with spin [10] and Dirac's treatment of angular momentum and the harmonic oscillator problem [11]. However, it should be noted that the roots of this method may be traced back to the great mathematician Cauchy. We can find some detailed lists of references illustrating the history from the book written by Schlesinger [12]. On the other hand, it is worth mentioning that in the 19th century a symmetry of second-order differential equations had been identified by Darboux [13]. The Darboux transformation relates the solutions of a pair of closely linked first order differential equations as studied by Schrödinger, Infeld, Hull and others. For instance, in Schrödinger's classical works [1–3], he made use of the factorization method to study the well known harmonic oscillator in non-relativistic quantum mechanics in order to avoid using the cumbersome mathematical tools. In Infeld and Hull's classical paper [8], the six factorization types A, B, C, D, E and F, the transition probabilities and the perturbation problems of some typical examples such as the spherical harmonics, hypergeometric functions, harmonic oscillator and Kepler problems have been studied in detail. It should be noted that there existed essential differences between those two methods even though the basic ideas of Infeld and Hull's factorization method are very closely related to those developed by Schrödinger. In Schrödinger's language, the basic difference between those two methods can be expressed as follows. Schrödinger used a finite number of finite ladders, whereas Infeld used an infinite number of finite ladders. All problems studied by Schrödinger using his method can be treated directly by

Infeld's method, but the opposite is not true. Such a fact becomes evident if we compare two different treatments of the Kepler problem in a Euclidean or spherical space. For example, the Kepler problem provides a direct application of the method proposed by Infeld [4]. However, this problem cannot be treated directly by Schrödinger's method. What Schrödinger did and what was usually done, was to use a mathematical transformation involving the coordinate and energy and to change the Kepler problem into a different one accessible to his factorization method. Nevertheless, the procedures of these two methods used to study the harmonic oscillator are almost similar, namely, all of them began by studying a given Hamiltonian, which is a second-order differential equation in essence. In fact, as it will be shown in Chapter 4, the expressions of the ladder operators for the harmonic oscillator can be easily obtained from its exactly normalized eigenfunctions expressed by the Hermite polynomials. By using the recursion relations among the Hermite polynomials, it is not difficult to obtain the ladder operators as defined in almost all quantum mechanics textbooks.

We now make a few remarks on the Infeld-Hull factorization method since it has played an important role in exactly solvable quantum mechanical problems during the past half century. It is a common knowledge that the creation and annihilation operators assumed as A^+ and A^- can be obtained by the Infeld-Hull factorization method for a second-order differential operator [8]. They have shown that a second-order differential equation with the form

$$\left[\frac{d^2}{dx^2} + r(x, m) + \lambda \right] \psi_m(x) = 0 \tag{1.1}$$

may be replaced by a pair of following first-order equations

$$A_m^+ \psi_m \equiv \left[k(x, m+1) - \frac{d}{dx} \right] \psi_m = \sqrt{\lambda - L(m+1)} \psi_{m+1}, \tag{1.2}$$

$$A_m^- \psi_m \equiv \left[k(x, m) + \frac{d}{dx} \right] \psi_m = \sqrt{\lambda - L(m)} \psi_{m-1}, \tag{1.3}$$

which mean that A_m^+ and A_m^- become the required ladder operators. It is worth noting that these two operators depend on the parameter m which they step. Four years later, Weisner removed this dependence by introducing a spurious variable [14]. Later on, Joseph published his influential series of three papers about the self-adjoint ladder operators in the late 1960s [15–17]. In Joseph's papers, the main aim was not so much to derive those unknown solutions of eigenvalue problems, but to show the considerable simplification, unification and generalization of many aspects of the systems with which he was concerned. Joseph first reviewed the theory of self-adjoint ladder operators and made a comparison with the more usual type of ladder operator, and then applied such a method to the orbital angular momentum problem in arbitrary D dimensions,

the isotropic harmonic oscillator, the pseudo-rotation group $O(D, 1)$, the non-relativistic and relativistic Dirac Kepler problems in a space of D dimensions as well as the solutions of the generalized angular momentum problem. In his first contribution [15], it is shown that the dependence on m is from the separation of variables necessary in deriving Eq. (1.1) from the Schrödinger equation.

No matter what form $r(x, m)$ is taken, it should be pointed out that not all functions $k(x, m)$ and $L(m)$ permit factorization of equation (1.1). Those that classify the different six types of factorization can occur. Upper and lower bounds to the ladder permit the explicit form of the eigenvalues and the eigenfunctions to be decided in a rather elegant fashion.

However, the limitation of the Infeld-Hull factorization method is that it requires a particular representation of quantum mechanical problem. As a result, the ladder operators cannot be expressed as an abstract algebraic form. It should be noted that Coish [18] extended the connection between Infeld factorization operators and angular momentum operators well known as spherical harmonics Y_{lm} to other factorization problems, such as the symmetric top, electronmagnetic pole system, Weyl's spherical harmonics with spin, free particle on a hypersphere and Kepler problem, by explicitly recognizing them as angular momentum problems.

Later on, Miller [19–21] recast the classification of the different types of factorization into the classification of the Lie groups generated by the ladder operators. A detailed investigation of the factorization types led him to the idea that this elegant method is a particular case of the representation theory of the Lie algebras [20]. It is illustrated in Miller's work that this technique developed to solve quantum mechanical eigenvalue problems is also a very powerful tool for studying recurrence formulas obeyed by the special functions of hypergeometric type, which are the solutions of linear second-order ordinary differential equations and satisfy differential recurrence relations. On the other hand, Miller enlarged the Infeld-Hull factorization method to differential equations and established a connection to the orthogonal polynomials of a discrete variable [21]. On the other hand, Kaufman investigated the special functions from the viewpoint of the Lie algebra [22], in which the families of special functions such as the Bessel, Hermite, Gegenbauer functions and the associated Legendre polynomials were defined by their recursion relations. The operators which raise and lower indices in those functions are considered as the generators of a Lie algebra. The "addition theorem" was obtained by using the powerful concepts of the Lie algebra without any recourse to any analytical methods and found that this theorem coincided with that derived by analytical methods [23]. Many other expansion theorems were then derived from the addition theorems. However, the disadvantage of the Kaufman's work [22] is its restriction to the study of 2- and 3-parameter Lie group. Additionally, it should

be noted that Deift further developed the scheme of the factorization method by constructing the deformed factorizations [24].

From the 1970s to the early 1980s, it seemed that the factorization method had been completely explored. Nevertheless, Mielnik made an additional contribution to the traditional factorization method in 1984 [25]. In that work, he did not consider the particular solution of the Riccati type differential equation related to the Infeld-Hull factorization method approach, but the general solution to that equation. Mielnik used the modified factorization method to study the harmonic oscillator and obtained a one-parameter family of new exactly solvable potentials, which are different from the harmonic oscillator potential but have the same spectrum as that of the harmonic oscillator. In the same year, Fernández applied this method to study the hydrogen-like radial differential equation and constructed a one-parameter family of new exactly solvable radial potentials, which are isospectral to those of the hydrogen-like radial equation [26]. In addition, Bagrov, Andrianov, Samsonov and others [27–33] established a connection between this modified method and Darboux transformation [13, 34–41]. The further investigation of Darboux transformations[1] related to other interesting topics such as the supersymmetric quantum mechanics, the intertwining operators, the inverse scattering method can be found in recent publications [43–69]. For example, Rosas employed the intertwining technique proposed by Mielnik to generalize the traditional Infeld-Hull factorization method for the radial hydrogen-like Hamiltonian and to derive n-parametric families of potentials, which are almost isospectral to the radial hydrogen-like Hamiltonian even though the similar topic had been carried out by Fernández in 1984 [66, 67]. In addition, Fernández *et al.* applied such a technique to the higher-order supersymmetric quantum mechanics [70].

It should be noted that other related and derived methods have been brought forward with the development of the traditional factorization method. For example, in the early 1980s Witten noticed the possibility of arranging the second-order differential equations such as the Schrödinger Hamiltonian into isospectral pairs, the so-called supersymmetric partners [71]. More recent developments, which have generated some interest in many solvable potentials, were the introduction of the supersymmetric quantum mechanics (SUSYQM) and shape invariance [72–101]. It was Gendenshtein who established a bridge between the theory of solvable potentials in one-dimensional quantum system and SUSYQM by introducing the concept of a discrete reparametrization invariance, usually called shape invariance [72].

Due to the importance of the SUSYQM and shape invariance, let us give them a brief review. The SUSY was originally constructed as a non-trivial unification of space-time and internal symmetries with four-dimensional relativistic quantum field theory. Up to now, the SUSYQM has been a useful technique to construct exact solutions in quantum mechanics and attracted much

attention of many authors. The concept of shape invariance introduced by Gendenshtein has become a key ingredient in this field. Generally speaking, all ordinary Schrödinger equations with shape invariant potentials can be solved algebraically with the SUSY method. If the potentials $V_\pm$ are related to each other by

$$V_+(x, a_1) = V_-(x, a_2) + R(a_1), \tag{1.4}$$

where a_1, a_2 are two parameters, then these potentials $V_\pm$ are called "shape invariant". It should be mentioned that, up to now, the problem of the general characterization of all such shape invariant potentials with arbitrary relationship between these two parameters a_1 and a_2 has remained unsolved [98]. If these two parameters can be connected by a translation, then we may obtain all usual well-known solvable potentials like the Coulomb-like potential, the Morse potential, the shifted oscillator, the harmonic oscillator, the Scarf I and Scarf II potentials, the Rosen-Morse I and Rosen-Morse II potentials, the Eckart and Pöschl-Teller potentials and others [73, 100]. That the parameters a_2 and a_1 are related by scaling is other solvable potentials. In fact, more general relationships have been studied only partially so far. The method of shape invariant supersymmetric potentials in some sense also throws light on the earlier Schrödinger-Infeld-Hull factorization method.

On the other hand, the SUSYQM can be recognized as the reformulation of the factorization method [102]. It is also considered as an application of the Darboux transformation method to solve a second order differential equation. It should be noted that most of these approaches mentioned above could be formulated by rewriting them as some transformations to map the original wave equations into some second order ordinary differential equations, whose solutions are the special functions like the hypergeometric type functions and others. For some well known solvable potentials with the shape invariance properties [72], however, it has turned out that those shape invariance potentials are exactly same as the ones which can be obtained from factorization method. Recently, Andrianov *et al.* [30–33], Sukumar [74–78] and Nieto [103] have put the method on its natural background discovering the links between the SUSYQM, the factorization method and the Darboux algorithm, causing then a renaissance of the related algebraic methods. We suggest the reader to consult the references [70, 73, 100, 104] for more information on the relations among them. Specially, the implications of supersymmetry for the solutions of the Schrödinger equation, the Dirac equation, the inverse scattering theory and the multi-soliton solutions of the Korteweg-de Vries (KdV) equation are examined by Sukumar [104].

Additionally, the group theoretical method is closely related to the factorization method (see, e. g. [105, 106]). Moreover, it is well known that the coherent states of quantum systems are also closely related to the ladder operators, which can be obtained from the factorization method [107]. For example, the beautiful

properties of the harmonic oscillator coherent states have motivated many authors to look for them in other physical systems [49–51, 108–124]. Therefore, we may say that the factorization method has become the milestone of these approaches like the SUSYQM, the group theoretical method and the shape invariance approach. That is to say, although the methods of solution usually focus on different aspects of solvable potentials, they are not independent from each other. When studying all these related subjects, we are really impressed by the almost complete ubiquity of some specific Riccati equations appearing in the theory [125], in which the appropriate use of the mathematical properties of the Riccati equation is very useful in obtaining a deep insight into the theory of factorization problems in quantum mechanics and in the particular class given by shape invariant Hamiltonian. In addition to them, other two approximation methods in supersymmetric quantum mechanics, namely, the supersymmetric WKB (SWKB) approximation and perturbation theory, are essentially based on the factorization method [73, 88, 100, 126–128].

Up to now, the seminal idea proposed by Witten has been developed to the subject of the SUSYQM: the study of quantum mechanical systems governed by an algebra becomes identical to that of supersymmetry in field theory. Recently, many people have made a lot of contributions to this subject. It will not be possible to do full justice to all the people who have contributed. We would like to keep a chronological order of how the ideas have developed and refer to the papers that act as markers in this progression. The detailed information can be found in the review articles [70, 73, 100, 104, 125].

Except for the traditional Schrödinger-Infeld-Hull factorization method, it is worth noting that Inui used an alternative factorization method to investigate a unified theory of recurrence formulas in 1948 [129, 130]. However, there are no more applications to physical problems. For this approach, the "up-stair" (creation) and "down-stair" (annihilation) operators are not obtained from a direct factorization of the studied second-order differential operator itself, but from some difference or contiguous relations which are satisfied by their eigenfunctions given in a generally priori known form. In fact, Inui generalized Infeld's method [4] so that the results are applicable to all transcendental functions of hypergeometric and confluent hypergeometric types [131]. It is shown from his work that the key to magic factorization of the traditional factorization method is in his hands so long as the corresponding differential equations have three regular singularities of the Fuchsian type or those with one regular singularity and one irregular singularity.

We are now in the position to briefly review some interesting topics and studies related to the factorization method as follows. For example, Lorente has employed the Rodrigues formula to construct the creation and annihilation operators for orthogonal polynomials of continuous and discrete variables on a uniform lattice [132]. Moreover, it is worth mentioning that the contributions

made by Nikiforov and co-authors to the classical orthogonal polynomials of continuous and discrete variables have opened the way to a rigorous and systematic approach to the factorization method [133, 134].

On the other hand, it is well known that the matrix elements for some physical functions can be calculated by the ladder operator method. Many investigations along this line have been carried out. For example, the matrix element calculations for the rotating Morse oscillator were studied by López and Moreno [135], in which the authors described a simple method in terms of the hypervirial theorem along with a second-quantization formalism to obtain recurrence relations without using explicit wave functions for the calculations of some matrix elements of related physical functions for the rotating Morse potential. The algebraic recursive solution of the perturbed Morse oscillator eigenequation was obtained by Bessis *et al.* [136], in which they used the perturbed ladder-operator method to derive its solution. Such a method used in their work is an extension of the original Schrödinger-Infeld-Hull traditional factorization method. The perturbed factorization technique which has been first used to study the Stark effect calculations in principle is more attractive and interesting [1, 8]. Actually, once the perturbed ladder operators are found, one can use the usual factorization scheme to obtain the analytical expressions of the perturbed eigenvalues and eigenfunctions. Some interesting investigations on the perturbed operator technique have been done by Bessis *et al.* [137–141]. In 1987, Berrondo and his co-workers Palma and López-Bonilla utilized the ladder operator approach to obtain the matrix elements for the Morse potential [142], in which they first mapped the Morse potential system into a two-dimensional harmonic oscillator and then used the corresponding algebra belonging to the harmonic oscillator to obtain its matrix elements. In the early 1990s, Moreno and his co-authors used the ladder operator technique together with the hypervirial theorem to derive the recurrence formulas of some useful radial matrix elements for the hydrogenic radial Schrödinger equation [143]. The advantage of this method is that the closed-form expressions are well suited to compute the diagonal and off-diagonal matrix elements for any values of quantum numbers n and l.

By the way, let us mention $N = 1$ superalgebra and its realization and relation to shape invariance. For example, Filho and Ricotta studied the ladder operators for subtle hidden shape invariant potentials and constructed the ladder operators for two exactly solvable potentials like the free particle in a box and the Hulthén potential that present a subtle hidden shape invariance using the superalgebra of supersymmetric quantum mechanics [144]. Other studies have also been carried out in this field [145].

Another interesting topic related to the factorization method is the point canonical transformation method and its invariant potential classes. As we know, the potentials with dynamic symmetries associated with any one of the

hidden dynamic algebras for the studied quantum systems can be grouped into different classes. All potentials in a given class, along with their corresponding eigenvalues and eigenfunctions can be mapped into one another by point canonical transformation [146–151]. Recently, Alhaidari has extended such a method to the Dirac equation case [152–154].

With the recent development of the quantum group, the q-deformed ladder operators for some interesting quantum systems were carried out [155], in which the authors Gupta and Cooper used the quantum deformation algebra $so_q(2, 1)$ to derive the q-analogues of the ladder and shift operators for the radial hydrogenic, radial harmonic oscillator and Morse oscillator potentials.

It is worth pointing out that we shall concentrate more attention on the factorization method than the topics related to those like the supersymmetric quantum mechanics, shape invariance, supersymmetric WKB approximation, the coherent states and other related topics, but we are going to study them in the due Chapters in order to show how they are related to the traditional factorization method.

Among almost all contributions to the factorization method mentioned above, the creation and annihilation operators obtained from the factorization method are directly based on the Hamiltonian of a given quantum system. In order to realize a suitable dynamic Lie group, sometimes, the ladder operators can be constructed by introducing an extra auxiliary parameter as shown by Berrondo and Palma [156]. Recently, we have used another new approach to the factorization method [105, 106] to obtain the ladder operators of some quantum systems and to construct a suitable Lie algebras, as will be addressed below. The main difference between them is that we derive the ladder operators only from the physical variable without introducing any auxiliary variable. Also, we may investigate the controllability of the quantum systems using some basic theories in quantum control as shown in our recent publications [157, 158].

Heretofore, we may say that the factorization method has become the cornerstone of those different approaches through the above introduction. The relations among them can be simply shown in Fig. 1.1.

2. Motivations and aims

The motivations of this work are as follows. Since the literature is inundated with scattered articles on this topic we try to give a comprehensive review of the traditional factorization method and its wide spread applications in quantum mechanics, which complements the traditional coverage found in the existing quantum mechanics textbooks. In particular, we want to introduce a new approach to the factorization method and apply this method to some important quantum systems. As an important generalized application of the factorization method, we shall study the quantum control. In this book, we attempt to put the mathematical and physical concepts and techniques like the
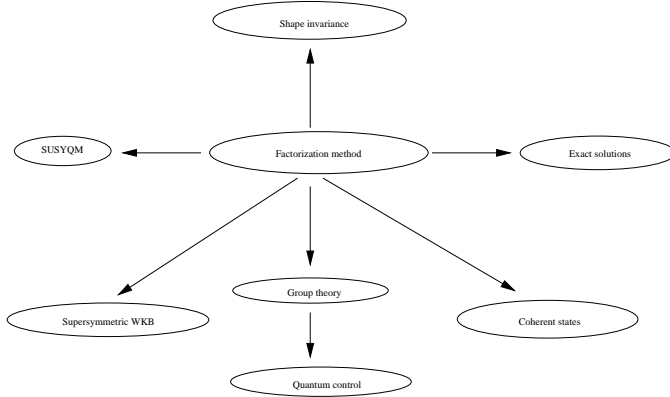
Figure 1.1.   The relations among factorization method, exact solutions, group theory, coherent states, SUSYQM, shape invariance, supersymmetric WKB and quantum control.

factorization method, Lie algebras, matrix elements and quantum control at the reader's disposal and to pave the reader's way into this territory as rapidly as possible.

Notes

1   We want to give a brief review for Darboux transformations. As we know, Darboux transformations are very closely related to the SUSYQM, intertwining operators and inverse scattering techniques as well as other topics. Darboux's result had not been used and recognized as important for a long time. This result was only mentioned as an exercise by Ince in 1926 [36], when he published Darboux theorem in a section of "Miscellaneous examples" in page 132 together with two other particular examples, the free particle and the Pöschl-Teller potential. In 1941, Schrödinger factorized the hypergeometric equation and found that there were a few ways of factorizing it [1–3]. His idea actually originated from the well known treatment of the harmonic oscillator by Dirac's creation and annihilation operators for it. Later on, the important contributions to the factorization method were from Infeld-Hull's work [4–6]. In 1955, Crum published a very important iterative generalization of Darboux's result [35], in which the Darboux's result in 1882 can be regarded as the special case $N = 1$. Specifically, he presented the successive Darboux transformations in compact formulas.   In 1979, Matveev extended the range of applicability of the concept to differential-difference and difference-difference evolution equations [38, 39]. Recently, Yurov has used the Darboux transformation for Dirac equation with $(1 + 1)$ potentials and obtained the exact solutions for the adiabatic external field [42]. The detailed information is found in the work by Rosu [55].

PART II

METHOD

Chapter 2

THEORY

1.   Introduction

Let us assume that for some self-adjoint operator H, there exists a pair of mutually adjoint operators L^+ and L^- satisfying

$$[H, L^+] \equiv HL^+ - L^+H = L^+, \quad [H, L^-] = -L^-. \tag{2.1}$$

If denoting the eigenfunctions of the operator H by Φ_l with the following property

$$H\Phi_l = l\Phi_l, \tag{2.2}$$

it is not difficult to find from the above relations (2.1) and (2.2) that

$$H(L^+\Phi_l) = (l+1)(L^+\Phi_l), \quad H(L^-\Phi_l) = (l-1)(L^-\Phi_l), \tag{2.3}$$

which can be interpreted as

$$L^+\Phi_l \sim \Phi_{l+1}, \quad L^-\Phi_l \sim \Phi_{l-1}. \tag{2.4}$$

Due to this relations we call the operators $L^\pm$ as ladder operators. Additionally, if there exist upper and lower bounds to the ladder operators, then the exact eigenvalues and eigenfunctions of operator H can be obtained by consideration of the wave function Φ_l corresponding to these bounds and subsequent use of the formulas (2.4). As shown in the traditional factorization method, its main task is to obtain the exact eigenvalues and eigenfunctions of the given quantum system. The ladder operators can be obtained directly by factorizing the quantum system Hamiltonian.

2.   Formalism

Let us introduce a new formalism for the factorization method to be used in this work. For this method, we intend to find the ladder operators $L_\pm$ with the

following properties

$$L_n^{\pm} \Phi_n(\xi) = l_n^{\pm} \Phi_{n\pm1}(\xi). \tag{2.5}$$

Specifically, we are going to look for the ladder operators of the form

$$L_n^{\pm} = A_n^{\pm}(\xi) \frac{d}{d\xi} + B_n^{\pm}(\xi), \tag{2.6}$$

where we stress that these ladder operators only depend on the physical variable ξ, which is different for different quantum systems.

Based on Eq. (2.5), we can obtain the following expressions

$$L_{n+1}^- L_n^+ \Phi_n(\xi) = l_n^+ l_{n+1}^- \Phi_n(\xi), \ \ L_n^+ L_{n+1}^- \Phi_{n+1}(\xi) = l_n^+ l_{n+1}^- \Phi_{n+1}(\xi), \tag{2.7}$$

from which we find that the products of the operators $L_{n+1}^- L_n^+$ and $L_n^+ L_{n+1}^-$ acting on the given wave functions $\Phi_n(\xi)$ and $\Phi_{n+1}(\xi)$, respectively, have the same constant

$$c_n \equiv l_n^+ l_{n+1}^-, \tag{2.8}$$

which is independent of the arbitrarily multiplying constant appearing in the front of wave functions $\Phi_n(\xi)$.

It is worth pointing out that some features of this new approach can be summarized as follows. First, the procedure of this new approach is converse to that of the traditional Schrödinger-Infeld-Hull factorization method, whose main task is to obtain the unknown exact eigenfunctions and eigenvalues of the studied quantum system. For the present approach, however, we assume that the exact solutions of the quantum systems can be obtained from the standard quantum mechanical method. Once the exact solutions which, sometimes, can be expressed by the associated Laguerre functions, confluent hypergeometric functions and other special functions are known, we may construct the creation and annihilation operators by acting the first differential operator $d/d\xi$ on the normalized eigenfunctions and then by using the recursion relations among those special functions. Second, we may construct a suitable Lie algebra in terms of the obtained ladder operators so that we may study other properties of quantum system based on the Lie algebra. Third, we can obtain the analytical expressions of matrix elements for some related physical functions directly from the ladder operators. It is shown that this method represents an elegant and simple approach to obtain those matrix elements. Up to now, we have established ladder operators and constructed suitable Lie algebras for some interesting quantum systems [105, 106, 159–167], and studied some interesting properties such as the controllabilities of quantum systems in terms of the basic properties of the Lie algebras and some known theorems on the control theory [157, 158].

Chapter 3

LIE ALGEBRAS SU(2) AND SU(1, 1)

1. Introduction

Since the exactly solvable one-dimensional quantum systems with certain central potentials are usually related to the dynamic groups SU(2) and SU(1, 1), we want to briefly review some of their basic properties in order to study some interesting and typical quantum systems based on the monographs and textbooks [20, 168, 169].

We use groups throughout mathematics and the sciences often to capture the internal symmetry of other structures in the form of automorphism groups. It is well-known that the internal symmetry of the structure is usually related to an invariant mathematical property and the set of transformations that preserve this kind of invariant mathematical property together with the operation of composition of transformations form a group named as a symmetry group.

It should be noted that Galois theory is the historical origin of the group concept. He used groups to describe the symmetries of the equations satisfied by the solutions of a polynomial equation. The solvable groups are thus named due to their prominent role in this theory.

The concept of the Lie group named for mathematician Sophus Lie plays a very important role in the study of differential equations and manifolds; they combine analysis and group theory and are therefore the proper objects for describing symmetries of analytical structures.

An understanding of group theory is also important in the physical and chemical sciences. For example, in chemistry, groups are used to classify crystal structures, regular polyhedra, and the symmetries of molecules. In physics, groups are also very important because they describe the symmetries which the laws of physics seem to obey. On the other hand, physicists are very interested in group representations, especially of the Lie groups, since these representations

often point the way to the possible physical theories and they play an essential role in the algebraic method of solving quantum mechanics problems.

As a common knowledge, the study of the groups is always related to the corresponding algebraic method. Up to now, the algebraic method has become the subject of interest in various fields of physics. Here we give a brief review of its development in order to make the reader recognize its importance both in physics and in chemistry.

The elegant algebraic method was first introduced in the context of the new matrix mechanics around 1925. Since the introduction of the angular momentum in quantum mechanics, which was intimately connected with the representations of the rotation group SO(3) associated with the rotational invariance of central potentials, its importance was soon recognized and the necessary formalism was developed principally by some pioneering scientists like Wigner, Weyl, Racah and others [10, 170–173]. Up to now, the algebraic method to treat the angular momentum theory can be found in almost all textbooks of quantum mechanics. On the other hand, it often runs parallel to the differential equation approach due to the great scientist Schrödinger. Even though Pauli used the algebraic method to treat the hydrogen atom in 1926 [174] and Schrödinger also solved the same problem almost at the same time [175], their fates were quiet different. This is because the standard differential equation approach was more accessible to the physicists than the algebraic method. As a result, the algebraic approach to determine the eigenvalue of the hydrogen atom was largely forgotten and the algebraic techniques went into abeyance for a few decades. Until the mid-1950s, the algebraic techniques revived with the development of quantum mechanics of the elementary particles since the explicit forms of the Hamiltonian for those elementary particle systems are unknown and the physicists have to make certain assumptions on the internal symmetries of those elementary particles. Among various attempts to solve this difficult problem, the particle physicists examined some non-compact Lie algebras and hoped that they would provide a clue to the classification of the elementary particles. Unfortunately, this hope did not materialize. Nevertheless, it is found that the Lie algebras of the compact Lie groups enable such a classification[1] for the elementary particles[2] [176] and the non-compact groups are relevant for the dynamic groups in atomic physics [184] and the non-classical properties of quantum optical systems involving coherent and squeezed states as well as the beam splitting and linear directional coupling devices [185–189].

It is worth mentioning that one of the reasons why the algebraic techniques were accepted very slowly and the original group theoretical and algebraic methods proposed by Pauli [174] was neglected is undoubtedly related to the abstract character and inherent complexity of group theory. Even though the proper understanding of group theory requires an intimate knowledge of the standard theory of finite groups and of the topology and manifold theory, the

basic concepts of group theory are quite simple, specially when we present them in the context of physical applications. Basically, we attempt to introduce them as simple as possible so that the common reader can master the basic ideas and essence of group theory. The detailed information on the group theory can be found in the textbooks [183, 190, 191].

On the other hand, during the development of the algebraic method, Racah algebra techniques played a very important role both in physics and in chemistry. The main power of Racah algebra for practical computations is that it enables us to deal with the integration over the angular coordinates of a complex many-particle system analytically. Generally speaking, we can reduce the number of independent variables greatly by choosing the proper coordinates and using the rotational symmetries of the quantum system. In practical applications, the Racah algebra techniques typically lead to the expressions written in terms of the generalized Clebsch-Gordon coefficients, Wigner n-j symbols, tensor spherical harmonics and/or rotation matrices. With the developments of algebraic method in the late 1950s and early 1960s, the algebraic method proposed by Pauli was systematized and simplified greatly by using the concepts of the Lie algebras. Up to now, the algebraic method has been widely applied to various fields of physics such as nuclear physics [192], field theory and particle physics [176, 177, 182, 193], atomic and molecular physics [194–197], quantum chemistry [198], solid state physics [199], quantum optics [124, 185, 200–206] and others.

2.　Abstract groups

We now give some basic definitions about the groups based on textbooks by Weyl, Wybourne, Miller and others [10, 168, 207].

Definition: A **group** $\mathcal{G}$ is a set of elements $\{f, g, h, k, \ldots\}$ together with a binary operation. This binary operation named as the group multiplication is subject to the following four requirements:

- **Closure**: if f, g are in $\mathcal{G}$ then fg is also in $\mathcal{G}$,

- **Identity element**: there exists an identity element e in $\mathcal{G}$ (a unit) such that $ef = fe = f$ for any $f \in \mathcal{G}$,

- **Inverses**: for every $f \in \mathcal{G}$ there exists an inverse element $f^{-1} \in \mathcal{G}$ such that $ff^{-1} = f^{-1}f = e$,

- **Associative law**: the identity $f(hk) = (fh)k$ is satisfied for all elements $f, h, k \in \mathcal{G}$.

It should be noted that there existed two kinds of different meanings of the term "abstract group" during the first half of the 20th century. The first meaning was that of a group defined by four axioms given above, but the second one was that of a group defined by generators and commutation relations. Essentially, they are the two sides of the same coin.

Abelian group: if $fg = gf$, we say that the elements f and g commute. If all elements of $\mathcal{G}$ commute, then $\mathcal{G}$ is a commutative or Abelian group. If $\mathcal{G}$ has a finite number of elements, it has finite order $n(\mathcal{G})$, where $n(\mathcal{G})$ is the number of elements. Otherwise, $\mathcal{G}$ has infinite order.

Subgroup: a subgroup of $\mathcal{G}$ is a subset $\mathcal{S} \in \mathcal{G}$, which is itself a group under the group multiplication defined in $\mathcal{G}$, i.e., $f; h \in \mathcal{S} \longrightarrow f\,h \in \mathcal{S}$.

Homomorphism: a homomorphism of groups $\mathcal{G}$ and $\mathcal{H}$ is a mapping from a group $\mathcal{G}$ into a group $\mathcal{H}$, which transforms products into products, i.e., $\mathcal{G} \to \mathcal{H}$.

Isomorphism: an isomorphism is a homomorphism which is one-to-one and "onto" [207]. From the viewpoint of the abstract group theory, isomorphic groups can be identified. In particular, isomorphic groups have identical multiplication tables.

Representation: a representation of a group $\mathcal{G}$ is a homomorphism of the group into the group of invertible operators on a certain (most often complex) Hilbert space V (called representation space). If the representation is to be finite-dimensional, it is sufficient to consider homomorphisms $\mathcal{G} \to \mathcal{G}L(n)$, where $\mathcal{G}L(n)$ is the group of non-singular matrices of dimension n. Usually, the image of the group in this homomorphism is called a representation as well.

Irreducible representation: an irreducible representation is a representation whose representation space contains no proper subspace invariant under the operators of the representation.

Commutation relation: since a Lie algebra has an underlying vector space structure we are able to choose a basis set $\{L_i\}(i = 1, 2, 3, \ldots, N)$ for the Lie algebra. In general, the Lie algebra can be completely defined by specifying the commutators of these basis elements:

$$[L_i, L_j] = \sum_k c_{ijk} L_k, \quad i, j, k = 1, 2, 3, \ldots, N, \tag{3.1}$$

which are called the defining commutation relations for the Lie algebra and the coefficients c_{ijk} are called the structure constants. The elements L_i are called the generators of the Lie algebra. It is worth noting that the set of operators which commute with all elements of the Lie algebra are called Casimir operators, which are very useful in studying Lie algebras.

Hereupon, we want to give two typical examples to indicate the variety of mathematical objects with the structure of groups. For more examples, we refer the reader to the textbook by Miller [207].

Example 1: For the real numbers R, we consider the **addition** as the group product. The product of two elements a, b is their sum $a + b$. We may take 0 as an **identity element**. The **inverse** of an element c is its negative $-c$. The set odd real number R constructs an infinite Abelian group. Among the subgroups of R are the integers, the even integers and the group consisting of the element zero alone.

Example 2: For a given group $\mathcal{G}$, two elements $\{0, 1\} \in \mathcal{G}$, the group multiplication is given by $0 \cdot 0 = 0, 0 \cdot 1 = 1 \cdot 0 = 1, 1 \cdot 1 = 0$. We may take 0 as the **identity element**. This is an Abelian group with order $n = 2$. It has only two subgroups, $\{0\}$ and $\{0, 1\}$.

3. Matrix representation

For a given Lie algebra with the commutation relations (3.1), we may consider the generators L_i as operators which act on the n-dimensional vector space V. If $\{|j\rangle\}(j = 1, 2, 3, \ldots)$ is a basis set for V, then we have

$$L_k|i\rangle = \sum_j |j\rangle\langle j|L_k|i\rangle, \tag{3.2}$$

with

$$
\begin{aligned}
i, j &= 1, 2, 3, \ldots, n, \\
k &= 1, 2, 3, \ldots, N.
\end{aligned}
\tag{3.3}
$$

Here $\langle j|L_k|i\rangle$ denotes the matrix element of the operator L_k, and $|i\rangle, |j\rangle$ are two different states of the system. If denoting by $\mathbf{L}_k$ the matrix representing L_k, we may show that

$$[\mathbf{L}_i, \mathbf{L}_j] = \sum_k c_{ijk}\mathbf{L}_k, \tag{3.4}$$

where the matrices $\mathbf{L}_i$ generate a matrix representation of the Lie algebra because they have the same defining commutation relations as the relations (3.1).

As we know, once the irreducible representations are obtained, then any matrix representation can be constructed by using the irreducible representations as building blocks. In general, for a given matrix representation, we can obtain an identical block diagonal structure by applying a similarity transformation to all the matrices. If so, we say that the representation is reducible since the block matrices can form smaller dimensional matrix representations of the Lie algebra. For example, if each $\mathbf{L}_i$ has the form

$$\mathbf{L}_i = \begin{pmatrix} \mathbf{C}_i & \mathbf{0} \\ \mathbf{0} & \mathbf{D}_i \end{pmatrix}, \tag{3.5}$$

where $\mathbf{C}_i$ and $\mathbf{D}_i$ represent $m \times m$ and $l \times l$ matrices, respectively, then it is very easy to prove that the $\mathbf{C}_i$ forms a matrix representation and so does the $\mathbf{D}_i$.

On the contrary, if we cannot obtain such a reduction by applying any similarity transformation then we say that the representation is irreducible.

We will introduce in the following parts some basic properties of the non-compact so(2, 1)$\simeq$ su(1, 1) algebra alongside the well known compact so(3)$\simeq$ su(2) Lie algebra of the angular momentum theory, with which the reader is familiar due to their applications in successive Chapters. In addition, it is worth addressing that a detailed knowledge of the Lie groups or algebras is not essential to the understanding of the applications we will consider, because all of results are presented in a simple and acceptable manner using only the familiar concepts such as the commutators, eigenvalues and vector spaces, etc. The detailed information about the group theory can be consulted in the textbooks by Weyl, Wigner, Hamermesh, Gilmore, Wybourne, Miller, Saletan, Cromer, Ma and others [10, 168, 173, 183, 190, 191, 207, 208].

4.   Properties of groups SU(2) and SO(3)

It is well known that both groups SO(3) and SU(2), and also their Lie algebras so(3) and su(2), have been widely applied both in physics and in chemistry. The former describes the rotations of three-dimensional space and is closely related to the conservation of the angular momentum of quantum systems, but the latter is related to the spin operators in quantum mechanics. On the other hand, the theory of the spin and isotopic spin of elementary particles is intimately associated with the representation theory of the rotation group SO(3), which is locally isomorphic to the Lie group SU(2). This leads to the isomorphic relation between the Lie algebras so(3) and su(2) [207], to which the reader is referred for more detailed information.

Both of Lie algebras su(2) and so(3) are spanned over the vector spaces R by three generators $L_i(i = 1, 2, 3)$ of rotations with respect to three mutually orthogonal axes. The communication relations of these generators are given by

$$[L_i, L_j] = \epsilon_{ijk}L_k, \tag{3.6}$$

where ϵ_{ijk} is the Levi-Civita symbol.

As we know, the group SO(3) can be described by a convenient coordinate system-Euler angles (θ, ϕ, ψ)

$$\theta \in (0, \pi), \quad \phi \in [0, 2\pi), \quad \psi \in [0, 2\pi), \tag{3.7}$$

while for the SU(2) group, the Euler angles become

$$\theta \in (0, \pi), \quad \phi \in [0, 2\pi), \quad \psi \in [-2\pi, 2\pi). \tag{3.8}$$

On the other hand, both of them are connected but only the SU(2) group is simply connected because the groups SU(2) and SO(3) are different in their topological properties. For example, the SU(2) group is homeomorphic to the

unit sphere S_4 in four-dimensional space. That is to say, if element $a \in \mathrm{SU}(2)$ is a point on this sphere, then $-a$ is the point on the other end of the diameter of S_4 passing through a. However, the rotation group SO(3) is homeomorphic to the projective space obtained by identifying opposite ends of each diameter in unit sphere S_4. Therefore, we say that the group SU(2) is a covering group of the rotation group SO(3) and it covers the rotation group SO(3) twice. Additionally, it is worth mentioning that there exists a one-to-one relationship between the representations of linear groups and the representations of their corresponding algebras.

It should be addressed that the global representations of the Lie algebras su(2) and so(3) have an important feature. Let us consider a representation of the Lie algebra su(2) or so(3), say $\mu(L_i) = S_i$, which corresponds to a global representation of the respective group. Suppose that ℓ is the eigenvalue of the S_i, then $e^{i\beta\ell}$ is the eigenvalue of $e^{i\beta S_i}$. However, this has to be periodical in β with the period 2π or 4π for SO(3) and SU(2), respectively, since we require the representation to be globally analytical. As a result, if h is the eigenvector belonging to the eigenvalue ℓ, we have

$$h = e^{i\beta_0 S_i}h = e^{i\beta_0\ell}h, \tag{3.9}$$

which implies that

$$e^{i\beta_0\ell} = 1, \tag{3.10}$$

where $\beta_0 = 2\pi$ for SO(3) group and $\beta_0 = 4\pi$ for SU(2) group. Hence, we find that ℓ must be integer for group SO(3) and 2ℓ for group SU(2). This important property will be useful in constructing the quantum mechanical Hamiltonian by using the Lie algebra generators.

5. Properties of non-compact groups SO(2, 1) and SU(1, 1)

We now give a brief review of non-compact Lie groups SO(2, 1) and SU(1, 1). As we know, the group SO(2, 1) is locally isomorphic to the SU(1, 1) group; their commutation relations are analogous to those of groups SU(2) and SO(3), and can be expressed as

$$[L_1, L_2] = -L_3, \quad [L_2, L_3] = L_1, \quad [L_3, L_1] = L_2, \tag{3.11}$$

where the operator L_3 is considered as the generator of the geometrical rotation, while L_1 and L_2 are the Lorentz transformation.

6. Generators of Lie groups SU(2) and SU(1, 1)

Let us introduce some basic properties of the Lie groups SU(2) and SU(1, 1) in detail. We suggest the reader refer to [117] for more information.

For a set of three-dimensional real matrices satisfying the following determinant

$$R^T E R = E, \quad E = \mathrm{diag}\{1, 1, \sigma\}, \tag{3.12}$$

where we associate the case $\sigma = 1$ to the SU(2) group, and associate the case $\sigma = -1$ to the SU(1, 1) group. Due to $R_{33}^2 = 1 - \sigma(R_{13}^2 + R_{23}^2)$, then we say that SU(2) is a compact Lie group and SU(1, 1) is a non-compact Lie group.

When expanding the generators around the identity element

$$R = \mathbf{1} - i\,X, \quad R^T E R = E - i\{X^T E + EX\}, \quad \det R = 1 - i\,\mathrm{Tr}X, \quad (3.13)$$

we have

$$\mathrm{Tr}X = 0, \quad X = -EX^T E = \sum_{i=1}^{3} \omega_i L_i, \quad (3.14)$$

where the matrix expressions of the generators $L_i (i = 1, 2, 3)$ in their own representations can be taken as

$$L_1 = \begin{pmatrix} 0 & 0 & 0 \\ 0 & 0 & -i\sigma \\ 0 & i & 0 \end{pmatrix},$$

$$L_2 = \begin{pmatrix} 0 & 0 & i\sigma \\ 0 & 0 & 0 \\ -i & 0 & 0 \end{pmatrix}, \quad (3.15)$$

$$L_3 = \begin{pmatrix} 0 & -i & 0 \\ i & 0 & 0 \\ 0 & 0 & 0 \end{pmatrix},$$

from which we may obtain the following commutation relations

$$[L_1, L_2] = i\sigma\, L_3, \quad [L_2, L_3] = iL_1, \quad [L_3, L_1] = iL_2. \quad (3.16)$$

Furthermore, if we introduce the ladder operators

$$L_{\pm} = L_1 \pm iL_2, \quad (3.17)$$

then we have

$$[L_3, L_{\pm}] = \pm L_{\pm}, \qquad [L_+, L_-] = 2\sigma L_3, \quad (3.18)$$

where $\sigma = 1$ corresponds to SU(2) group, and $\sigma = -1$ corresponds to SU(1, 1) group.

The corresponding Casimir operator can be calculated as

$$\begin{aligned} L^2 &= \sigma(L_1^2 + L_2^2) + L_3^2 \\ &= \sigma\, L_+ L_- + L_3(L_3 - 1) \\ &= \sigma\, L_- L_+ + L_3(L_3 + 1), \end{aligned} \quad (3.19)$$

with the following properties

$$[L^2, L_i] = 0, \qquad i = 1, 2, 3. \tag{3.20}$$

It is well-known that a set of mutually commuting operators can be simultaneously diagonalized. For the non-compact Lie group SU(1, 1) and compact Lie group SU(2), the maximum number of such operators is two. For SU(2) group, we may choose any of pairs $\{L^2, L_i\}(i = 1, 2, 3)$ and the representation theory would be same in each case. The unitary irreducible representations can be characterized by a single quantum number. For the non-compact Lie group SU(1, 1), however, each choice of a pair of mutually commuting operators will lead to a different set of inequivalent representations.

7. Irreducible representations

In this section we attempt to present a simple unified approach to the matrix representation theory of the Lie algebras so(2, 1) and so(3) based on Refs. [168, 169, 209–211].

As we know, the Lie algebras so(3) and so(2, 1) have a similar structure and their general representation theories are very closely related to each other. Nevertheless, if specializing to the unitary representations by requiring that their generators be Hermitian, we shall find that the properties of the Lie algebras so(3) and so(2, 1) are essentially different. In fact, all unitary irreducible representations of the Lie algebra so(3) are finite dimensional [212]. Additionally, all nontrivial unitary irreducible representations of the Lie algebra so(2, 1) are infinite dimensional [210]. On the other hand, we find that the unitary irreducible representations of the Lie algebra so(2, 1) are not as well known as those of the Lie algebra so(3), but as a spectrum generating algebra, the Lie algebra so(2, 1) has played an important role in many simple quantum systems [168, 169, 209]. Important examples are the so(2, 1) for the radial Coulomb and su(2) for the bound states of the Morse and PT potentials. Other different approaches to the realization of the Lie algebra so(2, 1) generators in terms of the coordinate and momentum operators were studied with a number of applications [213, 214]. Since the Lie algebras su(2) and su(1, 1) are isomorphic to the Lie algebras so(3) and so(2, 1), respectively, we will not normally distinguish them in the following discussion.

In this work, what are we interested in is the bound states of simple quantum systems, and not in the scattering states. Thus, we may choose $\{L^2, L_3\}$ to describe the bound states of quantum systems, but the other choices will be more suitable for describing the continuous states in the scattering theory [168]. Therefore, we may choose a representation space of state $|Q, m\rangle$, on which L^2 and L_3 are simultaneously diagonal:

$$L^2|Q, m\rangle = Q|Q, m\rangle, \qquad L_3|Q, m\rangle = m|Q, m\rangle. \tag{3.21}$$

For simplicity, we take

$$Q = j(j + 1), \tag{3.22}$$

from which we find that the state $|Q, m\rangle$ remains invariant if replacing j by $-j - 1$. Thus, the state $|Q, m\rangle$ plays the same role as the state $|lm\rangle$ in the angular momentum theory.

Based on equations (3.17)- (3.21), we have

$$L_3 L_\pm |Q, m\rangle = (m \pm 1) L_\pm |Q, m\rangle, \tag{3.23}$$

$$L^2 L_\pm |Q, m\rangle = Q L_\pm |Q, m\rangle. \tag{3.24}$$

Therefore, we may obtain a set of states by raising and lowering the eigenvalue m in unit steps if acting the ladder operators $L_\pm$ on a given state $|Q, m_0\rangle$ till the coefficients A_{Qm} or B_{Qm} is equivalent to zero,

$$L_+|Q, m - 1\rangle = A_{Qm}|Q, m\rangle, \quad m > m_0, \tag{3.25}$$

$$L_-|Q, m\rangle = B_{Qm}|Q, m - 1\rangle, \quad m \leq m_0. \tag{3.26}$$

It should be noted that these states are the common eigenfunctions of the operators L^2 and L_3. When $m > m_0$, we obtain the following expression

$$\begin{aligned} L^2|Q, m - 1\rangle &= [\sigma L_- L_+ + L_3(L_3 + 1)]|Q, m - 1\rangle \\ &= \sigma A_{Qm} L_-|Q, m\rangle + (m^2 - m)|Q, m - 1\rangle \\ &= Q|Q, m - 1\rangle, \end{aligned} \tag{3.27}$$

from which, together with (3.26), we have

$$\begin{aligned} A_{Qm}B_{Qm} &= \sigma(Q - m^2 + m) \\ &= \sigma(j + m)(j - m + 1), \end{aligned} \tag{3.28}$$

which also holds for $m \leq m_0$.

We find that the state $|Q, m\rangle$ is determined by Eqs. (3.25) and (3.26). As we know, the coefficients A_{Qm} and B_{Qm} can be changed with the arbitrarily multiplying constant appearing in the front of the state $|Q, m\rangle$, but this state is also the eigenfunction of the operators $L_+ L_-$ and $L_- L_+$, whose eigenvalues are $A_{Qm}B_{Qm}$ and $A_{Q(m+1)}B_{Q(m+1)}$, respectively.

Now, let us briefly review the irreducible representations of the Lie algebras so(2, 1) and so(3) [169]. In general, there exist four kinds of irreducible representations except for the identity representation such as the unbounded spectrum

$D(Q, m_0)$, spectrum bounded below $D^+(j)$, spectrum bounded above $D^-(j)$ and bounded spectrum $D(j)$.

- **Unbounded spectrum** $D(Q, m_0)$: If $j \pm m_0 \neq$ integer, the parameter m_0 is continuous and can be uniquely chosen so that we have $m_0 \in [-\frac{1}{2}, \frac{1}{2})$. Thus, each such m_0 will give a different L_3 eigenvalue spectrum. On the other hand, from (3.28) we may take $A_{Qm} = B_{Qm} = [\sigma(j + m)(j - m + 1)]^{\frac{1}{2}}$ for convenience, then the coefficients A_{Qm} and B_{Qm} are not equivalent to zero for $j \neq \pm m$. Therefore, we have

$$m = m_0 \pm k, \quad m_0 \in [-1/2, 1/2), \quad j \pm m_0 \neq \text{integer}, \qquad (3.29)$$

  where k is a non-negative integer.

- **Spectrum bounded below** $D^+(j)$: If acting the lowering operator L_- on the state $|Q, m\rangle$, we have $L_-|Q, m\rangle = 0$ for some m, but $L_+|Q, m\rangle \neq 0$ for any m, then we may obtain infinite dimensional irreducible representations, whose L_3 eigenvalue spectra are bounded from below. In mathematical language, we have

$$m = -j + k, \quad 2j \neq 0, 1, 2, \dots. \qquad (3.30)$$

- **Spectrum bounded above** $D^-(j)$: This case is similar to the spectrum bounded below $D^+(j)$ except that the L_3 spectrum is bounded above, i.e.,

$$m = j - k, \quad 2j \neq 0, 1, 2, \dots. \qquad (3.31)$$

- **Bounded spectrum** $D(j)$: Combining the spectrum bounded below $D^+(j)$ and spectrum bounded above $D^-(j)$, we obtain finite dimensional irreducible representations denoted by $D(j)$ with L_3 spectrum $m = -j + k$, where $0 \leq k \leq 2j = 0, 1, 2, \dots$. They are the only finite dimensional irreducible representations, i.e.,

$$m = -j + k, \quad 0 \leq k \leq 2j = 0, 1, 2, \dots. \qquad (3.32)$$

It should be pointed out that these classifications apply to both Lie algebras so(2, 1) and so(3). Also, we find that in the bounded spectrum $D(j)$ case, j can be an integer or a half-odd integer. For the latter case, we are really studying the Lie algebras su(1, 1) or su(2) of the special unitary groups SU(1, 1) and SU(2), respectively, because we can only have the integer values of the angular momentum for the three-dimensional rotation group SO(3).

For simplicity, we summarize the classifications of the irreducible representations of so(2, 1) as follows (see Table 3.1):

Table 3.1.   Classifications of irreducible representations of Lie algebras so(2, 1) and so(3), where k is a non-negative integer.

$D(Q, m_0)$	$m = m_0 \pm k, m_0 \in [-\frac{1}{2}, \frac{1}{2})$	$j \pm m_0 \neq$ integer
$D^+(j)$	$m = -j + k$	$2j \neq 0, 1, 2, \ldots$
$D^-(j)$	$m = j - k$	$2j \neq 0, 1, 2, \ldots$
$D(j)$	$m = -j + k$	$0 \leq k \leq 2j = 0, 1, 2, \ldots$

8.   Irreducible unitary representations

We now study the irreducible unitary representations of the Lie groups due to their applications in physics. This requires that the representation matrices of operators L_+ and L_- are mutually conjugate matrices.

Since the representation matrices of the operators L_i and L^2 are Hermitian so both Q and m are real numbers. This leads to the following two restrictions on the general irreducible representations:

- Q and m must be real eigenvalues,

- L_+L_- and L_-L_+ are positive definite Hermitian operators, then their eigenvalues must be non-negative real numbers.

The first restriction implies that m_0 is real and either j is real or $j = -\frac{1}{2} + i\alpha(\alpha \neq 0)$ in terms of Eq. (3.22). On the other hand, it is shown from the second restriction and Eqs. (3.18) and (3.28) that

$$\sigma(Q - m^2 \pm m) = \sigma(j \pm m)(j \mp m + 1) \geq 0, \qquad (3.33)$$

which must be satisfied by any irreducible unitary representation. The sign of these inequalities is different for so(2, 1) ($\sigma = -1$) and so(3) ($\sigma = 1$). In other words, for different σ the parameters j and m of two Lie algebras so(3) and so(2, 1) are different. The relation (3.33) can be illustrated conveniently by the graph in Fig. 8.2, where the regions in the (j, m) plane are bounded by the lines $j \mp m = 0$ and $j \pm m + 1 = 0$. The regions for these two Lie algebras are denoted in this figure. Here we shall consider so(3) and so(2, 1) separately as done by Adams, Čižek and Paldus [169].

As far as the irreducible unitary representations of the Lie algebra so(3), the case $j = -\frac{1}{2} + i\alpha$ is impossible. This is because $Q = j(j + 1) < -\frac{1}{4}$, the fundamental inequalities (3.33) cannot be satisfied for real m and α. Thus, j must be real and it follows that equation (3.33) can be satisfied only for a finite number of values of m. The L_3 eigenvalue spectra lie on the region above the m axis, they start on the lines $j \pm m = 0$. From Fig. 8.2, it is

clear that for each eigenvalue spectrum in the so(3) region below the m axis, there is an identical one in the upper so(3) region, i.e., they start on the lines $j \mp m + 1 = 0$. The corresponding irreducible unitary representations $D(j)$ and $D(-j-1)$ are equivalent because they have the same L_3 eigenvalue spectrum so that a complete set of inequivalent irreducible unitary representations is given, e.g., by those corresponding to the upper so(3) region only. Therefore, we say that the irreducible unitary representations of the Lie algebraso(3) are finite dimensional,

$$|m| \leq j, \quad 2j = 0, 1, 2, \ldots. \tag{3.34}$$

We now study the irreducible unitary representations of the Lie algebra so(2, 1). For this Lie algebra, the situation is different from that of the so(3). It is shown that there are four series of irreducible unitary representations for the su(1, 1) Lie algebra except for the identity representation [169].

For the irreducible unitary representations of types $D^+(j)$ and $D^-(j)$ given in Table. 3.2, for simplicity, the fundamental inequalities can only be satisfied for $j < 0$. For example, for the irreducible unitary representations of type $D^+(j)$, the L_3 eigenvalue spectra start on the line OA in Fig. 8.2 and extend in unit steps to the right into the allowed region AEB. In a similar way, for the irreducible unitary representations of type $D^-(j)$, the L_3 eigenvalue spectra start on the line OF and extend to the left into the allowed region CGF.

The irreducible unitary representations of the so(2, 1) having unbounded L_3 eigenvalues spectra are from the general class $D(Q, m_0)$ given by $D^\pm(j)$. In general, they can be divided into two types: supplementary series of irreducible unitary representations $D_s(Q, m_0)$ and the principal series $D_p(Q, m_0)$. The supplementary series arise for $-1 < j < 0$ and $m_0 \in [-\frac{1}{2}, \frac{1}{2}]$. For this case, j and m_0 lie within the diamond-shaped region OBDC in Fig. 8.2. The boundaries of this region cannot be included because $j + m_0$ is not equal to an integer. The interior of this region can be concisely described by either of the inequalities $|j + \frac{1}{2}| < \frac{1}{2} - |m_0|$ and $Q < |m_0|(|m_0| - 1)$, and it also follows that $-\frac{1}{4} < Q < 0$. If starting at an arbitrary point in this region, the operator L_3 eigenvalue spectrum extends in unit steps to the right and left into the allowed regions CFG and AEB. Finally, the principal series $D_p(Q, m_0)$ arises for $j = -\frac{1}{2} + i\alpha$ and $m_0 \in (-\frac{1}{2}, \frac{1}{2})$. In this case, we have $Q = -\alpha^2 - \frac{1}{4} < -\frac{1}{4}$. Therefore, for any such m_0 on the line segment CB in Fig. 3.1, the operator L_3 eigenvalue spectrum extends to the left and right along the dashed line and each inequivalent irreducible unitary representation of this type is characterized by α^2 and m_0.

For any irreducible unitary representations of so(2, 1) of types $D^\pm(j)$ or $D_s(Q, m_0)$, the dashed line $j = -\frac{1}{2}$ is a line of symmetry dividing the allowed regions into two parts. For any such irreducible unitary representation there is an equivalent one on the opposite side of this line with the same L_3 eigenvalue

spectrum. Hence, there are a few ways to describe a complete set of inequivalent irreducible unitary representations of each type. For instance, for type $D^+(j)$ we can choose a) all $D^+(j)$ with spectra starting on OA, b) all $D^+(-j-1)$ with spectra starting on DE and c) all $D^+(-j-1)$ with spectra starting on DB and all $D^+(j)$ starting on BA, or d) all $D^+(j)$ with spectra beginning on OB and all $D^+(-j-1)$ beginning on BE. In a similar way, we may choose lines OF, DG, DCF or OCG for type $D^-(j)$. However, for type $D_s(Q, m_0)$ we may choose either those arising from the triangle OCB or those from the triangle BDC.

To summarize, we classify the eigenvalue spectra and irreducible unitary representations of the so(2, 1) as follows (see Table 3.2):

Table 3.2. Classifications of irreducible unitary representations of the Lie algebras so(2, 1), where k is a non-negative integer.

identify representation	$Q = 0$	$m = j = 0$
$D^+(j)$	$j < 0$	$m = -j + k$
$D^-(j)$	$j < 0$	$m = j - k$
$D_S(Q, m_0)$	$-\frac{1}{4} \leq Q < 0$	$m = m_0 \pm k, Q < |m_0|(|m_0| - 1)$
$D_p(Q, m_0)$	$\alpha > 0, Q = -\frac{1}{4} - \alpha^2$	$m = m_0 \pm k, m_0 \in (-\frac{1}{2}, \frac{1}{2})$

9.   Concluding remarks

In this Chapter we have given a basic review for some basic properties of the Lie groups SU(2) and SU(1, 1) as well as their corresponding Lie algebras in order to apply them in the successive Chapters. In particular, we have paid much attention to the non-compact Lie group SU(1, 1) and its Lie algebra su(1, 1), as well as their irreducible unitary representations, since the bound states of many quantum systems can be described by its irreducible unitary representations. To illustrate the differences between the compact Lie algebra su(2) and non-compact Lie algebra su(1, 1), we have demonstrated them in Fig. 8.2. The more information about the properties of the Lie groups and Lie algebras, in particular the SU(2) and SO(2, 1) groups as well as their corresponding Lie algebras can refer to the textbooks [10, 117, 169, 183, 208].
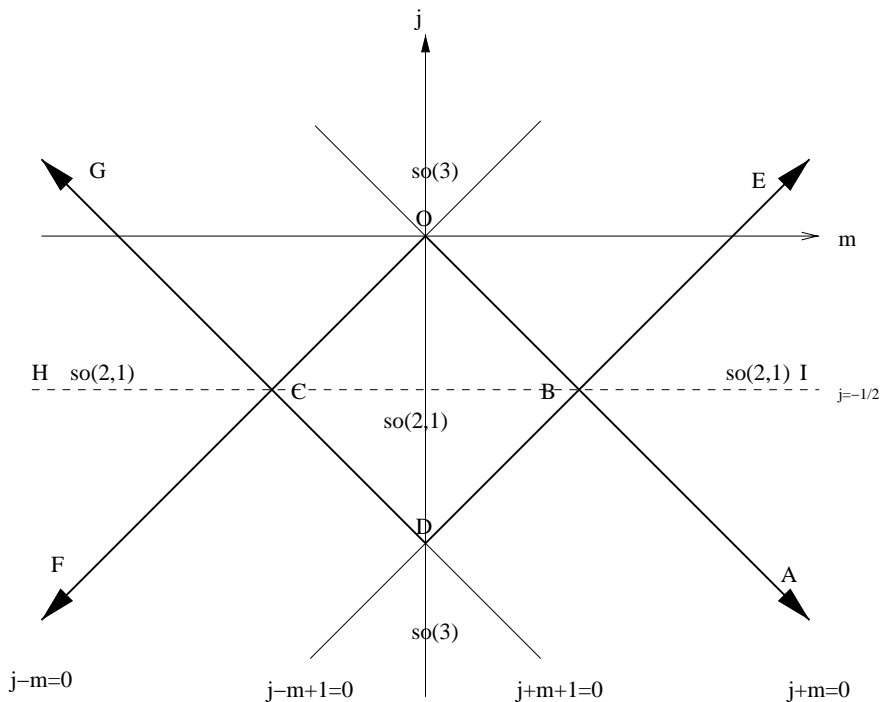
Figure 3.1. The change regions of parameters j and m for the irreducible unitary representations of the Lie algebras so(3) and so(2, 1).

Notes

1 For example, the particle physicists use the compact Lie group SU(3) to classify elementary particles. Throughout the 1960s, in order to explain the ever-growing number of subatomic particles which were observed in experiments, theoretical physicists considered the possibility that protons and neutrons were composed of smaller units of matter. Based on the symmetry group SU(3) which describes strongly interacting particles in terms of building blocks, Gell-Mann and Ne'eman proposed a particle classification scheme called "the Eightfold Way" in 1961 [176]. Three years later, Gell-Mann introduced the concept of quarks as a physical basis for the scheme, adopting the fanciful term from a passage in James Joyce's novel "Finnegans Wake" [177]. It should be noted that another American physicist George Zweig developed a similar theory independently in 1964 and called his fundamental particles "aces" [178–180].

2 Gell-Mann's physical model provided a simple picture in which all mesons
   are shown as consisting of a quark and an antiquark and all baryons as
   composed of three quarks. It postulated the existence of three types of
   quarks, distinguished by distinctive "flavors". These three quark types are
   now commonly designated as "u" (up) quark, "d" (down) quark, and "s"
   (strange) quark. Each carries a fractional electric charge (i.e., a charge less
   than that of the electron). The "u" and "d" quarks are thought to make up
   protons and neutrons and are thus the ones observed in ordinary matter. The
   "s" quarks occur as components of K mesons and various other extremely
   short-lived subatomic particles which were first observed in cosmic rays
   but which play no part in ordinary matter. Theoretical physicists consider
   the Lie group SU(3) as the internal symmetry of hadrons. Its fundamental
   representation is a triplet. The simplest possibility consists of a triplet with
   spin $\frac{1}{2}$, baryon number $\frac{1}{3}$, and containing a strong-isospin doublet with
   electric charges $\frac{2}{3}$ and $\frac{1}{3}$ as well as a singlet with electric charge $-\frac{1}{3}$. Baryons
   and mesons are arranged in those multiplets of SU(3) that the products
   $3 \otimes 3 \otimes 3$ and $3 \otimes \overline{3}$ of the triplet 3 and its conjugate $\overline{3}$ decompose to:
   $3 \otimes 3 \otimes 3 = 1 \oplus 8 \oplus 8 \oplus 10$ and $3 \otimes \overline{3} = 1 \oplus 8$. The introduction of SU(3)$_F$
   as an internal flavor symmetry and its fundamental representation of 3 quarks
   brought great simplification and some understanding to the known baryons
   and mesons. We suggest the reader to consult the textbooks [181–183] for
   more information on the classifications of the elementary particles with the
   aid of the powerful group theory mathematical tool.

PART III

APPLICATIONS IN NON-RELATIVISTIC
QUANTUM MECHANICS

Chapter 4

HARMONIC OSCILLATOR

1.   Introduction

It is well known that the quantum harmonic oscillator is the analogue of the classical harmonic oscillator. It is one of the most important model systems in quantum mechanics [215, 216]. There are several reasons for its pivotal role. First, it represents one of few quantum mechanical systems for which the simple exact solutions are known. Second, as in classical mechanics, a wide variety of physical situations can be reduced to it either exactly or approximately. In particular, more complicated quantum systems can always be analyzed in terms of normal modes[1] of motion whenever the interaction forces are linear functions of the relative displacements. Therefore, it is not surprising that the one-dimensional harmonic oscillator has become very important for the quantum mechanical treatment of such physical problems as the vibrations of individual atoms in molecules and in crystals, in which the linear harmonic oscillator describes vibrations in molecules and their counterparts in solids, the phonons. Third, the most eminent role of the harmonic oscillator is its linkage to the boson, one of the conceptual building blocks of microscopic physics. For example, bosons describe the modes of the electromagnetic field, providing the basis for its quantization. Even though the linear harmonic oscillator may represent rather non-elementary objects like a solid and a molecule, it provides a window into the most elementary structure of the physical world. The most likely reason for this connection with fundamental properties of matter is that the harmonic oscillator Hamiltonian is symmetric in momentum and position, both operators appearing as quadratic terms. On the other hand, the harmonic oscillator also provides the key to the quantum theory of the electromagnetic field, whose vibrations in a cavity can be analyzed into harmonic normal modes, each of which has energy levels of the harmonic oscillator type.

2.   **Exact solutions**

For completeness we briefly study the exact solutions of the harmonic oscillator quantum system by solving the second-order differential equation even though such an investigation can be found in almost all quantum mechanical textbooks.

For a given harmonic oscillator

$$V(x) = \frac{1}{2}m\omega^2 x^2, \tag{4.1}$$

where m and ω represent the mass of the particle and the frequency of the oscillator.

The Schrödinger equation with the harmonic oscillator is given by

$$H\Phi(x) = -\frac{\hbar^2}{2m}\frac{d^2\Phi(x)}{dx^2} + \frac{1}{2}m\omega^2 x^2\Phi(x) = E\Phi(x). \tag{4.2}$$

In general, it is convenient to deal with such a differential equation by rewriting it in dimensionless form. For this purpose, we introduce the following dimensionless parameters

$$\xi = \alpha x, \quad \tau = \frac{2E}{\hbar\omega}, \quad \alpha = \sqrt{\frac{m\omega}{\hbar}}. \tag{4.3}$$

Substitution of them into Eq. (4.2) allows us to obtain

$$\frac{d^2\Phi(\xi)}{d\xi^2} + (\tau - \xi^2)\Phi(\xi) = 0. \tag{4.4}$$

From the behaviors of the wave functions at the origin and at infinity, we take the following ansatz for the wave functions

$$\Phi(\xi) = e^{-\frac{1}{2}\xi^2}H(\xi). \tag{4.5}$$

Substituting this equation (4.5) into (4.4) yields the following equation for $H(\xi)$

$$\frac{d^2H(\xi)}{d\xi^2} - 2\xi\frac{dH(\xi)}{d\xi} + (\tau - 1)H(\xi) = 0, \tag{4.6}$$

whose solutions are nothing but the Hermite polynomials $H_n(\xi)$ with the following relation

$$\tau - 1 = 2n, \qquad n = 0, 1, 2, 3, \ldots, \tag{4.7}$$

from which we can obtain the eigenvalues as

$$E_n = \hbar\omega\left(n + \frac{1}{2}\right). \tag{4.8}$$

The corresponding eigenfunctions of this quantum system can be written as

$$\Phi_n(x) = N_n e^{-\frac{1}{2}\alpha^2 x^2} H_n(\alpha x), \tag{4.9}$$

where the normalization constant N_n can be derived by the normalization condition

$$\int_{-\infty}^{\infty} |\Phi_n(x)|^2 dx = 1 \tag{4.10}$$

as

$$N_n = \left(\frac{\alpha}{\pi^{\frac{1}{2}} 2^n n!} \right)^{\frac{1}{2}}. \tag{4.11}$$

3. Ladder operators

Before introducing how to construct the ladder operators for the harmonic oscillator in terms of our new approach, let us show the traditional method to establish the ladder operators as shown in almost all quantum mechanics textbooks. In general, the creation and annihilation operators $a^\dagger$ and a are defined directly from the given Hamiltonian (4.2) as

$$a^\dagger = \frac{1}{\sqrt{2}} \left(x - \frac{d}{dx} \right), \quad a = \frac{1}{\sqrt{2}} \left(x + \frac{d}{dx} \right), \tag{4.12}$$

where the natural units $m = \hbar = \omega = 1$ are taken for simplicity if not stated otherwise.

However, the reader will ask why the creation and annihilation operators of the harmonic oscillator are taken as the forms of the expressions (4.12). In theory, they can be obtained from the standard factorization method. The advantage of this approach is that we need not know what are the exact solutions of this quantum system.

To make the reader clearly know how to obtain the results (4.12), we are going to consider this problem following our approach, i.e. we can construct the ladder operators by first acting the first order differential operator d/dx on the harmonic oscillator wave functions $\Phi_n(x)$ and then using the recurrence relations among the Hermite polynomials.

For this purpose, by acting the differential operator d/dx on the wave functions $\Phi_n(x)$ given in Eq. (4.9), we have

$$\frac{d\Phi_n(x)}{dx} = -x\,\Phi_n(x) + N_n e^{-\frac{1}{2}x^2} \frac{d}{dx} H_n(x). \tag{4.13}$$

Consider the recurrence relations among the Hermite polynomials $H_n(x)$

$$\frac{d}{dx} H_n(x) = 2n\,H_{n-1}(x), \tag{4.14}$$

$$2x\, H_n(x) = 2n\, H_{n-1}(x) + H_{n+1}(x). \tag{4.15}$$

Substitutions of them into Eq. (4.13) allow us to obtain the following expressions

$$\left(\frac{d}{dx} + x\right) \Phi_n(x) = 2n \frac{N_n}{N_{n-1}} \Phi_{n-1}(x), \tag{4.16}$$

$$\left(-\frac{d}{dx} + x\right) \Phi_n(x) = \frac{N_n}{N_{n+1}} \Phi_{n+1}(x). \tag{4.17}$$

If considering the normalization constant N_n given in Eq. (4.11), we have

$$\frac{1}{\sqrt{2}} \left(-\frac{d}{dx} + x\right) \Phi_n(x) = \sqrt{n+1} \Phi_{n+1}(x), \tag{4.18}$$

$$\frac{1}{\sqrt{2}} \left(\frac{d}{dx} + x\right) \Phi_n(x) = \sqrt{n} \Phi_{n-1}(x), \tag{4.19}$$

from which we may define the creation and annihilation operators exactly as those (4.12) with the following properties

$$a^\dagger\, \Phi_n(x) = \sqrt{n+1} \Phi_{n+1}(x), \tag{4.20}$$

$$a\, \Phi_n(x) = \sqrt{n} \Phi_{n-1}(x). \tag{4.21}$$

The corresponding Hamiltonian can be simply expressed as

$$H = \left(a^\dagger a + \frac{1}{2}\right) = \left(\hat{N} + \frac{1}{2}\right), \tag{4.22}$$

where we have introduced the number operator

$$\hat{N} = a^\dagger a, \tag{4.23}$$

which is clearly positive and Hermitian. It has the property

$$\hat{N} \Phi_n(x) = n\, \Phi_n(x). \tag{4.24}$$

The commutation relations among $\hat{N}$, $a^\dagger$ and a are given by

$$[a, a^\dagger] = 1, \quad [\hat{N}, a] = -a, \quad [\hat{N}, a^\dagger] = a^\dagger, \tag{4.25}$$

where we have used the formula for the operators A, B and C

$$[AB, C] = A[B, C] + [A, C]B. \tag{4.26}$$

It is found that Eq. (4.25) is the well known Weyl-Heisenberg algebra $\mathcal{H}_2$. On the other hand, based on the commutation relations (4.25), we can obtain the following two useful formulas

$$\hat{N} a = a(\hat{N} - 1), \qquad \hat{N} a^\dagger = a^\dagger (\hat{N} + 1). \qquad (4.27)$$

Repeated use of the relations (4.27) allows us to obtain

$$\hat{N} a^j = a^j (\hat{N} - j), \qquad \hat{N} a^{\dagger j} = a^{\dagger j} (\hat{N} + j), \quad j = 0, 1, 2, \ldots, \qquad (4.28)$$

which can be proved as follows:

$$
\begin{aligned}
[\hat{N}, a^j]\phi &= a[\hat{N}, a^{j-1}]\phi + [\hat{N}, a]a^{j-1}\phi \\
&= a\{a[\hat{N}, a^{j-2}] + [\hat{N}, a]a^{j-2}\}\phi + [\hat{N}, a]a^{j-1}\phi \\
&= \ldots = a\{a^{j-2}[\hat{N}, a] + \ldots + [\hat{N}, a]a^{j-2}\}\phi + [\hat{N}, a]a^{j-1}\phi \\
&= a[-(j-1)a^{j-1}]\phi - a^j\phi \\
&= -ja^j\phi,
\end{aligned}
\qquad (4.29)
$$

$$
\begin{aligned}
[\hat{N}, a^{\dagger j}]\phi &= a^\dagger[\hat{N}, a^{\dagger(j-1)}]\phi + [\hat{N}, a^\dagger]a^{\dagger(j-1)}\phi \\
&= a^\dagger\{a^\dagger[\hat{N}, a^{\dagger(j-2)}] + [\hat{N}, a^\dagger]a^{\dagger(j-2)}\}\phi + [\hat{N}, a^\dagger]a^{\dagger(j-1)}\phi \\
&= \ldots = a^\dagger\{a^{\dagger(j-2)}[\hat{N}, a^\dagger] + \ldots + [\hat{N}, a^\dagger]a^{\dagger(j-2)}\}\phi \\
&\quad + [\hat{N}, a^\dagger]a^{\dagger(j-1)}\phi \\
&= a^\dagger[(j-1)a^{\dagger(j-1)}]\phi + a^{\dagger j}\phi \\
&= ja^{\dagger j}\phi,
\end{aligned}
\qquad (4.30)
$$

from which we obtain Eq. (4.28).

Similarly, we can obtain another useful formula

$$a^{\dagger j} a^j = \hat{N}(\hat{N} - 1)(\hat{N} - 2)\ldots(\hat{N} - [j-1]), \quad j \geq 1. \qquad (4.31)$$

The obvious positive nature number of the left side of equation (4.31) for all j rules out the possibility that the number operator $\hat{N}$ has any continuous distribution for its energy levels.

Here we want to make a remark about equation (4.22). As we know, the Hamiltonian H can be expressed by number operator $\hat{N} = a^\dagger a$. Our question is what the operator $aa^\dagger$ is. We want to answer it from another starting point

by acting this operator on the arbitrary wave function $f(x)$. If so, we have

$$
\begin{aligned}
(aa^\dagger)f(x) &= a\,\frac{1}{\sqrt{2}}\left(x - \frac{d}{dx}\right)f(x)\\
&= \frac{1}{2}\left(x + \frac{d}{dx}\right)\left[xf(x) - \frac{df(x)}{dx}\right]\\
&= \frac{1}{2}\left(-\frac{d^2}{dx^2} + x^2 + 1\right)f(x),
\end{aligned}
\tag{4.32}
$$

from which we have

$$
aa^\dagger = \frac{1}{2}\left(-\frac{d^2}{dx^2} + x^2\right) + \frac{1}{2}.
\tag{4.33}
$$

This means that

$$
\left(aa^\dagger - \frac{1}{2}\right)\Phi_n(x) = E_n\Phi_n(x).
\tag{4.34}
$$

Likewise, we have

$$
a^\dagger a = \frac{1}{2}\left(-\frac{d^2}{dx^2} + x^2\right) - \frac{1}{2},
\tag{4.35}
$$

which implies that

$$
\left(aa^\dagger + \frac{1}{2}\right)\Phi_n(x) = E_n\Phi_n(x),
\tag{4.36}
$$

which coincides with the result (4.22).

On the other hand, from Eqs. (4.33) and (4.35) we are able to obtain

$$
aa^\dagger - a^\dagger a = [a, a^\dagger] = 1,
\tag{4.37}
$$

which is consistent with the result (4.25).

Let us analyze the properties of the harmonic oscillator wave functions in terms of Eqs. (4.16)- (4.19). It is known from Eq. (4.19) that the normalized solution of ground state is calculated as

$$
\Phi_0(x) = \sqrt{\frac{1}{\pi^{1/2}}}\,\exp\left(-\frac{1}{2}x^2\right),
\tag{4.38}
$$

where the factor $\alpha = 1$ is taken. If substituting Eq. (4.38) into Eq. (4.17), we find

$$
\Phi_1(x) = \sqrt{\frac{2}{\pi^{1/2}}}\,x\exp\left(-\frac{1}{2}x^2\right).
\tag{4.39}
$$

Therefore, it is found that the ground state $\Phi_0(x)$ and the first excited state $\Phi_1(x)$ are even and odd functions of the variable x, respectively. That is to say, they are eigenfunctions of the parity with eigenvalues $+1$ and -1. Generally speaking, equations (4.18) and (4.19) transform between eigenfunctions of opposite parity.

In fact, we can consider the transformations between states of the same parity [101]. This can be performed by applying Eq. (4.18) to Eq. (4.38), i.e.,

$$\Phi_n(x) = \frac{1}{\sqrt{\pi^{1/2}2^n n!}} \left(x - \frac{d}{dx} \right)^n \exp\left(-\frac{1}{2}x^2 \right). \tag{4.40}$$

Making use of the following identity

$$\left(x - \frac{d}{dx} \right) g(x) = -e^{\frac{1}{2}x^2} \frac{d}{dx} e^{-\frac{1}{2}x^2} g(x), \tag{4.41}$$

we may obtain the following result

$$\left(x - \frac{d}{dx} \right)^n g(x) = (-1)^n e^{\frac{1}{2}x^2} \frac{d^n}{dx^n} e^{-\frac{1}{2}x^2} g(x). \tag{4.42}$$

From Eqs. (4.40) and (4.42), we have

$$\Phi_n(x) = \frac{1}{\sqrt{\pi^{1/2}2^n n!}} \exp\left(-\frac{1}{2}x^2 \right) H_n(x), \tag{4.43}$$

where we have used the definition of the Hermite polynomials

$$H_n(x) = (-1)^n e^{x^2} \frac{d^n}{dx^n} e^{-x^2}. \tag{4.44}$$

Based on the relations between the Hermite polynomial and confluent hypergeometric functions.

$$H_{2n}(x) = (-1)^n \frac{(2n)!}{n!} F\left(-n, \frac{1}{2}; x^2 \right), \tag{4.45}$$

$$H_{2n+1}(x) = (-1)^n 2x \frac{(2n+1)!}{n!} F\left(-n, \frac{3}{2}; x^2 \right), \tag{4.46}$$

we are able to obtain the even and odd functions of the harmonic oscillator as following [101]

$$\Phi_{2n}(x) = (-1)^n \sqrt{\frac{(2n)!}{\pi^{1/2}2^{2n}(n!)^2}} e^{-\frac{1}{2}x^2} F\left(-n, \frac{1}{2}, x^2 \right), \tag{4.47}$$

$$\Phi_{2n+1}(x) = (-1)^n x \sqrt{\frac{(2n+1)!}{\pi^{1/2}2^{2n-1}(n!)^2}} e^{-\frac{1}{2}x^2} F\left(-n, \frac{3}{2}, x^2 \right), \tag{4.48}$$

where $n = 0, 1, 2, \ldots$. It should be noted that this method for determining the normalized wave functions can be used to study other physical problems.

4.   Bargmann-Segal transform

In this section we review the Bargmann-Segal transformation for the harmonic oscillator. Fock proposed an operator solution to the commutation relation $[a, a^\dagger] = 1$ almost 80 years ago [217], where the operator a and $a^\dagger$ refer to the annihilation and creation operators related to the harmonic oscillator. This solution can be formulated in the field of the complex numbers z if one considers

$$\left[\frac{d}{dz}, z\right] = 1, \tag{4.49}$$

from which we have the following transformation

$$z \rightarrow a^\dagger, \qquad \frac{d}{dz} \rightarrow a. \tag{4.50}$$

As a result, the Hamiltonian written in the second quantization language (4.22) can be transformed to the Bargmann-Segal space by applying this rule. For example, the harmonic oscillator Hamiltonian (4.22) can be transformed as

$$H = z\frac{d}{dz} + \frac{1}{2}, \tag{4.51}$$

whose eigenfunctions can be easily obtained as

$$\phi_n(z) = z^n, \tag{4.52}$$

with the following property

$$H\phi_n(z) = \left(n + \frac{1}{2}\right)\phi_n(z) = E_n\phi_n(z). \tag{4.53}$$

It should be noted that the quantization arises not from a boundary condition as in the configuration space[2] but from the analysis of the complex variable function. The rigorous mathematical justification of the transformation rule has been studied quite well by Bargmann, Segal and Cook [218–220]. Recently, Palma *et al.* have employed this property to study the harmonic oscillator Floquet states in the Bargmann-Segal space [221, 222]. They used the second quantization algebraic technique to obtain the Floquet quasienergies and eigenfunctions for a particle in the harmonic oscillator potential when the particle is simultaneously subjected to a monochromatic electric field.

5.   Single mode realization of dynamic group SU(1, 1)

As shown above, the Hamiltonian H and the creation and annihilation operators $a^\dagger$, a and unit one 1 form a closed Lie algebra, which makes it possible to find the spectrum of the Hamiltonian H and gives the dynamic group of the

harmonic oscillator. Because the four parameter Lie group obtained in this way has a complicated structure, Barut constructed the dynamic algebra in a simpler way based on the following operators [223]:

$$L_+ = \sqrt{\hat{N}} a^\dagger, \quad L_- = a\sqrt{\hat{N}}, \quad L_0 = H = \hat{N} + \frac{1}{2}, \qquad (4.54)$$

which satisfy the following commutation relations

$$[L_0, L_\pm] = \pm L_\pm, \quad [L_-, L_+] = 2L_0, \qquad (4.55)$$

which correspond to the commutation relations of the generators of an non-compact Lie algebra su(1, 1).

The Casimir operator in this case can be calculated as

$$\begin{aligned} C &= L_+ L_- - L_0(L_0 - 1) \\ &= L_- L_+ - L_0(L_0 + 1) \\ &= \frac{1}{4}. \end{aligned} \qquad (4.56)$$

On the other hand, Goshen and Lipkin studied this problem from another approach [224]. They have found that the operators $(a^\dagger)^2$, a^2 and $a^\dagger a$ satisfy the following commutation relations

$$[a^\dagger a, (a^\dagger)^2] = 2(a^\dagger)^2, \quad [a^\dagger a, a^2] = -2a^2, \quad [a^2, (a^\dagger)^2] = 2 + 4a^\dagger a. \ (4.57)$$

However, upon introducing the following set of operators

$$L_+ = \frac{1}{2}(a^\dagger)^2, \quad L_- = \frac{1}{2}a^2, \quad L_3 = \frac{1}{4}(1 + 2a^\dagger a), \qquad (4.58)$$

we find that they satisfy the commutation relations of the su(1, 1) algebra, i.e.

$$[L_+, L_-] = -2L_3, \quad [L_3, L_\pm] = \pm L_\pm. \qquad (4.59)$$

As we know, there are four irreducible representations of the non-compact Lie algebra su(1, 1) as shown in Chapter 3. Since there exists the ground state for the harmonic oscillator, this system corresponds to the irreducible representation $D^+(j)$ of the su(1, 1) with the eigenvalues of the operator L_0 that are bounded below and equal to $n - j = n + \frac{1}{2}$ ($j = -\frac{1}{2}$). Therefore, all levels of the linear oscillator realize one irreducible representation of the non-compact Lie algebra su(1, 1).

6.   Matrix elements

In this section we study the matrix elements of some related physical functions as done in our previous work [105, 106, 161]. It is shown from Eqs. (4.12) that the related physical functions x and d/dx can be expressed as

$$x = \frac{1}{\sqrt{2}}(a^\dagger + a),\tag{4.60}$$

$$\frac{d}{dx} = \frac{1}{\sqrt{2}}(a - a^\dagger),\tag{4.61}$$

from which, together with the results (4.20) and (4.21), we can obtain their analytical matrix elements

$$
\begin{aligned}
\langle m|x|n\rangle &\equiv \int_{-\infty}^{\infty} u_m(x)\, x\, \Phi_n(x)dx \\
&= \frac{1}{\sqrt{2}}(\sqrt{n+1}\,\delta_{m,n+1} + \sqrt{n}\,\delta_{m,n-1}),
\end{aligned}\tag{4.62}
$$

$$
\begin{aligned}
\langle m|\tfrac{d}{dx}|n\rangle &\equiv \int_{-\infty}^{\infty} u_m(x)\frac{d}{dx}\Phi_n(x)dx \\
&= \frac{1}{\sqrt{2}}(\sqrt{n}\,\delta_{m,n-1} - \sqrt{n+1}\,\delta_{m,n+1}),
\end{aligned}\tag{4.63}
$$

which are consistent with the conclusions $\langle m|x|m\rangle = 0$ and $\langle m|d/dx|m\rangle = 0$. If introducing the momentum operator $p = -i\hbar\frac{d}{dx}$, we may know its analytical matrix element immediately.

In addition, we find that the eigenfunctions of the harmonic oscillator can be simply obtained by acting the creation operator $a^\dagger$ on the ground state $\Phi_0(x)$

$$\Phi_n(x) = \frac{1}{\sqrt{n!}}(a^\dagger)^n\Phi_0(x),\tag{4.64}$$

which can also be simply obtained from Eq. (4.40). On the other hand, from this equation we may obtain two important useful formulas

$$
\begin{aligned}
a^m|n\rangle &= \frac{\sqrt{n!}}{(n-m)!}(a^\dagger)^{n-m}|0\rangle \\
&= \sqrt{\frac{n!}{(n-m)!}}\,|n-m\rangle,
\end{aligned}\tag{4.65}
$$

and

$$
\begin{aligned}
(a^\dagger)^m|n\rangle &= \frac{(a^\dagger)^{n+m}}{\sqrt{n!}}|0\rangle \\
&= \sqrt{\frac{(n+m)!}{n!}}\,|n+m\rangle,
\end{aligned}\tag{4.66}
$$

which are helpful in the calculation of matrix element. It is shown from Eq. (4.64) that all states of this quantum system can be easily obtained from the fundamental ground state by successively applying $a^\dagger$ on the ground state.

Finally, if taking the summation and subtraction between the formulas (4.18) and (4.19), we have

$$\sqrt{2}x\Phi_n(x) = \sqrt{n+1}\Phi_{n+1}(x) + \sqrt{n}\Phi_{n-1}(x), \tag{4.67}$$

$$\sqrt{2}\frac{d}{dx}\Phi_n(x) = -\sqrt{n+1}\Phi_{n+1}(x) + \sqrt{n}\Phi_{n-1}(x). \tag{4.68}$$

As shown above, we find that the present approach can be more easily accepted by the beginner and/or common reader than the traditional factorization method. Thus, they may know the reason why the creation and annihilation operators can be defined as the forms of Eqs. (4.12). From this simple example, it is found that the present factorization method is more elegant and reasonable than the traditional factorization method. However, they have different advantages and features when dealing with different physical problems.

7.   Coherent states

In this section let us review the coherent states of the harmonic oscillator in order to display the role of the ladder operators in coherent states. As we know, the coherent states of the harmonic oscillator in quantum mechanical textbooks are known as Glauber [3] states [225]. They are known as single harmonic oscillator prototypes of the coherent states of the oscillating electromagnetic field, which are the model of the ideal continuous wave laser field, or an electromagnetic field of unmodulated radio waves.

Following the notations used by Glauber, we are able to define coherent states as eigenstates of the annihilation operator a

$$a|\alpha\rangle = \alpha|\alpha\rangle, \tag{4.69}$$

from which we have

$$\langle\alpha'|a|\alpha\rangle = \alpha\langle\alpha'|\alpha\rangle. \tag{4.70}$$

Taking its complex conjugate yields

$$\langle\alpha|a^\dagger|\alpha'\rangle = \alpha^*\langle\alpha|\alpha'\rangle, \tag{4.71}$$

which is convenient to express this relation by the formal statement for adjoint states

$$\langle\alpha|a^\dagger = \alpha^*\langle\alpha|. \tag{4.72}$$

Here we make a remark about this definition. It is natural to ask whether there exists any state $|\iota\rangle$ with the following property [116]

$$a^\dagger|\iota\rangle = \iota|\iota\rangle. \tag{4.73}$$

In terms of equation (4.21) we have

$$\langle n|a^\dagger|\iota\rangle = \sqrt{n}\langle n-1|\iota\rangle = \iota\langle n|\iota\rangle, \tag{4.74}$$

for $n = 1, 2, 3, \ldots$; and for $n = 0$, equation (4.74) implies that

$$\langle 0|a^\dagger|\iota\rangle = \iota\langle 0|\iota\rangle = 0. \tag{4.75}$$

Let us discuss the special case $\iota = 0$. If so, then equation (4.74) results in

$$\langle n-1|\iota\rangle = 0, \tag{4.76}$$

for $n = 1, 2, 3, \ldots$, namely, $|\iota\rangle = 0$. However, if $\iota \neq 0$, then $\langle 0|\iota\rangle = 0$, which implies that

$$\langle n|\iota\rangle = 0, \tag{4.77}$$

for $n = 1, 2, 3, \ldots$ by repeated use of equation (4.74). Therefore, we draw a conclusion that $|\iota\rangle = 0$. That is to say, there is no nonzero state satisfying the supposition (4.73).

In addition, if $F(a)$ represents a rather general function of the annihilation operator a, then it follows from (4.69) that

$$F(a)|\alpha\rangle = F(\alpha)|\alpha\rangle. \tag{4.78}$$

In a similar way, for rather general functions $G(a^\dagger)$, it follows from (4.72) that

$$\langle \alpha|G(a^\dagger) = G(\alpha^*)\langle \alpha|. \tag{4.79}$$

On the other hand, it is well known that the state $|\alpha\rangle$ can be expanded in terms of the harmonic oscillator eigenstates $|n\rangle$ as

$$|\alpha\rangle = \sum_{n=0}^{\infty} g_n|n\rangle = \sum_{n=0}^{\infty} |n\rangle\langle n|\alpha\rangle. \tag{4.80}$$

Substitution of this into Eq. (4.69) yields the following recurrence relation

$$g_{n+1} = \frac{\alpha}{\sqrt{n+1}}g_n \tag{4.81}$$

for the expansion coefficients. From this we can obtain the relation between g_n and g_0

$$g_n = \frac{\alpha^n}{\sqrt{n!}}g_0, \tag{4.82}$$

where g_0 is determined by the following normalization condition

$$
\begin{aligned}
\langle \alpha | \alpha \rangle &= \sum_{n=0}^{\infty} |g_n|^2 \\
&= \sum_{n=0}^{\infty} \frac{|\alpha|^{2n}}{n!} |g_0|^2 \\
&= e^{|\alpha|^2} |g_0|^2 \\
&= 1,
\end{aligned} \tag{4.83}
$$

from which we have

$$
|g_0| = e^{-\frac{1}{2}|\alpha|^2}. \tag{4.84}
$$

Generally speaking, the definition of the coherent states g_0 is chosen to be a real number. Therefore, the expansion of the $|\alpha\rangle$ in eigenstates of the harmonic oscillator $|n\rangle$ can be written as

$$
|\alpha\rangle = e^{-\frac{1}{2}|\alpha|^2} \sum_{n=0}^{\infty} \frac{\alpha^n}{\sqrt{n!}} |n\rangle. \tag{4.85}
$$

On the other hand, the coherent states can be frequently introduced by using the displacement operator

$$
D(\alpha) = e^{\alpha a^\dagger - \alpha^* a}, \tag{4.86}
$$

with the relation

$$
|\alpha\rangle = D(\alpha)|0\rangle, \tag{4.87}
$$

where $|0\rangle$ is the ground state of the harmonic oscillator. This definition was actually used by Feynman and Glauber in 1951 in their studies of quantum transitions caused by the classical currents [226, 227]. From the following discussion, we find that this definition is equivalent to equation (4.85).

Using the Baker-Campbell-Hausdorff (BCH) formula for any two operators A and B which commute with the commutator of A and B

$$
e^{-\frac{1}{2}[A,B]} e^A e^B = e^{A+B} \tag{4.88}
$$

and the relation

$$
[\alpha a^\dagger, \alpha^* a] = |\alpha|^2, \tag{4.89}
$$

we find from equation (4.87)

$$
|\alpha\rangle = e^{-\frac{1}{2}|\alpha|^2} e^{\alpha a^\dagger} e^{-\alpha^* a} |0\rangle. \tag{4.90}
$$

Due to $a|0\rangle = 0$, we have $e^{-\alpha^*}|0\rangle = |0\rangle$. Thus, equation (4.90) can be simplified as

$$|\alpha\rangle = e^{-\frac{1}{2}|\alpha|^2}e^{\alpha a^\dagger}|0\rangle. \tag{4.91}$$

When expanding the operator $e^{\alpha a^\dagger}$ in power series form, we can obtain the same result as (4.85).

We now proceed to calculate the overlap between the coherent states using equation (4.85)

$$\begin{aligned}\langle\alpha|\beta\rangle &= e^{-\frac{1}{2}|\alpha|^2 - \frac{1}{2}|\beta|^2} \sum_{n=0}^{\infty} \frac{(\alpha^*\beta)^n}{n!} \\ &= \exp(-\tfrac{1}{2}|\alpha|^2 - \tfrac{1}{2}|\beta|^2 + \alpha^*\beta).\end{aligned} \tag{4.92}$$

Similarly, we have

$$\langle\beta|\alpha\rangle = \exp\left(-\frac{1}{2}|\alpha|^2 - \frac{1}{2}|\beta|^2 + \beta^*\alpha\right). \tag{4.93}$$

From Eqs. (4.92) and (4.93), we have

$$\begin{aligned}|\langle\alpha|\beta\rangle|^2 &= \langle\alpha|\beta\rangle\langle\beta|\alpha\rangle \\ &= \exp(-|\alpha|^2 - |\beta|^2 + \alpha^*\beta + \alpha\beta^*) \\ &= \exp(-|\alpha - \beta|^2).\end{aligned} \tag{4.94}$$

Considering $\langle\alpha|\beta\rangle \neq 0$ for $\alpha \neq \beta$, we see that the coherent states are not orthogonal. However, the set of coherent states is complete, and it may provide a continuous, non-orthogonal basis for the Hilbert space of the oscillator. Actually, the coherent states are overcomplete: any state of the harmonic oscillator can be expanded in terms of a subset of $\{|\alpha\rangle\}$.

Additionally, the time evolution of a state is given by the time evolution operator $U(t)$. The coherent states in this case can be expressed as

$$\begin{aligned}|\alpha, t\rangle &= U(t,0)|\alpha(0)\rangle \\ &= e^{-iHt}|\alpha(0)\rangle \\ &= e^{-iHt}e^{-\frac{1}{2}|\alpha(0)|^2} \sum_{n=0}^{\infty} \frac{[\alpha(0)]^n}{\sqrt{n!}}|n\rangle.\end{aligned} \tag{4.95}$$

Using Eq. (4.64), we obtain

$$|\alpha, t\rangle = e^{-\frac{1}{2}|\alpha(0)|^2} \sum_{n=0}^{\infty} \frac{[\alpha(0)]^n}{\sqrt{n!}} e^{-i(n+\frac{1}{2})t} \frac{(a^\dagger)^n}{\sqrt{n!}}|0\rangle, \tag{4.96}$$

which can be further modified as

$$
\begin{aligned}
|\alpha, t\rangle &= e^{-\frac{1}{2}|\alpha(0)|^2} e^{-\frac{i}{2}t} \sum_{n=0}^{\infty} \frac{[\alpha(0)e^{-i\,t}a^{\dagger}]^n}{n!} |0\rangle \\
&= \exp[-\tfrac{1}{2}|\alpha(0)|^2 - \tfrac{i}{2}t + \alpha(0)e^{-i\,t}a^{\dagger}]|0\rangle.
\end{aligned}
\tag{4.97}
$$

In the calculation, we have taken $\omega = \hbar = 1$.

Before ending this section, two remarks are appropriate. First, the coherent states defined by means of equations (4.69) and (4.85) were used by Schwinger in 1953 as auxiliary states to simplify some calculations [228]. Later on, Rashevskiy, Klauder and Bargmann developed independently their mathematical properties [229–231]. Second, it is found from this typical example that we have to use the ladder operators to construct the coherent states. Therefore, the factorization method also becomes the cornerstone of the coherent states since the ladder operators can be obtained from it. Third, the multi-dimensional harmonic oscillator also possesses the coherent states. This can be performed by generalizing the one-dimensional case to arbitrary dimensional one. It should be addressed that these states are sometimes regarded as Cartesian coherent states in order to distinguish them from an alternative set of states known as the coherent angular momentum states for $D \geq 2$, which are the superposition of the kets of an angular momentum basis. We do not study this case for simplicity.

8.   Franck-Condon factors

It is well known that the calculations of the Franck-Condon factors have been important in the analysis of the radiative and non-radiative transitions of different electronic states in molecules [232]. Considering the fact that both the equilibrium internuclear distances and the harmonic vibration frequencies in two electronic states between which the transitions occur are very different, the calculations of the Franck-Condon factors thus become very complicated. Further complications are from the anharmonic terms of the potential functions and also from the distortion of the molecules in the excited states. As a result, all these complications make systematic and reliable analysis of the experimental results rather difficult. It is worth noting that even though the calculations of the Franck-Condon factors can be obtained numerically, it may be convenient to develop explicit formulas for the overlap integrals which lead to a straightforward and less computer-intensive calculations. Because the harmonic oscillators are usually good approximations to the potential energy surfaces of molecules near the potential wells, the calculation of the Franck-Condon factors becomes very important.

Let us briefly review the development of this subject. In 1925, Franck established his famous principle which enables us to estimate the intensities of vibrational electronic transitions between two different electronic states in diatomic molecules [233]. Condon immediately extended its scope in his two

well-known papers to rationalize the shapes of absorption and fluorescence bands [234, 235]. In Condon's second paper [235], the principle was given its final quantitative formulation by means of the newly discovered wave mechanics. Condon himself gave an excellent review of this subject in 1947 [236]. Hutchisson first gave an explicit evaluation of Condon's intensity formula for the case of a harmonic vibrator in 1930 [237] and also showed how his method could be extended to an anharmonic vibrator in 1931 [238]. It is found that Hutchisson's results are finite series expansions and very complicated. The complication will increase rapidly with the vibrational quantum numbers. Nevertheless, Hutchisson's method was successfully applied to several molecules and also gave rise to attention and interest from astrophysicists [239–241]. Later on, a simple recurrence procedure developed by Manneback in 1951 to compute the matrix of the amplitudes of probabilities (transition moment) was used to calculate the intensities of the vibrational spectrum in electronic bands of diatomic molecules [242]. But the results given by him were limited to the case of harmonic motion in both excited and ground states. In 1959, Wagner applied the analysis method to obtain closed-form formulas for calculating the Franck-Condon integrals [243]. In the same year Ansbacher [244] evaluated the Franck-Condon overlap integrals in terms of a finite sum of polynomials and recovered those integrals obtained by Wagner [243]. Ansbacher found that the results given by Wagner can be stated in a more concise form which is more easily derived by means of the generating functions of the Hermite polynomials. Additionally, the first general expressions of the calculations of the Franck-Condon factors for polyatomic molecules were published in a paper by Sharp and Rosenstock in 1964 [245]. A little more than a decade later, Cederbaum and Domcke made important contributions to the generalization of the theory to arbitrary electronic transitions [246]. In the late 1990s, Malmqvist, Forsberg and Islampour *et al.* have obtained a general expression of multidimensional Franck-Condon integrals for the harmonic oscillators [247, 248]. Recently, Chang has made use of the basic properties of the Hermite polynomials and Gaussian integrals to obtain the Franck-Condon factors for the harmonic oscillator with a double summation [249].

It is worth pointing out that these contributions to the Franck-Condon factors are mainly based on the so-called analytical method (integro-differential procedures), i.e., the Franck-Condon factors can be derived by direct integral of the known wave functions of the harmonic oscillator. Even though such an approach can be easily accessible to many scientists, we want to study this problem with the algebraic method, which is closely related to the ladder operator approach. The contributions to the calculations of the Franck-Condon factors using the algebraic method can be summarized as follows. For example, Koide proposed an algebraic method to calculate the electronic transitions accompanied by the excitation of molecular or crystal vibrations, namely, he expressed

the Hamiltonian of the normal vibrations in terms of the ladder operators and also used the transformations which are also expressed by those ladder operators to represent the change in the equilibrium nuclear distances and vibrational frequencies [250]. The square of the Franck-Condon overlap was obtained by him [250]. Later, Katriel and Adam generalized this method and calculated not only the Franck-Condon factors but also matrix elements of the coordinate and kinetic energy operators. On the other hand, he also reproduced Ansbacher's formulas as a triple summation [251, 252]. In 1984, Ozkän [253] proposed an algebraic method to calculate the Franck-Condon factors following Katriel's idea [252]. Nishikawa used the coherent states technique to study the Franck-Condon factors and also obtained the generalized matrix elements of $x^j, e^{-\alpha x}$ and $e^{-\beta x^2}$ [254]. In terms of the BCH theorem and Cauchy's integral formula for complex variable, Palma *et al.* applied the second quantization formalism via a proper definition and use of the creation and annihilation operators of the harmonic oscillator to obtain all Ansbacher's formulas completely [255–258]. It should be noted that the second quantization formalism has been used since 1960 to calculate the matrix elements [250], but all these methods require the definition of complicated operators and algebras. Recently, other calculations of the Franck-Condon factors for the harmonic oscillator have also been carried out by using analytical methods [259]. For example, Hsue used operator manipulations in a two-step method [260] to derive an explicit expression of the Franck-Condon factors for the harmonic oscillator in the general case of displaced origins and shifted frequencies and also discussed the case of the rotated coordinates in the excited states of two dimensional transitions. In particular, Iachello and Ibrahim evaluated the Franck-Condon overlap integrals by means of the analytical and algebraic methods [261], in which they have used the translation (also named as displacement) and dilation operators to calculate the Franck-Condon factors for the harmonic oscillator and then generalized this elegant method to other anharmonic oscillators such as the Morse oscillator. In this work, we want to give a brief review of the calculations of the Franck-Condon factors for the harmonic oscillator following the procedure used by Nishikawa, Iachello and Ibrahim [254, 261].

Before proceeding further, it is necessary to introduce two important operators known as displacement and dilation operators, in order to derive the Franck-Condon factors for the harmonic oscillator [254, 261].

Let us first consider the displacement operator $D(d)$

$$
\begin{aligned}
D(d) \; &= \exp[d\tfrac{d}{dx}] \\
&= \exp[\gamma(a - a^\dagger)],
\end{aligned}
\tag{4.98}
$$

where

$$
\gamma = \frac{d}{\sqrt{2}},
\tag{4.99}
$$

with the property

$$D(-d)\Phi(x) = \Phi(x - d). \tag{4.100}$$

In the calculation we have used the formula (4.61).

We are now in the position to calculate the matrix elements of the displacement operator $D(-d)$. That is to say, we are going to calculate the following expression

$$
\begin{aligned}
\langle n|D(-d)|m\rangle &= \frac{1}{\sqrt{n!m!}}\langle 0|a^n \exp[\gamma(a^\dagger - a)](a^\dagger)^m|0\rangle \\
&= \frac{e^{-\frac{\gamma^2}{2}}}{\sqrt{n!m!}}\langle 0|a^n \exp(\gamma a^\dagger)\exp(-\gamma a)(a^\dagger)^m|0\rangle \\
&= \frac{e^{-\frac{\gamma^2}{2}}}{\sqrt{n!m!}}\sum_{s=0}^{n}\sum_{s'=0}^{m}\frac{\gamma^s(-\gamma)^{s'}}{s'!s!}\langle 0|a^n(a^\dagger)^s a^{s'}(a^\dagger)^m|0\rangle,
\end{aligned}
\tag{4.101}
$$

where we have chosen the normal form for the displacement operator $D(-d)$ as shown by Nishikawa [254]

$$
D(-d) = \begin{cases}
e^{-\frac{\gamma^2}{2}} e^{\gamma a^\dagger} e^{-\gamma a}, & \text{normal form}, \\[2mm]
e^{\frac{\gamma^2}{2}} e^{-\gamma a} e^{\gamma a^\dagger}, & \text{antinormal form}.
\end{cases}
\tag{4.102}
$$

The different choices of $D(-d)$ arise from the arbitrary choice of the operators A and B when we use the BCH formula (4.88) to derive the formula (4.102). As we know, once the normal form of the unitary operator is given, the overlap integral for the displacement operator can be evaluated directly by using the properties of the normally ordered operators as done by Klauder and Louisell *et al.* [200, 262]. Calculating the remaining matrix elements and simplifying, we may obtain the following expression for the matrix element of the displacement operator as [243, 250, 254]

$$
\begin{aligned}
\langle n|D(-d)|m\rangle &= e^{-\frac{\gamma^2}{2}}\sqrt{n!m!}(-1)^n\gamma^n\gamma^m\sum_{s=0}^{\min[m,n]}\frac{(-\gamma^2)^s}{(m-s)!(n-s)!s!} \\
&= \begin{cases}
e^{-\frac{\gamma^2}{2}}(\gamma)^{n-m}\sqrt{\dfrac{m!}{n!}}L_m^{n-m}(\gamma^2), & \text{for } n > m, \\[4mm]
e^{-\frac{\gamma^2}{2}}(-\gamma)^{m-n}\sqrt{\dfrac{n!}{m!}}L_n^{m-n}(\gamma^2), & \text{for } n < m,
\end{cases}
\end{aligned}
\tag{4.103}
$$

where we have used the following definition of the associated Laguerre polynomial [263]

$$
L_n^\alpha(x) = \sum_{i=0}^{n}\binom{\alpha+n}{n-i}\frac{(-x)^i}{i!}. \tag{4.104}
$$

On the other hand, we may obtain the Franck-Condon overlap integral for the antinormal form of the displacement operator [252, 254]

$$
\begin{aligned}
\langle n|D(-d)|m\rangle &= \frac{e^{\frac{\gamma^2}{2}}}{\sqrt{n!m!}}\langle 0|a^n \exp(-\gamma a)\exp(\gamma a^\dagger)(a^\dagger)^m|0\rangle \\
&= e^{\frac{\gamma^2}{2}}\sqrt{n!m!}(\gamma)^{n-m}\sum_{s=0}^{\min[m,n]}\frac{(-\gamma^2)^s(n+s)!}{s!(n-m+s)!}.
\end{aligned}
\tag{4.105}
$$

However, this expression is less convenient for actual calculation than that of the normal form of the displacement operator. It should be pointed out that the result (4.105) for the antinormal form can be transformed into the result (4.103) for the normal form through the Kummer's transformation formula for the confluent hypergeometric functions [264].

We now treat the frequency shift case. Such a problem was investigated by Katriel [252] through introducing two kinds of creation and annihilation operators corresponding to two different harmonic oscillators. This problem was restudied by Nishikawa, Iachello and Ibrahim [254, 261]. Nevertheless, their treatment methods are essentially the same except for the slightly different expressions and notations. Following the procedure used by Iachello and Ibrahim, we start by considering the following identity

$$
e^{\alpha x\frac{d}{dx}}g(x) = g(e^\alpha x),
\tag{4.106}
$$

from which we can obtain the following expression in terms of the wave functions (4.10) for the harmonic oscillator

$$
\Phi_n(\alpha, x) = \sqrt{\alpha}e^{(\ln\alpha)x\frac{d}{dx}}\Phi_n(x),
\tag{4.107}
$$

from which we can define the dilation operator [254, 261]

$$
\begin{aligned}
V(\alpha) &= \sqrt{\alpha}e^{(\ln\alpha)x\frac{d}{dx}} \\
&= \sqrt{\alpha}\exp\left[\ln\alpha\left(\frac{a^2-(a^\dagger)^2}{2}-\frac{1}{2}\right)\right] \\
&= \exp\left[\frac{\ln\alpha(a^2-(a^\dagger)^2)}{2}\right],
\end{aligned}
\tag{4.108}
$$

where we have used the relations (4.60) and (4.61). As shown in Eqs. (4.58), when using the BCH factorization formula for the SU(1, 1) group, we have [261]

$$
e^{\eta(L_--L_+)} = e^{-\tanh\eta L_+}e^{-2[\ln\cosh\eta]L_3}e^{\tanh\eta L_-},
\tag{4.109}
$$

where $\eta = \ln\alpha$. As a result, the dilation operator can be further arranged as

$$
V(\alpha) = e^{-\ln\cosh\eta/2}e^{-(\tanh\eta)(a^\dagger)^2/2}e^{-(\ln\cosh\eta)a^\dagger a}e^{(\tanh\eta)a^2/2}.
\tag{4.110}
$$

In a similar way to calculate the Franck-Condon overlap integral for the displacement operator $D(-d)$, we may calculate the Franck-Condon overlap integral for the dilation operator as [261]

$$
\begin{aligned}
\langle n|V(\alpha)|m\rangle \; &= \left[\frac{\alpha n!m!}{2^{n+m-1}(1+\alpha^2)}\right]^{\frac{1}{2}}\sqrt{\frac{1}{(1+\alpha^2)^{n+m}}} \\
&\times \sum_{\substack{j=n=m\,\mathrm{mod}\,2 \\ j\in[0,\min(n,m)]}} \frac{2^{2j}(1-\alpha^2)^{\frac{n-j}{2}}(\alpha^2-1)^{\frac{m-j}{2}}\alpha^j}{j!\left(\dfrac{n-j}{2}\right)!\left(\dfrac{m-j}{2}\right)!}.
\end{aligned}
\tag{4.111}
$$

We now study the Franck-Condon factors for the harmonic oscillator with different equilibrium coordinates and frequencies. The complete Franck-Condon factors can be obtained by combining the matrix elements of the displacement and dilation operators as

$$
\langle n|V(\alpha)^\dagger D(-d)V(\alpha')|m\rangle = \langle n|D(-d\alpha)V(\alpha'/\alpha)|m\rangle,
\tag{4.112}
$$

where we have used the relations

$$
\begin{aligned}
D(d)V(\alpha) &= D(\alpha)V(\alpha d), \\
V(\alpha)^\dagger &= V(\alpha)^{-1} = V(1/\alpha), \\
V(\alpha)V(\alpha') &= V(\alpha\alpha').
\end{aligned}
\tag{4.113}
$$

Making use of the results (4.101) and (4.110) as well as the BCH factorization formula, we have [261]

$$
\begin{aligned}
\langle n|D(-d\alpha)V(\alpha'/\alpha)|m\rangle \; &= \exp\left[-\frac{d^2\alpha^2\alpha'^2}{2(\alpha^2+\alpha'^2)}\right]\sqrt{\frac{n!m!}{2^{n+m}}\frac{2\alpha\alpha'}{\alpha^2+\alpha'^2}} \\
&\sqrt{\left(\frac{\alpha^2}{\alpha^2+\alpha'^2}\right)^{(n+m)}}\sum_{j=0}^{\min[n,m]}\frac{1}{j!\left(-\dfrac{d^2\alpha^2\alpha'^2}{\alpha^2+\alpha'^2}\right)^j} \\
&\times \sum_{\substack{l\in[j,n] \\ l=n\,\mathrm{mod}\,2}}\;\sum_{\substack{l'\in[j,m] \\ l'=m\,\mathrm{mod}\,2}}\left[\frac{\left(\dfrac{\alpha'^2-\alpha^2}{\alpha^2}\right)^{\frac{m-l'}{2}}\left(\dfrac{\alpha^2-\alpha'^2}{\alpha^2}\right)^{\frac{n-l}{2}}}{\left(\dfrac{\alpha'^2+\alpha^2}{\alpha^2}\right)^{\frac{l+l'}{2}}}\right.
\end{aligned}
$$

$$\times \frac{\left(\frac{\alpha'}{\alpha}\right)^{l'} \left(-\frac{\alpha'^2}{\alpha^2}\right)^{l} (-2d\alpha)^{l+l'}}{(l-j)!(l'-j)! \left(\frac{n-l}{2}\right)! \left(\frac{m-l'}{2}\right)!}\Bigg]. \tag{4.114}$$

It should be noted that in the calculation we have used the following BCH formula in its most general form

$$e^C e^D = e^{\left\{C+D+\frac{1}{2}[C,D]+\frac{1}{12}([C,[C,D]]+[D,[D,C]])+\ldots\right\}} \tag{4.115}$$

to obtain

$$e^{-\eta\theta\, a^\dagger} e^{\eta\, a} e^{\theta(a^\dagger)^2} = e^{\eta^2\theta} e^{\eta\theta\, a^\dagger} e^{\theta(a^\dagger)^2} e^{\eta\, a}, \tag{4.116}$$

which is valid for any arbitrary number η and θ.

9.   Concluding remarks

In this Chapter we have studied the harmonic oscillator in detail by means of the algebraic method due to its crucial role in quantum mechanics. The creation and annihilation operators have been constructed by our present factorization method. That is to say, we have obtained them directly from the well known eigenfunctions by acting the operator d/dx on the normalized eigenfunctions. On the other hand, we have found that this method is elegant and simple to obtain the analytical expressions of the matrix elements and construct the Weyl-Heisenberg algebra. On the other hand, we have carried out the coherent states of the harmonic oscillator. In addition, we have studied its Bargmann-Segal transformation. It is found that we can easily obtain the eigenvalues from this transformation. Finally, we have studied the Franck-Condon factors of the harmonic oscillator with algebraic method after a detailed introduction of its development. Before ending this Chapter, we want to give a remark here. From the above study we have found that the factorization method hinges on expressing the harmonic oscillator Hamiltonian as a product of creation and annihilation operators $a^\dagger$ and a, which can also be used to construct the desired eigenfunctions. For such a simple quantum system, it is not difficult to factorize the Hamiltonian into the product of the creation and annihilation operators by means of the traditional Schrödinger-Infeld-Hull factorization method. For the other quantum systems, however, the constructions of the ladder operators by the traditional factorization method, undoubtedly, will become very complicated. Such complications can be overcome and become easier if using our present factorization method. Therefore, we prefer to apply this new method to study those complicated quantum systems as to be shown in the successive Chapters.

Notes

1   These normal modes are formally equivalent to harmonic oscillators.

2 For example, we may obtain the quantization condition by considering the finiteness of wave functions at infinity when we treat the central potential problems.

3 The term "coherent states" was initially used by Glauber in the field of quantum optics. Due to the understanding contributions to the quantum theory of optical coherence and to the development of laser-based precision spectroscopy, including the optical frequency comb technique, the Nobel Prize of Physics in 2005 was awarded to him and other two scientists John L. Hall (American physicist) and Theodor W. Hänsch (German physicist).

Chapter 5

INFINITELY DEEP SQUARE-WELL POTENTIAL

1. Introduction

Due to its importance in quantum mechanics, the square-well potential has been studied in almost all textbooks in quantum mechanics. Generally speaking, it has been treated traditionally by solving the Schrödinger equation in the configuration space. For example, some authors used this analysis method to investigate many interesting topics such as the quantum revivals versus the classical periodicity [265], the revival of wave packets in the infinite square well [266–268], the general series solution for finite square-well energy levels in wave-packet studies [269], the application of renormalization to the dynamics of a particle moving in this potential well driven by an external field [270], the time-independent and time-dependent wave packets for the Wigner quasi-probability distribution for the square well [271, 272], the evolution and collision of Bose-Condensed gases in it [273], the quantum dots [274] and quantum wells [275, 276], and so on.

On the other hand, the algebraic method has been used to study this problem [161, 277–284]. It is found that this model potential satisfies the commutation relations of the generators for the non-compact Lie algebra su(1, 1).

In this Chapter we shall pay more attention to the algebraic method than the analysis method since the algebraic method is, sometimes, related to the factorization method. We attempt to construct a suitable Lie algebra su(1, 1) based on our present factorization method. On the other hand, the matrix elements of the physical quantities $\cos(\pi x/L)$ and $[\sin(\pi x/L)]p$, where L represents the width of the potential well, are obtained analytically from the creation and annihilation operators.

This Chapter is organized as follows. Section 2 is devoted to constructing the ladder operators for the infinitely deep square well potential. In Section 3

we study the dynamic group for this system and obtain the matrix elements. In Section 4 we briefly deal with the infinitely deep symmetric well potential case. In Section 5 we attempt to study this problem by means of the SUSYQM approach. In Section 6 we shall investigate the Perelomov coherent states for the infinitely deep square well potential. The Barut-Girardello coherent states are carried out in Section 7. The concluding remarks are given in Section 8.

2.   Ladder operators for infinitely deep square-well potential

Let us first study the exact solutions of this quantum system. The Hamiltonian for a single particle moving in a one-dimensional infinitely deep square-well potential is given by

$$H = \frac{p^2}{2\mu} + V(x), \tag{5.1}$$

where the potential $V(x)$ is taken as

$$V(x) = \begin{cases} 0, & \text{for } x \in [0, L], \\ \infty, & \text{otherwise.} \end{cases} \tag{5.2}$$

The well known exact solutions of the Schrödinger equation (5.1) can be expressed as

$$|n\rangle \equiv \Psi_n(z) = \begin{cases} N_L \sin(nz), & \text{for } z \in [0, \pi], \\ 0, & \text{otherwise,} \end{cases} \tag{5.3}$$

where

$$z = \frac{\pi x}{L}, \quad N_L = \sqrt{\frac{2}{L}}. \tag{5.4}$$

Here n is a positive integer, and $|1\rangle$ is the ground state. The eigenvalues of this system are given by

$$E_n = \hbar \omega n^2, \quad n = 1, 2, 3, \ldots, \tag{5.5}$$

with

$$\omega = \frac{\hbar \pi^2}{2\mu L^2}, \tag{5.6}$$

where μ is the mass of the moving particle.

For convenience we define the number operator $\hat{n}$ and its inverse $\hat{n}^{-1}$ [161]:

$$\hat{n}|n\rangle = n|n\rangle, \quad \hat{n}^{-1}|n\rangle = n^{-1}|n\rangle. \tag{5.7}$$

With the same spirit of obtaining the ladder operators for the harmonic oscillator, let us study the creation and annihilation operators for the present system with our new factorization method.

We now address the problem of finding creation and annihilation operators $\hat{M}_\pm$ for the wave functions (5.3)

$$\hat{M}_\pm|n\rangle \sim |n \pm 1\rangle. \tag{5.8}$$

Because the ground state $|1\rangle$ has to be annihilated by the annihilation operator $\hat{M}_-$, we define

$$\hat{M}_-|n\rangle = (n-1)|n-1\rangle, \quad \hat{M}_+|n\rangle = n|n+1\rangle, \tag{5.9}$$

where we assume that the matrix of $\hat{M}_+$ in the bases $|n\rangle$ is the transpose of the annihilation operator $\hat{M}_-$.

Now, we want to make use of the eigenfunctions (5.3) to study the creation and annihilation operators with the factorization method. By applying the first differential operator d/dz on the eigenfunctions (5.3), we have

$$\frac{d}{dz}\Psi_n(z) = n\sqrt{\frac{2}{L}}\cos(nz). \tag{5.10}$$

As a result, we may express $\hat{M}_\pm$ in terms of z, d/dz, $\hat{n}$ and $\hat{n}^{-1}$ as follows:

$$\hat{M}_- = \left[(\cos z)\hat{n} - (\sin z)\frac{d}{dz}\right]\hat{n}^{-1}(\hat{n}-1), \tag{5.11}$$

$$\hat{M}_+ = (\cos z)\hat{n} + (\sin z)\frac{d}{dz}, \tag{5.12}$$

with the properties (5.9).

The commutator $[\hat{M}_-, \hat{M}_+]$ can be calculated in the basis $|n\rangle$:

$$[\hat{M}_-, \hat{M}_+]|n\rangle = (2n-1)|n\rangle = 2\hat{M}_0|n\rangle, \tag{5.13}$$

where we have introduced the following operator

$$\hat{M}_0 = \hat{n} - \frac{1}{2}. \tag{5.14}$$

3. Realization of dynamic group SU(1, 1) and matrix elements

In this section let us study the dynamic group. As we know, in the space spanned by $|n\rangle$ the operators $\hat{M}_{\pm}$ and $\hat{M}_0$ satisfy the commutation relations of an su(1, 1) algebra, which is isomorphic to the so(2, 1) algebra:

$$[\hat{M}_-, \hat{M}_+] = 2\hat{M}_0, \qquad [\hat{M}_0, \hat{M}_\pm] = \pm\hat{M}_\pm. \tag{5.15}$$

Therefore, we conclude that the non-compact Lie group SU(1, 1) is the dynamic group for this system.

As introduced in Chapter 3, there are four series of irreducible unitary representations for the su(1, 1) algebra except for the identity representation [169]. Since there exists the ground state for this quantum system, the eigenfunctions for the bound states of this system belong to the representation $D^+(j)$ of the non-compact Lie group SU(1, 1)

$$
\begin{aligned}
&I_0|j, m\rangle = m|j, m\rangle, \\
&I_-|j, m\rangle = [(m + j)(m - j - 1)]^{\frac{1}{2}}\,|j, m - 1\rangle, \\
&I_+|j, m - 1\rangle = [(m + j)(m - j - 1)]^{\frac{1}{2}}\,|j, m\rangle, \\
&m = -j + k, \qquad k = 0, 1, 2, \ldots, \qquad j < 0.
\end{aligned}
\tag{5.16}
$$

By comparing with Eqs. (5.9) and (5.14), we have $j = -\frac{1}{2}$, $m = n - \frac{1}{2}$, and $|n\rangle = |-\frac{1}{2}, n - \frac{1}{2}\rangle$.

On the other hand, the Hamiltonian can be simply expressed as

$$\hat{H}|n\rangle = \hbar\omega\hat{M}_-\hat{M}_+|n\rangle. \tag{5.17}$$

In addition, the corresponding Casimir operator can be calculated as

$$
\begin{aligned}
C &= [\hat{M}_+\hat{M}_- - \hat{M}_0(\hat{M}_0 - 1)] \\
&= [\hat{M}_-\hat{M}_+ - \hat{M}_0(\hat{M}_0 + 1)] \\
&= \frac{1}{4},
\end{aligned}
\tag{5.18}
$$

with the property

$$C|n\rangle = \frac{1}{4}|n\rangle. \tag{5.19}$$

We are now in the position to calculate the matrix elements of some related physical functions. From Eqs. (5.11) and (5.12) we obtain

$$\cos z(\hat{n} - 1) = \frac{1}{2}\left[\hat{M}_+\hat{n}^{-1}(\hat{n} - 1) + \hat{M}_-\right], \tag{5.20}$$

$$\sin z \frac{d}{dz}(\hat{n}-1) = \frac{1}{2}\left[\hat{M}_+(\hat{n}-1) - \hat{M}_-\hat{n}\right]. \tag{5.21}$$

When $|n\rangle$ is not the ground state, i.e. $n \neq 1$, we have

$$\langle m| \cos z |n\rangle = \frac{1}{2}\left[\delta_{m,(n+1)} + \delta_{m,(n-1)}\right], \tag{5.22}$$

$$\langle m| \sin z \frac{d}{dz}|n\rangle = \frac{n}{2}\left[\delta_{m,(n+1)} - \delta_{m,(n-1)}\right]. \tag{5.23}$$

For $n = 1$, we have

$$\cos z |1\rangle = \sin z \frac{d}{dz}|1\rangle = \frac{1}{2}\hat{M}_+|1\rangle. \tag{5.24}$$

Because there is no state with $m = 0$, equation (5.23) also holds for $n = 1$.

4. Ladder operators for infinitely deep symmetric well potential

In this section we are going to briefly study the dynamic group for the infinitely deep symmetric square well potential taken as

$$V(x) = \begin{cases} 0, & \text{for } x \in [-\frac{L}{2}, \frac{L}{2}], \\ \infty, & \text{otherwise.} \end{cases} \tag{5.25}$$

The exact solutions of the Schrödinger equation with this potential are given by

$$|n\rangle \equiv \Psi_n(z) = \begin{cases} N_L \sin(nz), & \text{when } n = \text{even}, \\ N_L \cos(nz), & \text{when } n = \text{odd}, \end{cases} \tag{5.26}$$

where N_L is given in Eq. (5.4).

For simplicity, we give the corresponding results only since the derivation procedure is similar to that of the infinitely deep square well potential case. Consequently, we have

$$\hat{L}_- = \left[\sin z\, \hat{n} + \cos z \frac{d}{dz}\right]\frac{\hat{n}-1}{\hat{n}}, \tag{5.27}$$

$$\hat{L}_+ = \left[\sin z\, \hat{n} - \cos z \frac{d}{dz}\right], \tag{5.28}$$

$$\hat{L}_0 = \hat{n} - \frac{1}{2}, \tag{5.29}$$

with the following properties

$$\hat{L}_-|n\rangle = l_-|n-1\rangle = (-1)^n(n-1)|n-1\rangle, \tag{5.30}$$

$$\hat{L}_+|n\rangle = l_+|n+1\rangle = (-1)^{n+1}n|n+1\rangle, \tag{5.31}$$

$$\hat{L}_0|n\rangle = l_0|n\rangle = \left(n - \frac{1}{2}\right)|n\rangle. \tag{5.32}$$

After careful calculations, we find that these operators $\hat{L}_{\pm,0}$ satisfy the following commutation relations

$$[\hat{L}_-, \hat{L}_+] = 2\hat{L}_0, \quad [\hat{L}_0, \hat{L}_\pm] = \pm\hat{L}_\pm, \tag{5.33}$$

which also correspond to an su(1, 1) Lie algebra. It is found that the ladder operators $\hat{L}_\pm$ will change the even wave functions into the odd ones and *vice versa*.

On the other hand, through similar calculations we have

$$\sin z = \frac{1}{2}\left(\hat{L}_+\frac{1}{\hat{n}} + \hat{L}_-\frac{1}{\hat{n}-1}\right), \tag{5.34}$$

$$\cos z\frac{d}{dz} = \frac{1}{2}\left(\hat{L}_-\frac{\hat{n}}{\hat{n}-1} - \hat{L}_+\right). \tag{5.35}$$

By using Eqs. (5.30)-(5.32), we may obtain their matrix elements as follows

$$\langle m|\sin z|n\rangle = \frac{(-1)^n}{2}(\delta_{m,n-1} - \delta_{m,n+1}), \tag{5.36}$$

$$\langle m|\cos z\frac{d}{dz}|n\rangle = \frac{(-1)^n}{2}n(\delta_{m,n-1} + \delta_{m,n+1}). \tag{5.37}$$

As studied above, we find that the dynamic groups for both the infinitely deep asymmetric and symmetric square-well potentials are the non-compact Lie group SU(1, 1).

5.   SUSYQM approach to infinitely deep square well potential

We study in the following this problem from the viewpoint of the SUSYQM [279]. It is well-known that SUSYQM provides us an elegant and powerful tool for obtaining the exact eigenvalues and eigenfunctions of a large class of one-dimensional solvable quantum mechanical problems. In general, the SUSYQM

naturally imposes an algebraic structure on all exactly solvable physical potentials in quantum mechanics. In fact, the infinitely deep square well potential can be seen as a special case of the Eckart potential, whose group theoretical properties have been investigated in detail [97, 285–288]. Thus, it is possible to establish a connection between the SUSYQM method and the group theoretical potential algebra method.

In SUSYQM, each superpotential $W(x, a)$ produces two partner potentials as follows:

$$V_{\pm}(x) = W^2(x, a) \pm \frac{d}{dx} W(x, a), \tag{5.38}$$

and the ladder operators are defined as

$$L^{\mp}(x, a) = W(x, a) \pm \frac{d}{dx}, \tag{5.39}$$

from which we may express the Hamiltonian as

$$H = L^+ L^-. \tag{5.40}$$

A subset of all possible superpotentials $W(x, a)$ has the properties of shape invariance. Generally speaking, the partner potential $V_-(x)$ can be adjusted to make the ground state energy level $E_0 = 0$. Each of the excited state energies is thus shifted from the Schrödinger value by $-E_0$. The ground state eigenfunction $\Psi_0^{(-)}(x, a) \sim \exp[-\int_{x_0}^x W(x, a)dx]$ can be obtained from the superpotential $W(x, a)$. For example, for $W(x, a) = -a \cot x$, we have $\Psi_0^{(-)}(x, a) \sim \sin^a x$. For the infinitely deep square well potential, if we take $a = 1$, then the ground state $\Psi_0^{(-)}(x, 1) \sim \sin x$. If applying the creation operator $L^+(x, 1)$ successively on the ground state, then we can obtain the excited states $\sin nx$ ($x = z$ in this case). The corresponding eigenvalues $E_n^{\pm}$ can be obtained from the shape invariance condition, which represents them as a simple sum of algebraic remainders from the difference of the values of the two partner potentials $V_{\pm}(x)$. They are the shifted eigenvalues $E_n^- = \hbar\omega n^2 - E_0$, $E_n^+ = E_{n+1}^-$, where ω is defined by Eq. (5.6). The connection between the shape invariant potentials and the non-compact Lie algebra so(2, 1) has been established well in [279].

6.   Perelomov coherent states

Even though the Gazeau-Klauder coherent states for the infinitely deep square well potential have been discussed in [289, 290], we are going to deal with the same problem using different approaches, specifically the Perelomov and Barut-Girardello coherent states.

First, we use the Perelomov's notation to study the Perelomov coherent states [117]

$$|\beta, k\rangle = D(\beta)|0, k\rangle = N_\beta \sum_{n=0}^{\infty} \sqrt{\frac{\Gamma(2k+n)}{n!\Gamma(2k)}} \beta^n |n, k\rangle, \qquad (5.41)$$

where $D(\beta) = \exp(\beta \hat{M}_+ - \beta^* \hat{M}_-)$. The factor N_β can be calculated by the normalization condition as

$$N_\beta = (1 - |\beta|^2)^{\frac{1}{2}}, \qquad (5.42)$$

which implies that the constraint condition is $|\beta| < 1$ and this limits the range of the parameter $|\beta|$.

In terms of the irreducible unitary representations of the non-compact Lie algebra su(1, 1), which is the hidden dynamic group of this quantum system, it is known that the Bargmann index k [291] can be taken as $\frac{1}{2}, 1, \frac{3}{2}, 2, \ldots$. For simplicity, taking $k = \frac{1}{2}$ and considering the local basis x, we derive the analytical expression of coherent states $|\beta x\rangle$,

$$
\begin{aligned}
|\beta x\rangle &= \sqrt{2(1 - |\beta|^2)} \sum_{n=0}^{\infty} \beta^n \sin(n+1)\pi\, x \\
&= \sqrt{2(1 - |\beta|^2)} \frac{i(e^{2i\pi x} - 1)}{2(e^{i\pi x} - \beta)(e^{i\pi x}\beta - 1)} \\
&= \sqrt{\frac{1 - |\beta|^2}{2}} \frac{i(e^{2i\pi x} - 1)}{(e^{i\pi x} - \beta)(e^{i\pi x}\beta - 1)} \cdot \frac{e^{-i\pi x}}{e^{-i\pi x}} \\
&= \sqrt{2(1 - |\beta|^2)} \frac{\sin(\pi x)}{(1 + |\beta|^2) - 2\beta \cos(\pi x)},
\end{aligned}
\qquad (5.43)
$$

where we have taken $L = 1$ for simplicity and denoted the shifted eigenfunctions as $\sin(n+1)x$ with $n = 0, 1, 2, 3, \ldots$ for convenience.

In the following we will use the coherent sates $|\beta x\rangle$ to obtain some interesting results. For example, we can evaluate the mean value of the energy as

$$
\begin{aligned}
E_\beta &= \langle \beta, \tfrac{1}{2}|H|\beta, \tfrac{1}{2}\rangle \\
&= \hbar\omega N^2 \sum_{n=0}^{\infty} \beta^{2n}(n+1)^2 \\
&= \hbar\omega \frac{(1 + |\beta|^2)}{(1 - |\beta|^2)^2},
\end{aligned}
\qquad (5.44)
$$

from which we may study the relation between the mean value of energy levels E_β and $|\beta|$ as shown in Fig. 5.1. It is found that the mean value of energy levels E_β will increase as $|\beta|$ increases. However, its value almost remains invariant when $|\beta| < 0.3$.
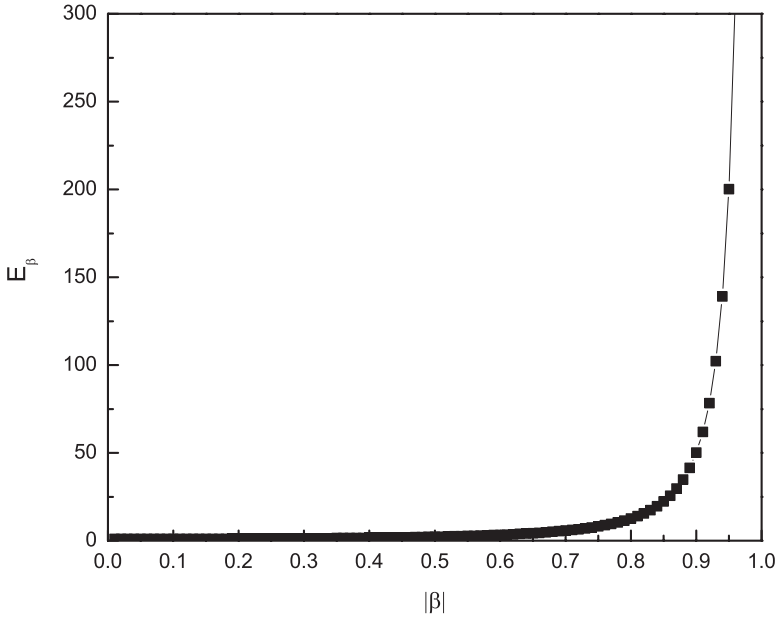
Figure 5.1. The mean value of the energy levels E_β as a function of the parameter $|\beta|$. The natural units $\hbar = \omega = 1$ are taken.

On the other hand, let us study the uncertainty relation $\langle \Delta x \rangle \langle \Delta p \rangle$. In the coherent sates $|\beta x\rangle$, it is found that the mean value of x can be obtained analytically; unfortunately, its expression is too complicated to write it down explicitly except for the numerical calculation. The corresponding mean value of x^2 cannot be obtained analytically. However, the mean values of $p = -i\hbar \frac{d}{dx}$ and $p^2 = -\hbar^2 \frac{d^2}{dx^2}$ can be analytically evaluated as

$$\langle \beta x|p|\beta x \rangle = 0, \tag{5.45}$$

and

$$\langle \beta x|p^2|\beta x \rangle = \hbar^2 \frac{\pi^2 (1 + |\beta|^2)(1 - |\beta|)}{(1 + |\beta|)^5 \left[\frac{(-1 + |\beta|)^2}{(1 + |\beta|)^2} \right]^{3/2}}$$

$$= \hbar^2 \frac{(1 + |\beta|^2)\pi^2}{(1 - |\beta|^2)^2}, \tag{5.46}$$

from which we can obtain the expectation value of the momentum p as

$$\langle \Delta p \rangle = \pi \hbar \sqrt{\frac{(1 + |\beta|^2)}{(1 - |\beta|^2)^2}}. \tag{5.47}$$

We show the relation between $\langle \Delta p \rangle$ and $|\beta|$ in Fig. 5.2. We find that $\langle \Delta p \rangle$ also increases with the $|\beta|$ and $\langle \Delta p \rangle$ tends to infinity when $|\beta| \rightarrow 1$. On the other hand, it increases very slowly when $\beta < 0.3$.
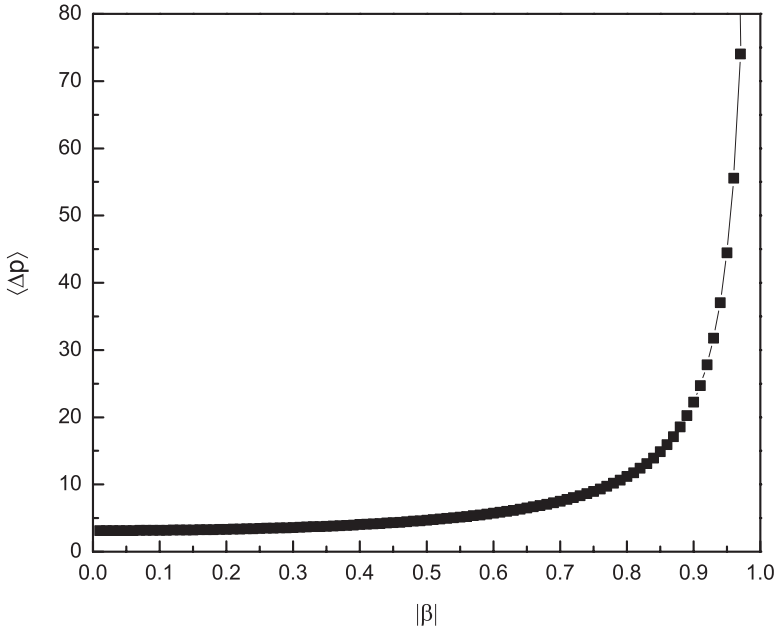
Figure 5.2.   The uncertainty $\langle \Delta p \rangle$ as a function of the parameter $|\beta|$. The natural unit $\hbar = 1$ is taken.

We now study the corresponding relation between $\langle \Delta x \rangle$ and $|\beta|$ as shown in Fig. 5.3, in which the uncertainty $\langle \Delta x \rangle$ decreases as the parameter $|\beta|$ increases.

Finally, let us consider the uncertainty relation $\langle \Delta x \rangle \langle \Delta p \rangle$. From the numerical calculation, we find that

$$\langle \Delta x \rangle \langle \Delta p \rangle \geq \frac{\hbar}{2} \tag{5.48}$$

has a minimum corresponding to $|\beta| = 0$, for which it takes the value $0.567862\hbar \geq \frac{1}{2}\hbar$. Therefore, we may say that the Perelomov coherent states are not minimum uncertainty states. We find from Fig. 5.4 that the uncertainty $\langle \Delta x \rangle \langle \Delta p \rangle$ increases with the parameter $|\beta|$. Similarly, it almost remains invariant for the small values of the parameter $|\beta| < 0.3$.

Let us mention the temporal properties of the coherent states. In quantum mechanics the time evolution can be expressed as

$$
\begin{aligned}
|\beta, \tfrac{1}{2}, t\rangle &= \exp[-iHt] \\
&= N_\beta \sum_{n=0}^{\infty} \beta^n \exp[-iE_n t]|\beta, \tfrac{1}{2}\rangle,
\end{aligned}
\tag{5.49}
$$
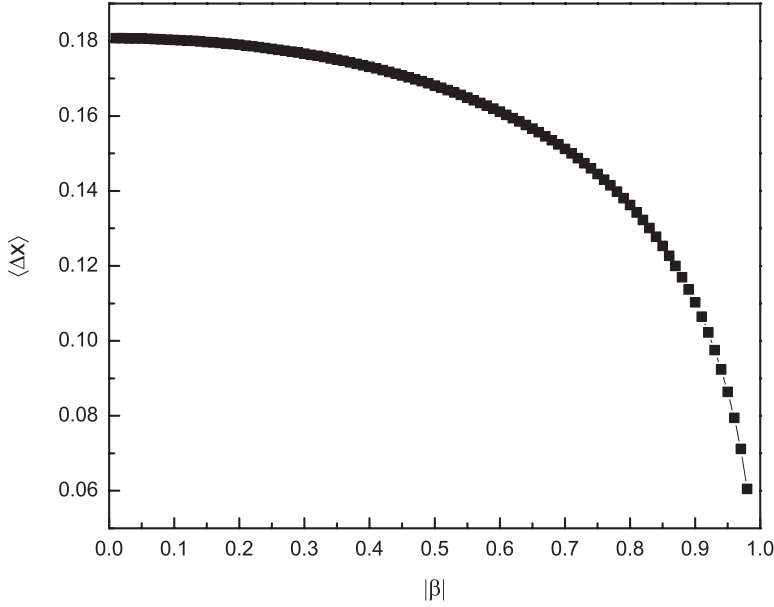
where E_n are the shifted eigenvalues given by $\hbar\omega(n+1)^2$ $(n = 0, 1, 2, \ldots)$ and $|\beta, \frac{1}{2}\rangle$ is given in Eq. (5.43). Generally speaking, the time evolution of the coherent states does not keep its initial form. It is found that the states will deform with time t when $|\beta|$ increases as shown by the uncertainty relation in Fig. 8.6.

7. Barut-Girardello coherent states

In this section we briefly study the Barut-Girardello coherent states of the particle moving in the infinitely deep square well potential [282]. Recently, a similar study has been carried out by Antoine and Klauder [278], but their method is slightly different from ours. In particular, it is found that the Barut-Girardello coherent states for this potential can be obtained analytically and explicitly as shown below.

The Barut-Girardello coherent states are the eigenstates of the annihilation operator $\hat{M}_-$

$$\hat{M}_-|\beta, k\rangle = \beta|\beta, k\rangle, \tag{5.50}$$

where the Barut-Girardello coherent states $|\beta, k\rangle$ are given by [209]

$$|\beta, k\rangle = N \sum_{n=0}^{\infty} \frac{\beta^n}{\sqrt{n!\Gamma(n+2k)}}|n, k\rangle, \quad N = \sqrt{\frac{|\beta|^{2k-1}}{I_{2k-1}(2|\beta|)}}, \tag{5.51}$$
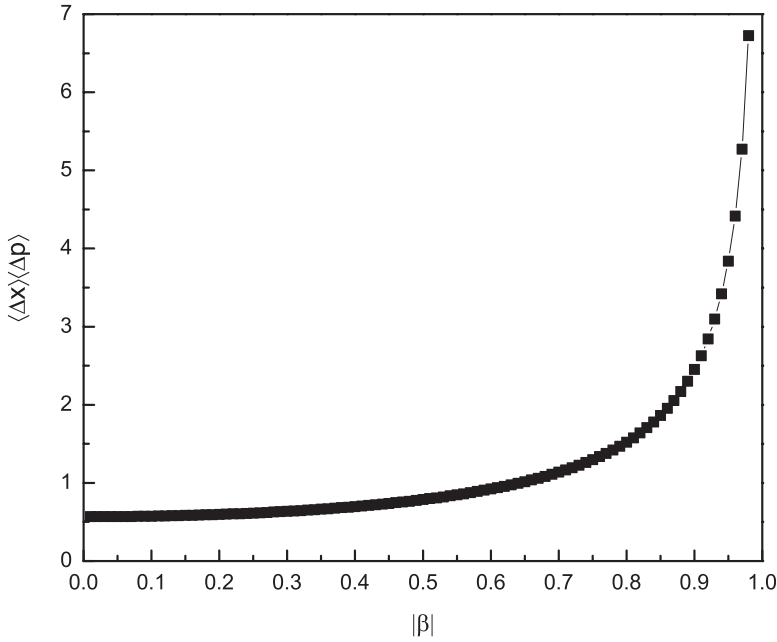
Figure 5.4. The uncertainty relation $\langle \Delta x \rangle \langle \Delta p \rangle$ as a function of the parameter $|\beta|$. The natural unit $\hbar = 1$ is taken.

where $I_\nu(x)$ is the ν-order modified Bessel function of the first kind.

It is found from [209, 292] that these states are normalized but not orthogonal and that the following resolution of the identity holds

$$\int d\mu(\beta, k)|\beta, k\rangle\langle\beta, k| = 1, \qquad (5.52)$$

with

$$d\mu(\beta, k) = \frac{2}{\pi} K_{2k-\frac{1}{2}}(2|\beta|) I_{2k-\frac{1}{2}}(2|\beta|) d^2\beta, \qquad (5.53)$$

$$d^2\beta = d(\operatorname{Re} \beta)d(\operatorname{Im} \beta), \qquad (5.54)$$

where K_ν is the ν-order Bessel function of the second kind [263].

For the same reason, if taking $k = \frac{1}{2}$, then we may simplify Eq. (5.51) as

$$\begin{aligned} |\beta, \tfrac{1}{2}\rangle \quad &= \sqrt{\frac{2}{I_0(2|\beta|)}} [\cosh(|\beta| \cos \pi x) + \sinh(|\beta| \cos \pi x)] \\ &\times [\cos(|\beta| \sin \pi x) \sin \pi x + \sin(|\beta| \sin \pi x) \cos \pi x]. \end{aligned} \qquad (5.55)$$

As we know, once the coherent states are obtained, we may calculate the mean values of some physical observables. First, let us study the mean value

of the energy levels in the Barut-Girardello states

$$
\begin{aligned}
E_\beta &= \langle \beta, \tfrac{1}{2}|H|\beta, \tfrac{1}{2}\rangle \\
&= \hbar\omega N^2 \sum_{n=0}^{\infty} \frac{|\beta|^{2n}(n+1)^2}{(n!)^2} \\
&= \hbar\omega \left[1 + |\beta|^2 + 2|\beta| \frac{I_1(2|\beta|)}{I_0(2|\beta|)} \right].
\end{aligned}
\tag{5.56}
$$

Before ending this part, let us give some remarks on both different types of coherent states. First, we make comparison of the uncertainty relations $\langle\Delta x\rangle\langle\Delta p\rangle$ between the Perelomov coherent states and the Barut-Girardello ones as shown in Fig. 5.5. We find that both coherent states almost keep undeformed for a small range of the parameter $|\beta| < 0.3$. On the other hand, it is found that the Perelomov coherent states will increase with the parameter $|\beta| > 0.3$, while the Barut-Girardello coherent states evolve over time almost resembling its initial state for the large values of the parameter $|\beta|$. That is to say, the Barut-Girardello coherent states almost keep invariant with the increment of the parameter $|\beta|$. Roughly speaking, the increment amplitudes of the uncertainty relations obtained by the Perelomov coherent states will be much greater than those obtained by the Barut-Girardello coherent states . Therefore, this type of coherent states can be seen to approximate the behavior of the minimum uncertainty states for a wide range of the parameter $|\beta|$. The similar behaviors also occur among the mean values of the energy levels, the uncertainties $\langle\Delta x\rangle$ and $\langle\Delta p\rangle$ for two different Perelomov and Barut-Girardello coherent states . We do not show their differences for simplicity. In addition, the Perelomov coherent states are limited by the value of the parameter $|\beta| < 1$, but the Barut-Girardello coherent states have no such a limit. Thus, it seems that the Barut-Girardello coherent states can be used to describe the uncertainty states of the moving particle for a wide range of the parameter $|\beta|$. On the contrary, the Perelomov coherent states cannot be adequately pertinent.

Second, it is surprising to find that the uncertainty relation $\langle\Delta x\rangle\langle\Delta p\rangle$ in the Barut-Girardello coherent states does not always increase with the increment of the parameter $|\beta|$ as shown in Fig. 5.6. We find that there exist two turning points for $|\beta| = 0.6, 1.3$. That is to say, the $\langle\Delta x\rangle\langle\Delta p\rangle$ first increases for $|\beta| \in (0, 0.6)$ and then decreases for $|\beta| \in (0.6, 1.3)$ and finally it always increases with the parameter $|\beta| \geq 1.3$. Likewise, $\langle\Delta x\rangle\langle\Delta p\rangle \geq \frac{\hbar}{2}$ corresponds to a minimum value for $|\beta| = 0$, to which it also takes the value $0.567862\hbar \geq \frac{1}{2}\hbar$. Thus, the Barut-Girardello coherent states are not either minimum uncertainty states.

Finally, it should be noted that under certain conditions, details of which are studied by Gazeau and Klauder [289], the Gazeau-Klauder coherent states which are applicable to the nondegenerate discrete part of the infinite quantum well spectrum will reduce to the Barut-Girardello coherent states.
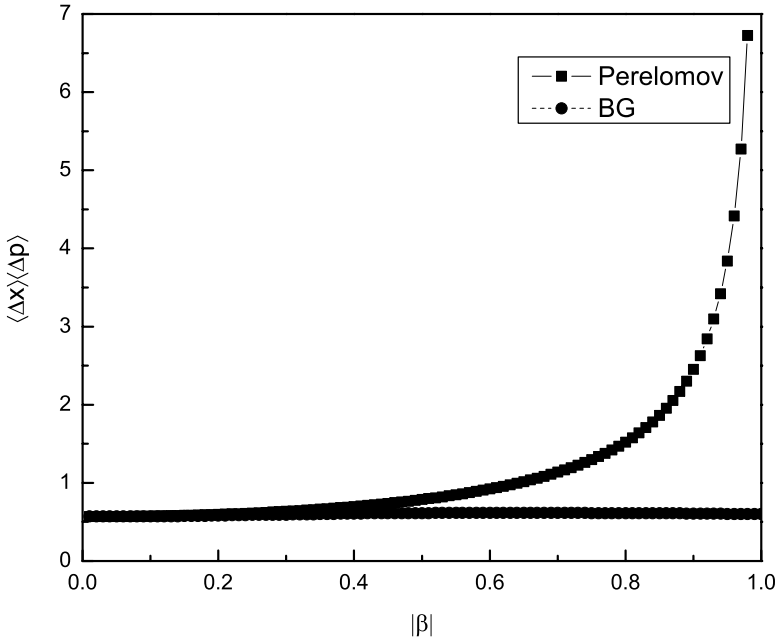
Figure 5.5.   Comparison of the uncertainty relation $\langle\Delta x\rangle\langle\Delta p\rangle$ between Perelomov coherent states and Barut-Girardello coherent states. The natural unit $\hbar = 1$ is taken.

8.   Concluding remarks

In this Chapter we have studied the dynamic group structure of the one-dimensional quantum system with an infinitely deep square-well potential and established the creation and annihilation operators from the factorization method. It is found that the Lie group $SU(1, 1)$ is the dynamic group for this system. The representation for the bound states of this system can be described by the representation $D^+(-\frac{1}{2})$ with a spectrum bounded from below. The matrix elements of the physical quantities $\cos(\pi x/L)$ and $[\sin(\pi x/L)]p$ have been analytically obtained from the ladder operators. On the other hand, we have carried out the Perelomov coherent states and the Barut-Girardello coherent states . In particular, we have studied the former coherent states in detail. The uncertainties $\langle\Delta x\rangle$ and $\langle\Delta p\rangle$ have been investigated. The relation between the mean value of the energy levels and the parameter $|\beta|$ is discussed.

On the other hand, we have made some comparisons of the uncertainty relations $\langle\Delta x\rangle\langle\Delta p\rangle$ between the Perelomov coherent states and the Barut-Girardello ones. We have found that both coherent states almost keep undeformed for a small range of the parameter $|\beta| < 0.3$. However, the Perelomov coherent states will increase with the parameter $|\beta| > 0.3$, while the Barut-Girardello coherent states evolve over time almost resembling its initial state
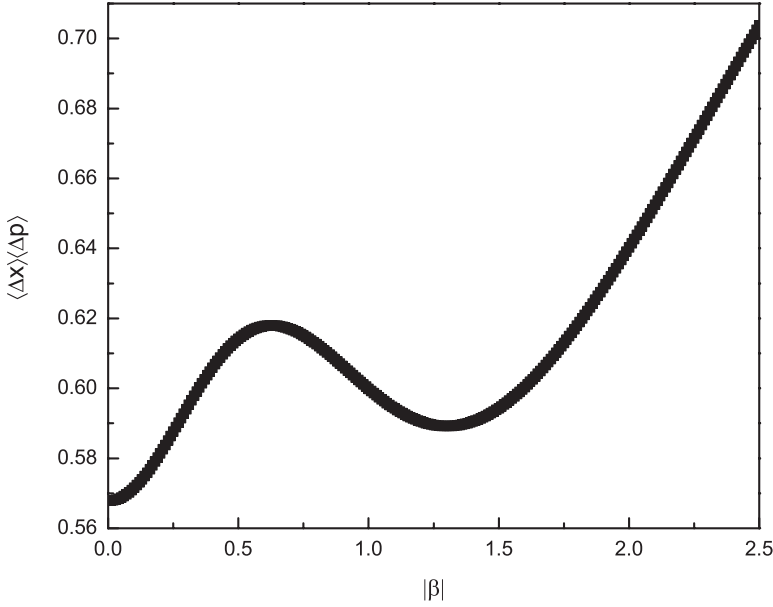
Figure 5.6. Uncertainty relation $\langle \Delta x \rangle \langle \Delta p \rangle$ in the Barut-Giradello coherent states.

for the large values of the parameter $|\beta|$. That is to say, the Barut-Girardello coherent states almost remain invariant with the increment of the parameter $|\beta|$. The similar behaviors also occur among the mean values of the energy levels, the uncertainties $\langle \Delta x \rangle$ and $\langle \Delta p \rangle$ for two different Perelomov and Barut-Girardello coherent states . Additionally, the Perelomov coherent states will be limited by the value of the parameter $|\beta| < 1$, but the Barut-Girardello coherent states have no such a limit. Thus, it seems that the Barut-Girardello coherent states can be used to describe the uncertainty states of the moving particle for a wide range of the parameter $|\beta|$, but the Perelomov coherent states cannot be adequate.

Finally, it is surprising to find that the uncertainty relation $\langle \Delta x \rangle \langle \Delta p \rangle$ in the Barut-Girardello coherent states does not always increase with the increment of the parameter $|\beta|$. We find that there exist two turning points for $|\beta| = 0.6, 1.3$. That is to say, the uncertainty $\langle \Delta x \rangle \langle \Delta p \rangle$ first increases for $|\beta| \in (0, 0.6)$, and then decreases for $|\beta| \in (0.6, 1.3)$ and finally it always increases with the parameter $|\beta| \geq 1.3$. Likewise, we have also found that the Barut-Girardello coherent states are not either minimum uncertainty states.

Chapter 6

MORSE POTENTIAL

1.   Introduction

The study of exactly solvable problems has attracted much attention of many authors since the early development of quantum mechanics. To our knowledge, the exact solvable physical problems are few in quantum mechanics except for several well-known exactly solvable quantum systems like the hydrogen atom, harmonic oscillator and others. Due to its mathematical advantages, the harmonic oscillator model has been widely used to describe the interaction force of the diatomic molecule. Nevertheless, it is well known that the real molecular vibrations are anharmonic. Among many molecular potentials, the Morse potential as an ideal and typical anharmonic potential permits an exactly mathematical treatment and it has been the subject of interest since it was proposed by Morse in 1929 [293]. In particular, the Morse potential will reduce to the harmonic oscillator in the harmonic limit.

Up to now, the Morse potential has been widely used both in physics and in chemistry [294–296]. Undoubtedly, there have been hundreds of papers appearing in the literature since 1929. Considering its importance in various fields of physics and chemistry, we are going to give a brief review of this potential. Generally speaking, there are two methods to obtain the eigenfunctions and eigenvalues of the Morse potential. The first method is the analytical method. That is to say, its exact solutions can be obtained by solving the Schrödinger equation as treated by Morse [293], Landau and Lifshitz [297] and others. Another method is the SUSYQM method, which is also related to the algebraic method [298–301]. For example, Panigrahi and Sukhatme presented the partner potentials of the ground state and the first excited state of the Morse potential [298]. Filho and Ricotta derived the energy spectrum of the Morse potential using the variational method and the SUSYQM method [299]. Molnár,

Földi, Benedict and Bartha employed the SUSYQM technique to treat the NO molecular vibrations in the Morse potential perturbed by an external field and calculated the dissociation probability of this molecule excited by appropriate series of chirped laser pulses [300]. Han, Song and Yang obtained the eigenfunctions and eigenvalues by the SUSYQM approach and found that the Morse potential is shape invariant [301].

In fact, among hundreds of contributions to the Morse potential, most of them have paid much attention to its wide applications in physics, chemistry and other related fields, but not to how to solve it using different methods. Roughly speaking, there are a few main applications of the Morse potential in various fields. First, it is about the calculations of the transition probabilities and corresponding matrix elements. For example, Fraser and Jarmain have calculated the vibrational transition probabilities of diatomic molecules by integrating the vibrational wave functions of the Morse potential [302, 303], the exactly solvable quantum mechanical vibrational transition probabilities for a collinear collision of an atom and a Morse oscillator was studied by Clark and Dickinson [304], who were enlightened by the early contributions made by Mies [305] and Hunding [306]. On the other hand, one has to calculate some necessary matrix elements [307–323] when one calculates the transition probabilities even though such a task can be easily obtained numerically. It should be noted that many authors employed the explicit Morse eigenfunctions expressed in terms of the associated Laguerre polynomials to calculate the matrix elements. For example, Vasan and Cross generalized the calculations of the matrix elements to the exponential-type function and the product of the coordinate and the exponential-type function in terms of the exact solutions of the Morse potential [307]. Naccache used the Heisenberg's form of the correspondence principle for non-relativistic matrix elements to evaluate matrix elements of the position, momentum and the kinetic energy for the Morse potential [308]. Gallas applied the Morse eigenfunctions to obtain the matrix elements of any power of the coordinate [311]. Sage began by considering some basic properties of the associated Laguerre functions to calculate some matrix elements of the bound states of the Morse potential and also gave model calculations for the local model of the CH stretch in aromatic hydrocarbons [318]. On the other hand, many authors used some quantum theorems like the hypervirial and Hellmann-Feynman theorems to obtain simple recursion relations between different matrix elements. The advantage of this method is that we need not use the explicit eigenfunctions of the Morse potential. The typical contributions are made by Tipping, Moreno and Zúñiga *et al.* [312–314]. Recently, we have proposed a generalized expression of the second hypervirial for arbitrary central potential wave functions in arbitrary dimension D and demonstrated that the new proposed second hypervirial formula is powerful in deriving the general Blanchard's and Krammers' recurrence relations among the radial matrix

elements [316, 317]. For example, we have obtained the recurrence relation and identity between the exponential functions and the powers of the radial function for the Morse potential even though its solutions cannot be obtained exactly. In addition, Iwamoto and Matsumoto have studied the dipole matrix elements for vibration-rotation transitions between discrete and continuous states of the Morse molecules [324], in which the continuous wave functions of the Morse potential were obtained as done by others [325]. Second, the Morse potential was considered in the thermodynamics. For example, Dallwig, Weese, Weiss and Schlier studied the statistical properties of the resonance states in a double Morse potential well [326]. Völkel, Cuccoli, Spicci and Tognetti presented the calculations of equilibrium thermodynamic properties of the quantum Morse chain using a variational method [327]. Talukdar, Chatterji and Banerjee have studied the phase shift contributions to the partition function of a diatomic molecular system described by the Morse potential [328]. The third is about the study of the Wigner distribution function for the Morse potential [329–333]. It should be noted that the contribution made by Dahl and Springborg played an important role in its study. The fourth is related to the modified Morse potential [334–338]. The main aim is to find a more suitable diatomic potential to describe the vibrational spectrum. For example, Deng and Fan proposed an electronic energy function for diatomic molecules in 1957 expressed as [334]

$$V(r) = D \left[1 - \frac{e^{ar_e} - 1}{e^{ar-1}} \right]^2,$$

(6.1)

which implies that this potential approaches infinite as the internuclear distance r tends to zero and the Schrödinger equation with this potential is exactly solvable. Recently, Rong, Kjaergaard and Sage have used the Morse and Deng-Fan potentials to treat the X-H stretching motion in small molecules and calculated transition frequencies and intensities of overtones of X-H stretching vibrations. Finally, they compared the results by using different molecular potentials [339]. The fifth is on the study of rotation-vibration spectra for the Morse potential. The first contribution to this field was made by Pekeris in 1934 [340]. After that, some works along this line have been developed [341–346]. For example, Berkdemir and Han used the Nikiforov-Uvarov method and Pekeris approximation to study the Morse quantum system for any l-state solutions [341]. Killingbeck used the hypervirial perturbation method to study the similar problem. Sixth, the Morse potential was also applied to solid state physics. To our knowledge, the application of the Morse potential function is widespread during the past several decades in the study of various physical properties of the solids which include the harmonic, anharmonic and also defect properties, e.g., the second and third order elastic constants in cubic metals studied by Girifalco, Weizer, Lincoln, Koliwad and Ghate [347, 348], the binding energies and stability of FCC and BCC type metals [347, 349, 350], the thermal expansion

in cubic and hexagonal metals at room temperature [351, 352], the point defect [353], line defect [354], grain boundary phenomena [355] and volume change in some low-concentration substitutional alloys [356]. For instance, Roy, Manna and Sen Gupta have used the Morse potential functions to study the ordered Cu_3Au and Au_3Cu alloys as well as thermal expansion and the equation of state [357, 358] and others [359]. Additionally, the Morse potential was used to study the lattice sums in cubic crystals [360] and the multiphonon absorption in alkali halides [361]. The seventh is about the calculations of the Franck-Condon factors [362–377]. For example, Chau used an iterative method for the Franck-Condon factor calculations by using the Morse potential functions to estimate equilibrium bond lengths of diatom [367]. Palma, Rivas-Silva, Durand and Sandoval have used the algebraic method to study the Franck-Condon factors[368]. López *et al.* employed the properties of the Morse eigenfunctions to calculate the Franck-Condon factors with the aid of the MATHEMATICA tool [374]. Furthermore, Ley-Koo, Mateos-Cortes and Villa-Torres studied this problem including rotation contributions in the quantum system [375, 376].

Other various investigations have been performed apart from the main applications of the Morse potential in various fields of physics and chemistry as mentioned above. For example, Carvajal *et al.* used the configuration localized Morse wave functions to study the vibrational transitions in anharmonic diatomic molecules [378]. Cooper applied the algebraic method to study the molecular spectra [379, 380]. Alhaidari studied the solution of the relativistic Dirac-Morse problem [381]. The large-N approach to study the Morse potential was also carried out [382–384]. Tošić and Popov presented a method to solve the Bloch equation for the Morse potential [385]. Recently, the series solutions for both the traditional and position-dependent Schrödinger equations with the Morse quantum system have been investigated [386–388].

It should be pointed out that most contributions to the Morse potential are related to the analysis method. As another important method, algebraic method has played a crucial role in its study [389–392]. For example, the coherent states of the Morse potential have been discussed since they are closely related to the algebraic technique [393–400]. Due to the fact that the Morse potential is solvable, hence the interest is to deal with it using different approaches. On the basis of these methods, an su(1, 1) algebra has been identified [97, 136, 213, 370, 401–406]. On the other hand, it was recognized that the SU(2) group was the dynamic group associated with the bounded region of the spectrum [156]. Therefore, a natural question which arises is the one concerned with obtaining creation and annihilation operators satisfying the su(2) algebra for the discrete part of the spectrum. The Morse potential has been studied in terms of both SO(2, 1) [97, 136, 213, 401–406] and SU(2) groups [105, 197]. The latter description has been exploited in the development of an algebraic treatment of molecular vibrations in polyatomic molecules which incorporates

anharmonic effects at the local mode level, while the former turned out to be relevant for the algebraic determination of S-matrix under scattering conditions. The fundamental difference between these approaches is that SO(2, 1) is a non-compact group, which involves either unitary continuous representations or infinite-dimensional discrete ones. Thus, the raising and lowering operators of the SO(2, 1) are associated with step variations of the potential depth, keeping a fixed energy [401], while the SU(2) formulation involves the description of the bound states only, a finite number [105, 197]. On the other hand, in SO(2, 1) the Morse Hamiltonian is associated with the Casimir invariant (the potential group approach) [407–409], in the case of the SU(2) the Hamiltonian is a simple function of the generators [105, 156]. The connection of the SU(2) group with the Morse system can be directly established by means of a coordinate transformation applied to the radial equation of the two-dimensional harmonic oscillator [142, 410]. This procedure, however, does not provide us with an explicit realization of the SU(2) generators in terms of the physical coordinate. This realization was explored further in [411, 412], where a comparison of the Morse matrix elements with those of the SU(2) leads to a series expansion of the coordinate and momentum in terms of the SU(2) generators. Other investigations have used a realization of these operators which involve an auxiliary variable [156], while Nieto and Simmons constructed the raising and lowering operators which were not, however, linked with a group structure [413].

The aims of this Chapter are the following. First, we derive a realization of the dynamic group for the Morse potential using the factorization method and show that together with a weight generator they exactly satisfy the SU(2) commutation relations. Second, we shall verify our results by calculating matrix elements of certain functions of the Morse coordinate and momentum, and study the harmonic limit, and indicate some other possible applications of these operators.

This Chapter is organized as follows. From Section 2 to 4, we shall first study the exact solutions of the Morse quantum system and then establish the raising and lowering operators directly from the eigenfunctions of the Morse potential with the factorization method and construct a dynamic Lie algebra su(2). In Section 5 the matrix elements of the operators $1/y$ and d/dy are obtained from the ladder operators. Section 6 is devoted to showing how the harmonic limit is attained. In Section 7 we shall briefly address the Franck-Condon factors. Section 8 is devoted to the study of the transition probabilities. In Section 9 we shall study the realization of the dynamic group SU(1, 1) for the Morse potential. Finally, in Section 10 we present our summary and conclusions.

2. Exact solutions

Choosing the separated atoms limit as the zero of energy, the Morse potential has the following form [293]

$$V(x) = V_0(e^{-2\beta x} - 2e^{-\beta x}), \tag{6.2}$$

where $V_0 > 0$ corresponds to its depth, β is related to the range of the potential, and x gives the relative distance from the equilibrium position of the atoms.

The solutions of the Schrödinger equation associated to the Morse potential are given in Ref. [297]

$$\Psi_n^\nu(y) = N_n^\nu e^{-\frac{y}{2}} y^s L_n^{2s}(y), \tag{6.3}$$

where $L_n^{2s}(y)$ are the associated Laguerre functions and the argument y is related to the physical displacement coordinate x by

$$y = \nu e^{-\beta x}. \tag{6.4}$$

The factor N_n^ν is the normalization constant

$$N_n^\nu = \sqrt{\frac{\beta(\nu - 2n - 1)\Gamma(n + 1)}{\Gamma(\nu - n)}}, \tag{6.5}$$

and the variables ν and s are related with the potential and the energy, respectively, through

$$\nu = \sqrt{\frac{8\mu V_0}{\beta^2 \hbar^2}}, \quad s = \sqrt{\frac{-2\mu E}{\beta^2 \hbar^2}}, \tag{6.6}$$

with the constraint condition

$$2s = \nu - 2n - 1. \tag{6.7}$$

Here μ is the reduced mass of the molecule.

It should be noted that Landau and Lifshitz did not show how to derive the exact solutions of the Morse system in detail. In order to make it clear to obtain the constraint condition (6.7), let us derive it briefly below.

We begin by considering the new variables given in Eqs. (6.4) and (6.6). Substitutions of them into the Schrödinger equation

$$-\frac{1}{2\mu} \frac{d^2}{dx^2} \Psi(x) + V(x)\Psi(x) = E\Psi(x) \tag{6.8}$$

allow us to obtain the following modified second-order differential equation

$$\frac{d^2}{dy^2} \Psi(y) + \frac{1}{y} \frac{d}{dy} \Psi(y) + \left(\frac{\nu}{2y} - \frac{s^2}{y^2} - \frac{1}{4} \right) \Psi(y) = 0, \tag{6.9}$$

where we have used the relation

$$\frac{d}{dx} = (-\beta y)\frac{d}{dy}. \tag{6.10}$$

From the behaviors of the wave functions at the origin and at infinity, we take the wave functions as

$$\Psi(y) = e^{-\frac{y}{2}} y^s F(y). \tag{6.11}$$

Substitution of this into Eq. (6.9) leads to

$$y\frac{d^2}{dy^2}F(y) + (2s + 1 - y)\frac{d}{dy}F(y) - \left(s + \frac{1-\nu}{2}\right)F(y) = 0, \tag{6.12}$$

whose solutions are nothing but the confluent hypergeometric functions as

$$F(y) = N\,F\left(s + \frac{1-\nu}{2}, 2s + 1; y\right). \tag{6.13}$$

Thus, we are able to obtain the quantum condition

$$s + \frac{1-\nu}{2} = -n, \quad n = 0, 1, 2, ..., \tag{6.14}$$

from which we obtain Eq. (6.7).

On the other hand, making use of the relation between the confluent hypergeometric functions and the associated Laguerre functions, we may obtain the exact solutions of this quantum systems as given in Eq. (6.3).

3. Ladder operators for the Morse potential

We address in this part the problem of finding creation and annihilation operators for the Morse wave functions (6.3) based on the basic idea proposed by Avram and Drăgănescu [370], but following a different approach. In other words, we intend to find differential operators $\hat{K}_\pm$ with the following property

$$\hat{K}_\pm \Psi_n^\nu(y) = k_\pm \Psi_{n\pm1}^\nu(y). \tag{6.15}$$

Specifically, we look for operators of the form

$$\hat{K}_\pm = A_\pm(y)\frac{d}{dy} + B_\pm(y), \tag{6.16}$$

which only depend on the physical variable y.

For this purpose, we begin by acting the differential operator d/dy on the Morse wave functions

$$\frac{d}{dy}\Psi_n^\nu(y) = -\frac{1}{2}\Psi_n^\nu(y) + \frac{1}{y}s\Psi_n^\nu(y) + N_n^\nu e^{-\frac{y}{2}} y^s \frac{d}{dy}L_n^{2s}(y). \tag{6.17}$$

One possible relation for the derivative of the associated Laguerre functions is given in [263]

$$\frac{d}{dy}L_n^\alpha(y) = -\frac{1}{(\alpha+1)}\left[yL_{n-1}^{\alpha+2}(y) + nL_n^\alpha(y)\right].$$ (6.18)

Substitution of this expression into Eq. (6.17) leads to the following relation between the Morse functions belonging to the same potential

$$\left[\frac{d}{dy}(2s+1) - \left(\frac{1}{y}s - \frac{1}{2}\right)(2s+1) + n\right]\Psi_n^\nu(y) = -\frac{N_n^\nu}{N_{n-1}^\nu}\Psi_{n-1}^\nu(y),$$ (6.19)

from which we can define the annihilation operator

$$\hat{K}_- = -\left[\frac{d}{dy}(2s+1) - \frac{1}{y}s(2s+1) + \frac{\nu}{2}\right]\sqrt{\frac{s+1}{s}}$$ (6.20)

with the following effect over the wave functions

$$\hat{K}_-\Psi_n^\nu(y) = k_-\Psi_{n-1}^\nu(y),$$ (6.21)

where

$$k_- = \sqrt{n(\nu - n)}.$$ (6.22)

As we see, this operator annihilates the ground state $\Psi_0^\nu(y)$, as expected from a step-down operator. In Eq. (6.20) the variable s is to be understood as a diagonal operator depending on n, according to the constraint condition $2s = \nu - 2n - 1$. Note also that the order of the different terms in Eq. (6.20) is important, as these operators do not commute.

We now proceed to find the corresponding creation operator. First, we should keep in mind that we need obtain a relation between $\frac{d}{dy}L_n^\alpha(y)$ and $L_{n+1}^{\alpha-2}(y)$ since this implies a relation between $\frac{d}{dy}\Psi_n^\nu(y)$ and the Morse wave functions $\Psi_{n-1}^\nu(y)$. To achieve this task we start with the relation

$$y\frac{d}{dy}L_n^\alpha(y) = nL_n^\alpha(y) - (n+\alpha)L_{n-1}^\alpha(y),$$ (6.23)

which, when taking into account that [263]

$$(n+1)L_{n+1}^\alpha(y) - (2n+\alpha+1-y)L_n^\alpha(y) + (n+\alpha)L_{n-1}^\alpha(y) = 0$$ (6.24)

can be transformed into

$$y\frac{d}{dy}L_n^\alpha(y) = (-n-\alpha-1+y)L_n^\alpha(y) + (n+1)L_{n+1}^\alpha(y).$$ (6.25)

On the other hand, the relation

$$L_n^{\alpha-1}(y) = L_n^{\alpha}(y) - L_{n-1}^{\alpha}(y), \tag{6.26}$$

together with Eq. (6.24), allows us to set up the following relation

$$\frac{(\alpha-1)}{(n+\alpha)} L_{n+1}^{\alpha}(y) = \frac{(\alpha+y-1)}{(\alpha+n)} L_n^{\alpha}(y) + L_{n+1}^{\alpha-2}(y). \tag{6.27}$$

Here, we want to show how to derive this formula in detail. It is shown from Eqs. (6.24) and (6.26) that

$$(n+1)L_{n+1}^{\alpha}(y) - 2(n+\alpha)L_n^{\alpha}(y) + (\alpha+y-1)L_n^{\alpha}(y)$$
$$+(n+\alpha)[L_n^{\alpha}(y) - L_n^{\alpha-1}(y)] = 0, \tag{6.28}$$

which can be further simplified as

$$(n+1)L_{n+1}^{\alpha}(y) - (n+\alpha)L_n^{\alpha}(y) - (n+\alpha)L_n^{\alpha-1}(y) + (\alpha+y-1)L_n^{\alpha}(y) = 0, \tag{6.29}$$

from which, together with Eq. (6.26) again, we have

$$(n+1)L_{n+1}^{\alpha}(y) - (n+\alpha)[L_{n+1}^{\alpha}(y) - L_{n+1}^{\alpha-1}(y)]$$
$$-(n+\alpha)L_n^{\alpha-1}(y) + (\alpha+y-1)L_n^{\alpha}(y) = 0, \tag{6.30}$$

which can be further rewritten as

$$(\alpha-1)L_{n+1}^{\alpha}(y) + (n+\alpha)[L_n^{\alpha-1}(y) - L_{n+1}^{\alpha-1}(y)] - (\alpha+y-1)L_n^{\alpha}(y) = 0. \tag{6.31}$$

Using Eq. (6.26) again, we have

$$(\alpha-1)L_{n+1}^{\alpha}(y) - (n+\alpha)L_{n+1}^{\alpha-2}(y) - (\alpha+y-1)L_n^{\alpha}(y) = 0, \tag{6.32}$$

which is nothing but Eq. (6.27). Equation (6.27) in turn can be substituted into Eq. (6.25) to give

$$(\alpha-1)\frac{d}{dy}L_n^{\alpha}(y) = \left[(\alpha+n) - \frac{\alpha(\alpha-1)}{y}\right] L_n^{\alpha}(y)$$
$$+ \frac{(n+1)(n+\alpha)}{y} L_{n+1}^{\alpha-2}(y). \tag{6.33}$$

Finally, when this equation is substituted into (6.17), we obtain

$$\frac{d}{dy}\Psi_n^{\nu}(y) = \left[-\frac{1}{2} - \frac{s}{y} + \frac{(2s+n)}{(2s-1)}\right] \Psi_n^{\nu}(y)$$
$$+ \frac{N_n^{\nu}}{N_{n+1}^{\nu}} \frac{(n+1)(n+2s)}{(2s-1)} \Psi_{n+1}^{\nu}(y), \tag{6.34}$$

which allows us to define the creation operator as

$$\hat{K}_+ = \left[\frac{d}{dy}(2s - 1) + \frac{1}{y}s(2s - 1) - \frac{\nu}{2} \right] \sqrt{\frac{s - 1}{s}} \qquad (6.35)$$

satisfying the equation

$$\hat{K}_+ \Psi_n^\nu(y) = k_+ \Psi_{n+1}^\nu(y), \qquad (6.36)$$

with

$$k_+ = \sqrt{(n + 1)(\nu - n - 1)}. \qquad (6.37)$$

Since $\hat{K}_+$ is a raising operator it is expected to annihilate the last bounded state. Indeed, for such a state $s = 1$ and the square root in (6.35) makes the operator vanish.

4. Realization of dynamic group SU(2)

We now study the dynamic group associated with the ladder operators $\hat{K}_+$ and $\hat{K}_-$. Based on the results (6.21), (6.22), (6.36) and (6.37), we can calculate the commutator $[\hat{K}_+, \hat{K}_-]$:

$$[\hat{K}_+, \hat{K}_-]\Psi_n^\nu(y) = 2k_0 \, \Psi_n^\nu(y), \qquad (6.38)$$

where we have introduced the eigenvalue

$$k_0 = -\left(\frac{\nu - 1}{2} - n \right). \qquad (6.39)$$

We can thus define the operator

$$\hat{K}_0 = -\left(\frac{\nu - 1}{2} - \hat{n} \right). \qquad (6.40)$$

This operator can be rewritten in terms of differential operators with the help of the differential equation for the Morse wave functions [414]

$$\left(y\frac{d^2}{dy^2} + \frac{d}{dy} - \frac{s^2}{y} - \frac{y}{4} + \frac{\nu}{2} \right) \Psi_n^\nu(y) = 0, \qquad (6.41)$$

from which we can establish the identity

$$\hat{K}_0 = -\left(y\frac{d^2}{dy^2} + \frac{d}{dy} - \frac{s^2}{y} - \frac{y}{4} + n + \frac{1}{2} \right). \qquad (6.42)$$

Thus, the operators $\hat{K}_\pm$ and $\hat{K}_0$ satisfy the commutation relations

$$[\hat{K}_+, \hat{K}_-] = 2\hat{K}_0, \quad [\hat{K}_0, \hat{K}_\pm] = \pm\hat{K}_\pm, \tag{6.43}$$

which correspond to the SU(2) group for the Morse potential. As mentioned earlier, this result is consistent with the description of a finite discrete spectrum and in accordance with previous algebraic descriptions of the bound states of the Morse potential [411, 412]. The operators $\hat{K}_\pm$ and $\hat{K}_0$ are thus equivalent to $\hat{J}_\mp$ and $\hat{J}_0$ used in [411, 412], respectively, where the number of bosons N introduced there is related to ν through $N = \nu - 1$.

The Casimir operator can be calculated as

$$\begin{aligned} C\,\Psi_n^\nu(y) &= \left[\hat{K}_0^2 + \frac{1}{2}(\hat{K}_+\hat{K}_- + \hat{K}_-\hat{K}_+)\right]\Psi_n^\nu(y) \\ &= j(j+1)\Psi_n^\nu(y), \end{aligned} \tag{6.44}$$

where j, the label of the irreducible representations of the Lie algebra su(2), is given by

$$j = \frac{\nu - 1}{2} = \frac{N}{2}. \tag{6.45}$$

From the commutation relations (6.43) we know that $\hat{K}_0$ is the projection of the angular momentum m, and consequently

$$n - \frac{\nu - 1}{2} = m. \tag{6.46}$$

Therefore, the ground state corresponds to $m = -j$, while the maximum number of states $n_{\max} = \frac{\nu-3}{2}$ and accordingly $m_{\max}|_{n_{\max}} = -1$. The Morse wave functions are then associated with one branch (in this case to $m \leq -1$) of the su(2) representations, as expected in [407]. Finally, we should notice that in terms of the su(2) algebra the Hamiltonian acquires a simple form

$$H = -\frac{\hbar\omega}{\nu}\hat{K}_0^2, \tag{6.47}$$

where

$$\omega = \frac{\hbar\beta^2\nu}{2\mu}. \tag{6.48}$$

On the other hand, the Morse wave functions can be simply expressed as

$$\Psi_n^\nu(y) = \mathcal{N}_n^\nu\,\hat{K}_+^n\,\Psi_0^\nu(y), \tag{6.49}$$

where the normalization constant can be obtained as

$$\mathcal{N}_n^\nu = \sqrt{\frac{(\nu - n - 1)!}{n!(\nu - 1)!}}. \tag{6.50}$$

5. Matrix elements

For further calculations, we find from Eqs. (6.20) and (6.35) that the following physical functions can be obtained by the creation and annihilation operators $\hat{K}_{\pm}$ as

$$
\begin{aligned}
\frac{d}{dy} &= \hat{K}_{+}\left(\frac{1}{2(2s-1)}\sqrt{\frac{s}{s-1}}\right) - \hat{K}_{-}\left(\frac{1}{2(2s+1)}\sqrt{\frac{s}{s+1}}\right) \\
&+ \frac{\nu}{2(2s+1)(2s-1)},
\end{aligned}
\tag{6.51}
$$

and

$$
\begin{aligned}
\frac{1}{y} &= \hat{K}_{+}\left(\frac{1}{2s(2s-1)}\sqrt{\frac{s}{s-1}}\right) + \hat{K}_{-}\left(\frac{1}{2s(2s+1)}\sqrt{\frac{s}{s+1}}\right) \\
&+ \frac{\nu}{(2s+1)(2s-1)}.
\end{aligned}
\tag{6.52}
$$

Their matrix elements can be analytically obtained by means of Eqs. (6.21), (6.22), (6.36) and (6.37) as

$$
\begin{aligned}
\left\langle m\left|\frac{1}{y}\right|n\right\rangle &= \frac{1}{(\nu-2n-2)}\sqrt{\frac{(n+1)(\nu-n-1)}{(\nu-2n-1)(\nu-2n-3)}}\delta_{m,n+1} \\
&+ \frac{1}{(\nu-2n)}\sqrt{\frac{n(\nu-n)}{(\nu-2n-1)(\nu-2n+1)}}\delta_{m,n-1} \\
&+ \frac{\nu}{(\nu-2n-2)(\nu-2n)}\delta_{m,n},
\end{aligned}
\tag{6.53}
$$

and

$$
\begin{aligned}
\left\langle m\left|\frac{d}{dy}\right|n\right\rangle &= \frac{1}{2(\nu-2n-2)}\sqrt{\frac{(n+1)(\nu-n-1)(\nu-2n-1)}{(\nu-2n-3)}}\delta_{m,n+1} \\
&- \frac{1}{2(\nu-2n)}\sqrt{\frac{n(\nu-n)(\nu-2n-1)}{(\nu-2n+1)}}\delta_{m,n-1} \\
&+ \frac{\nu}{2(\nu-2n)(\nu-2n-2)}\delta_{m,n}.
\end{aligned}
\tag{6.54}
$$

It is shown that this method is elegant and simple to calculate the matrix elements of some related physical functions.

6. Harmonic limit

We turn our attention in this section to the harmonic limit in which the Morse potential approaches a harmonic oscillator potential. In the limits $\beta \to 0$ and

$V_0 \to \infty$, but keeping the product $k = 2\beta^2 V_0$ finite[1], so that the expansion of the exponential functions in (6.2), leads to the harmonic limit

$$\lim_{V_0 \to \infty} V_{\text{Morse}} = \frac{1}{2} k x^2. \tag{6.55}$$

We now proceed to analyze the contraction of the su(2) algebra

$$G_{\text{su}(2)} = \{\hat{K}_+, \hat{K}_-, \hat{K}_0\} \tag{6.56}$$

in this limit. We first note that according to the relation $2s = \nu - 2n - 1$, we have

$$\lim_{\nu \to \infty} \frac{2s}{\nu} = \lim_{\nu \to \infty} \sqrt{\frac{s-1}{s}} = \lim_{\nu \to \infty} \sqrt{\frac{s+1}{s}} = 1. \tag{6.57}$$

If we expand the exponential function of the variable y and keep in mind that in the harmonic limit $\beta \to 0$, then we are able to obtain the following approximations

$$y \simeq \nu(1 - \beta x), \quad \frac{1}{y} \simeq \frac{1}{\nu}(1 + \beta x), \tag{6.58}$$

which can be used to obtain the corresponding approximation for the derivative

$$\frac{d}{dy} = -\frac{1}{\beta} \frac{1}{y} \frac{d}{dx}, \tag{6.59}$$

whose harmonic limit turns out to be

$$\lim_{\nu \to \infty} \frac{d}{dy} = \lim_{\nu \to \infty} \left[-\frac{1}{\beta} \frac{1}{\nu} (1 + \beta x) \frac{d}{dx} \right] = -\frac{1}{\beta \nu} \frac{d}{dx}. \tag{6.60}$$

We are now ready to study the harmonic limit of the operators (6.56), but before doing so it is convenient to introduce the renormalization operators

$$b^\dagger = \frac{\hat{K}_+}{\sqrt{\nu}}, \quad b = \frac{\hat{K}_-}{\sqrt{\nu}}, \quad b_0 = \frac{-2\hat{K}_0}{\nu}, \tag{6.61}$$

which, when considering Eqs. (6.20) and (6.35), leads to

$$\lim_{\nu \to \infty} b^\dagger = \frac{\sqrt{\nu}\beta}{2} x - \frac{1}{\beta\sqrt{\nu}} \frac{d}{dx} = \sqrt{\frac{\mu\omega}{2\hbar}} x - \sqrt{\frac{\hbar}{2\mu\omega}} \frac{d}{dx} = a^\dagger, \tag{6.62}$$

$$\lim_{\nu \to \infty} b = \sqrt{\frac{\mu\omega}{2\hbar}} x + \sqrt{\frac{\hbar}{2\mu\omega}} \frac{d}{dx} = a, \tag{6.63}$$

$$\lim_{\nu \to \infty} b_0 = 1, \tag{6.64}$$

where ω is given in (6.48). The operators $a^\dagger$ and a satisfy the bosonic commutation relations

$$[a, a^\dagger] = 1, \quad [a, a] = [a^\dagger, a^\dagger] = 0, \tag{6.65}$$

as expected. Thus, in the harmonic limit the su(2) algebra contracts to the Weyl algebra, i.e.,

$$\lim_{\nu \to \infty} G_{\mathrm{su}(2)} = \{a^\dagger, a, 1\}. \tag{6.66}$$

Finally, in terms of the operators (6.61) the Morse wave functions take a simple form

$$\Psi_n^\nu(y) = \sqrt{\frac{\nu^n(\nu - n - 1)!}{n!(\nu - 1)!}} \, (b^\dagger)^n \, \Psi_0^\nu(y), \tag{6.67}$$

whose harmonic limit is given by

$$\lim_{\nu \to \infty} \Psi_n^\nu(y) = \frac{1}{\sqrt{n!}} \, (a^\dagger)^n \, \Phi_0(y), \tag{6.68}$$

where $\Phi_0(y)$ is the ground state of the harmonic oscillator.

Before ending this section, it is interesting to note that the operators $\hat{b}$ and $\hat{b}^\dagger$ can be explicitly expressed in terms of the physical coordinate x and its corresponding momentum p as follows:

$$\hat{b}^\dagger = \left[\frac{e^{\beta x}}{\nu} \left(-\frac{ip}{\beta \hbar} + s \right) (2s - 1) - \frac{\nu}{2} \right] \sqrt{\frac{s - 1}{\nu s}}, \tag{6.69}$$

$$\hat{b} = \left[\frac{e^{\beta x}}{\nu} \left(\frac{ip}{\beta \hbar} + s \right) (2s + 1) - \frac{\nu}{2} \right] \sqrt{\frac{s + 1}{\nu s}}, \tag{6.70}$$

which essentially correspond to the inverse of the expansions obtained in [411].

7.   Franck-Condon factors

It is well known that the intensity of vibronic spectra can be computed in first order approximation in terms of the Franck-Condon factors. Up to now, different approximate methods to compute the Franck-Condon factors for the Morse potential have been proposed [261, 364–376]. In general, the Franck-Condon factors can be calculated by using the explicit Morse eigenfunctions. For example, the closed analytic expression of the Franck-Condon factors was obtained by Matsumoto and Iwamoto [372, 373] and others [367, 371–376]. Here, we shall give a brief review of the approximation method to study the Franck-Condon factors following the approach by Meléndez, Sandoval and Palma [369]. Before proceeding further, let us analyze the complexity of this system.

As we know, the relation between the variables y and y' is nonlinear as shown below

$$y' = b_0 \nu' \nu^{-\frac{\beta'}{\beta}} y^{\frac{\beta'}{\beta}}, \tag{6.71}$$

from which we have

$$\frac{d}{dy'} = \frac{\beta \nu^{\frac{\beta'}{\beta}}}{b_0 \nu' \beta'} y^{1-\frac{\beta'}{\beta}} \frac{d}{dy}, \tag{6.72}$$

where $y' = b_0 \nu' e^{-\beta' x}$ and $y = \nu e^{-\beta x}$ with $b_0 = e^{-\beta' x_0}$.

Since the relation between the variables y' and y is nonlinear, we expect to obtain $\hat{K}'_{\pm,0}$ as an expansion in powers of $\hat{K}_{\pm,0}$. A linear relation can be obtained only for the special case in which $\beta = \beta'$, and $x_0 = 0$, for which the relation is independent of β. Let us study this problem in this special case. To this end, we obtain the relation between $\hat{K}'_{\pm,0}$ and $\hat{K}_{\pm,0}$ as the set of equations

$$
\begin{aligned}
\hat{K}'_- &= \hat{K}_+ \frac{\nu'}{\nu} \sqrt{\frac{s(s'+1)}{s'(s-1)} \frac{(2s'+1)(s'-s)}{2s(2s-1)}} \\
&+ \hat{K}_- \frac{\nu'}{\nu} \sqrt{\frac{s(s'+1)}{s'(s+1)} \frac{(2s'+1)(s'+s)}{2s(2s+1)}} \\
&+ \left[\frac{\nu'(2s'+1)(2s'-1)}{2(2s-1)(2s+1)} - \frac{\nu'}{2} \right] \sqrt{\frac{s'+1}{s'}},
\end{aligned} \tag{6.73}
$$

and

$$
\begin{aligned}
\hat{K}'_+ &= \hat{K}_+ \frac{\nu'}{\nu} \sqrt{\frac{s(s'-1)}{s'(s-1)} \frac{(2s'-1)(s'+s)}{2s(2s-1)}} \\
&+ \hat{K}_- \frac{\nu'}{\nu} \sqrt{\frac{s(s'-1)}{s'(s+1)} \frac{(2s'-1)(s'-s)}{2s(2s+1)}} \\
&+ \left[\frac{\nu'(2s'-1)(2s'+1)}{2(2s-1)(2s+1)} - \frac{\nu'}{2} \right] \sqrt{\frac{s'-1}{s'}},
\end{aligned} \tag{6.74}
$$

which show that the relation between them is very complicated.

We are now going to give a brief review of the approximation method to study the Franck-Condon factors [369]. If we make a power expansion of the Morse potential (6.2) up to the fourth order,

$$V(x) = \mathcal{A}x^2 + \mathcal{B}x^3 + \mathcal{C}x^4, \tag{6.75}$$

where

$$\mathcal{A} = V_0\beta^2, \quad \mathcal{B} = -V_0\beta^3, \quad \mathcal{C} = \frac{7}{12}V_0\beta^4, \tag{6.76}$$

then we can express the Hamiltonian of the system as

$$H = \frac{p^2}{2\mu} + \frac{1}{2}\mu\omega^2 x^2 + \mathcal{B}x^3 + \mathcal{C}x^4. \tag{6.77}$$

By using the creation and annihilation operators of the harmonic oscillator (4.12) and keeping only the linear and quadratic terms, the Hamiltonian (6.77) can be written as

$$H = \hbar\omega(N + 1/2) + 3\kappa(a^\dagger + a) + 6\lambda[a^2 + 2a^\dagger a + (a^\dagger)^2 + 1/2], \tag{6.78}$$

with the constants

$$\kappa = -\sqrt{\left(\frac{\hbar}{2\mu\omega}\right)^3}V_0\beta^3, \quad \lambda = \frac{7}{12}\left(\frac{\hbar}{2\mu\omega}\right)^2 V_0\beta^4. \tag{6.79}$$

It is shown that Eq. (6.78) can be diagonalized by using the Bogoliubov-Tyablikov transformation [415], for which we may calculate the commutator

$$[H, a^\dagger] = (\hbar\omega + 12\lambda)a^\dagger + 12\lambda a + 3\kappa. \tag{6.80}$$

By applying the same notations as in [415] to identity the coefficients $\mathcal{A}$ and $\mathcal{B}$ from Eq. (6.78), we may obtain the matrix $\mathbf{M}$ straightforwardly as [369]

$$\mathbf{M} = \hbar\omega(\hbar\omega + 24\lambda) \tag{6.81}$$

with

$$\mathcal{B} = \hbar\omega + 12\lambda, \quad \mathcal{C} = 12\lambda. \tag{6.82}$$

The energy is therefore given by

$$E = \sqrt{\mathbf{M}} = \hbar\omega\sqrt{1 + \frac{24\lambda}{\hbar\omega}}, \tag{6.83}$$

which means that the new frequency includes the anharmonic corrections through the formula

$$\omega' = \omega\sqrt{1 + \frac{24\lambda}{\hbar\omega}}, \tag{6.84}$$

which implies that the spectroscopic harmonic frequency ω' defining the Morse oscillator parameters is only perturbed by the fourth-order coefficient λ. Making use of λ given in (6.79), we may know the new frequency ω'. The merit of this formalism allows us to algebraically obtain the frequencies associated with each one of the vibrational molecular states. On the other hand, using the recurrence

relations for the Franck-Condon factors derived by Palma and Morales [255], one may calculate any Franck-Condon factors for the Morse eigenstates. In their work [369], some typical diatomic molecules were evaluated, showing that the results obtained by such an approximation agreed well with those obtained by other approaches.

8.   Transition probability

We now study the transition probability between two eigenstates. As shown in [393], the electric dipole operator for the transition probability can be expressed as

$$V = -q\epsilon_0 x e^{i\omega t} = F e^{i\omega t}, \tag{6.85}$$

where the q, ω and ϵ_0 denote electric charge of the molecule, the angular frequency and the intensity of the electric field, respectively. Consequently, the transition probability between two eigenstates can be calculated by

$$\omega_{n\to m} = \frac{2\pi}{\hbar} q^2\omega^2 |\langle m|x|n\rangle|^2 \delta(E_m - E_n \pm \hbar\omega), \tag{6.86}$$

whose result cannot be obtained simply as addressed in [368, 369, 372, 373].

If expressing $\langle m|x|n\rangle$ by $y = \nu e^{-\beta x}$ instead of x, then we have

$$\omega_{n\to m} = \frac{2\pi}{\hbar} \frac{q^2\omega^2}{\beta^2} |\langle m|\ln y|n\rangle|^2 \delta(E_m - E_n \pm \hbar\omega), \tag{6.87}$$

from which we can obtain the expected result

$$
\begin{aligned}
\omega_{n\to m} &= \frac{2\pi}{\hbar} \frac{q^2\omega^2}{\beta^2} \sum_{\ell=1}^{\infty} \frac{1}{\ell} \\
&\times \left| \left\langle m \left| \left\{ 1 - \left(\hat{K}_+ \left[\frac{1}{2s(2s-1)} \sqrt{\frac{s}{s-1}} \right] \right. \right. \right. \right. \right. \\
&\left. \left. \left. \left. + \hat{K}_- \left[\frac{1}{2s(2s+1)} \sqrt{\frac{s}{s+1}} \right] + \frac{\nu}{(2s+1)(2s-1)} \right) \right\}^{\ell} \right| n \right\rangle \right|^2 \\
&\times \delta(E_m - E_n \pm \hbar\omega),
\end{aligned}
\tag{6.88}
$$

where we have used Eq. (6.52) and the Taylor series expansion formula

$$\ln y = \sum_{\ell=1}^{\infty} \frac{1}{\ell} \left(1 - \frac{1}{y} \right)^{\ell}. \tag{6.89}$$

9.   Realization of dynamic group SU(1, 1)

As shown above, we have used the factorization method to obtain the ladder operators directly from the Morse wave functions and then constructed a suitable Lie algebra su(2). However, the Morse potential can also be recognized as an SU(1, 1) group for fixed energy but with different potential strength, i.e., the potential group approach.

We now construct the dynamic group SU(1, 1) for the Morse potential following Refs. [156, 401]. The eigenvalues E of the quantum system are well known as [293]

$$\varepsilon_n = -\left(v - n - \frac{1}{2}\right)^2, \tag{6.90}$$

with the anharmonicity constant v and the dimensionless energy ε

$$v = \sqrt{\frac{2\mu V_0}{\beta^2 \hbar^2}}, \quad \varepsilon = \frac{2\mu E}{\hbar^2 \beta^2}, \tag{6.91}$$

where $v = \nu/2$. Likewise, we only discuss the bound states spectrum $E < 0$. Equation (6.90) implies that ε depends on the quantum number n and the v (the depth of the potential well). The quantum number n representing the number of anharmonic phonons is taken as $n = 0, 1, ..., [v - \frac{1}{2}]$, with $[v - \frac{1}{2}]$ being the largest integer not exceeding $(v - \frac{1}{2})$.

Before proceeding to construct the dynamical group SU(1, 1), we define a dimensionless distance $u = \beta x$. Thus, the Schrödinger equation for $\psi_n^v(u)$ can be expressed as

$$\frac{d^2}{du^2}\psi_n^v(u) + [\varepsilon + v^2(2e^{-u} - e^{-2u})]\psi_n^v(u) = 0. \tag{6.92}$$

For convenience, we take

$$y = ve^{-u}, \quad y \in [0, \infty). \tag{6.93}$$

Substitution of this into Eq. (6.92) leads to

$$y^2 \frac{d^2}{dy^2}\psi_n^v(y) + y\frac{d}{dy}\psi_n^v(y)(2vy + \varepsilon - y^2)\psi_n^v(y) = 0. \tag{6.94}$$

On the other hand, we define

$$\phi_n^v(y) = e^{-\frac{u}{2}}\psi_n^v(y) = v^{-\frac{1}{2}}y^{\frac{1}{2}}\psi_n^v(y). \tag{6.95}$$

Substitution of this into Eq. (6.92) allows us to obtain

$$\frac{d^2}{dy^2}\phi_n^v(y) + \left(\frac{\varepsilon + \frac{1}{4}}{y^2} + \frac{2v}{y} - 1\right)\phi_n^v(y) = 0, \tag{6.96}$$

which can be rearranged as

$$\left(-y\frac{d^2}{dy^2} - \frac{\varepsilon + \frac{1}{4}}{y} + y\right)\phi_n^v(y) = 2v\phi_n^v(y). \tag{6.97}$$

We define

$$\hat{K}_1 = y, \quad \hat{K}_2 = -i\,y\frac{d}{dy}, \quad \hat{K}_3 = -y\frac{d^2}{dy^2} - \frac{\varepsilon + \frac{1}{4}}{y}, \tag{6.98}$$

from which we can obtain the following relations

$$[\hat{K}_1, \hat{K}_2] = i\,\hat{K}_1, \quad [\hat{K}_2, \hat{K}_3] = i\,\hat{K}_3, \quad [\hat{K}_1, \hat{K}_3] = 2\,i\,\hat{K}_2, \tag{6.99}$$

where we have used an important commutation relation $[y, -i\frac{d}{dy}] = i$.

By further defining

$$\hat{L}_0 = \frac{1}{2}(\hat{K}_1 + \hat{K}_3), \quad \hat{L}_1 = \frac{1}{2}(\hat{K}_3 - \hat{K}_1), \quad \hat{L}_2 = \hat{K}_2, \tag{6.100}$$

we find that these operators satisfy the commutation relations of the generators of the non-compact group SU(1, 1), i.e.,

$$[\hat{L}_1, \hat{L}_2] = -i\hat{L}_0, \quad [\hat{L}_2, \hat{L}_0] = i\hat{L}_1, \quad [\hat{L}_0, \hat{L}_1] = i\hat{L}_2. \tag{6.101}$$

However, it is convenient to construct the transition operators [2] with the form

$$\hat{L}_\pm = \frac{1}{2}(\hat{K}_3 - \hat{K}_1) \pm i\,\hat{K}_2 = \hat{L}_1 \pm i\,\hat{L}_2, \tag{6.102}$$

from which, together with $\hat{L}_0$, one can obtain another expression of the commutation relation of the non-compact group SU(1, 1)

$$[\hat{L}_0, \hat{L}_\pm] = \pm\hat{L}_\pm, \quad [\hat{L}_+, \hat{L}_-] = -2\hat{L}_0. \tag{6.103}$$

On the other hand, it is shown from Eqs. (6.97), (6.98) and (6.102) that the transition operators $\hat{L}_\pm$ can be obtained as

$$\hat{L}_+ = y\frac{d}{dy} + v - y, \quad \hat{L}_- = -y\frac{d}{dy} + v - y. \tag{6.104}$$

We now calculate the eigenvalues of transition operators $\hat{L}_\pm$ acting on the wave functions $\phi_n^v(y)$. It is shown from Eqs. (6.97) and (6.100) that

$$\hat{L}_0\phi_n^v(y) = v\phi_n^v(y). \tag{6.105}$$

In addition, it is found from Eq. (6.103) that

$$\hat{L}_0\hat{L}_\pm = \hat{L}_\pm(\hat{L}_0 \pm 1), \tag{6.106}$$

from which, together with Eq. (6.105), we have

$$\hat{L}_0[\hat{L}_\pm\phi_n^v(y)] = (v \pm 1)[\hat{L}_\pm\phi_n^v(y)]. \tag{6.107}$$

On the other hand, since the energy is a constant we must have

$$\hat{L}_\pm\phi_n^v(y) = l_\pm\phi_{n\pm1}^{v\pm1}(y), \tag{6.108}$$

where $l_\pm$ are the corresponding eigenvalues of the transition operators $\hat{L}_\pm$ to be determined below.

As an important physical quantity, the Casimir operator can be obtained as

$$\begin{aligned}
C &= \hat{L}_0^2 - \hat{L}_1^2 - \hat{L}_2^2 \\
&= \hat{L}_0^2 - \hat{L}_0 - \hat{L}_+\hat{L}_- \\
&= \hat{L}_0^2 + \hat{L}_0 - \hat{L}_-\hat{L}_+ \\
&= -(\varepsilon + 1/4).
\end{aligned} \tag{6.109}$$

In the calculation, we have used Eqs. (6.98) and (6.100). This result coincides with that of Refs. [156, 401]. Moreover, it is shown from Eq. (6.109) that the system Hamiltonian H can be expressed as

$$H = -\frac{1}{4} - \hat{L}_0^2 + \hat{L}_0 + \hat{L}_+\hat{L}_- = -(C + 1/4), \tag{6.110}$$

where we have considered the negative value of the eigenvalues $E = \frac{\hbar^2\beta^2}{2\mu}\varepsilon < 0$.

We now determine the eigenvalues $l_\pm$ of the transition operators $\hat{L}_\pm$. It is found from Eq. (6.109) that

$$\begin{aligned}
\hat{L}_\pm\hat{L}_\mp &= \hat{L}_0^2 \mp \hat{L}_0 - C \\
&= v^2 \mp v + \frac{1}{4} - \left(v - n - \frac{1}{2}\right)^2,
\end{aligned} \tag{6.111}$$

from which we have

$$\begin{aligned}
\hat{L}_+\hat{L}_-\phi_n^v(y) &= (\hat{L}_0^2 - \hat{L}_0 - C)\phi_n^v(y) \\
&= (2vn - n^2 - n)\phi_n^v(y).
\end{aligned} \tag{6.112}$$

Hence, by choosing a phase factor of unity, we have

$$\begin{aligned}
\hat{L}_-\phi_n^v(y) &= l_-\phi_{n-1}^{v-1}(y) \\
&= \sqrt{n(2v - n - 1)}\phi_{n-1}^{v-1}(y).
\end{aligned} \tag{6.113}$$

Likewise, we have

$$
\begin{aligned}
\hat{L}_- \hat{L}_+ \phi_n^v(y) &= (\hat{L}_0^2 + \hat{L}_0 - C)\phi_n^v(y) \\
&= (2vn + 2v - n^2 - n)\phi_n^v(y),
\end{aligned}
\tag{6.114}
$$

from which we have

$$
\begin{aligned}
\hat{L}_+ \phi_n^v(y) &= l_+ \phi_{n+1}^{v+1}(y) \\
&= \sqrt{(n+1)(2v-n)}\, \phi_{n+1}^{v+1}(y).
\end{aligned}
\tag{6.115}
$$

Therefore, we find that the transition operators $\hat{L}_\pm$ shift the value of $v \to v \pm 1$ and $n \to n \pm 1$ for a given constant energy ε. This means that these transition operators change the potential parameters V_0, but not the energy E.

We make some remarks here. First, it is shown from Eq. (6.105) that the eigenvalue of the operator $\hat{L}_0$ represents the potential well depth parameter, whereas the eigenvalue of the Casimir operator C of the dynamic group SU(1, 1) determines the energy ε. Second, the irreducible representations of this dynamic algebra correspond to the constant energy ε of the Morse potential. This forms the basis of the potential group approach to the Morse potential. This means that the present quantum system evolves on a manifold that gives access to the bound states with the same constant energy and different potential strengths. Finally, we should mention that the wave functions can be obtained as

$$
\psi_n^v(y) = N_n^v\, e^{-y}\, (2y)^{v-n-\frac{1}{2}}\, L_n^{2v-2n-1}(2y),
\tag{6.116}
$$

with

$$
N_n^v = \sqrt{\frac{\beta(2v - 2n - 1)\Gamma(n+1)}{\Gamma(2v - n)}},
\tag{6.117}
$$

where v and y are given in Eqs. (6.91) and (6.93), respectively. Thus, there exists a common dense invariant domain D_ω for these transition operators $\hat{L}_\pm$ and $\hat{L}_0$ spanned by analytical functions $\psi_n^v(y)$ with the same constant energy and different potential strengths.

10.   Concluding remarks

In this Chapter we have established the creation and annihilation operators for the Morse wave functions by the factorization method. We have obtained them only from the physical variable y. We have also shown that the SU(2) is the appropriate dynamic group for the bound states of the Morse potential. We have used the su(2) algebra to express the Morse wave functions by successively acting the creation operator $\hat{K}_+$ on the ground state. The matrix elements of the related physical functions $1/y$ and d/dy have been analytically obtained from

the ladder operators $\hat{K}_\pm$. This method can be generalized to other quantum systems as to be shown in following Chapters and represents a simple and elegant approach to obtain these matrix elements in comparison with the traditional techniques in configuration space. The harmonic limit has also been analyzed, showing that the su(2) algebra contracts to the appropriate Weyl algebra in this limit. The Franck-Condon factors and transition probability are studied briefly. Finally, we have realized the dynamic group SU(1, 1) for the Morse potential due to its wide applications in physics. In fact, this approach is the so-called potential group approach, namely, the energy of the quantum system remains invariant for potentials with different strengths.

Notes

1 Here we have shifted the Morse potential (6.2) as $V(x) + V_0$ in order to reduce it to the harmonic oscillator. However, such a modification does not affect the nature of the problem.

2 We prefer to use the term "transition operator" under the case of the SU(1, 1) group in comparison with the "ladder operator" under the case of the SU(2) group.

Chapter 7

PÖSCHL-TELLER POTENTIAL

1.   Introduction

As mentioned before, algebraic methods have been applied to a wide variety of fields both in physics and in chemistry. Systems displaying a dynamic symmetry can be treated with algebraic techniques. In particular, the Morse [293] and Pöschl-Teller (PT) potentials [416, 417] represent two of the most studied anharmonic ones, both having in common their relation with the SO(2, 1) [153, 156, 213, 406, 409] and SU(2) [106, 197] groups. The latter description has been exploited to describe the vibrational excitations of molecular systems, while the former arises in the potential group approach, where wave functions associated with different potentials but with the same energy are connected.

The PT potential introduced by Pöschl and Teller [416] and by Rosen and Morse [417] has been the subject of several studies [297, 418–422], although it has not attracted as much attention as the Morse potential [136, 295, 319, 404, 405, 423, 424]. A recent application of the PT potential was given in the framework of the su(2) vibron model, where it turned out to be associated with the vibrational excitations of the molecular bending modes [425–427]. As we know, the Morse potential can be used to describe the vibrational spectrum of the stretching degrees of freedom since the energy level expression for one simple Morse oscillator reproduces the observed energy levels for highly excited stretching for many molecules. The potential along each bond is represented as a Morse potential. Even though the Morse potential facilitates the treatment of the anharmonicity of the stretching degrees of freedom very nicely, it is not easy to know how to treat other degrees of freedom–bending motions. The PT potential is pertinent for describing the vibration of the bending degrees of freedom [425]. The basic idea behind the vibron model consists of describing algebraically the stretching and bending degrees of freedom in a unified framework, keeping

track of the nature of the wave functions in configuration space. The su(2) approach to vibrational excitations is based on the homomorphism between the one-dimensional Morse or PT eigenfunctions and the states associated with the SU(2)⊃ SO(2) chain. This connection has been given through a transformation applied to the radial component of a two-dimensional harmonic oscillator.

Recently, Alhassid *et al.* have established the connection between the dynamic algebra su(2) and the PT potential by using the basic properties of the angular momentum [407]. On the other hand, it is known that the Schrödinger equation with this potential plays a very important role in the soliton mathematics, from which the multi-soliton solutions of the nonlinear Korteweg-de Vries (KdV) equation can be explicitly constructed [428].

Before proceeding with our approach to treat this potential, let us review the approach used by Alhassid *et al.* in order to show how to connect this realization with the angular momentum . For the fixed integer j, the simultaneous eigenfunctions χ_j^m of I^2 and I_z have been defined by them. The dynamic symmetries are characterized by the group chain U(2)⊃ O(2). They satisfy

$$I^2\chi_j^m = j(j+1)\chi_j^m, \quad I_z\chi_j^m = m\chi_j^m, \tag{7.1}$$

with

$$\chi_j^m(\theta, \phi) = u_j^m(\theta)e^{im\phi}, \tag{7.2}$$

where $u_j^m(\theta)$ satisfies

$$\left[-\frac{1}{\sin\theta}\frac{\partial}{\partial\theta}\left(\sin\theta\frac{\partial}{\partial\theta}\right) + \frac{m^2}{\sin^2\theta}\right]u_j^m(\theta) = j(j+1)u_j^m(\theta). \tag{7.3}$$

The substitution $\cos\theta = \tanh y$ into above equation allows us to obtain

$$\left[-\frac{d^2}{dy^2} - \frac{j(j+1)}{\cosh^2 y}\right]u_j^m(y) = -m^2 u_j^m(y), \quad m = 0, \pm 1, \pm 2, \ldots, j. \tag{7.4}$$

The spectrum is given by

$$E_m = -\beta m^2, \tag{7.5}$$

where the scale factor β is inserted to provide the appropriate dimensions. It is shown that I^2 is the square of the angular momentum which satisfies the commutation relations

$$[I_i, I_j] = i\epsilon_{ijk}I_k, \tag{7.6}$$

which makes us interpret the operators $I_i(i = 1, 2, 3)$ as the generators of the dynamic group SU(2) for the PT system for integer j. In comparison with the result given in Eq. (7.56) below, it is found that $j = N/2$ coincides with that of Ref. [407].

Nevertheless, we shall present the connection of the modified Pöschl-Teller potential (MPT) with the su(2) algebra using the factorization method as shown in our recent work [106], which allows us to define creation and annihilation operators satisfying the su(2) commutation relations. In addition, the PT and MPT potentials have been analyzed in [297, 416–422, 425–427], but the normalization constant for the MPT was only discussed in [421].

Recently, Zúñiga *et al.* have presented different approaches to calculate matrix elements of several functions for the MPT potential [429] and also obtained the raising and lowering operators for the MPT potential with the factorization method, but the connection of these operators with the su(2) algebraic structure was not established.

The aims of this Chapter are the following. First, we study the exact solutions of the MPT potential and obtain the normalization constant. Second, we show that the creation and annihilation operators with the appropriate weight factors satisfy the su(2) commutation relations. It should be noted that our treatment method in this work differs from that used in Refs. [421, 429].

This Chapter is organized as follows. In Section 2 we present the normalized wave functions for the MPT potential. Section 3 is devoted to the construction of the appropriate raising and lowering operators. In Section 4 the dynamic group SU(2) is established from these ladder operators and the matrix elements of the operators $\frac{u}{\sqrt{1-u^2}}$ and $\sqrt{1-u^2}\frac{d}{du}$ are calculated from them. In Section 5 we employ an alternative approach to derive the ladder operators. Section 6 is to study the harmonic limit. In Section 7 we study the expansions of the coordinate x and the momentum p from the SU(2) generators. Finally in Section 8 we present our conclusions.

2. Exact solutions

We now study the normalization constant for the MPT potential following two different methods. We first use a relation between the hypergeometric functions and the associated Legendre polynomials as shown by Landau *et al.* [297]. The second procedure is to use the relation between the Gegenbauer polynomials and the hypergeometric functions.

Let us study its exact solutions following Ref. [297], where the normalization constant was not presented. The MPT potential is given by [418]

$$V(x) = -\frac{D}{\cosh^2(\alpha x)}, \qquad (7.7)$$

where D is the depth of the well, α is related to the range of the potential and x gives the relative distance from the equilibrium position.

The Schrödinger equation associated with this potential takes the form

$$\frac{d^2\Psi_n^q(x)}{dx^2} + \frac{2\mu}{\hbar^2}\left(E + \frac{D}{\cosh^2(\alpha x)}\right)\Psi_n^q(x) = 0, \qquad (7.8)$$

where μ is the reduced mass of the molecule and q is related to the depth of the potential as shown below. In accordance with Ref. [297] we introduce the following definitions

$$\epsilon = \sqrt{\frac{-2\mu E}{\alpha^2\hbar^2}}, \quad q(q+1) = \frac{2\mu D}{\alpha^2\hbar^2}, \quad q = \frac{1}{2}(-1+2k), \qquad (7.9)$$

with

$$k = \sqrt{\frac{1}{4} + \frac{2\mu D}{\alpha^2\hbar^2}}, \qquad \nu = 2k = 2q+1, \qquad (7.10)$$

where we have introduced the variable ν because, as we shall see, it turns out to be relevant for the identification of the creation and annihilation operators with the su(2) algebra. Using these definitions and the change of variable $u = \tanh(\alpha x)$, equation (7.8) becomes

$$\frac{d}{du}\left[(1-u^2)\frac{d\Psi_n^q(u)}{du}\right] + \left[q(q+1) - \frac{\epsilon^2}{1-u^2}\right]\Psi_n^q(u) = 0, \qquad (7.11)$$

where we have used the formulas

$$\frac{du}{dx} = \frac{\alpha}{\cosh^2(\alpha x)}, \qquad \frac{1}{\cosh^2(\alpha x)} + \tanh^2(\alpha x) = 1. \qquad (7.12)$$

By introducing the variable

$$\xi = \frac{1}{2}(1-u), \qquad (7.13)$$

then equation (7.11) becomes

$$\xi(1-\xi)\frac{d^2\Psi_n^q(u)}{d\xi^2} + (1-2\xi)\frac{d\Psi_n^q(u)}{d\xi} + \left[q(q+1) - \frac{\epsilon^2}{4\xi(1-\xi)}\right]\Psi_n^q(u) = 0. \qquad (7.14)$$

If making the substitution

$$\Psi_n^q(u) = (1-u^2)^{\epsilon/2}w(u) = [4\xi(1-\xi)]^{\epsilon/2}w(\xi), \qquad (7.15)$$

then we obtain

$$\xi(1-\xi)\frac{d^2w(\xi)}{d\xi^2} + (1+\epsilon)(1-2\xi)\frac{dw(\xi)}{d\xi} - (\epsilon-q)(1+q+\epsilon)w(\xi) = 0. \qquad (7.16)$$

In comparison with the hypergeometric differential equation

$$x(1-x)\frac{d^2y(x)}{dx^2} + [c-(a+b+1)x]\frac{dy(x)}{dx} - aby(x) = 0, \qquad (7.17)$$

where a, b and c are three constants, we find that the finite solutions for $u = 1$ are given by

$$\Psi_n^q(u) = N(1-u^2)^{\epsilon/2}F[\epsilon-q, \epsilon+q+1, \epsilon+1; \frac{1}{2}(1-u)], \qquad (7.18)$$

where the hypergeometric functions are defined by

$$F(a,b,c;x) = 1 + \frac{ab}{1!c}x + \frac{a(a+1)b(b+1)}{2!c(c+1)}x^2 + \dots. \qquad (7.19)$$

For $\Psi_n^q(u)$ to remain finite for $u = -1$, we find that the quantum condition is given by

$$\epsilon - q = -n, \quad n = 0, 1, 2, \dots, \qquad (7.20)$$

from which we are able to obtain the eigenvalues as

$$E_n = -\frac{\alpha^2\hbar^2}{2\mu}(q-n)^2, \qquad (7.21)$$

where $\epsilon = q - n > 0$. The number of bound states is determined by the dissociation limit $\epsilon = q - n = 0$, giving rise to $n_{\max} = q = k - \frac{1}{2}$. The normalization constant N, however, was not given in Eq. (7.18) and must be determined.

The relation between the hypergeometric functions and the associated Legendre polynomials (see 8. 751 in [263]) can be written as

$$P_\nu^m(x) = \frac{(-1)^m\Gamma(\nu+m+1)(1-x^2)^{\frac{m}{2}}}{2^m\Gamma(\nu-m+1)m!}F[m-\nu, m+\nu+1, m+1; \frac{1}{2}(1-x)]. \qquad (7.22)$$

Substitution of this into (7.18) allows us to write the solutions of the form

$$\Psi_n^q(u) = (-1)^{(q-n)}Q_n^q(P)P_q^{q-n}(u), \qquad (7.23)$$

where $Q_n^q(P)$ is a normalization constant to be determined from the associated Legendre polynomials $P_q^{q-n}(u)$. Taking into account the formula (see 7. 122 in [263]),

$$\int_0^1 \frac{[P_n^m(x)]^2}{1-x^2}dx = \frac{1}{2m}\frac{(n+m)!}{(n-m)!}, \quad 0 < m < n, \qquad (7.24)$$

we obtain

$$Q_n^q(P) = \sqrt{\frac{\alpha n!(q-n)}{(2q-n)!}}. \tag{7.25}$$

The wave functions of the MPT potential acquire thus the final form in terms of the associated Legendre polynomials

$$\Psi_n^q(u) = N_n^q(P)P_q^{q-n}(u), \tag{7.26}$$

where

$$N_n^q(P) = (-1)^{(q-n)}\sqrt{\frac{\alpha n!(q-n)}{(2q-n)!}}. \tag{7.27}$$

This normalization constant will be used to establish the ladder operators.

We now calculate the normalization constant based on the Gegenbauer polynomials, which are related to the same hypergeometric functions given in Eq. (7.18). The relation between them is given in Ref. [430] by

$$C_n^\lambda(x) = \frac{\Gamma(2\lambda+n)}{n!\Gamma(2\lambda)}F[-n, 2\lambda+n, \frac{1}{2}+\lambda; \frac{1}{2}(1-x)]. \tag{7.28}$$

In terms of this expression, the wave functions (7.18) take the form

$$\Psi_n^q(u) = N_n^q(C)(1-u^2)^{\frac{\epsilon}{2}}C_n^{q+\frac{1}{2}-n}(u), \tag{7.29}$$

where $N_n^q(C)$ stands for the normalization constant to be determined by the following normalization condition

$$\int_{-\infty}^{+\infty}[\Psi_n^q(x)]^2dx = \frac{[N_n^q(C)]^2}{\alpha}\int_{-1}^{1}(1-u^2)^{q-n-1}[C_n^{q-n+\frac{1}{2}}(u)]^2du$$
$$= 1. \tag{7.30}$$

This integral can be calculated from Eq. (7. 314) in [263], which becomes clear if expressed in the following form

$$\int_{-1}^{1}(1-x^2)^{\nu-\frac{3}{2}}(1+x)\,[C_n^\nu(x)]^2dx = \frac{\pi^{\frac{1}{2}}\Gamma(\nu-\frac{1}{2})\Gamma(2\nu+n)}{n!\Gamma(\nu)\Gamma(2\nu)}, \quad [\Re e\,\nu > \frac{1}{2}], \tag{7.31}$$

which in turn can be transformed into

$$\int_{-1}^{1}(1-x^2)^{\nu-\frac{3}{2}}\,[C_n^\nu(x)]^2dx = \frac{\pi^{\frac{1}{2}}\Gamma(\nu-\frac{1}{2})\Gamma(2\nu+n)}{n!\Gamma(\nu)\Gamma(2\nu)}, \tag{7.32}$$

since the function $(1 - x^2)^{\nu - \frac{3}{2}} x \, [C_n^\nu(x)]^2$ is odd and consequently its integral vanishes in the interval [-1, 1]. Taking into account Eq. (7.32), we are able to obtain the normalization constant as

$$N_n^q(C) = \sqrt{\frac{\alpha n! (q - n - \frac{1}{2})! (2q - 2n)!}{\pi^{\frac{1}{2}} (q - n - 1)! (2q - n)!}}.$$ (7.33)

We now establish the relation between the associated Legendre polynomials and the Gegenbauer polynomials. Since these two polynomials are connected with the hypergeometric functions, from Eqs. (7.22) and (7.28) we obtain

$$C_n^{q + \frac{1}{2} - n}(x) = (-1)^{n-q} \frac{2^{q-n}(q - n)!}{(2q - 2n)!} (1 - x^2)^{\frac{n-q}{2}} P_q^{q-n}(x),$$ (7.34)

where we note that the phase factor $(-1)^{n-q}$ appears between these two polynomials with real argument. This expression can be used to convert the solution (7.26) into Eq. (7.29) and *vice versa*, taking into account the formula [430],

$$2^{2z} z! (z - \frac{1}{2})! = \pi^{\frac{1}{2}} (2z)!,$$ (7.35)

in order to identify the normalization factor. It is more convenient, however, to use Eq. (7.26) to establish the ladder operators.

3. Ladder operators

In this section we address the problem of finding creation and annihilation operators for the MPT potential with the factorization method. In other words, we intend to find differential operators $\hat{M}$ with the following property

$$\hat{M}_\pm \Psi_n^q(u) = m_\pm \Psi_{n\pm1}^q(u).$$ (7.36)

Specifically, we look for operators with the form

$$\hat{M}_\pm = A_\pm(u) \frac{d}{du} + B_\pm(u),$$ (7.37)

where we remark that these operators only depend on the physical variable u.

We start by acting the differential operator $\frac{d}{du}$ on the MPT wave functions (7.26). This can be achieved by using the following formulas (see Eq.8. 733 in [263])

$$(1 - x^2) \frac{dP_\nu^\mu(x)}{dx} = -\sqrt{1 - x^2} P_\nu^{\mu+1}(x) - \mu x P_\nu^\mu(x),$$ (7.38)

$$(1 - x^2) \frac{dP_\nu^\mu(x)}{dx} = (\nu - \mu + 1)(\nu + \mu)\sqrt{1 - x^2} P_\nu^{\mu-1}(x) + \mu x P_\nu^\mu(x).$$ (7.39)

By using Eq. (7.38), we have

$$\frac{d\Psi_n^q(u)}{du} = \frac{u(n-q)}{1-u^2}\Psi_n^q(u) - \frac{1}{\sqrt{1-u^2}}\frac{N_n^q(P)}{N_{n-1}^q(P)}\Psi_{n-1}^q(u). \qquad (7.40)$$

If introducing the explicit form of the normalization constant, we can obtain

$$\sqrt{1-u^2}\left(\frac{d}{du} - \frac{u(n-q)}{1-u^2}\right)\sqrt{\frac{q-n+1}{q-n}}\,\Psi_n^q(u) = \sqrt{n(2q-n+1)}\,\Psi_{n-1}^q(u). \qquad (7.41)$$

Therefore, we can define the annihilation operator $\hat{M}_-$ as

$$\hat{M}_- = \sqrt{1-u^2}\left(\frac{d}{du} + \frac{u(q-n)}{1-u^2}\right)\sqrt{\frac{q-n+1}{q-n}}, \qquad (7.42)$$

or in terms of Eq. (7.20)

$$\hat{M}_- = \sqrt{1-u^2}\left(\frac{d}{du} + \frac{u}{1-u^2}\,\epsilon\right)\sqrt{\frac{\epsilon+1}{\epsilon}}, \qquad (7.43)$$

where in order to simplify the notation we have taken into account that $2\epsilon = \nu - 2n - 1 = 2q - 2n$.

The action of the operator (7.43) on the wave functions $\Psi_n^\nu(u)$ leads to

$$\hat{M}_-\Psi_n^\nu(u) = m_-\Psi_{n-1}^\nu(u), \qquad (7.44)$$

with

$$m_- = \sqrt{n(\nu - n)}, \qquad (7.45)$$

where we have considered the relation $\nu = 2q + 1$ as given in Eq. (7.10). As we can see, this operator annihilates the ground state $\Psi_0^\nu(u)$, as expected from a lowering operator.

We now proceed to find the corresponding creation operator $\hat{M}_+$. To this end, using Eq. (7.39) we have

$$\frac{d\Psi_n^q(u)}{du} = \frac{u(q-n)}{1-u^2}\Psi_n^q(u) + \frac{(n+1)(2q-n)}{\sqrt{1-u^2}}\frac{N_n^q(P)}{N_{n+1}^q(P)}\Psi_{n+1}^q(u), \quad (7.46)$$

from which, after introducing the parameter ν, we obtain

$$-\sqrt{1-u^2}\left[\frac{d}{du} - \frac{u(\nu-2n-1)}{2(1-u^2)}\right]\sqrt{\frac{(\nu-2n-3)}{(\nu-2n-1)}}\,\Psi_n^\nu(u) \qquad (7.47)$$
$$= \sqrt{(n+1)(\nu-n-1)}\,\Psi_{n+1}^\nu(u).$$

Furthermore, based on the constraint condition $2\epsilon = \nu - 2n - 1$, we can define the creation operator $\hat{M}_+$ as

$$\hat{M}_+ = \sqrt{1-u^2}\left(-\frac{d}{du} + \frac{u}{1-u^2}\epsilon\right)\sqrt{\frac{\epsilon - 1}{\epsilon}}, \qquad (7.48)$$

with the following effect over the wave functions

$$\hat{M}_+ \Psi_n^\nu(u) = m_+ \Psi_{n+1}^\nu(u), \qquad (7.49)$$

where

$$m_+ = \sqrt{(n+1)(\nu - n - 1)}. \qquad (7.50)$$

We find that the ladder operators obtained here are equivalent, except for the weight factor, to those presented in Ref. [429].

4. Realization of dynamic group SU(2)

We now establish the dynamic Lie algebra associated with the operators $\hat{M}_+$ and $\hat{M}_-$. Based on the results (7.44), (7.45), (7.49) and (7.50) we can calculate the commutator $[\hat{M}_-, \hat{M}_+]$:

$$[\hat{M}_+, \hat{M}_-]\Psi_n^\nu(u) = 2m_0\,\Psi_n^\nu(u), \qquad (7.51)$$

where we have introduced the eigenvalue

$$m_0 = -\left(\frac{\nu - 1}{2} - n\right). \qquad (7.52)$$

We can thus define the operator

$$\hat{M}_0 = -\left(\frac{\nu - 1}{2} - \hat{n}\right). \qquad (7.53)$$

The operators $\hat{M}_\pm$ and $\hat{M}_0$ satisfy the commutation relations

$$[\hat{M}_+, \hat{M}_-] = 2\hat{M}_0, \qquad [\hat{M}_0, \hat{M}_\pm] = \pm\hat{M}_\pm, \qquad (7.54)$$

which correspond to an su(2) algebra. This result is consistent with the description of a finite discrete spectrum, in accordance with previous algebraic description of the bounded states of the MPT potential [411, 412]. The operators $\hat{M}_{\pm,0}$ are thus equivalent to $\hat{J}_{\mp,0}$ used in Refs. [411, 412], respectively. The number of bosons N introduced here is related to ν by $N = \nu - 1$.

The Casimir operator is given by

$$\begin{aligned} C\Psi_n^\nu(u) &= [\hat{M}_0^2 + \tfrac{1}{2}(\hat{M}_+\hat{M}_- + \hat{M}_-\hat{M}_+)]\Psi_n^\nu(u) \\ &= [\hat{M}_0^2 + \hat{M}_0 + \hat{M}_-\hat{M}_+]\Psi_n^\nu(u) \qquad (7.55) \\ &= j(j+1)\Psi_n^\nu(u), \end{aligned}$$

where j, the label of the irreducible representations of the Lie algebra su(2), is given by

$$j = \frac{\nu - 1}{2} = \frac{N}{2}.$$

(7.56)

From the commutation relations (7.54), we know that $\hat{M}_0$ is the projection of the angular momentum m, and consequently

$$n - \frac{\nu - 1}{2} = m.$$

(7.57)

The ground state thus corresponds to $m = -j$, while the maximum number of states $n_{\max} = \frac{\nu - 3}{2}$ and accordingly $m_{\max}|_{n_{\max}} = -1$, in accordance with the condition $\epsilon = q - n = 1$. The MPT wave functions are then associated with one branch (in this case to $m \leq -1$) of the su(2) representations, as expected. Finally, we should notice that, in terms of the su(2) algebra, the Hamiltonian has a simple form

$$\hat{H} = -\frac{\hbar \omega}{\nu} \hat{M}_0^2,$$

(7.58)

with eigenvalues

$$\begin{aligned} E_n &= -\frac{\hbar \omega}{\nu} \left(n - \frac{\nu - 1}{2} \right)^2 \\ &= -\frac{\hbar \omega}{2} \frac{\nu}{2} + \hbar \omega (n + 1/2) - x\omega (n + 1/2)^2, \end{aligned}$$

(7.59)

where the spectroscopic constants are given by

$$\omega = \frac{\hbar \alpha^2 \nu}{2\mu}, \qquad x\omega = \frac{\hbar^2 \alpha^2}{2\mu}.$$

(7.60)

It should be noted that Eq. (7.59) can be redefined to absorb the constant term, but we prefer to keep it in order to reproduce Eq. (7.21). On the other hand, the wave functions can be expressed as

$$\Psi_n^\nu(u) = \mathcal{N}_n^\nu \hat{M}_+^n \Psi_0^\nu(u), \qquad \mathcal{N}_n^\nu = \sqrt{\frac{(\nu - n - 1)!}{n!(\nu - 1)!}}.$$

(7.61)

For other calculations one can obtain the following expressions in terms of the raising and lowering operators $\hat{M}_\pm$

$$\begin{aligned} \frac{u}{\sqrt{1 - u^2}} &= \hat{M}_- \sqrt{\frac{1}{(\nu - 2n - 1)(\nu - 2n + 1)}} \\ &+ \hat{M}_+ \sqrt{\frac{1}{(\nu - 2n - 1)(\nu - 2n - 3)}}, \end{aligned}$$

(7.62)

$$\sqrt{1-u^2}\frac{d}{du} = \frac{1}{2}\left(\hat{M}_-\sqrt{\frac{\nu-2n-1}{\nu-2n+1}} - \hat{M}_+\sqrt{\frac{\nu-2n-1}{\nu-2n-3}}\right). \qquad (7.63)$$

We can thus calculate their matrix elements in a straightforward way by means of Eqs. (7.44), (7.45), (7.49) and (7.50):

$$\left\langle \Psi_{n'}^{\nu}(u)\left|\frac{u}{\sqrt{1-u^2}}\right|\Psi_n^{\nu}(u)\right\rangle = \langle \Psi_{n'}^{\nu}(u)|\sinh(\alpha x)|\Psi_n^{\nu}(u)\rangle$$

$$= \sqrt{\frac{n(\nu-n)}{(\nu-2n-1)(\nu-2n+1)}}\delta_{n',n-1}$$

$$+\sqrt{\frac{(n+1)(\nu-n-1)}{(\nu-2n-1)(\nu-2n-3)}}\delta_{n',n+1}, \qquad (7.64)$$

$$\left\langle \Psi_{n'}^{\nu}(u)\left|\sqrt{1-u^2}\frac{d}{du}\right|\Psi_n^{\nu}(u)\right\rangle = \left\langle \Psi_{n'}^{\nu}(u)\left|\frac{\cosh(\alpha x)}{\alpha}\frac{d}{dx}\right|\Psi_n^{\nu}(u)\right\rangle$$

$$= \frac{1}{2}\sqrt{\frac{n(\nu-n)(\nu-2n-1)}{(\nu-2n+1)}}\delta_{n',n-1}$$

$$-\frac{1}{2}\sqrt{\frac{(n+1)(\nu-n-1)(\nu-2n-1)}{(\nu-2n-3)}}\delta_{n',n+1}. \qquad (7.65)$$

The ladder operators can also be properly combined to obtain recursion relations among the matrix elements for the MPT potential [429].

5. Alternative approach to derive ladder operators

As shown above, we have established the ladder operators by using the recursion relations among the Legendre polynomials. In this section we are going to employ the recursion relations among the Gegenbauer polynomials to obtain the ladder operators with the factorization method. That is, we may obtain them by acting the differential operator $\frac{d}{du}$ on the MPT wave functions expressed by the Gegenbauer polynomials (7.29).

Before proceeding further, let us recall the following formula [263]

$$\frac{dC_n^{\lambda}(t)}{dt} = 2\lambda C_{n-1}^{\lambda+1}(t), \qquad (7.66)$$

from which together with Eq. (7.29), we may obtain

$$\frac{d\Psi_n^q(u)}{du} = -\frac{u(q-n)}{1-u^2}\Psi_n^q(u) + \frac{2q-2n+1}{\sqrt{1-u^2}}\frac{N_n^q}{N_{n-1}^q}\Psi_{n-1}^q(u). \qquad (7.67)$$

By introducing the explicit form of the normalization constant, equation (7.67) becomes

$$\sqrt{1-u^2}\left(\frac{d}{du}+\frac{u(q-n)}{1-u^2}\right)\sqrt{\frac{q-n+1}{q-n}}\Psi_n^q(u)=\sqrt{n(2q-n+1)}\Psi_{n-1}^q(u),$$
(7.68)

from which we can define the annihilation operator[1] as

$$\hat{P}_-=\sqrt{1-u^2}\left(\frac{d}{du}+\frac{u(q-n)}{1-u^2}\right)\sqrt{\frac{q-n+1}{q-n}},$$
(7.69)

or in terms of Eq. (7.20)

$$\hat{P}_-=\sqrt{1-u^2}\left(\frac{d}{du}+\frac{u}{1-u^2}\,\epsilon\right)\sqrt{\frac{\epsilon+1}{\epsilon}},$$
(7.70)

where we have considered $2\epsilon=\nu-2n-1=2q-2n$. The action of the operator (7.70) on the wave functions allows us to obtain

$$\hat{P}_-\Psi_n^\nu(u)=p_-\Psi_{n-1}^\nu(u),$$
(7.71)

with

$$p_-=\sqrt{n(\nu-n)}.$$
(7.72)

It is demonstrated that this operator annihilates the ground state $\Psi_0^\nu(u)$, as expected from an annihilation operator.

We now proceed to find the corresponding creation operator $\hat{P}_+$. To this end, we consider the formula [see (10. 43) of Ref. [431]]

$$\begin{aligned}2(\lambda-1)(2\lambda-1)xC_n^\lambda(x)&=4\lambda(\lambda-1)(1-x^2)C_{n-1}^{\lambda+1}(x)\\&\quad+(2\lambda+n-1)(n+1)C_{n+1}^{\lambda-1}(x).\end{aligned}$$
(7.73)

This recurrence relation can be used together with Eq. (7.66) to obtain

$$\frac{d\Psi_n^q(u)}{du}=\frac{u(q-n)}{1-u^2}\Psi_n^q(u)-\frac{(n+1)(2q-n)}{\sqrt{1-u^2}(2q-2n-1)}\frac{N_n^q}{N_{n+1}^q}\Psi_{n+1}^q(u).$$
(7.74)

If we use the explicit form of the normalization constant (7.33), the equation (7.74) becomes

$$\begin{aligned}-\sqrt{1-u^2}\left(\frac{d}{du}-\frac{u(q-n)}{1-u^2}\right)&\sqrt{\frac{(q-n-1)}{(q-n)}}\Psi_n^q(u)\\&=\sqrt{(n+1)(2q-n)}\Psi_{n+1}^q(u).\end{aligned}$$
(7.75)

Likewise, in terms of Eq. (7.20), we can define the creation operator $\hat{P}_+$ as

$$\hat{P}_+ = \sqrt{1 - u^2} \left(-\frac{d}{du} + \frac{u}{1 - u^2} \epsilon \right) \sqrt{\frac{\epsilon - 1}{\epsilon}}, \tag{7.76}$$

with the following effect on the wave functions

$$\hat{P}_+ \Psi_n^\nu(u) = p_+ \Psi_{n+1}^\nu(u), \tag{7.77}$$

where

$$p_+ = \sqrt{(n + 1)(\nu - n - 1)}. \tag{7.78}$$

In a similar way, we find that $\hat{P}_{\pm,0}$ ($\hat{P}_0 = \hat{M}_0$) construct a compact Lie group SU(2) as $\hat{M}_{\pm,0}$. We do not show other properties of this group for simplicity.

6. Harmonic limit

We turn our attention in this section to the harmonic limit, in which the MPT potential approaches a harmonic oscillator potential. In the limits $\alpha \to 0$ and $D \to \infty$, but keeping the product $k = 2\alpha^2 D$ finite, the expansion of the exponential functions in Eq. (7.7), leads to the harmonic limit

$$\lim_{D \to \infty} V_{\mathrm{MPT}} = \frac{1}{2} k x^2. \tag{7.79}$$

We now proceed to analyze the contraction of the su(2) algebra in this limit

$$G_{\mathrm{su}(2)} = \{\hat{M}_+, \hat{M}_-, \hat{M}_0\}. \tag{7.80}$$

We first note that according to the relation $2\epsilon = \nu - 2n - 1$, we have

$$\lim_{\nu \to \infty} \sqrt{\frac{\epsilon + 1}{\epsilon}} = \lim_{\nu \to \infty} \sqrt{\frac{\epsilon - 1}{\epsilon}} = 1. \tag{7.81}$$

On the other hand, we make the following approximations in the harmonic limit $\alpha \to 0$

$$\cosh(\alpha x) \simeq 1, \quad \sinh(\alpha x) \simeq \alpha x. \tag{7.82}$$

By making use of the following identities

$$\sqrt{1 - u^2} \frac{d}{du} = \frac{\cosh(\alpha x)}{\alpha} \frac{d}{dx}, \quad \frac{u}{\sqrt{1 - u^2}} = \sinh(\alpha x), \tag{7.83}$$

we can obtain the harmonic limit.

Similar to the Morse potential case, it is convenient to introduce the following renormalizations

$$\hat{b}^\dagger = \frac{\hat{M}_+}{\sqrt{\nu}}, \quad \hat{b} = \frac{\hat{M}_-}{\sqrt{\nu}}, \quad \hat{b}_0 = \frac{-2\hat{M}_0}{\nu}, \tag{7.84}$$

which, together with (7.42) and (7.48), leads to

$$\lim_{\nu \to \infty} \hat{b}^\dagger = \left(-\frac{1}{\sqrt{\nu}\alpha}\frac{d}{dx} + \frac{\sqrt{\nu}\alpha}{2}x\right) = \sqrt{\frac{\mu\omega}{2\hbar}}x - \sqrt{\frac{\hbar}{2\mu\omega}}\frac{d}{dx} = a^\dagger, \tag{7.85}$$

$$\lim_{\nu \to \infty} \hat{b} = \left(\frac{1}{\sqrt{\nu}\alpha}\frac{d}{dx} + \frac{\sqrt{\nu}\alpha}{2}x\right) = \sqrt{\frac{\mu\omega}{2\hbar}}x + \sqrt{\frac{\hbar}{2\mu\omega}}\frac{d}{dx} = a, \tag{7.86}$$

$$\lim_{\nu \to \infty} \hat{b}_0 = 1, \tag{7.87}$$

with

$$\omega = \frac{\hbar\alpha^2}{2\mu}\nu \simeq \sqrt{\frac{2D\alpha^2}{\mu}}, \tag{7.88}$$

where we have used the relation

$$\frac{\nu}{2} = k \simeq \sqrt{\frac{2\mu D}{\alpha^2\hbar^2}} \tag{7.89}$$

in the harmonic limit $D \to \infty$.

The operators $a^\dagger$ and a satisfy the bosonic commutation relations

$$[a, a^\dagger] = 1, \quad [a, a] = [a^\dagger, a^\dagger] = 0, \tag{7.90}$$

as expected. Therefore, the su(2) algebra will contract to the Weyl algebra in the harmonic limit

$$\lim_{\nu \to \infty} G_{\mathrm{su}(2)} = \{a^\dagger, a, 1\}. \tag{7.91}$$

Finally, in terms of the operators given in Eq. (7.84), the MPT wave functions can be simply expressed as

$$\Psi_n^\nu(u) = \sqrt{\frac{\nu^n(\nu - n - 1)!}{n!(\nu - 1)!}}\,(\hat{b}^\dagger)^n\,\Psi_0^\nu(u), \tag{7.92}$$

whose harmonic limit is given by

$$\lim_{\nu \to \infty} \Psi_n^\nu(u) = \frac{1}{\sqrt{n!}}\,(a^\dagger)^n\,\Phi_0(u), \tag{7.93}$$

where $\Phi_0(u)$ is the ground state of the harmonic oscillator.

7. Expansions of the coordinate x and momentum p from the SU(2) generators

In this section we obtain the expansions of the coordinate x and momentum $\hat{p}$ in terms of the operators $\hat{b}^\dagger$ and $\hat{b}$ as given above, namely,

$$\hat{b} = \sqrt{1 - u^2}\left(\frac{d}{du} + \frac{u}{1 - u^2}\,\epsilon\right)\sqrt{\frac{\epsilon + 1}{\nu\epsilon}}, \tag{7.94}$$

where we remark that the relation $2\epsilon = \nu - 2n - 1 = 2q - 2n$ was used. The action of the operator (7.94) on the wave functions is given by

$$\hat{b}\,\Psi_n^q(u) = b_-\Psi_{n-1}^q(u), \tag{7.95}$$

where

$$b_- = \sqrt{n(1 - n/\nu)}. \tag{7.96}$$

For the creation operator we have

$$\hat{b}^\dagger = \sqrt{1 - u^2}\left(-\frac{d}{du} + \frac{u}{1 - u^2}\,\epsilon\right)\sqrt{\frac{\epsilon - 1}{\nu\epsilon}}, \tag{7.97}$$

with the following effect on the wave functions

$$\hat{b}^\dagger\,\Psi_n^q(u) = b_+\Psi_{n+1}^q(u), \tag{7.98}$$

where

$$b_+ = \sqrt{(n+1)[1 - (n+1)/\nu]}. \tag{7.99}$$

We now obtain the expansion of the coordinate x and momentum p from these two operators $\hat{b}^\dagger$ and $\hat{b}$ since they play a very important role in this system. Extracting the coordinate x and momentum p from Eqs. (7.62) and (7.63), we obtain

$$\sinh \alpha x = \frac{1}{2}\left(\hat{b}\sqrt{\frac{\nu}{\epsilon(\epsilon + 1)}} + \hat{b}^\dagger\sqrt{\frac{\nu}{\epsilon(\epsilon - 1)}}\right), \tag{7.100}$$

$$\frac{\cosh(\alpha x)}{\alpha}\frac{d}{dx} = \frac{1}{2}\left(\hat{b}\sqrt{\frac{\nu\epsilon}{\epsilon + 1}} - \hat{b}^\dagger\sqrt{\frac{\nu\epsilon}{\epsilon - 1}}\right). \tag{7.101}$$

If taking into account the Taylor series expansions

$$\operatorname{arcsinh}(x) = x - \frac{x^3}{6} + \frac{3x^5}{40} + ..., \tag{7.102}$$

$$\operatorname{sech}(x) = 1 - \frac{x^2}{2} + \frac{5x^4}{24} + ..., \tag{7.103}$$

and retaining up to the second terms, we obtain the following expansions in terms of Eqs. (7.100) and (7.101)

$$
\begin{aligned}
x \;=\;& \frac{1}{2\alpha}(\hat{b}^\dagger f_n + \hat{b} g_n) - \frac{1}{48\alpha}(\hat{b}^\dagger f_n \hat{b}^\dagger f_n \hat{b}^\dagger f_n + \hat{b}^\dagger f_n \hat{b}^\dagger f_n \hat{b} g_n \\
&+ \hat{b}^\dagger f_n \hat{b} g_n \hat{b}^\dagger f_n + \hat{b}^\dagger f_n \hat{b} g_n \hat{b} g_n + \hat{b} g_n \hat{b}^\dagger f_n \hat{b}^\dagger f_n + \hat{b} g_n \hat{b}^\dagger f_n \hat{b} g_n \quad (7.104) \\
&+ \hat{b} g_n \hat{b} g_n \hat{b}^\dagger f_n + \hat{b} g_n \hat{b} g_n \hat{b} g_n) + \dots
\end{aligned}
$$

$$
\begin{aligned}
p \;=\;& \frac{i\hbar\alpha}{2}(\hat{b}^\dagger h_n - \hat{b} q_n) + \frac{i\hbar\alpha}{16}(\hat{b}^\dagger f_n \hat{b}^\dagger f_n \hat{b}^\dagger h_n - \hat{b}^\dagger f_n \hat{b}^\dagger f_n \hat{b} q_n \\
&+ \hat{b}^\dagger f_n \hat{b} g_n \hat{b}^\dagger h_n - \hat{b}^\dagger f_n \hat{b} g_n \hat{b} q_n + \hat{b} g_n \hat{b}^\dagger f_n \hat{b}^\dagger h_n - \hat{b} g_n \hat{b}^\dagger f_n \hat{b} q_n \quad (7.105) \\
&+ \hat{b} g_n \hat{b} g_n \hat{b}^\dagger h_n + \hat{b} g_n \hat{b} g_n \hat{b} q_n) + \dots
\end{aligned}
$$

where we have introduced the notations

$$
f_n = \sqrt{\frac{\nu}{\epsilon(\epsilon - 1)}}, \;\; g_n = \sqrt{\frac{\nu}{\epsilon(\epsilon + 1)}}, \;\; h_n = \sqrt{\frac{\nu\epsilon}{\epsilon - 1}}, \;\; q_n = \sqrt{\frac{\nu\epsilon}{\epsilon + 1}}, \;\; (7.106)
$$

as well as the momentum operator $p = -i\hbar \frac{d}{dx}$.

   On the other hand, it should be noted that, because of the symmetry of the MPT potential, the expansions of x and p involve only odd powers of the operators $\hat{b}^\dagger(\hat{b})$; x and p are odd functions under inversion.

8.   Concluding remarks

   In this Chapter we have obtained the normalization constant associated with the wave functions of the MPT potential and established the ladder operators only from the physical variable $u = \tanh(\alpha x)$ with the factorization method. We have found that these ladder operators can be identified as an su(2) algebra, which is consistent with the description of the bounded region of the spectrum analyzed in the framework of a two-dimensional harmonic oscillator. It is found that the su(2) dynamic algebra allows us to express the MPT wave functions in closed form by acting the operator $\hat{b}^\dagger$ on the ground state. The matrix elements of some physical operators have been analytically obtained from the ladder operators $\hat{M}_{\pm,0}$. The harmonic limit has also been studied. It is shown that the su(2) algebra will contract to the Weyl algebra in this limit. The expansions of the coordinate x and the momentum p are evaluated from the operators of the Lie group SU(2).

Notes

1   Here we use operator $\hat{P}_-$ to differ $\hat{M}_-$.

Chapter 8

PSEUDOHARMONIC OSCILLATOR

1.   Introduction

As shown in previous Chapters, with the factorization method we have constructed the ladder operators for some important physical potentials. From these operators we can construct a suitable dynamic group and obtain closed-form analytical expressions of matrix elements for some related functions. Even though we may obtain those matrix elements using other approaches such as the direct integration for some special functions, the advantage of the use of the ladder operators lies in its elegance and intuitivity.

As we know, the real molecular vibrations are anharmonic even though the harmonic oscillator model is widely used. For example, some anharmonic oscillator molecular potentials such as the Morse, PT potentials represent two typical model potentials to describe the molecular vibrations. In this Chapter, we want to study another anharmonic potential, the so-called pseudoharmonic oscillator, which is the sum of the harmonic oscillator and the inversely quadratic potential. This singular central potential was proposed by Goldman and Krivchenkov in the early 1960s and expressed as $V = V_0(x/a - a/x)^2$ [419], where V_0 and a are two parameters. It should be noted that the inverse square interaction potential was first proposed by Post in 1956 when he studied the one-dimensional many identical particles problem in the case of the pair-force interaction between the particles (see Appendix II in [432]). Since 1961 such a quantum system has been studied by many authors [297, 419, 432–444]. For example, Landau and Lifshitz studied its exact solutions in three dimensions [297]. Hurley found that this kind of pseudoharmonic oscillator interaction between the particles can be exactly solved by separation of variables when he studied the three-body problem in one dimension [434]. A few years later, Calogero studied the one-dimensional three- and N-body problems interacting pairwise via

harmonic and inverse square (centrifugal) potential [435, 436]. On the other hand, this potential was generalized by Camiz and Dodonov *et al.* to the nonstationary (varying frequency) pseudoharmonic oscillator potential [437–439]. In addition, such a physical problem was also studied in arbitrary dimension D [437–441]. Recently, Sage has studied the vibrations and rotations of the pseudogaussian oscillator in order to describe the diatomic molecule [444], in which he briefly reinvestigated some properties of the pseudoharmonic oscillator to study the pseudogaussian oscillator. On the other hand, we have studied its dynamic group in two dimensions [162].

The purposes of this Chapter are the following. First, we are going to study this problem in one-dimensional space. The ladder operators, the dynamic group and the Barut-Girardello coherent states are to be developed. Second, we generalize this problem to arbitrary dimensional case. We do not study the three dimensional case since Popov has investigated the similar problem when he studied its coherent states [443], in which the pseudoharmonic oscillator is taken as

$$V_{\text{PH}}(r) = \frac{1}{8}\kappa r_0^2 \left(\frac{r}{r_0} - \frac{r_0}{r} \right)^2, \tag{8.1}$$

where κ is a force constant and the r_0 represents the equilibrium bond length. It should be noted that the potential taken here is slightly different from that of Ref. [443], but they are essentially same except for an unimportant constant.

This Chapter is organized as follows. In Section 2 we study exact solutions of this system in one dimension. Section 3 is devoted to constructing the ladder operators and obtaining the analytical expressions of matrix elements for some related functions ρ and $\rho\frac{d}{d\rho}$ with $\rho = x^2$. The Barut-Girardello coherent states are carried out in Section 4. Section 5 is devoted to the study of the thermodynamic properties. In Section 6 we generalize this quantum system to arbitrary dimensional case. The recurrence relations among the matrix elements are derived in Section 7. Some concluding remarks are given in Section 8.

2.   Exact solutions in one dimension

The motivation for a physicist to investigate one-dimensional problem [445] may be best illustrated by the story of the man who was scanning the ground for his key under a lamppost when he returned home very late at night after an alcoholic evening. He was pretty sure that he had dropped the key somewhere else, but only under the lamppost was there enough light to conduct a proper search [435]. In some sense, the exact solutions even of oversimplified physical models might provide some possibility to assess the reliability of approximation techniques to be used in more realistic contexts.

Let us begin by considering the one-dimensional Schrödinger equation with this potential. The Schrödinger equation for the pseudoharmonic oscillator

$$\left(-\frac{\hbar^2}{2m}\frac{d^2}{dx^2} + V(x)\right)\Phi(x) = E\Phi(x),\tag{8.2}$$

with the potential [446]

$$V(x) = \frac{1}{2}m\omega^2 x^2 + \frac{\hbar^2}{2m}\frac{\alpha}{x^2},\tag{8.3}$$

where m, ω and α represent the mass of the particle, the frequency and the strength of the external field, respectively.

By defining a new variable $\rho = x^2$, we may rearrange Eq. (8.2) as ($\hbar = m = \omega = 1$)

$$\frac{d^2}{d\rho^2}\Phi(\rho) + \frac{1}{2\rho}\frac{d}{d\rho}\Phi(\rho) - \left(\frac{1}{4} + \frac{\alpha}{4\rho^2} - \frac{E}{2\rho}\right)\Phi(\rho) = 0.\tag{8.4}$$

Take the wave functions of the form

$$\Phi(\rho) = \rho^s e^{-\frac{\rho}{2}}\omega(\rho), \quad s = \frac{1 + \sqrt{1 + 4\alpha}}{4}.\tag{8.5}$$

Substituting Eq. (8.5) into Eq. (8.4) leads to

$$\rho\frac{d^2}{d\rho^2}\omega(\rho) + (2s + 1/2 - \rho)\frac{d}{d\rho}\omega(\rho) + (E/2 - s - 1/4)\,\omega(\rho) = 0,\tag{8.6}$$

whose solutions are nothing but the confluent hypergeometric functions $F(s - E/2 + 1/4, 2s + 1/2; \rho)$. Thus, we may obtain the eigenfunctions as

$$\Phi(\rho) = N\rho^s e^{-\frac{\rho}{2}}F(s - E/2 + 1/4, 2s + 1/2; \rho),\tag{8.7}$$

from which we are able to obtain the general quantum condition as

$$s - E/2 + 1/4 = -n.\tag{8.8}$$

Thus, we can obtain the eigenvalues as

$$E_n = 1 + 2n + \sqrt{\alpha + 1/4}, \quad n = 0, 1, 2, \ldots,\tag{8.9}$$

which implying that the energy levels are equidistant.

When $E/2 - s - 1/4$ is a non-negative integer, considering the following two useful relations [263]

$$L_n^\beta(x) = \frac{\Gamma(\beta + n + 1)}{n!\Gamma(\beta + 1)}F(-n, \beta + 1; x),\tag{8.10}$$

$$\int_0^\infty x^\beta e^{-x} L_n^\beta(x) L_m^\beta(x) dx = \frac{\Gamma(n+\beta+1)}{n!} \delta_{nm}, \tag{8.11}$$

we can finally obtain the normalized wave functions as

$$\Phi_n^s(\rho) = N_n \rho^s e^{-\frac{\rho}{2}} L_n^{2s-1/2}(\rho), \quad N_n = \sqrt{\frac{n!}{\Gamma(n+2s+1/2)}}. \tag{8.12}$$

We make an interesting remark here. As discussed in Ref. [447], we find that the eigenfunctions (8.12) ($\rho = x^2$) vanish not only as $x \to \infty$, but also as $x \to i\infty$. The substitution $x \to ix$ demonstrates intimate connections between the eigenvalues $E(x)$ and $E(ix)$, namely, we find that the substitution $x \to ix$ reverses the sign of E in Eq. (8.2), leaving the parameter β invariant. Accordingly, we have $E(x) = -E(ix)$.

3.   Ladder operators

We now turn to construct the ladder operators with the factorization method. That is to say, we intend to find the ladder operators $\hat{L}_\pm$ with the properties

$$\hat{L}_\pm = A_\pm(\rho) \frac{d}{d\rho} + B_\pm(\rho), \quad \hat{L}_\pm \Phi_n(\rho) = l_\pm \Phi_{n\pm 1}(\rho), \tag{8.13}$$

where these ladder operators only depend on the physical variable ρ.

For this purpose, we start by applying the differential operator $\frac{d}{d\rho}$ to the wave functions (8.12)

$$\frac{d}{d\rho} \Phi_n(\rho) = \left(\frac{s}{\rho} - \frac{1}{2} \right) \Phi_n(\rho) + N_n \rho^s e^{-\frac{\rho}{2}} \frac{d}{d\rho} L_n^{2s-1/2}(\rho). \tag{8.14}$$

We shall use this important expression to construct the ladder operators $\hat{L}_\pm$ by using the recursion relations among the associated Laguerre functions so that we may establish the relations between $\Phi_n(\rho)$ and $\Phi_{n\pm 1}(\rho)$.

To this end, let us recall two useful relations [263]

$$x \frac{d}{dx} L_n^\beta(x) = \begin{cases} n L_n^\beta(x) - (n+\beta) L_{n-1}^\beta(x), \\ (n+1) L_{n+1}^\beta(x) - (n+\beta+1-x) L_n^\beta(x). \end{cases} \tag{8.15}$$

Their substitutions into (8.14) enable us to obtain the following relations

$$\left(\frac{d}{d\rho} - \frac{n+s}{\rho} + \frac{1}{2} \right) \Phi_n(\rho) = -\frac{n+2s-1/2}{\rho} \frac{N_n}{N_{n-1}} \Phi_{n-1}(\rho), \tag{8.16}$$

$$\left(\frac{d}{d\rho} + \frac{n+s+1/2}{\rho} - \frac{1}{2} \right) \Phi_n(\rho) = \frac{n+1}{\rho} \frac{N_n}{N_{n+1}} \Phi_{n+1}(\rho), \tag{8.17}$$

from which, together with N_n given in Eq. (8.12), we can define the following operators

$$\hat{L}_- = -\rho\frac{d}{d\rho} + s + \hat{n} - \frac{\rho}{2}, \quad \hat{L}_+ = \rho\frac{d}{d\rho} + s + \hat{n} + 1/2 - \frac{\rho}{2}, \quad (8.18)$$

introducing the number operator $\hat{n}$ with the property

$$\hat{n}\Phi_n(\rho) = n\Phi_n(\rho). \quad (8.19)$$

The ladder operators $\hat{L}_\pm$ have the following properties

$$\hat{L}_-\Phi_n(\rho) = l_-\Phi_{n-1}(\rho), \quad \hat{L}_+\Phi_n(\rho) = l_+\Phi_{n+1}(\rho), \quad (8.20)$$

where

$$l_- = \sqrt{n(n + 2s - 1/2)}, \quad l_+ = \sqrt{(n + 1)(n + 2s + 1/2)}. \quad (8.21)$$

Moreover, we find that the wave functions can be directly obtained by applying the creation operator $\hat{L}_+$ to the ground state $\Phi_0(\rho)$, i.e.

$$\Phi_n(\rho) = \mathcal{N}_n\hat{L}_+^n\Phi_0(\rho), \quad (8.22)$$

with

$$\mathcal{N}_n = \sqrt{\frac{\Gamma(2s + 1/2)}{n!\Gamma(n + 2s + 1/2)}}, \quad \Phi_0(\rho) = \sqrt{\frac{1}{\Gamma(2s + 1/2)}}\rho^s e^{-\frac{\rho}{2}}. \quad (8.23)$$

We now study the dynamic group associated with the operators $\hat{L}_+$ and $\hat{L}_-$. Based on the results (8.20) and (8.21), we can calculate the commutator $[\hat{L}_-, \hat{L}_+]$:

$$[\hat{L}_-, \hat{L}_+]\Phi_n(\rho) = 2l_0\Phi_n(\rho), \quad (8.24)$$

where we have introduced the eigenvalue

$$l_0 = \left(n + s + \frac{1}{4}\right). \quad (8.25)$$

Thus, we can define the operator

$$\hat{L}_0 = \left(\hat{n} + s + \frac{1}{4}\right). \quad (8.26)$$

The operators $\hat{L}_\pm$ and $\hat{L}_0$ thus satisfy the following commutation relations

$$[\hat{L}_-, \hat{L}_+] = 2\hat{L}_0, \quad [\hat{L}_0, \hat{L}_\pm] = \pm\hat{L}_\pm, \quad (8.27)$$

which correspond to an su(1, 1) algebra for the wave functions.

The Casimir operator is calculated by

$$C\Phi_n(\rho) = [\hat{L}_0(\hat{L}_0 - 1) - \hat{L}_+\hat{L}_-]\Phi_n(\rho) = \frac{4\alpha - 3}{16}\Phi_n(\rho). \qquad (8.28)$$

As we know, there are four series of irreducible unitary representations for the SU(1, 1) group except for the identity representation [169]. Since this quantum system has ground state, the representation of the dynamic algebra su(1, 1) belongs to $D^+(j)$:

$$
\begin{aligned}
I_0|j, \nu\rangle &= \nu|j, \nu\rangle, \\
I_-|j, \nu\rangle &= [(\nu + j)(\nu - j - 1)]^{1/2}|j, \nu - 1\rangle, \\
I_+|j, \nu - 1\rangle &= [(\nu + j)(\nu - j - 1)]^{1/2}|j, \nu\rangle, \\
\nu &= -j + n, \quad n = 0, 1, 2, \ldots, \quad j < 0.
\end{aligned}
\qquad (8.29)
$$

In comparison with Eqs. (8.20), (8.21), (8.25) and (8.26), we have $j = -(s + 1/4)$, $\nu = n + s + 1/4$, and $\Phi_n(\rho) = |j, \nu\rangle$.

As a byproduct, we may obtain the following two expressions from Eq. (8.18)

$$\rho = 2\hat{L}_0 - \hat{L}_- - \hat{L}_+, \quad \rho\frac{d}{d\rho} = \frac{1}{2}\left(\hat{L}_+ - \hat{L}_- - \frac{1}{2}\right), \qquad (8.30)$$

from which, together with Eqs. (8.20), (8.21), (8.25) and (8.26), we have

$$
\begin{aligned}
\langle\Phi_m(\rho)|\rho|\Phi_n(\rho)\rangle &\equiv \int_{-\infty}^{\infty}\Phi_m(x)x^2\Phi_n(x)dx \\
&= (2n + 2s + 1/2)\delta_{m,n} \\
&\quad - \sqrt{n(n + 2s - 1/2)}\delta_{m,(n-1)} \\
&\quad - \sqrt{(n + 1)(n + 2s + 1/2)}\delta_{m,(n+1)},
\end{aligned}
\qquad (8.31)
$$

and

$$
\begin{aligned}
\langle\Phi_m(\rho)|\rho\frac{d}{d\rho}|\Phi_n(\rho)\rangle &\equiv \int_{-\infty}^{\infty}\Phi_m(x)\frac{x}{2}\frac{d}{dx}\Phi_n(x)dx \\
&= \frac{1}{2}\sqrt{(n + 1)(n + 2s + 1/2)}\delta_{m,(n+1)} \\
&\quad - \frac{1}{2}\sqrt{n(n + 2s - 1/2)}\delta_{m,(n-1)} \\
&\quad - \frac{1}{4}\delta_{m,n}.
\end{aligned}
\qquad (8.32)
$$

4.   Barut-Girardello coherent states

Following Ref. [114, 292], we may construct the eigenstates of the annihilation operator $\hat{L}_-$

$$\hat{L}_-|z,s\rangle = z|z,s\rangle, \tag{8.33}$$

where z is an arbitrary complex number.

In addition, we may represent the eigenstates $|z,s\rangle$ as the superposition of the complete orthogonal basis $|n,s\rangle$

$$|z,s\rangle = \sum_{n=0}^{\infty} \langle n,s|z,s\rangle |n,s\rangle. \tag{8.34}$$

By applying the annihilation operator $\hat{L}_-$ on (8.34) and using Eqs. (8.20), (8.21), (8.33) as well as the following relations[1]

$$\langle n,s|n',s\rangle = \delta_{nn'}, \quad \sum_{n=0}^{\infty} |n,s\rangle\langle n,s| = 1, \tag{8.35}$$

we may obtain

$$\langle n,s|z,s\rangle = \frac{z}{\sqrt{n(n+2s-1/2)}} \langle n-1,s|z,s\rangle, \tag{8.36}$$

which, after the recurrence procedure, becomes

$$\langle n,s|z,s\rangle = z^n \sqrt{\frac{\Gamma(2s+1/2)}{n!\Gamma(n+2s+1/2)}} \langle 0,s|z,s\rangle. \tag{8.37}$$

By normalizing the states $|z,s\rangle$ to unity and using the relation [263]

$$\frac{I_\nu(2x)}{x^\nu} = \sum_{n=0}^{\infty} \frac{x^{2n}}{n!\Gamma(n+\nu+1)}, \tag{8.38}$$

where $I_\nu(2x)$ is the modified Bessel function of order ν, we have

$$\langle 0,s|z,s\rangle = \sqrt{\frac{|z|^{2s-1/2}}{I_{2s-1/2}(2|z|)\Gamma(2s+1/2)}}. \tag{8.39}$$

Substitution of Eqs. (8.39) and (8.37) into Eq. (8.34) yields

$$|z,s\rangle = \sqrt{\frac{|z|^{2s-1/2}}{I_{2s-1/2}(2|z|)}} \sum_{n=0}^{\infty} \frac{z^n}{\sqrt{n!\Gamma(n+2s+1/2)}} |n,s\rangle. \tag{8.40}$$

Also, the following resolution of the identity holds

$$\int d\mu(z,s)|z,s\rangle\langle z,s| = 1 \qquad (8.41)$$

with

$$d\mu(z,s) = \frac{2}{\pi}K_{2s-1/2}(2|z|)I_{2s-1/2}(2|z|)d^2z,$$
$$d^2z = d(\mathrm{Re}\,z)d(\mathrm{Im}\,z), \qquad (8.42)$$

where K_ν is the ν-order Bessel function of the second kind [263].

It should be mentioned that all integrals are performed over the whole complex z plane, i.e., $z = r\exp(i\phi), r \in [0,\infty), \phi \in [0,2\pi]$. By using the following relation [263]

$$\int_0^\infty dx\, x^\mu K_\nu(ax) = 2^{\mu-1}a^{-\mu-1}\Gamma[(1+\mu+\nu)/2]\Gamma[(1+\mu-\nu)/2], \quad (8.43)$$

with $\Re e(\mu + 1 \pm \nu) > 0$ and $\Re e\, a > 0$. It is not difficult to demonstrate the resolution of the identity (8.41).

On the other hand, we find that these states are not orthogonal

$$\langle\lambda,s|z,s\rangle = \frac{I_{2s-1/2}(2\sqrt{\lambda^*z})}{\sqrt{I_{2s-1/2}(2|\lambda|)I_{2s-1/2}(2|z|)}}, \qquad (8.44)$$

where λ is an arbitrary complex number.

5.   Thermodynamic properties

We now study the thermodynamic properties of this system based on our recent work [446]. For this purpose, it is necessary to obtain the vibrational partition function calculated by

$$Z = \sum_{n=0}^\infty e^{-\beta E_n}, \quad \beta = \frac{1}{kT}, \qquad (8.45)$$

where k is the Boltzmann factor. Substituting Eq. (8.9) into Eq. (8.45) enables us to obtain its exact expression

$$Z = \frac{1}{2\sinh\beta}e^{-\beta\sqrt{\alpha+1/4}}, \qquad (8.46)$$

which means that the partition function Z depends on the parameters α and β. All of related thermodynamic functions can be derived from partition function Z. For a given β, the dependence of Z on α is shown in Fig. 8.1. It is found that the Z monotonically decreases as α and β increase. On the other

hand, for the weak potential strength $\alpha = 10$, we find that the vibrational partition function of harmonic oscillator Z_{HO} tends to zero more slowly with the increasing parameter β than that of the pseudoharmonic oscillator Z_{PH}. For fixed β, the Z_{PH} is smaller than that of $Z_{\mathrm{HO}} = e^{\beta/2}/(e^{\beta} - 1)$ as shown in Fig. 8.2.
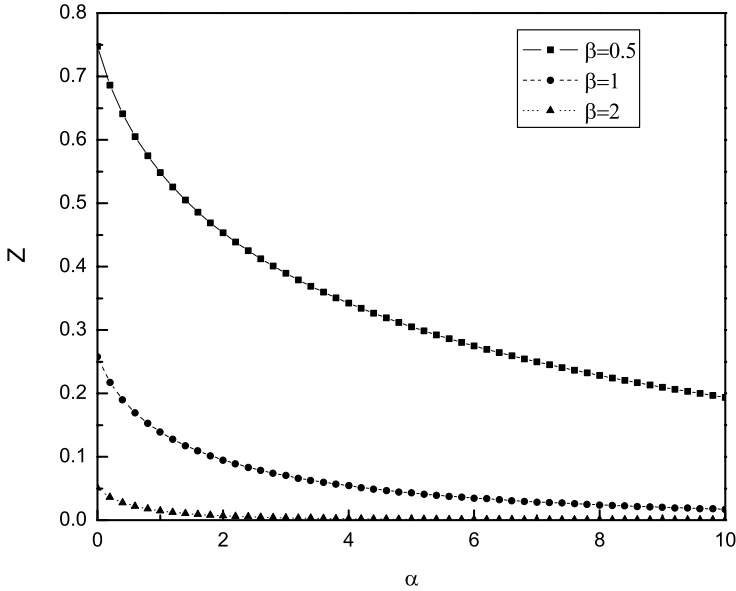

Figure 8.1. Vibrational partition function Z as function of α for different β (0. 5, 1 and 2).

The vibrational mean energy U can be obtained as

$$
\begin{aligned}
U &= -\frac{\partial}{\partial \beta} \ln Z \\
&= -\frac{\partial}{\partial \beta} \left(\ln \frac{e^{-\sqrt{\alpha+1/4}\beta}}{2} - \ln \sinh \beta \right) \\
&= \sqrt{\alpha + 1/4} + \coth \beta,
\end{aligned} \tag{8.47}
$$

which implies that

$$
U = \begin{cases} \sqrt{\alpha + 1/4} + 1/\beta, & \text{for } \beta \ll 1, \\ 1 + \sqrt{\alpha + 1/4}, & \text{for } \beta \to \infty, \end{cases} \tag{8.48}
$$

from which it is clear that U for $\beta \ll 1$ (high temperature) is different from that of the U_{HO} by an extra factor $\sqrt{\alpha + 1/4}$. It is shown in Fig. 8.3 that the U monotonically increases with the increasing parameter α, but for fixed α it decreases with the increasing β.
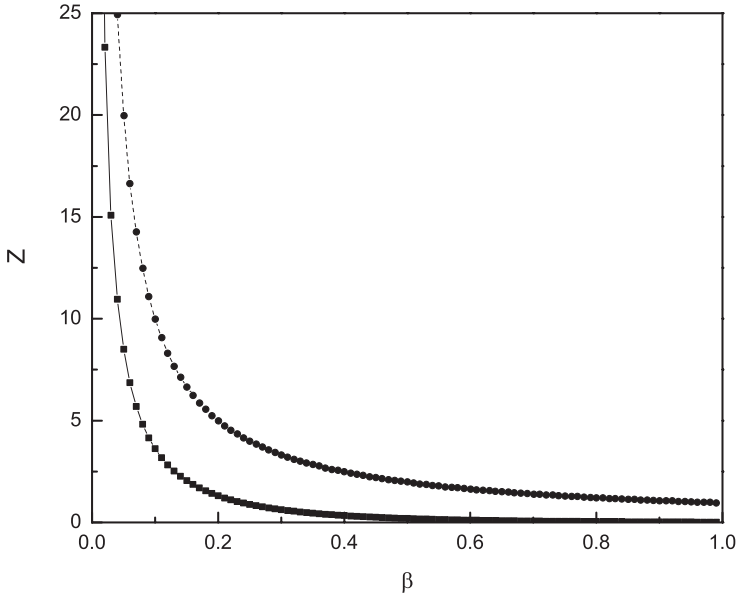
Figure 8.2.   The comparison of the vibrational partition functions between Z_{PH} (solid squared line) and Z_{HO}(dashed dotted line) for the weak potential strength $\alpha = 10$.
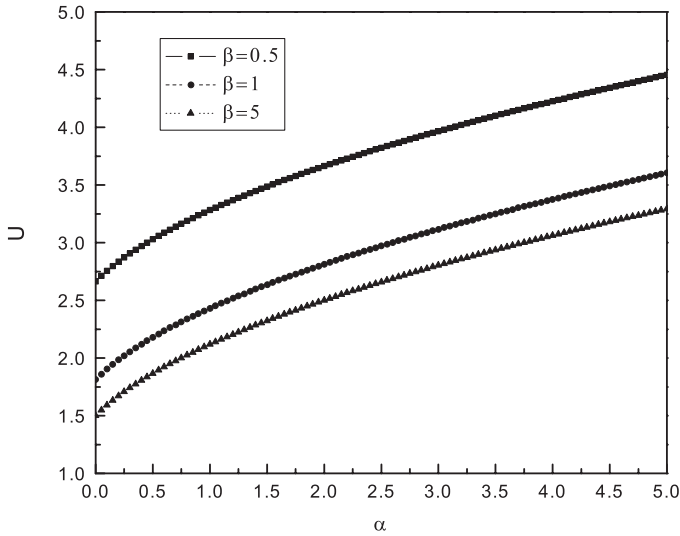

Figure 8.3.   Vibrational mean energy U as function of α for different β (0. 5, 1 and 5).

On the other hand, it is found that the potential strength α plays an important role in the U_{PH}. Basically, the difference between them increases with the α since $U_{PH} - U_{HO} = \frac{1}{2}[\sqrt{1 + 4\alpha} + \tanh(\beta/2)]$. Basically, when $\beta > 2$ the
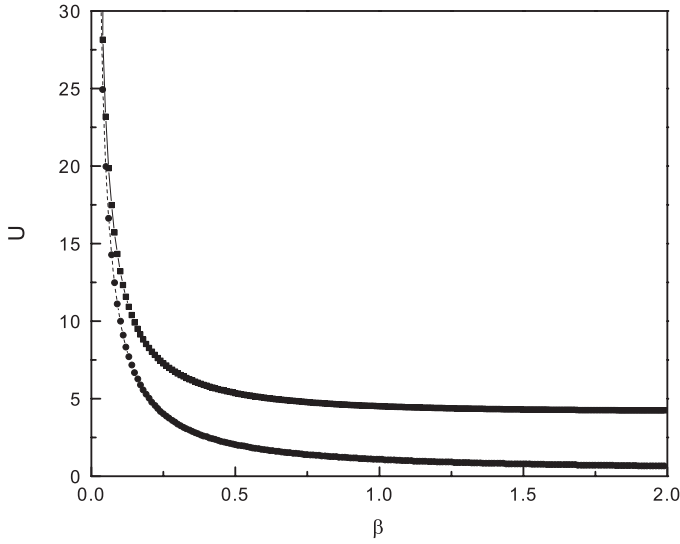
Figure 8.4. The comparison of the vibrational mean energy between U_{PH} (solid squared line) and U_{HO} (dashed dotted line) for the weak potential strength $\alpha = 10$.

difference between them becomes a constant, namely, their changes are parallel (see Fig. 8.4).

The vibrational specific heat C is obtained as

$$
\begin{aligned}
C &= \frac{\partial}{\partial T} U \\
&= \frac{\partial}{\partial T} \left[\sqrt{\alpha + 1/4} + \coth \beta \right] \\
&= \frac{k\beta^2}{\sinh^2 \beta}
\end{aligned}
\tag{8.49}
$$

which implies that

$$
C = \begin{cases} k, & \text{for } \beta \ll 1, \\ 0, & \text{for } \beta \to \infty. \end{cases}
\tag{8.50}
$$

This means that the potential strength α does not give any contribution to the vibrational specific heat C.

Let us consider the vibrational free energy F, which can be calculated as

$$
\begin{aligned}
F &= -\frac{1}{\beta} \ln Z \\
&= \sqrt{\alpha + 1/4} + \frac{\ln 2 \sinh \beta}{\beta}
\end{aligned}
\tag{8.51}
$$

which implies that

$$
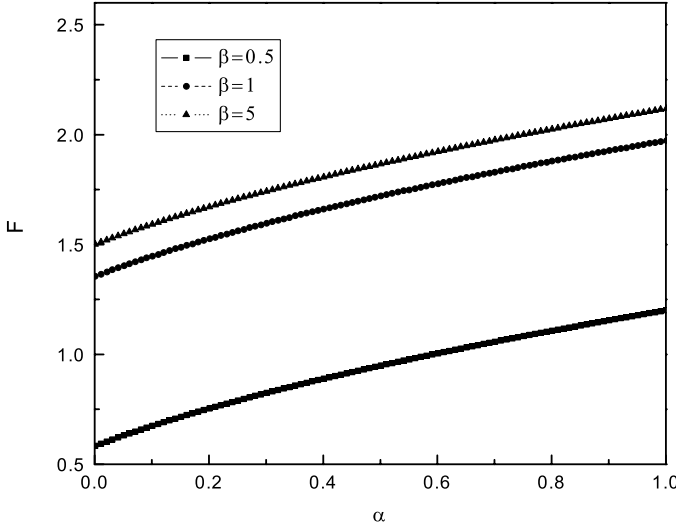F = 1 + \sqrt{\alpha + 1/4}, \quad \beta \to \infty.
\tag{8.52}
$$

Figure 8.5. Vibrational free energy F as function of α for different β (0. 5, 1 and 5).

It is shown in Fig. 8.5 that the free energy F monotonically increases with the increasing parameters α and β. Moreover, we find that the potential strength α plays an important role in F_{PH}. Basically, the difference between F_{PH} and F_{HO} increases with the α since $F_{\mathrm{PH}} - F_{HO} = \sqrt{\alpha + 1/4} + \frac{1}{\beta}[\ln \frac{\sinh \beta}{\sinh(\beta/2)}]$. We find that, when $\beta > 2$ the difference between them is a constant, i.e., their changes are almost parallel as shown in Fig. 8.6.

Finally, we study the vibrational entropy S, which can be calculated by

$$
\begin{aligned}
S &= k \ln Z + kT \left(\frac{\partial \ln Z}{\partial T} \right) \\
&= k \ln Z - k\beta \left(\frac{\partial \ln Z}{\partial \beta} \right) \\
&= k \left[\beta \coth \beta - \ln 2 \sinh \beta \right],
\end{aligned} \tag{8.53}
$$

which implies that the S is also independent of the potential strength α. This is similar to that of the specific heat C. The results that the thermodynamic functions S and C are independent of the potential strength α are very surprising and interesting.

6. Pseudoharmonic oscillator in arbitrary dimensions

Due to the recent interest in the higher dimensional field theory [23, 316, 448–456], we are going to generalize this quantum system to the arbitrary dimensional D case.
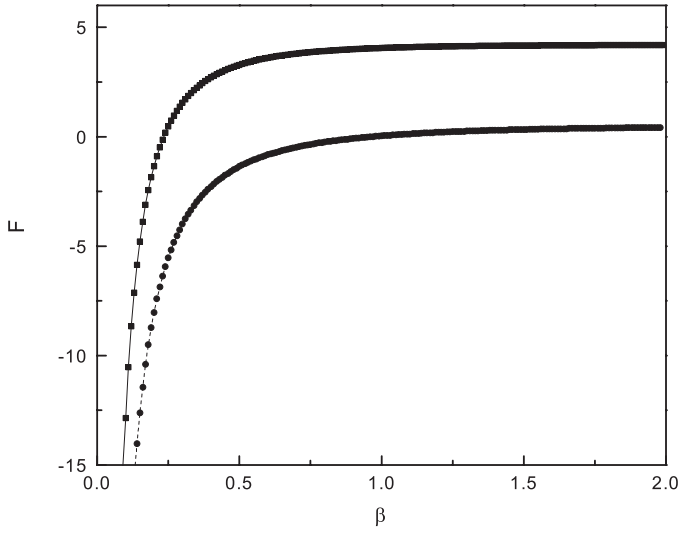
Figure 8.6. The comparison of the vibrational free energy between F_{PH} (solid squared line) and F_{HO} (dashed dotted line) for the weak potential strength $\alpha = 10$.

The D-dimensional Schrödinger equation for a physical potential $V(r)$ can be expressed as ($\mu = \hbar = 1$)

$$-\frac{1}{2} \nabla_D^2 \, \Psi(\mathbf{r}) = [E - V(r)]\Psi(\mathbf{r}), \tag{8.54}$$

where the $\mathbf{r}$ is a D-dimensional position vector with the Cartesian components $r_1, r_2, \ldots, r_D$. The Laplace operator ∇_D^2 is given by

$$\nabla_D^2 = \sum_{j=1}^{D} \frac{\partial^2}{\partial r_j^2}. \tag{8.55}$$

As shown by Erdelyi, Louck and Chatterjee [23, 449, 450], we introduce the hyperspherical coordinates as follows

$$
\begin{aligned}
r_1 &= r \cos\theta_1 \sin\theta_2 \ldots \sin\theta_{D-1}, \\
r_2 &= r \sin\theta_1 \sin\theta_2 \ldots \sin\theta_{D-1}, \\
r_b &= r \cos\theta_{b-1} \sin\theta_k \ldots \sin\theta_{D-1}, \quad 3 \leq b \leq D-1, \\
r_D &= r \cos\theta_{D-1} \\
\sum_{a=1}^{D} (r_a)^2 &= r^2.
\end{aligned}
\tag{8.56}
$$

The unit vector along **r** is usually denoted by $\hat{\mathbf{r}} = \mathbf{r}/r$. The volume element of the configuration space is given by

$$\prod_{a=1}^{D} dr_a = r^{D-1} dr d\Omega, \quad d\Omega = \prod_{a=1}^{D-1} (\sin \theta_a)^{a-1} d\theta_a, \qquad (8.57)$$

where

$$r \in [0, \infty), \quad \theta_1 \in [-\pi, \pi], \quad \theta_a \in [0, \pi], \quad a \in [2, D-1]. \qquad (8.58)$$

The angular momentum operators L_{ab} are defined as

$$L_{ab} = -ir_a \frac{\partial}{\partial r_b} + ir_b \frac{\partial}{\partial r_a}. \qquad (8.59)$$

A set of angular momentum operators are defined as

$$\begin{aligned}
&\mathbf{L}_1^2 = L_{12}^2 = -\frac{\partial^2}{\partial \theta_1^2}, \\
&\mathbf{L}_k^2 = \sum_{a<b=2}^{k+1} L_{ab}^2 = -\left\{ \frac{1}{\sin^{k-1}\theta_k} \frac{\partial}{\partial\theta_k} \sin^{k-1}\theta_k \frac{\partial}{\partial\theta_k} - \frac{\mathbf{L}_{k-1}^2}{\sin^2\theta_k} \right\}, \\
&2 \le k \le D-1, \quad \mathbf{L}^2 \equiv \mathbf{L}_{D-1}^2.
\end{aligned} \qquad (8.60)$$

Through a direct calculation by replacing variables, we express the Laplace operator in the hyperspherical coordinates

$$\nabla_D^2 = \frac{1}{r^{D-1}} \frac{\partial}{\partial r} r^{D-1} \frac{\partial}{\partial r} - \frac{\mathbf{L}^2}{r^2}. \qquad (8.61)$$

Define the generalized spherical harmonics $Y_{l_{D-2}\ldots l_1}^l(\theta_1 \ldots \theta_{D-1}) \equiv Y_{l_{D-2}\ldots l_1}^l(\hat{\mathbf{r}})$, which is the simultaneous eigenfunction of $\mathbf{L}_k^2$

$$\begin{aligned}
&\mathbf{L}_j^2 Y_{l_{D-2}\ldots l_1}^l(\hat{\mathbf{r}}) = l_j(l_j + j - 1) Y_{l_{D-2}\ldots l_1}^l(\hat{\mathbf{r}}), \\
&l \equiv l_{D-1} = 0, 1, \ldots, \qquad l_k = 0, 1, \ldots, l_{k+1}, \\
&l_1 = -l_2, -l_2 + 1, \ldots, l_2 - 1, l_2, \\
&j \in [1, D-1], \qquad k \in [2, D-2].
\end{aligned} \qquad (8.62)$$

Actually, $r^l Y_{l_{D-2}\ldots l_1}^l(\hat{\mathbf{r}})$ is a homogeneous polynomial of order l and satisfies the Laplace equation

$$\nabla_D^2 \left[r^l Y_{l_{D-2}\ldots l_1}^l(\hat{\mathbf{r}}) \right] = 0. \qquad (8.63)$$

For a given angular momentum l, the degeneracy of the eigenfunctions of $\mathbf{L}^2$ is given by

$$d_l(D) = \frac{(D + 2l - 2)(D + l - 3)!}{l!(D - 2)!}.$$

(8.64)

The explicit form of the generalized spherical harmonics $Y^l_{l_{D-2}\ldots l_1}(\hat{\mathbf{r}})$ with all $l_j = l$ is given by

$$Y^l_{l_{D-2}\ldots l_1}(\hat{\mathbf{r}}) = N_{D,l} r^{-l}(r_1 + ir_2)^l,$$

$$N_{D,l} = \begin{cases} 2^{-n-l}\left[\dfrac{(2l + 2n - 1)!}{\pi^n l!(l + n - 1)!}\right]^{1/2}, & \text{for } D = 2n + 1, \\[4mm] \left[\dfrac{(l + n - 1)!}{2\pi^n l!}\right]^{1/2}, & \text{for } D = 2n, \end{cases}$$

(8.65)

where $N_{D,l}$ is the normalization factor. The partners of $Y^l_{l_{D-2}\ldots l_1}(\hat{\mathbf{r}})$ can be calculated from it by the angular momentum operators L_{ab}. The wave functions $\Psi(\mathbf{r})$ with a given angular momentum l can be decomposed as a product of the radial function $R_l(r)$ and the generalized spherical harmonics $Y^l_{l_{D-2}\ldots l_1}(\hat{\mathbf{r}})$.

We are now in the position to study the quantum system for the pseudo-harmonic oscillator in arbitrary dimension D. Similarly, we take the potential $V(r)$ as follows:

$$V(r) = \frac{1}{2}m\omega^2 r^2 + \frac{\hbar^2}{2m}\frac{\alpha}{r^2}.$$

(8.66)

Following Refs. [23, 448, 449], we take the wave functions of the form

$$\Psi(\mathbf{r}) = r^{-(D-1)/2}R(r)Y^l_{l_{D-2}\ldots l_1}(\hat{\mathbf{x}}),$$

(8.67)

where the $Y^l_{l_{D-2}\ldots l_1}(\hat{\mathbf{x}})$ is the generalized spherical harmonics. Substitution of this into Eq. (8.54) allows us to obtain radial wave equation ($\hbar = m = \omega = 1$)

$$\frac{d^2}{dr^2}R(r) + \left(2E - r^2 - \frac{L(L+1)}{r^2}\right)R(r) = 0,$$

(8.68)

where

$$L \equiv -\frac{1}{2} + \sqrt{\alpha + (l - 1 + D/2)^2}.$$

(8.69)

By defining $\rho = r^2$, we can rearrange Eq. (8.68) as follows:

$$\frac{d^2}{d\rho^2}R(\rho) + \frac{1}{2\rho}\frac{d}{d\rho}R(\rho) - \left(\frac{1}{4} + \frac{L(L+1)}{4\rho^2} - \frac{E}{2\rho}\right)R(\rho) = 0.$$

(8.70)

Take the wave functions with the form

$$R(\rho) = \rho^\sigma e^{-\frac{\rho}{2}} F(\rho), \quad \sigma = (L+1)/2. \tag{8.71}$$

Substitution of this into Eq. (8.70) yields

$$\rho \frac{d^2}{d\rho^2} F(\rho) + (2\sigma + 1/2 - \rho) \frac{d}{d\rho} F(\rho) + (E/2 - \sigma - 1/4) F(\rho) = 0, \tag{8.72}$$

whose solutions are the confluent hypergeometric functions . Thus, one can obtain the eigenfunctions as

$$R(\rho) = N \rho^\sigma e^{-\frac{\rho}{2}} F(\sigma - E/2 + 1/4, 2\sigma + \frac{1}{2}; \rho). \tag{8.73}$$

Due to the finiteness of the solutions, we know from Eq. (8.73) that the general quantum condition is given by

$$\sigma - E/2 + 1/4 = -n, \tag{8.74}$$

from which we have

$$E_n = \frac{1}{2} + 2n + 2\sigma = 2n + L + 3/2, \quad n = 0, 1, 2, \ldots. \tag{8.75}$$

If $n = E/2 - \sigma - 1/4$ is taken as a non-negative integer, by making use of the formulas (8.10) and (8.11) we finally obtain the normalized radial wave functions as

$$R_n(\rho) = N_n \rho^\sigma e^{-\frac{\rho}{2}} L_n^{2\sigma - \frac{1}{2}}(\rho), \quad N_n = \sqrt{\frac{2n!}{\Gamma(2\sigma + n + \frac{1}{2})}}. \tag{8.76}$$

Now, we study the ladder operators $\hat{M}_\pm$ with the following properties

$$\hat{M}_\pm = A_\pm(\rho) \frac{d}{d\rho} + B_\pm(\rho), \quad \hat{M}_\pm R_n(\rho) = m_\pm R_{n\pm 1}(\rho), \tag{8.77}$$

where we stress that these operators only depend on the physical variable ρ.

For this purpose, we start by applying the operator $\frac{d}{d\rho}$ on the wave functions (8.76)

$$\frac{d}{d\rho} R_n(\rho) = \left(\frac{\sigma}{\rho} - \frac{1}{2} \right) R_n(\rho) + N_n \rho^\sigma e^{-\frac{\rho}{2}} \frac{d}{d\rho} L_n^{2\sigma - \frac{1}{2}}(\rho), \tag{8.78}$$

which is used to construct the ladder operators $\hat{M}_\pm$.

To this end, using the relations (8.15) and substituting them into (8.78) enable us to obtain the following relations

$$\left(\frac{d}{d\rho} - \frac{n+\sigma}{\rho} + \frac{1}{2}\right) R_n(\rho) = -\frac{n+2\sigma - \frac{1}{2}}{\rho} \frac{N_n}{N_{n-1}} R_{n-1}(\rho), \qquad (8.79)$$

$$\left(\frac{d}{d\rho} + \frac{n+\sigma+\frac{1}{2}}{\rho} - \frac{1}{2}\right) R_n(\rho) = \frac{n+1}{\rho} \frac{N_n}{N_{n+1}} R_{n+1}(\rho), \qquad (8.80)$$

from which, together with N_n given in Eq. (8.76), we can define the following operators

$$\hat{M}_- = -\rho\frac{d}{d\rho} + \sigma + \hat{n} - \frac{\rho}{2}, \quad \hat{M}_+ = \rho\frac{d}{d\rho} + \sigma + \hat{n} + \frac{1}{2} - \frac{\rho}{2}, \qquad (8.81)$$

where we have introduced the number operator $\hat{n}$ with the property

$$\hat{n} R_n(\rho) = n R_n(\rho). \qquad (8.82)$$

The ladder operators $\hat{M}_\pm$ have the following properties

$$\hat{M}_- R_n(\rho) = m_- R_{n-1}(\rho), \quad \hat{M}_+ R_n(\rho) = m_+ R_{n+1}(\rho), \qquad (8.83)$$

where

$$m_- = \sqrt{n(n+2\sigma-1/2)}, \quad m_+ = \sqrt{(n+1)(n+2\sigma+1/2)}. \qquad (8.84)$$

In a similar way, we find that the radial wave functions can be directly obtained by applying the creation operator $\hat{M}_+$ on the ground state $R_0(\rho)$, i.e.

$$R_n(\rho) = \mathcal{N}_n \hat{M}_+^n R_0(\rho), \qquad (8.85)$$

with

$$\mathcal{N}_n = \sqrt{\frac{\Gamma(2\sigma+\frac{1}{2})}{n!\Gamma(n+2\sigma+\frac{1}{2})}}, \quad R_0(\rho) = \sqrt{\frac{2}{\Gamma(2\sigma+\frac{1}{2})}}\rho^\sigma e^{-\frac{\rho}{2}}. \qquad (8.86)$$

We now study the algebra associated with the operators $\hat{M}_+$ and $\hat{M}_-$. Based on the results (8.83) and (8.84), we can calculate the commutator $[\hat{M}_-, \hat{M}_+]$:

$$[\hat{M}_-, \hat{M}_+] R_n(\rho) = 2m_0 R_n(\rho), \qquad (8.87)$$

where we have introduced the eigenvalue

$$m_0 = \left(n + \sigma + \frac{1}{4}\right). \qquad (8.88)$$

We can thus define the operator

$$\hat{M}_0 = \left(\hat{n} + \sigma + \frac{1}{4} \right).$$

$$(8.89)$$

The operators $\hat{M}_\pm$ and $\hat{M}_0$ thus satisfy the commutation relations

$$[\hat{M}_-, \hat{M}_+] = 2\hat{M}_0, \qquad [\hat{M}_0, \hat{M}_\pm] = \pm\hat{M}_\pm,$$

$$(8.90)$$

which correspond to an su(1, 1) algebra.

For the same reason, the representation of the Lie algebra su(1, 1) belongs to $D^+(j)$:

$$
\begin{aligned}
I_0|j, \nu\rangle &= \nu|j, \nu\rangle, \\
I_-|j, \nu\rangle &= \sqrt{(\nu + j)(\nu - j - 1)}|j, \nu - 1\rangle, \\
I_+|j, \nu - 1\rangle &= \sqrt{(\nu + j)(\nu - j - 1)}|j, \nu\rangle, \\
\nu &= -j + n, \qquad n = 0, 1, 2, \ldots, \qquad j < 0.
\end{aligned}
$$

$$(8.91)$$

In comparison with Eqs. (8.83), (8.84), (8.88) and (8.89), we have $j = -(\sigma + 1/4)$, $\nu = n + \sigma + 1/4$, and $R_n(\rho) = |j, \nu\rangle$.

Likewise, the following two related functions can be obtained from the ladder operators $\hat{M}_\pm$

$$\rho = 2\hat{M}_0 - \hat{M}_- - \hat{M}_+, \quad \rho\frac{d}{d\rho} = \frac{1}{2}\left(\hat{M}_+ - \hat{M}_- - \frac{1}{2} \right),$$

$$(8.92)$$

from which, together with Eqs. (8.83) and (8.84), we have

$$
\begin{aligned}
\int_0^\infty R_{n'}(r)r^2 R_n(r)dr = \ & (2n + 2\sigma + \tfrac{1}{2})\delta_{n',n} \\
& - \sqrt{n(n + 2\sigma - 1/2)}\, \delta_{n',(n-1)} \\
& - \sqrt{(n+1)(n + 2\sigma + 1/2)}\, \delta_{n',(n+1)},
\end{aligned}
$$

$$(8.93)$$

and

$$
\begin{aligned}
\int_0^\infty R_{n'}(r)\frac{r}{2}\frac{d}{dr}R_n(r)dr = \ & \frac{1}{2}\sqrt{(n+1)(n + 2\sigma + 1/2)}\, \delta_{n',(n+1)} \\
& - \frac{1}{2}\sqrt{n(n + 2\sigma - 1/2)}\, \delta_{n',(n-1)} \\
& - \frac{1}{4}\delta_{n',n}.
\end{aligned}
$$

$$(8.94)$$

7. Recurrence relations among matrix elements

As we know, the vibrational transitions involving two different electronic states require the calculation of matrix elements. Even though its calculation can be usually done by direct numerical integration or by an approximate method, the analytical expression of matrix elements is elegant and stands in its own right. For this purpose, we first derive a general calculation formula for off-diagonal matrix elements and then derive their recurrence relations.

By denoting $|n\rangle \equiv R_n(r)$, we can express the calculation formula for off-diagonal matrix elements of r^κ as

$$\langle n|r^\kappa|n'\rangle = \frac{N_n N_{n'}}{2} \int_0^\infty \rho^{(L+L'+\kappa+1)/2} e^{-\rho} L_n^{L+\frac{1}{2}}(\rho) L_{n'}^{L'+\frac{1}{2}}(\rho) d\rho, \quad (8.95)$$

where we have used the relation $2\sigma = L + 1$. Using the relation [430]

$$\int_0^\infty x^\tau e^{-x} L_n^u(x) L_{n'}^{u'}(x) dx = (-1)^{n+n'} \Gamma(1+\tau) \sum_i \cdot \begin{pmatrix} \tau - u \\ n - i \end{pmatrix} \begin{pmatrix} \tau - u' \\ n' - i \end{pmatrix} \begin{pmatrix} \tau + i \\ i \end{pmatrix}, \quad (8.96)$$

with the condition $\Re e(\tau) > -1$, we have

$$\langle n|r^\kappa|n'\rangle = \frac{(-1)^{n+n'} N_n N_{n'}}{2} \Gamma[(L+L'+\kappa+3)/2] \times \sum_i \begin{pmatrix} \frac{L'+\kappa-L}{2} \\ n-i \end{pmatrix} \begin{pmatrix} \frac{L+\kappa-L'}{2} \\ n'-i \end{pmatrix} \begin{pmatrix} \frac{1+L+L'+\kappa+2i}{2} \\ i \end{pmatrix}, \quad (8.97)$$

with the condition $\kappa > -(L+L'+3)$. From this, we obtain a simple calculation formula for diagonal matrix elements

$$\langle n|r^\kappa|n\rangle = \frac{N_n^2}{2} \Gamma[(2L+\kappa+3)/2] \sum_i \begin{pmatrix} \frac{\kappa}{2} \\ n-i \end{pmatrix}^2 \begin{pmatrix} \frac{1+2L+\kappa+2i}{2} \\ i \end{pmatrix}, \quad (8.98)$$

which implies that $\langle n|n\rangle = 1$ for $\kappa = 0$.

Now, let us derive their recurrence relations following the so-called Krammers' approach[2] [457]. For two different states $|n\rangle$ and $|n'\rangle$, we may rewrite Eq. (8.68) as

$$\frac{d^2 R_n(r)}{dr^2} + \left[(4n + 2L + 3) - r^2 - \frac{L(L+1)}{r^2}\right] R_n(r) = 0, \quad (8.99)$$

$$\frac{d^2 R_{n'}(r)}{dr^2} + \left[(4n' + 2L' + 3) - r^2 - \frac{L'(L'+1)}{r^2}\right] R_{n'}(r) = 0. \quad (8.100)$$

From the behaviors of wave functions (8.76) at the origin and at infinity,

$$
\begin{aligned}
R_n(r) &\to r^{L+1}, &&\text{when } r \to 0, \\
R_n(r) &\to e^{-r^2/2}, &&\text{when } r \to \infty,
\end{aligned}
\tag{8.101}
$$

and taking $\kappa > -(L + L' + 1)$, we have the following definite integral results

$$
\begin{aligned}
r^\kappa R_{n'}(r)\frac{dR_n(r)}{dr}\Big|_0^\infty &= 0, & r^{\kappa-1}R_{n'}(r)R_n(r)\big|_0^\infty &= 0, \\
r^\kappa \frac{dR_{n'}(r)}{dr}R_n(r)\Big|_0^\infty &= 0, & r^{\kappa+1}\frac{dR_{n'}(r)}{dr}\frac{dR_n(r)}{dr}\Big|_0^\infty &= 0.
\end{aligned}
\tag{8.102}
$$

First, if we multiply each term of Eq. (8.99) by $r^\kappa R_{n'}(r)$ and then doing the integration, then the three terms in the brackets are nothing but the matrix elements of r^κ, $r^{\kappa-1}$ and $r^{\kappa-2}$, respectively. Integrating the first term twice by parts and taking Eq. (8.102) into account, we may obtain

$$
\begin{aligned}
\int_0^\infty \kappa\, r^{\kappa-1} R_n(r)\frac{dR_{n'}(r)}{dr}dr &= \int_0^\infty r^\kappa \frac{dR_n(r)}{dr}\frac{dR_{n'}(r)}{dr}dr \\
&\quad + \langle n|r^{\kappa+2}|n'\rangle - (4n + 2L + 3)\langle n|r^\kappa|n'\rangle \\
&\quad + [L(L+1) - \kappa(\kappa - 1)]\langle n|r^{\kappa-2}|n'\rangle.
\end{aligned}
\tag{8.103}
$$

Here we make a remark about how to obtain this result in order to make the process of derivation understandable and readable. By multiplying each term of Eq. (8.99) by $r^\kappa R_{n'}(r)$ and doing the integration, we have

$$
\begin{aligned}
&\int_0^\infty r^\kappa R_{n'}(r)\frac{dR_n(r)}{dr}dr \\
&= -\int_0^\infty R_{n'}(r)r^\kappa \left[(4n + 2L + 3) - r^2 - \frac{L(L+1)}{r^2}\right] R_n(r)dr.
\end{aligned}
\tag{8.104}
$$

If taking

$$
\begin{aligned}
u &= r^\kappa R_{n'}(r), & dv &= \frac{d^2 R_n(r)}{dr^2}dr, \\
du &= \kappa r^{\kappa-1} R_{n'}(r) + r^\kappa \frac{dR_{n'}(r)}{dr}, & v &= \frac{dR_n(r)}{dr},
\end{aligned}
\tag{8.105}
$$

then we have

$$
\begin{aligned}
&r^\kappa R_{n'}(r)\frac{dR_n(r)}{dr}\Big|_0^\infty - \int_0^\infty \left[\kappa r^{\kappa-1} R_{n'}(r)\frac{dR_n(r)}{dr} + r^\kappa \frac{dR_{n'}(r)}{dr}\frac{dR_n(r)}{dr}\right]dr \\
&= -(4n + 2L + 3)\langle n|r^\kappa|n'\rangle + \langle n|r^{\kappa+2}|n'\rangle + [L(L+1)]\langle n|r^{\kappa-2}|n'\rangle,
\end{aligned}
\tag{8.106}
$$

from which together with Eq. (8.102), we obtain the following result

$$
\begin{aligned}
\int_0^\infty \kappa r^{\kappa-1} R_{n'}(r)\frac{dR_n(r)}{dr}dr \ &= -\int_0^\infty r^\kappa \frac{dR_{n'}(r)}{dr}\frac{dR_n(r)}{dr}dr \\
&+(4n+2L+3)\langle n|r^\kappa|n'\rangle - \langle n|r^{\kappa+2}|n'\rangle \\
&-[L(L+1)]\langle n|r^{\kappa-2}|n'\rangle.
\end{aligned}
\tag{8.107}
$$

Similarly, by taking

$$
\begin{aligned}
u &= \kappa\, r^{\kappa-1} R_{n'}(r), & dv &= \frac{dR_n(r)}{dr}dr, \\
du &= \kappa(\kappa-1)r^{\kappa-2}R_{n'}(r)+\kappa r^{\kappa-1}\frac{dR_{n'}(r)}{dr}, & v &= R_n(r),
\end{aligned}
\tag{8.108}
$$

and integrating the left side of this equation by parts, we are able to obtain

$$
\begin{aligned}
\int_0^\infty \kappa r^{\kappa-1} R_{n'}(r)\frac{dR_n(r)}{dr}dr \ &= \kappa r^{\kappa-1} R_{n'}(r)R_n(r)\Big|_0^\infty \\
&-\int_0^\infty \kappa(\kappa-1)r^{\kappa-2}R_{n'}(r)R_n(r)dr \\
&-\int_0^\infty \kappa r^{\kappa-1}\frac{R_{n'}(r)}{dr}R_n(r)dr.
\end{aligned}
\tag{8.109}
$$

If using Eq. (8.102) and combining Eq. (8.107) and (8.109), then we may obtain the final result (8.103).

In a similar way, we may multiply each term of Eq. (8.100) by $r^\kappa R_n(r)$ and then do the integration. If integrating the first term by parts and considering Eq. (8.102), we have

$$
\begin{aligned}
-\int_0^\infty \kappa\, r^{\kappa-1} R_n(r)\frac{dR_{n'}(r)}{dr}dr \ &= \int_0^\infty r^\kappa \frac{dR_n(r)}{dr}\frac{dR_{n'}(r)}{dr}dr + \langle n|r^{\kappa+2}|n'\rangle \\
&-(4n'+2L'+3)\langle n|r^\kappa|n'\rangle \\
&+L'(L'+1)\langle n|r^{\kappa-2}|n'\rangle.
\end{aligned}
\tag{8.110}
$$

Comparing Eq. (8.103) with Eq. (8.110) leads to

$$
\begin{aligned}
-\int_0^\infty r^\kappa \frac{dR_n(r)}{dr}\frac{dR_{n'}(r)}{dr}dr \ &= \langle n|r^{\kappa+2}|n'\rangle \\
&-(2n+2n'+L+L'+3)\langle n|r^\kappa|n'\rangle \\
&+\tfrac{1}{2}[L(L+1)+L'(L'+1) \\
&-\kappa(\kappa-1)]\langle n|r^{\kappa-2}|n'\rangle,
\end{aligned}
\tag{8.111}
$$

$$
\int_0^\infty \kappa\, r^{\kappa-1} R_n(r) \frac{dR_{n'}(r)}{dr} dr = \tfrac{1}{2}[L(L+1) - L'(L'+1)
$$
$$
-\kappa(\kappa-1)]\langle n|r^{\kappa-2}|n'\rangle
$$
$$
-(2n - 2n' + L - L')\langle n|r^\kappa|n'\rangle.
$$
$$
(8.112)
$$

Second, we multiply each term of Eq. (8.99) by $r^{\kappa+1}\frac{dR_{n'}(r)}{dr}$. Integrating the first term by parts and considering Eq. (8.102) again, we have

$$
-\int_0^\infty r^{\kappa+1} \frac{dR_n(r)}{dr} \frac{dR_{n'}(r)}{dr} dr = \int_0^\infty r^{\kappa+3} R_n(r) \frac{dR_{n'}(r)}{dr} dr
$$
$$
+ \int_0^\infty (1+\kappa) r^\kappa \frac{dR_n(r)}{dr} \frac{dR_{n'}(r)}{dr} dr
$$
$$
- (4n + 2L + 3) \int_0^\infty r^{\kappa+1} R_n(r) \frac{dR_{n'}(r)}{dr} dr
$$
$$
+ L(L+1) \int_0^\infty r^{\kappa-1} R_n(r) \frac{dR_{n'}(r)}{dr} dr.
$$
$$
(8.113)
$$

Likewise, we multiply each term of Eq. (8.100) by $r^{\kappa+1}\frac{dR_n(r)}{dr}$. Integrating the three terms in the brackets by parts and using the conditions Eq. (8.102) allow us to obtain

$$
\int_0^\infty r^{\kappa+1} \frac{dR_n(r)}{dr} \frac{dR_{n'}(r)}{dr^2} dr = -\int_0^\infty r^{\kappa+3} R_n(r) \frac{dR_{n'}(r)}{dr} dr
$$
$$
-(\kappa+3)\langle n|r^{\kappa+2}|n'\rangle
$$
$$
+ (4n' + 2L' + 3) \int_0^\infty r^{\kappa+1} R_n(r) \frac{dR_{n'}(r)}{dr} dr
$$
$$
+ (4n' + 2L' + 3)(\kappa+1)\langle n|r^\kappa|n'\rangle
$$
$$
- L'(L'+1)(\kappa-1)\langle n|r^{\kappa-2}|n'\rangle
$$
$$
- L'(L'+1) \int_0^\infty r^{\kappa-1} R_n(r) \frac{dR_{n'}(r)}{dr} dr.
$$
$$
(8.114)
$$

Incorporating this into (8.113) yields

$$
-\int_0^\infty (1+\kappa) r^\kappa \frac{dR_n(r)}{dr} \frac{dR_{n'}(r)}{dr} dr = -L'(L'+1)(\kappa-1)\langle n|r^{\kappa-2}|n'\rangle
$$
$$
-(\kappa+3)\langle n|r^{\kappa+2}|n'\rangle
$$
$$
+ [L(L+1) - L'(L'+1)]
$$

$$\times \int_0^\infty r^{\kappa-1} R_n(r) \frac{dR_{n'}(r)}{dr} dr$$
$$+ (1+\kappa)(4n' + 2L' + 3)\langle n|r^\kappa|n'\rangle$$
$$- (4n - 4n' + 2L - 2L')$$
$$\times \int_0^\infty r^{\kappa+1} R_n(r) \frac{dR_{n'}(r)}{dr} dr. \tag{8.115}$$

Replacing the third term integral on the right-hand side of Eq. (8.115) by Eq. (8.112), while replacing the fifth term integral by Eq. (8.112), in which κ is replaced by $\kappa + 2$ and then simplifying, we have

$$-\int_0^\infty r^\kappa \frac{dR_n(r)}{dr} \frac{dR_{n'}(r)}{dr} dr = \left\{ \frac{2[2(n-n') + L - L']^2}{(\kappa+1)(\kappa+2)} \right.$$
$$\left. - \frac{\kappa+3}{\kappa+1} \right\} \langle n|r^{\kappa+2}|n'\rangle$$
$$+ \left\{ \frac{[L(L+1) - L'(L'+1)]^2}{2\kappa(1+\kappa)} \right.$$
$$\left. - \frac{(\kappa-1)[L(L+1) + L'(L'+1)]}{2(1+\kappa)} \right\}$$
$$\times \langle n|r^{\kappa-2}|n'\rangle$$
$$+ \left\{ (2(n+n') + L + L' + 3) \right.$$
$$- \frac{2[L(L+1) - L'(L'+1)]}{\kappa(\kappa+2)}$$
$$\left. \times [2(n-n') + L - L'] \right\} \langle n|r^\kappa|n'\rangle. \tag{8.116}$$

In comparison Eq. (8.111) with Eq. (8.116), we obtain a very useful recurrence relation

$$\left\{ \frac{\kappa[L(L+1) + L'(L'+1)]}{2(\kappa+1)} - \frac{[L(L+1) - L'(L'+1)]^2}{4\kappa(1+\kappa)} \right.$$
$$\left. - \frac{\kappa(\kappa-1)}{4} \right\} \langle n|r^{\kappa-2}|n'\rangle + \left\{ -(2(n+n') + L + L' + 3) \right.$$
$$\left. + \frac{[L(L+1) - L'(L'+1)](2(n-n') + L - L')}{\kappa(\kappa+2)} \right\} \langle n|r^\kappa|n'\rangle$$
$$- \left\{ \frac{[2(n-n') + L - L']^2}{(\kappa+1)(\kappa+2)} - \frac{\kappa+2}{\kappa+1} \right\} \langle n|r^{\kappa+2}|n'\rangle = 0, \tag{8.117}$$

from which, we obtain a very simple recurrence relation among diagonal matrix elements

$$(\kappa + 2)\langle n|r^{\kappa+2}|n\rangle - (\kappa + 1)(4n + 2L + 3)\langle n|r^{\kappa}|n\rangle$$
$$+\frac{\kappa[(2L + 1)^2 - \kappa^2]}{4}\langle n|r^{\kappa-2}|n\rangle = 0. \tag{8.118}$$

In order to help the reader to understand effectively the recurrence relation (8.118), we give a few special expressions as follows

$$\langle n|r^2|n\rangle = 2n + L + 3/2, \tag{8.119}$$

$$\langle n|r^4|n\rangle = \frac{1}{8}[3(4n + 2L + 3)^2 - (2L + 1)^2 + 4], \tag{8.120}$$

$$\langle n|r^6|n\rangle = \frac{1}{48}(4n+2L+3)[15(4n+2L+3)^2 - 36L^2 - 36L + 75]. \tag{8.121}$$

In principle, we can obtain all analytical expressions of the diagonal matrix elements for even power of r. We do not give other expressions for the sake of space.

On the other hand, the diagonal matrix elements of the negative even powers of the r can also be obtained by using the integral formula of the confluent hypergeometric functions given by Landau *et al.*[297]

$$J_v = \int_0^\infty e^{-kz} z^{v-1} [F(-n, \gamma, kz)]^2 dz \tag{8.122}$$

and their recurrence relation

$$J_{\gamma+p} = \frac{(\gamma - p - 1)(\gamma - p)\dots(\gamma + p - 1)}{k^{2p+1}} J_{\gamma-p-1} \tag{8.123}$$

to obtain the recurrence relation between the positive powers and negative powers of the r as follows:

$$\langle nL|r^s|nL\rangle = (L + 1/2 - s/2)(L + 3/2 - s/2)\dots$$
$$\times(L + 1/2 + s/2)\langle nL|r^{-(s+2)}|nL\rangle, \tag{8.124}$$

from which, together with the results (8.119)-(8.121) we may obtain the following expressions

$$\langle nL|r^{-2}|nL\rangle = \frac{2}{2L + 1}, \tag{8.125}$$

$$\langle nL|r^{-4}|nL\rangle = \frac{4n + 2L + 3}{2(L - 1/2)(L + 1/2)(L + 3/2)}, \tag{8.126}$$

$$\langle nL|r^{-6}|nL\rangle = \frac{3(4n+2L+3)^2 - (2L+3)(2L-1)}{8(L-3/2)(L-1/2)(L+1/2)(L+3/2)(L+5/2)}.$$

(8.127)

Likewise, other matrix elements of the r^{-2s} ($s > 3$) can also be obtained.

To calculate the diagonal matrix elements of the odd powers of the r, we shall use Eq. (8.118). For example, we may obtain the following expression

$$\langle nL|r|nL\rangle = \frac{n!}{\Gamma(n+L+3/2)} \sum_{s=0}^{n} \frac{\pi(L+n-s+1)!}{4(1/2-s)!^2(n-s)!s!^2}.$$

(8.128)

On the other hand, if taking the odd power $k = 2s + 1$ we have

$$\langle 0L|r^{2s+1}|0L\rangle = \frac{\Gamma(L+s+2)}{\Gamma(L+3/2)}, \quad n = 0,$$

(8.129)

$$\langle 1L|r^{2s+1}|1L\rangle = \frac{\Gamma(L+s+2)}{\Gamma(L+5/2)}(L+s^2+2s+9/4), \quad n = 1,$$

(8.130)

from which we can easily obtain the diagonal matrix elements for the special case $s = 0$. Similarly, we may obtain other analytical expressions for large n.

For the special case $\alpha = 0$ and $D = 3$, however, we have $L = l$. Consequently, the results (8.97) and (8.117) reduce to those of the harmonic oscillator [458] and non-harmonic oscillator model potentials [459].

8. Concluding remarks

In this Chapter we have studied the exact solutions of the one-dimensional Schrödinger equation with the pseudoharmonic oscillator and obtained the ladder operators. We have found that these operators satisfy the commutation relations of the generators of the dynamic group SU(1, 1). The representation of the bound states can be described by the representation $D^+(j)$ with a spectrum bound below. The analytical matrix elements for some related functions ρ and $\rho\frac{d}{d\rho}$ have also been obtained from the ladder operators. On the other hand, we have constructed the Barut-Girardello coherent states following Ref. [114] and studied the thermodynamic properties. It is surprising and interesting to find that the thermodynamic functions S and C are independent of the potential strength α. Additionally, we have generalized this quantum system to the arbitrary dimensional case. Following Krammers' approach we have obtained the recurrence relations among the off-diagonal matrix elements.

Notes

1   Here, we are only interested in the irreducible unitary representations known
    as positive discrete series, where $s > 0$. The corresponding state is spanned
    by the complete orthogonal basis of the number state $|n, s\rangle$ ($n = 0, 1, 2, ...$,
    is the vibrational quantum number) of the pseudoharmonic oscillator Hilbert
    space.
2   This is a method that uses the Schrödinger equation multiplied by an appro-
    priate function, integral and differential operators and boundary conditions.

Chapter 9

ALGEBRAIC APPROACH TO AN ELECTRON IN A UNIFORM MAGNETIC FIELD

1.   Introduction

It is a common knowledge that the problem of an electron in the uniform magnetic field $\mathbf{H}$ is of importance in quantum mechanics. This is one of the simplest exactly solvable examples. This problem has been studied both in the non-relativistic Schrödinger equation and in the relativistic one [297, 460–462].

The purpose of this Chapter is the following. First, we shall review the exact solutions of the Schrödinger equation for a non-relativistic electron in the uniform magnetic field. Second, we establish the ladder operators directly from the eigenfunctions with the factorization method and then construct a suitable dynamic algebra.

This Chapter is organized as follows. In Section 2 we obtain the eigenvalues and eigenfunctions for a non-relativistic electron in the uniform magnetic field. Section 3 is devoted to the construction of the ladder operators. The matrix elements of the different functions ρ^2 and $\rho\frac{d}{d\rho}$ are obtained from these operators. The concluding remarks are given in Section 4.

2.   Exact solutions

For a particle in an electromagnetic field described by a vector potential $\mathbf{A}$ and a scalar potential V, the Schrödinger equation can be written as

$$\frac{1}{2\mu}(-i\hbar\nabla - Q\mathbf{A})^2\Psi = (E - V)\Psi, \qquad (9.1)$$

where μ is the electron mass and the charge Q is taken as $-e$ for the electron. In this Chapter, we are only interested in the case with the uniform magnetic field $\mathbf{H}$ and the electric field $V = 0$. As shown by Landau *et al.* [297], we discuss this problem in the cylindrical polar coordinates ρ, ϕ and z with the z-axis in the direction of the magnetic field, the vector potential has the components

$A_\phi = \frac{1}{2}H\rho$, $A_z = A_\rho = 0$, the Schrödinger equation can be expressed as

$$-\frac{\hbar^2}{2\mu}\left[\frac{1}{\rho}\frac{\partial}{\partial\rho}\left(\rho\frac{\partial\Psi}{\partial\rho}\right) + \frac{\partial^2\Psi}{\partial z^2} + \frac{1}{\rho^2}\frac{\partial^2\Psi}{\partial\phi^2}\right] - \frac{1}{2}i\hbar\omega_H\frac{\partial\Psi}{\partial\phi} + \frac{1}{8}\mu\omega_H^2\rho^2\Psi = E\Psi,$$
(9.2)

with $\omega_H = |e|H/\mu c$, where c is the velocity of the light.

We are now looking for the solutions in the form

$$\Psi = \frac{1}{\sqrt{2\pi}}R(\rho)e^{im\phi}e^{ip_z z/\hbar}, \quad m = 0, \pm 1, \pm 2, \ldots.$$
(9.3)

For simplicity, the natural units $\mu = c = \hbar = H = e = 1$ are employed if not stated elsewhere otherwise. Substitution of (9.3) into (9.2) allows us to obtain the following radial wave functions

$$\frac{1}{2}\left(\frac{d^2R(\rho)}{d\rho^2} + \frac{1}{\rho}\frac{dR(\rho)}{d\rho} - \frac{m^2}{\rho^2}R(\rho)\right) + \left(E' - \frac{1}{8}\rho^2\right)R(\rho) = 0,$$
(9.4)

where

$$E' = E - \frac{p_z^2}{2} - \frac{1}{2}m.$$
(9.5)

By defining a new independent variable $\zeta = \rho^2/2$, we can obtain the following simplified equation

$$\zeta\frac{d^2R(\zeta)}{d\zeta^2} + \frac{dR(\zeta)}{d\zeta} + \left(-\frac{1}{4}\zeta + E' - \frac{m^2}{4\zeta}\right)R(\zeta) = 0.$$
(9.6)

Let us consider the behaviors of this differential equation at the origin and at infinity. When $\zeta \to \infty$, the required wave functions behave as $e^{-\frac{1}{2}\zeta}$. When $\zeta \to 0$, they behave as $\zeta^{m/2}$. Consequently we may take the wave functions of the form

$$R(\zeta) = e^{-\zeta/2}\zeta^{m/2}\omega(\zeta).$$
(9.7)

Substitution of this into Eq. (9.6) leads to the following expression

$$\zeta\frac{d^2\omega(\zeta)}{d\zeta^2} + (m + 1 - \zeta)\frac{d\omega(\zeta)}{d\zeta} + \left(E' - \frac{m + 1}{2}\right)\omega(\zeta) = 0,$$
(9.8)

whose solutions are nothing but the confluent hypergeometric functions

$$\omega(\zeta) = F\left[-\left(E' - \frac{m + 1}{2}\right), m + 1; \zeta\right].$$
(9.9)

If the wave functions are finite everywhere, the quantity $(E' - \frac{m+1}{2})$ must be a non-negative integer n. Hence, the eigenvalues can be obtained as

$$E'_n = n + \frac{m+1}{2}, \quad n = 0, 1, 2, \ldots. \tag{9.10}$$

The corresponding radial wave functions are given by

$$R_n^m(\rho) = \frac{1}{m!} \left[\frac{(m+n)!}{2^m n!} \right]^{\frac{1}{2}} e^{-\rho^2/4} \rho^m F(-n, m+1; \rho^2/2), \tag{9.11}$$

where we have used the following normalized condition

$$\int_0^\infty R_n^m(\rho)^2 \rho d\rho = 1. \tag{9.12}$$

By using the relation between the associated Laguerre functions and the confluent hypergeometric functions (8.10), we can express the radial wave functions as

$$R_n^m(\rho) = N_n^m e^{-\rho^2/4} \rho^m L_n^m(\rho^2/2), \tag{9.13}$$

where

$$N_n^m = \sqrt{\frac{n!}{2^m (n+m)!}}. \tag{9.14}$$

3.   Ladder operators

In this section we address the problem of finding the creation and annihilation operators for the radial wave functions (9.13) with the factorization method. Likewise, we intend to find differential operators $\hat{\mathcal{L}}_\pm$ with the following property

$$\hat{\mathcal{L}}_\pm R_n^m(\rho) = \ell_\pm R_{n\pm 1}^m(\rho). \tag{9.15}$$

Specifically, we look for operators of the form

$$\hat{\mathcal{L}}_\pm = A_\pm(\rho) \frac{d}{d\rho} + B_\pm(\rho). \tag{9.16}$$

To this end we start by establishing the action of the differential operator $\frac{d}{d\rho}$ on the radial wave functions (9.13)

$$\frac{d}{d\rho} R_n^m(\rho) = -\frac{\rho}{2} R_n^m(\rho) + \frac{m}{\rho} R_n^m(\rho) + N_n^m \rho^m e^{-\rho^2/4} \frac{d}{d\rho} L_n^m(\rho^2/2). \tag{9.17}$$

Substitution of the first formula given in (8.15) into (9.17) enables us to obtain the following relation

$$\left(-\frac{d}{d\rho} + \frac{m}{\rho} - \frac{\rho}{2} + \frac{2n}{\rho}\right) R_n^m(\rho) = \frac{2(n+m)}{\rho} \frac{N_n^m}{N_{n-1}^m} R_{n-1}^m(\rho). \qquad (9.18)$$

Making use of Eq. (9.14), we can define the following operator

$$\hat{\mathcal{L}}_- = \frac{1}{2}\left[-\rho\frac{d}{d\rho} - \frac{1}{2}\rho^2 + (2n+m)\right], \qquad (9.19)$$

with the following effect on the radial wave functions

$$\hat{\mathcal{L}}_- R_n^m(\rho) = \ell_- R_{n-1}^m(\rho), \qquad (9.20)$$

where

$$\ell_- = \sqrt{n(m+n)}. \qquad (9.21)$$

As we can see, this operator annihilates the ground state $R_0^m(\rho)$, as expected from a step-down operator.

We now proceed to find the corresponding creation operator. Similarly, substitution of the second formula given in (8.15) into Eq. (9.17) allows us to obtain

$$\left[\frac{d}{d\rho} - \frac{m}{\rho} + \frac{\rho}{2} + \frac{2}{\rho}\left(n+m+1-\frac{\rho^2}{2}\right)\right] R_n^m(\rho) = \frac{2(n+1)}{\rho} \frac{N_n^m}{N_{n+1}^m} R_{n+1}^m(\rho), \qquad (9.22)$$

Using Eq. (9.14) again, we can define the following operator

$$\hat{\mathcal{L}}_+ = \frac{1}{2}\left[\rho\frac{d}{d\rho} - \frac{1}{2}\rho^2 + (2n+m+2)\right], \qquad (9.23)$$

satisfying the equation

$$\hat{\mathcal{L}}_+ R_n^m(\rho) = \ell_+ R_{n+1}^m(\rho), \qquad (9.24)$$

with

$$\ell_+ = \sqrt{(n+1)(m+n+1)}. \qquad (9.25)$$

We now study the dynamic algebra associated to the operators $\hat{\mathcal{L}}_+$ and $\hat{\mathcal{L}}_-$. Based on the results (9.20), (9.21), (9.24) and (9.25), we can calculate the commutator $[\hat{\mathcal{L}}_-, \hat{\mathcal{L}}_+]$:

$$[\hat{\mathcal{L}}_-, \hat{\mathcal{L}}_+] R_n^m(\rho) = 2\ell_0 R_n^m(\rho), \qquad (9.26)$$

where we have introduced the eigenvalue

$$\ell_0 = \left(n + \frac{m+1}{2}\right).$$ (9.27)

We can thus define the operator

$$\hat{\mathcal{L}}_0 = \left(\hat{n} + \frac{m+1}{2}\right),$$ (9.28)

with the number operator $\hat{n}$

$$\hat{n}R_n^m(\rho) = nR_n^m(\rho).$$ (9.29)

The operators $\hat{\mathcal{L}}_\pm$ and $\hat{\mathcal{L}}_0$ thus satisfy the commutation relations

$$[\hat{\mathcal{L}}_-, \hat{\mathcal{L}}_+] = 2\hat{\mathcal{L}}_0, \qquad [\hat{\mathcal{L}}_0, \hat{\mathcal{L}}_\pm] = \pm\hat{\mathcal{L}}_\pm,$$ (9.30)

which correspond to an su(1, 1) algebra for the radial wave functions. The Casimir operator can be expressed as

$$CR_n^m(\rho) = [\hat{\mathcal{L}}_0(\hat{\mathcal{L}}_0 - 1) - \hat{\mathcal{L}}_+\hat{\mathcal{L}}_-]R_n^m(\rho) = \frac{m^2 - 1}{4}R_n^m(\rho).$$ (9.31)

Similarly, we know that the representation of the dynamic algebra su(1, 1) belongs to $D^+(j)$:

$$\begin{aligned}
I_0|j, \nu\rangle &= \nu|j, \nu\rangle, \\
I_-|j, \nu\rangle &= [(\nu + j)(\nu - j - 1)]^{\frac{1}{2}}|j, \nu - 1\rangle, \\
I_+|j, \nu - 1\rangle &= [(\nu + j)(\nu - j - 1)]^{\frac{1}{2}}|j, \nu\rangle, \\
\nu &= -j + n, \quad n = 0, 1, 2, \ldots, \quad j < 0.
\end{aligned}$$ (9.32)

In comparison with Eqs. (9.20), (9.21), (9.24), (9.25), (9.27) and (9.28), we have $j = -(m + 1)/2$, $\nu = n + (m + 1)/2$, and $R_n^m(\rho) = |j, \nu\rangle$.

On the other hand, the following expressions in terms of the creation and annihilation operators $\hat{\mathcal{L}}_\pm$ can be obtained as

$$\rho^2 = 2[(2n + m + 1) - (\hat{\mathcal{L}}_+ + \hat{\mathcal{L}}_-)], \qquad \rho\frac{d}{d\rho} = (\hat{\mathcal{L}}_+ - \hat{\mathcal{L}}_-) - 1.$$ (9.33)

Their matrix elements can be analytically obtained from Eqs. (9.20), (9.21), (9.24), (9.25), (9.27) and (9.28) as

$$\begin{aligned}
\langle m|\rho^2|n\rangle &= 2[(2n + m + 1)\delta_{m,n} \\
&\quad - \sqrt{(n + 1)(n + m + 1)}\delta_{m,n+1} \\
&\quad - \sqrt{n(n + m)}\delta_{m,n-1}],
\end{aligned}$$ (9.34)

and

$$
\begin{aligned}
\langle m|\rho\tfrac{d}{d\rho}|n\rangle \ = \ & \sqrt{(n+1)(n+m+1)}\delta_{m,n+1} \\
& - \sqrt{n(n+m)}\delta_{m,n-1} \\
& - \delta_{m,n}.
\end{aligned}
\tag{9.35}
$$

4.   Concluding remarks

In this Chapter we have obtained the eigenvalues and eigenfunctions for a non-relativistic electron in the uniform magnetic field **H** and established the creation and annihilation operators directly from the eigenfunctions (9.13) with the factorization method. We have derived a realization of the dynamic group only in terms of the physical variable ρ. It is shown that these operators correspond to an SU(1, 1) dynamic group. The representation of the bound states of this quantum system is described by the representation $D^+(j)$ with a spectrum bound below. The analytical matrix elements of the different functions ρ^2 and $\rho\frac{d}{d\rho}$ are also obtained from the ladder operators $\hat{\mathcal{L}}_\pm$.

Chapter 10

RING-SHAPED NON-SPHERICAL OSCILLATOR

1.   Introduction

Up to now, the algebraic method has been a subject of the interest in various fields of physics. With the factorization method, we have established the ladder operators for quantum systems with some important potentials and constructed suitable Lie algebras. Recently, the quantum system for the ring-shaped non-spherical oscillator has been studied [463]. The purpose of this Chapter is to study its hidden symmetry.

This Chapter is organized as follows. In Section 2 we derive the eigenvalues and eigenfunctions of this system. Section 3 is devoted to establishing the ladder operators directly from the radial wave functions. In Section 4 we shall realize the dynamic group and obtain the analytical matrix elements of physical functions ρ and $\rho \frac{d}{d\rho}$ with $\rho = r^2$. Some conclusions are given in Section 5.

2.   Exact solutions

In this section we study the exact solutions of the Schrödinger equation with the ring-shaped non-spherical oscillator, which are necessary for constructing the ladder operators. Consider the Schrödinger equation with a potential $V(\mathbf{r})$

$$-\frac{\hbar^2}{2m}\nabla^2\Psi(\mathbf{r}) + V(\mathbf{r})\Psi(\mathbf{r}) = E\Psi(\mathbf{r}), \qquad (10.1)$$

where m is the mass of the particle. In the present work, the potential $V(\mathbf{r})$ is taken as a ring-shaped non-spherical oscillator,

$$V(r, \theta) = \frac{1}{2}m\omega^2 r^2 + \frac{\hbar^2}{2m}\left(\frac{\alpha}{r^2} + \frac{\beta}{r^2\sin^2\theta}\right), \qquad (10.2)$$

where the ω is the frequency; α and β are two dimensionless parameters.

For simplicity, the natural units $\hbar = m = \omega = 1$ are employed. Due to the symmetry of the potential, we take the wave functions with the form [463]

$$\Psi(r, \theta, \varphi) = \frac{R(r)}{r}\Theta(\theta)e^{\pm im\varphi}, \quad m = 0, 1, 2, \ldots. \tag{10.3}$$

Substitution of this into Eq. (10.1) allows us to obtain the radial equation and the angular one as follows:

$$\frac{d^2 R(r)}{dr^2} + \left(2E - r^2 - \frac{\alpha + \lambda}{r^2}\right) R(r) = 0, \tag{10.4}$$

$$\frac{1}{\sin\theta}\frac{d}{d\theta}\left(\sin\theta\frac{d\Theta(\theta)}{d\theta}\right) + \left(\lambda - \frac{\beta + m^2}{\sin^2\theta}\right)\Theta(\theta) = 0, \tag{10.5}$$

with the constant λ to be determined below.

Introduce

$$\xi = \sqrt{\beta + m^2}, \quad \lambda = \ell'(\ell' + 1), \quad x = \cos(\theta). \tag{10.6}$$

Substitution of Eq. (10.6) into Eq. (10.5) leads to

$$(1 - x^2)\frac{d^2\Theta(x)}{dx^2} - 2x\frac{d\Theta(x)}{dx} + \left[\ell'(\ell' + 1) - \frac{\xi^2}{1 - x^2}\right]\Theta(x) = 0, \tag{10.7}$$

which is called the so-called universal associated Legendre differential equation. Its normalized solutions can be obtained as

$$\begin{aligned}
\Theta_{\ell'\xi}(\theta) &= \sqrt{\frac{(2\ell' + 1)}{2}\frac{(\ell' - \xi)!}{\Gamma(\ell' + \xi + 1)}}(\sin\theta)^\xi \\
&\cdot \sum_{v=0}^{\left[\frac{\ell' - \xi}{2}\right]}\frac{(-1)^v\Gamma(2\ell' - 2v + 1)}{2^{\ell'}v!(\ell' - \xi - 2v)!\Gamma(\ell' - v + 1)}(\cos\theta)^{\ell' - \xi - 2v},
\end{aligned} \tag{10.8}$$

with

$$\ell' = \xi + k, \quad k = 0, 1, 2, \ldots. \tag{10.9}$$

Substitution of this into Eq. (10.4) allows us to obtain

$$\frac{d^2 R(r)}{dr^2} + \left(2E - r^2 - \frac{L(L + 1)}{r^2}\right) R(r) = 0, \tag{10.10}$$

with

$$L \equiv \frac{1}{2}\left[\sqrt{1 + 4\left[\alpha + \left(\sqrt{\beta + m^2} + k\right)\left(\sqrt{\beta + m^2} + k + 1\right)\right]} - 1\right]. \tag{10.11}$$

If we define a new variable $\rho = r^2$, then Eq. (10.10) can be rearranged as

$$\frac{d^2}{d\rho^2}R(\rho) + \frac{1}{2\rho}\frac{d}{d\rho}R(\rho) - \left(\frac{1}{4} + \frac{L(L+1)}{4\rho^2} - \frac{E}{2\rho}\right)R(\rho) = 0. \quad (10.12)$$

From the behaviors of the wave functions at the origin and at infinity, we can take the following ansatz for the wave functions

$$R(\rho) = \rho^\gamma e^{-\frac{\rho}{2}}F(\rho), \quad \gamma = \frac{L+1}{2}, \quad (10.13)$$

where another solution $\gamma = -\frac{L}{2}$ is not physically acceptable. Substitution of Eq. (10.13) into Eq. (10.12) yields

$$\rho\frac{d^2}{d\rho^2}F(\rho) + (2\gamma + 1/2 - \rho)\frac{d}{d\rho}F(\rho) + (E/2 - \gamma - 1/4)\,F(\rho) = 0, \quad (10.14)$$

whose solutions are nothing but the confluent hypergeometric functions $F(\gamma - E/2 + 1/4, 2\gamma + 1/2; \rho)$. One can finally obtain the eigenfunctions as

$$R(\rho) = N\rho^\gamma e^{-\frac{\rho}{2}}F(\gamma - E/2 + 1/4, 2\gamma + 1/2; \rho), \quad (10.15)$$

where the normalized factor N is to be determined below.

From consideration of the finiteness of the solutions, it is shown from Eq. (10.15) that the general quantum condition is given by

$$\gamma - E/2 + 1/4 = -n, \quad n = 0, 1, 2, \dots, \quad (10.16)$$

from which we have

$$E_n = 2(n + \gamma + 1/4) = \frac{1}{2} + 2n + 2\gamma, \quad (10.17)$$

which implies that the energy levels are equidistant.

When $n = E/2 - \gamma - 1/4$ is taken as a non-negative integer, based on the relations (8.10) and (8.11) we can finally obtain the normalized wave functions

$$R(\rho) = N_n\rho^\gamma e^{-\frac{\rho}{2}}L_n^{2\gamma-\frac{1}{2}}(\rho), \quad (10.18)$$

where

$$N_n = \sqrt{\frac{2n!}{\Gamma(2\gamma + n + \frac{1}{2})}}. \quad (10.19)$$

3.   Ladder operators

We now address the problem of finding the creation and annihilation operators for the radial wave functions (10.18) with the factorization method, which can be defined as

$$\hat{\mathcal{L}}_{\pm} R_n(\rho) = l_{\pm} R_{n_{\pm 1}}(\rho). \tag{10.20}$$

Specifically, we look for operators of the form

$$\hat{\mathcal{L}}_{\pm} = A_{\pm}(\rho)\frac{d}{d\rho} + B_{\pm}(\rho). \tag{10.21}$$

To this end we start by applying the differential operator $\frac{d}{d\rho}$ on the wave functions (10.18)

$$\frac{d}{d\rho} R_n(\rho) = \left(\frac{\gamma}{\rho} - \frac{1}{2}\right) R_n(\rho) + N_n \rho^{\gamma} e^{-\frac{\rho}{2}} \frac{d}{d\rho} L_n^{2\gamma - \frac{1}{2}}(\rho). \tag{10.22}$$

In a similar way, substitution of the first formula given in (8.15) into (10.22) enables us to obtain the following relation

$$\left(\frac{d}{d\rho} - \frac{n + \gamma}{\rho} + \frac{1}{2}\right) R_n(\rho) = -\frac{n + 2\gamma - \frac{1}{2}}{\rho} \frac{N_n}{N_{n-1}} R_{n-1}(\rho). \tag{10.23}$$

By making use of Eq. (10.19) and introducing the number operator $\hat{n}$ with the property

$$\hat{n} R_n(\rho) = n R_n(\rho), \tag{10.24}$$

we can define the following annihilation operator

$$\hat{\mathcal{L}}_- = -\rho\frac{d}{d\rho} + \gamma + \hat{n} - \frac{\rho}{2}, \tag{10.25}$$

with the following effect over the wave functions

$$\hat{\mathcal{L}}_- R_n(\rho) = l_- R_{n-1}(\rho), \tag{10.26}$$

where

$$l_- = \sqrt{n(n + 2\gamma - 1/2)}. \tag{10.27}$$

As we can see, this operator annihilates the ground state $R_0(\rho)$, as expected from a step-down operator.

We now proceed to find the corresponding creation operator. Substitution of the second formula (8.15) into Eq. (10.22) leads to

$$\left(\frac{d}{d\rho} + \frac{n + \gamma + \frac{1}{2}}{\rho} - \frac{1}{2}\right) R_n(\rho) = \frac{n + 1}{\rho} \frac{N_n}{N_{n+1}} R_{n+1}(\rho). \tag{10.28}$$

Using Eq. (10.19) again, we can define the following creation operator

$$\hat{\mathcal{L}}_+ = \rho \frac{d}{d\rho} + \gamma + \hat{n} + \frac{1}{2} - \frac{\rho}{2}, \tag{10.29}$$

satisfying the equation

$$\hat{\mathcal{L}}_+ R_n(\rho) = l_+ R_{n+1}(\rho), \tag{10.30}$$

with

$$l_+ = \sqrt{(n+1)(n+2\gamma+1/2)}. \tag{10.31}$$

Therefore, it is shown that the wave functions can be directly obtained from the creation operator $\hat{\mathcal{L}}_+$ acting on the ground state $R_0(\rho)$, namely,

$$R_n(\rho) = \mathcal{N}_n \hat{\mathcal{L}}_+^n R_0(\rho), \tag{10.32}$$

with

$$\mathcal{N}_n = \sqrt{\frac{\Gamma(2\gamma+\frac{1}{2})}{n!\Gamma(n+2\gamma+\frac{1}{2})}}, \qquad R_0(\rho) = \sqrt{\frac{2}{\Gamma(2\gamma+\frac{1}{2})}}\rho^\gamma e^{-\frac{\rho}{2}}. \tag{10.33}$$

4. Realization of dynamic group

We now study the dynamic algebra associated to the operators $\hat{\mathcal{L}}_+$ and $\hat{\mathcal{L}}_-$. Based on the results (10.26), (10.27), (10.30) and (10.31), we can calculate the commutator $[\hat{\mathcal{L}}_-, \hat{\mathcal{L}}_+]$:

$$[\hat{\mathcal{L}}_-, \hat{\mathcal{L}}_+] R_n(\rho) = 2l_0 R_n(\rho), \tag{10.34}$$

where we have introduced the eigenvalue

$$l_0 = \left(n + \gamma + \frac{1}{4}\right). \tag{10.35}$$

We can thus define the operator

$$\hat{\mathcal{L}}_0 = \left(\hat{n} + \gamma + \frac{1}{4}\right). \tag{10.36}$$

The operators $\hat{\mathcal{L}}_\pm$ and $\hat{\mathcal{L}}_0$ thus satisfy the commutation relations

$$[\hat{\mathcal{L}}_-, \hat{\mathcal{L}}_+] = 2\hat{\mathcal{L}}_0, \qquad [\hat{\mathcal{L}}_0, \hat{\mathcal{L}}_\pm] = \pm\hat{\mathcal{L}}_\pm, \tag{10.37}$$

which correspond to an su(1, 1) algebra for the radial wave functions.

The Casimir operator can be calculated as

$$CR_n(\rho) = [\hat{\mathcal{L}}_0(\hat{\mathcal{L}}_0 - 1) - \hat{\mathcal{L}}_+\hat{\mathcal{L}}_-]R_n(\rho) = \left(\gamma^2 - \frac{\gamma}{2} - \frac{3}{16}\right)R_n(\rho). \quad (10.38)$$

The hamiltonian H can be written as

$$H|n\rangle = 2\hat{L}_0|n\rangle = (2n + 2\gamma + \frac{1}{2})|n\rangle. \quad (10.39)$$

Likewise, we know that the representation of the dynamic group SU(1, 1) belongs to $D^+(j)$:

$$
\begin{aligned}
&I_0|j, \nu\rangle = \nu|j, \nu\rangle, \\
&I_-|j, \nu\rangle = [(\nu + j)(\nu - j - 1)]^{\frac{1}{2}}|j, \nu - 1\rangle, \\
&I_+|j, \nu - 1\rangle = [(\nu + j)(\nu - j - 1)]^{\frac{1}{2}}|j, \nu\rangle, \\
&\nu = -j + n, \quad n = 0, 1, 2, \ldots, \quad j < 0.
\end{aligned}
\quad (10.40)
$$

In comparison with Eqs. (10.26), (10.27), (10.30), (10.31), (10.35) and (10.36), we have $j = -(\gamma + 1/4)$, $\nu = n + \gamma + 1/4$, and $R_n(\rho) = |j, \nu\rangle$.

On the other hand, one can obtain the following expressions

$$\rho = 2\hat{\mathcal{L}}_0 - \hat{\mathcal{L}}_- - \hat{\mathcal{L}}_+, \quad \rho\frac{d}{d\rho} = \frac{1}{2}\left(\hat{\mathcal{L}}_+ - \hat{\mathcal{L}}_- - \frac{1}{2}\right). \quad (10.41)$$

Their matrix elements can be analytically obtained as

$$
\begin{aligned}
\langle R_m(\rho)|\rho|R_n(\rho)\rangle &\equiv \int_0^\infty R_m(r)r^2 R_n(r)dr \\
&= (2n + 2\gamma + \tfrac{1}{2})\delta_{m,n} \\
&\quad - \sqrt{n(n + 2\gamma - \tfrac{1}{2})}\delta_{m,(n-1)} \\
&\quad - \sqrt{(n + 1)(n + 2\gamma + \tfrac{1}{2})}\delta_{m,(n+1)},
\end{aligned}
\quad (10.42)
$$

and

$$
\begin{aligned}
\langle R_m(\rho)|\rho\tfrac{d}{d\rho}|R_n(\rho)\rangle &\equiv \int_0^\infty R_m(r)\frac{r}{2}\frac{d}{dr}R_n(r)dr \\
&= \tfrac{1}{2}\sqrt{(n + 1)(n + 2\gamma + \tfrac{1}{2})}\delta_{m,(n+1)} \\
&\quad - \tfrac{1}{2}\sqrt{n(n + 2\gamma - \tfrac{1}{2})}\delta_{m,(n-1)} \\
&\quad - \tfrac{1}{4}\delta_{m,n},
\end{aligned}
\quad (10.43)
$$

where the integral range $r \in [0, \infty)$. It should be noted that some results obtained above are essentially different from those in Chapiter 8 since the parameter γ is different from s used there.

5. Concluding remarks

In this Chapter we have studied the eigenvalues and eigenfunctions for the ring-shaped non-spherical oscillator and established the creation and annihilation operators directly from the eigenfunctions (10.18) with the factorization method. We have derived a realization of dynamic group only from physical variable ρ. It is shown that these operators satisfy an SU(1, 1) dynamic group. The representation of the bound states of this quantum system is described by the representation $D^+(j)$ with a spectrum bound below. The matrix elements of the different functions ρ and $\rho \frac{d}{d\rho}$ are also analytically obtained from the ladder operators $\hat{\mathcal{L}}_\pm$ and $\hat{\mathcal{L}}_0$. Before ending this Chapter, we make a remark about another anharmonic oscillator . Due to recent interest of the exact solutions of the Schrödinger equation for non-central potentials such as the non-central electromagnetic, Aharonov-Bohm and magnetic monopole potentials studied by Alhaidari [464–466] and our recently proposed new non-spherical potential [467] composed of the Coulomb potential and the angular-dependent potential $\frac{\cos^2 \theta}{(r \sin \theta)^2}$, we want to introduce another anharmonic oscillator [468], which is expressed as

$$V(r, \theta) = \frac{1}{2}\mu\omega^2 r^2 + \frac{\hbar^2}{2\mu}\frac{\alpha}{r^2} + \frac{\hbar^2}{2\mu}\frac{\beta \cos^2 \theta}{r^2 \sin^2 \theta}, \qquad (10.44)$$

where μ, ω, α and β denote the mass of the particle, the frequency and two dimensionless parameters, respectively.

After careful study, we find that the basic derivation is very similar to that of the ring-shaped non-spherical potential (10.2) discussed above. The detailed information can be found in Ref. [468], in which the ladder operators, dynamic group, the matrix elements of some related physical functions, the general calculation formula and recurrence relation for off-diagonal matrix elements have been investigated.

Chapter 11

GENERALIZED LAGUERRE FUNCTIONS

1. Introduction

It is well known that the factorization method plays an important role in physics. As shown in previous Chapters, we have obtained the ladder operators for some important potentials with the factorization method. Recently, the factorization method has been used to study some special functions [132]. The coherent states for generalized Laguerre functions have been worked out by Jellal, where the Klauder-Perelomov, Gazeau-Klauder and Barut-Girardello coherent states have been studied by using the su(1, 1) algebra [107]. Generally speaking, the exact solutions of the quantum systems with the central physical potentials can be expressed by the associated Laguerre functions as shown in previous some of Chapters. In this Chapter we want to systematically study the dynamic group for the generalized Laguerre functions with our approach since such a study shall be important for studying the quantum systems with the central physical potentials.

The plan of this Chapter is organized as follows. In Section 2 we study the properties of the generalized Laguerre functions. In Section 3 we construct the ladder operators by the factorization method and construct a suitable dynamic group. The matrix elements of some related operators x and $2x\frac{d}{dx}$ are calculated from the ladder operators. The concluding remarks are given in Section 4.

2. Generalized Laguerre functions

We begin with the definition of the generalized Laguerre functions [132]

$$|n\rangle \equiv \Psi_n^\beta(x) = N_n^\beta e^{-x/2} x^{\beta/2} L_n^\beta(x), \tag{11.1}$$

with

$$N_n^\beta = \sqrt{\frac{n!}{(n+\beta)!}}, \tag{11.2}$$

where β is integer.

The generalized Laguerre functions obey the following orthogonal condition

$$\int_0^\infty \Psi_n^\beta(x)\Psi_{n'}^\beta(x)dx = \delta_{nn'}. \tag{11.3}$$

Since the associated Laguerre functions $L_n^\beta(x)$ satisfy the following differential equation (see p. 1064 in [263])

$$x\frac{d^2}{dx^2}L_n^\beta(x) + (\beta+1-x)\frac{d}{dx}L_n^\beta(x) + nL_n^\beta(x) = 0, \tag{11.4}$$

we obtain the differential equation for the generalized Laguerre functions as

$$x\frac{d^2}{dx^2}\Psi_n^\beta(x) + \frac{d}{dx}\Psi_n^\beta(x) + \frac{1}{4}\left(2 + 2\beta - x - \frac{\beta^2}{x}\right)\Psi_n^\beta(x) + n\Psi_n^\beta(x) = 0. \tag{11.5}$$

Furthermore, we recall some recursion relations among the associated Laguerre functions (see p. 1062 in [263]) to be used to construct the ladder operators below

$$(n+1)L_{n+1}^\beta(x) + (n+\beta)L_{n-1}^\beta(x) + (x-2n-\beta-1)L_n^\beta(x) = 0,$$

$$x\frac{d}{dx}L_n^\beta(x) = nL_n^\beta(x) - (n+\beta)L_{n-1}^\beta(x),$$

$$x\frac{d}{dx}L_n^\beta(x) = (n+1)L_{n+1}^\beta(x) - (n+\beta+1-x)L_n^\beta(x). \tag{11.6}$$

By calculating the derivative of the generalized Laguerre functions $\Psi_n^\beta(x)$, we have

$$\frac{d}{dx}\Psi_n^\beta(x) = -\frac{1}{2}\Psi_n^\beta(x) + \frac{\beta}{2x}\Psi_n^\beta(x) + N_n^\beta e^{-x/2}x^{\beta/2}\frac{d}{dx}L_n^\beta(x), \tag{11.7}$$

which, together with Eq. (11.6), allows us to obtain the recursion relation among the generalized Laguerre functions

$$\sqrt{(n+1)(n+\beta+1)}\Psi_{n+1}^\beta + \sqrt{n(n+\beta)}\Psi_{n-1}^\beta = (2n+\beta+1-x)\Psi_n^\beta, \tag{11.8}$$

and

$$\left(-\frac{d}{dx} - \frac{1}{2} + \frac{\beta + 2n}{2x}\right) \Psi_n^\beta(x) = \frac{n+\beta}{x} \frac{N_n^\beta}{N_{n-1}^\beta} \Psi_{n-1}^\beta(x), \tag{11.9}$$

$$\left(\frac{d}{dx} - \frac{1}{2} + \frac{\beta + 2n + 2}{2x}\right) \Psi_n^\beta(x) = \frac{n+1}{x} \frac{N_n^\beta}{N_{n+1}^\beta} \Psi_{n+1}^\beta(x). \tag{11.10}$$

3. Ladder operators and realization of dynamic group SU(1, 1)

We now address how to construct the ladder operators for the generalized Laguerre functions by the factorization method and construct its dynamic group. We intend to find the differential operators $\hat{\mathcal{L}}_\pm$ with the property

$$\hat{\mathcal{L}}_\pm|n\rangle = \ell_\pm|n \pm 1\rangle. \tag{11.11}$$

For convenience we first define the number operator $\hat{n}$

$$\hat{n}|n\rangle = n|n\rangle. \tag{11.12}$$

The creation and annihilation operators $\hat{\mathcal{L}}_\pm$ can be obtained from Eqs. (11.9) and (11.10)

$$\hat{\mathcal{L}}_+ = x\frac{d}{dx} - \frac{x}{2} + \frac{\beta}{2} + \hat{n} + 1, \quad \hat{\mathcal{L}}_- = -x\frac{d}{dx} - \frac{1}{2}x + \frac{\beta}{2} + \hat{n}, \tag{11.13}$$

which satisfy

$$\hat{\mathcal{L}}_+|n\rangle = \ell_+|n+1\rangle = \sqrt{(n+1)(\beta+n+1)}|n+1\rangle,$$
$$\hat{\mathcal{L}}_-|n\rangle = \ell_-|n-1\rangle = \sqrt{n(\beta+n)}|n-1\rangle, \tag{11.14}$$

Obviously, the operator $\hat{\mathcal{L}}_-$ annihilates the ground state

$$|0\rangle = \sqrt{\frac{1}{\beta!}} x^{\beta/2} e^{-x/2}. \tag{11.15}$$

The commutator $[\hat{\mathcal{L}}_-, \hat{\mathcal{L}}_+]$ can be calculated in the basis $|n\rangle$

$$[\hat{\mathcal{L}}_-, \hat{\mathcal{L}}_+]|n\rangle = (2n + \beta + 1)|n\rangle. \tag{11.16}$$

We can thus define the operator $\hat{\mathcal{L}}_0$

$$\hat{\mathcal{L}}_0 = \hat{n} + \frac{\beta + 1}{2}, \tag{11.17}$$

with

$$\hat{\mathcal{L}}_0|n\rangle = \ell_0|n\rangle, \qquad \ell_0 = n + \frac{\beta + 1}{2}. \tag{11.18}$$

It is known that in the spaces spanned by the generalized Laguerre functions $|n\rangle$ the operators $\hat{\mathcal{L}}_\pm$ and $\hat{\mathcal{L}}_0$ satisfy the commutation relations of the su(1, 1) algebra, which is isomorphic to an so(2, 1) algebra:

$$[\hat{\mathcal{L}}_-, \hat{\mathcal{L}}_+] = 2\hat{\mathcal{L}}_0, \qquad [\hat{\mathcal{L}}_0, \hat{\mathcal{L}}_\pm] = \pm\hat{\mathcal{L}}_\pm. \tag{11.19}$$

Similarly, the representation of the dynamic algebra su(1, 1) belongs to $D^+(j)$

$$I_0|j, m\rangle = m|j, m\rangle,$$

$$I_-|j, m\rangle = [(m + j)(m - j - 1)]^{\frac{1}{2}} |j, m - 1\rangle,$$

$$I_+|j, m - 1\rangle = [(m + j)(m - j - 1)]^{\frac{1}{2}} |j, m\rangle, \tag{11.20}$$

$$m = -j + k, \qquad k = 0, 1, 2, \ldots, \qquad j < 0.$$

In comparison with Eqs. (11.14), (11.17) and (11.18) we have $j = -(\beta + 1)/2$, $m = n + (\beta + 1)/2$, and $|n\rangle = |j, m\rangle$.

The Casimir operator can be written as

$$C = \hat{\mathcal{L}}_0(\hat{\mathcal{L}}_0 - 1) - \hat{\mathcal{L}}_+\hat{\mathcal{L}}_-, \tag{11.21}$$

with the property

$$C|n\rangle = \frac{\beta^2 - 1}{4}|n\rangle. \tag{11.22}$$

Finally, we define the Hamiltonian as

$$H|n\rangle = \hat{\mathcal{L}}_+\hat{\mathcal{L}}_-|n\rangle = n(n + \beta)|n\rangle, \tag{11.23}$$

The generalized Laguerre functions can be expressed as

$$|n\rangle = \mathcal{N}_n^\beta \hat{\mathcal{L}}_+^n|0\rangle, \qquad \mathcal{N}_n^\beta = \sqrt{\frac{\beta!}{n!(n + \beta)!}}. \tag{11.24}$$

On the other hand, the following expressions can be easily obtained from the operators $\hat{\mathcal{L}}_\pm$ and $\hat{\mathcal{L}}_0$

$$x = 2\hat{\mathcal{L}}_0 - \hat{\mathcal{L}}_+ - \hat{\mathcal{L}}_-, \qquad 2x\frac{d}{dx} = \hat{\mathcal{L}}_+ - \hat{\mathcal{L}}_- - 1, \qquad (11.25)$$

from which we have

$$
\begin{aligned}
\langle m|x|n\rangle &= -\sqrt{(n+1)(n+\beta+1)}\delta_{m(n+1)} \\
&\quad -\sqrt{n(n+\beta)}\delta_{m(n-1)} \\
&\quad +(2n+\beta+1)\delta_{mn},
\end{aligned}
\qquad (11.26)
$$

and

$$
\begin{aligned}
\left\langle m\left|2x\frac{d}{dx}\right|n\right\rangle &= \sqrt{(n+1)(n+\beta+1)}\delta_{m(n+1)} \\
&\quad -\sqrt{n(n+\beta)}\delta_{m(n-1)} \\
&\quad -\delta_{mn}.
\end{aligned}
\qquad (11.27)
$$

Before ending this section, it is worth emphasizing that Eq. (11.8) can be reexpressed as

$$x|n\rangle = (2\hat{\mathcal{L}}_0 - \hat{\mathcal{L}}_+ - \hat{\mathcal{L}}_-)|n\rangle. \qquad (11.28)$$

4. Concluding remarks

In this Chapter we have established the creation and annihilation operators $\hat{\mathcal{L}}_\pm$ for the generalized Laguerre functions by the factorization method. It is shown that these operators $\hat{\mathcal{L}}_\pm$ and $\hat{\mathcal{L}}_0$ satisfy the commutation relations of an su(1, 1) algebra. The matrix elements of some operators x and $2x\frac{d}{dx}$ can be analytically calculated from these operators. Before ending this Chapter, we want to give a remark here. Generally speaking, the exact solutions of the Schrödinger equation with the central physical potentials can be expressed by the confluent hypergeometric functions or associated Laguerre functions, the dynamic group of such a quantum system will have the SU(1, 1) symmetry.

Chapter 12

NEW NONCENTRAL RING-SHAPED POTENTIAL

1. Introduction

The Hartmann potential [469] is a kind of noncentral physical potential, which is realized by adding a potential proportional to $(r \sin \theta)^{-2}$ to a Coulomb potential. In spherical coordinates, the Hartmann potential is defined by

$$V_q = \eta \sigma^2 \left(\frac{2a_0}{r} - q\eta \frac{a_o^2}{r^2 \sin^2 \theta} \right) \epsilon_0, \qquad (12.1)$$

where $a_0 = \hbar^2/me^2$ and $\epsilon_0 = -me^4/2\hbar^2$ represent the Bohr radius and the ground state energy of hydrogen atom, respectively, and η, σ, q are three dimensionless parameters. It should be pointed out that the parameter is taken as unit by Hartmann [469]. The introduction of the parameter q makes it possible to obtain the Coulomb-like potential by taking $q = 0$ and $\eta \sigma^2 = Z$ in Eq. (12.1).

Due to its possible applications to ring-shaped organic molecules like cyclic polyenes and benzene, many papers have been devoted to this potential since 1972 [469–489]. For example, the energy levels have been derived by standard analytical method [469]. The diamagnetic susceptibility of the ground state of this system and the spin-orbit coupling for the motion of a particle in the Hartmann potential have been studied [470, 471]. The contributions mentioned above have been realized by solving the Schrödinger equation through separating the variables both in spherical coordinates and in the parabolic ones. In addition to this standard approach, other methods to investigate this quantum system are the path integral approach [472–474], the nonbijective canonical transformation one [475], the SUSY quantum mechanics and the shape invariance method [476–479], the group theoretical method [475, 481–486], etc.

Based on these methods, the Green's function [482, 483], the accidental degeneracy and the hidden symmetry of this potential, the overlap coefficients [486] for two ring-shaped potentials have been studied. Recently, the properties of bound and continuous states as well as the recurrence relations among the matrix elements have been worked out by Chen *et al.* [487–489]. Additionally, some other interesting investigations related to the noncentral ring-shaped potentials have been carried out [464, 467, 490].

Recently, the ring-shaped non-spherical oscillator potential, which is composed of three terms–the harmonic oscillator term, the ring–shaped inverse square one and the dipole-like interaction term, has been discussed in our previous work [463, 491, 492]. Therefore, we want to propose another new ring-shaped non-spherical oscillator where the ring-shaped inverse square term is replaced by a new term $\beta(\cos^2\theta/r^2\sin^2\theta)$, which is expressed as [493]

$$V(r,\theta) = -\frac{\alpha}{r} + \frac{\sigma}{r^2} + \beta\frac{\cos^2\theta}{r^2\sin^2\theta}. \tag{12.2}$$

The purposes of this Chapter are the following. First, we study the exact bound state solutions and establish the ladder operators. In addition, we present the recurrence relations among diagonal matrix elements and some explicit expressions of mean values of r^k. Second, we study the exact solutions of continuous states and make some comments on the calculation formula of phase shifts and the analytical properties of scattering amplitude.

This Chapter is organized as follows. In Section 2 we present the eigenvalues and eigenfunctions of bound states. We construct the ladder operators directly from the radial wave functions in Section 3. We obtain two important recurrence relations and some explicit expressions of mean values of r^k in Section 4. In Section 5 we study the exact solutions of continuous states and make some comments on the calculation formula of phase shifts and analytical properties of scattering amplitude. Some concluding remarks are given in Section 6.

2.   Bound states

In spherical coordinates the Schrödinger equation with this new model potential (12.2) can be written as ($\hbar = \mu = e = 1$)

$$\left[-\frac{1}{2}\nabla^2 + V(r,\theta) - E\right]\Psi(r,\theta,\phi) = 0. \tag{12.3}$$

For a spherical potential, one may separate the wave functions as follows

$$\Psi(r,\theta,\phi) = \frac{1}{\sqrt{2\pi}}\frac{u(r)}{r}H(\theta)e^{\pm im\phi}, \quad m = 0, 1, 2, \ldots. \tag{12.4}$$

Substitution of this into Eq. (12.3) leads to a set of second order differential equations

$$\frac{d^2 u(r)}{dr^2} + \left(2E + \frac{2\alpha}{r} - \frac{\lambda + 2\sigma}{r^2}\right) u(r) = 0, \qquad (12.5)$$

$$\frac{1}{\sin \theta} \frac{d}{d\theta}\left[\sin \theta \frac{dH(\theta)}{d\theta}\right] + \left(\lambda - \frac{2\beta \cos^2 \theta + m^2}{\sin^2 \theta}\right) H(\theta) = 0, \qquad (12.6)$$

where λ is a separation constant. The boundary conditions for Eq. (12.5) require $u(0) = 0$ and the square-integrability of u on $(0, \infty)$, which implies that $u(\infty) = 0$ for the bound states. However, the boundary conditions for Eq. (12.6) require that $H(0)$ and $H(\pi)$ are taken as finite values. Let us study the exact solutions of Eqs. (12.5) and (12.6) below.

Take

$$m' = \sqrt{2\beta + m^2}, \qquad \lambda + 2\beta = l'(l' + 1), \qquad x = \cos \theta. \qquad (12.7)$$

Substitution of Eq. (12.7) into Eq. (12.6) allows us to obtain the following universal associated-Legendre differential equation [487–489]

$$(1 - x^2)\frac{d^2 H(x)}{dx^2} - 2x\frac{dH(x)}{dx} + \left[l'(l' + 1) - \frac{(m')^2}{1 - x^2}\right] H(x) = 0, \quad (12.8)$$

whose boundary condition is that $H|_{x=\pm 1}$ is finite and equal to a linear combination of the boundary values for Eq. (12.6). When l' and m' are positive integers or zero, equation (12.8) reduces to the usual associated Legendre differential equation. The solutions of Eq. (12.8) are given by

$$
\begin{aligned}
H_{l'm'}(\theta) &= \sqrt{\frac{(2l' + 1)}{2} \frac{(l' - m')!}{\Gamma(l' + m' + 1)}}(\sin \theta)^{m'} \\
&\quad \cdot \sum_{k=0}^{\left[\frac{l'-m'}{2}\right]} \frac{(-1)^k \Gamma(2l' - 2k + 1)}{2^{l'} k! (l' - m' - 2k)! \Gamma(l' - k + 1)}(\cos \theta)^{l'-m'-2k},
\end{aligned}
$$
$$(12.9)$$

where the relation between l' and m' is given by $l' = m' + k, k = 0, 1, 2, ...$

We now turn to study Eq. (12.5). Substitution of Eq. (12.7) and $l' = k + m'$ into Eq. (12.5) leads to

$$\frac{d^2 u(r)}{dr^2} + \left(2E + \frac{2\alpha}{r} - \frac{L(L + 1)}{r^2}\right) u(r) = 0, \qquad (12.10)$$

with

$$L \equiv \frac{1}{2}\left\{\sqrt{1 + 4\left[(m' + k)(m' + k + 1) + 2(\sigma - \beta)\right]} - 1\right\}, \qquad (12.11)$$

where m' is given in (12.7) and $m, k = 0, 1, 2, \ldots$.

We first discuss the bound states $E < 0$. By defining

$$\rho = \sqrt{-8E}r, \qquad \tau = \frac{\alpha}{\sqrt{-2E}}, \tag{12.12}$$

we may rearrange Eq. (12.10) as

$$\frac{d^2 u(\rho)}{d\rho^2} + \left[\frac{\tau}{\rho} - \frac{1}{4} - \frac{L(L+1)}{\rho^2}\right] u(\rho) = 0. \tag{12.13}$$

If we take the wave functions with the form

$$u(\rho) = \rho^{L+1} e^{-\rho/2} f(\rho), \tag{12.14}$$

then substitution of this into Eq. (12.13) yields

$$\rho \frac{d^2 f(\rho)}{d\rho^2} + [2(L+1) - \rho]\frac{df(\rho)}{d\rho} + [\tau - (L+1)]f(\rho) = 0, \tag{12.15}$$

whose solutions are confluent hypergeometric functions $F(L+1-\tau, 2L+2; \rho)$.

For the bound states, however, only the polynomial solutions are acceptable, which requires

$$L + 1 - \tau = -n_r, \qquad n_r = 0, 1, 2, \ldots. \tag{12.16}$$

From Eqs. (12.12) and (12.16), we are able to obtain the eigenvalues

$$E = -\frac{\alpha^2}{2(n_r + L + 1)^2} = -\frac{\alpha^2}{2(n')^2} \tag{12.17}$$

where

$$\begin{aligned}
n' &= n_r + L + 1 \\
&= \tfrac{1}{2}\left\{2n + 1 + \sqrt{1 + 4[(m'+k)(m'+k+1) + 2(\sigma - \beta)]}\right\}
\end{aligned} \tag{12.18}$$

and $m, k, n_r = 0, 1, 2, \ldots$.

When $n_r = \tau - L - 1$ is a non-negative integer, by using (8.10) we may obtain the corresponding radial eigenfunctions as

$$u_{n'L}(r) = N_{n'}^L \left(\frac{2\alpha r}{n'}\right)^{L+1} e^{-\alpha r/n'} L_{n_r}^{2L+1}(2\alpha r/n'), \tag{12.19}$$

where $N_{n'}^L$ is the normalization constant to be determined below. By using the recurrence relation among the generalized Laguerre polynomials [263]

$$(n+1)L_{n+1}^\alpha(z) + (z - \alpha - 2n - 1)L_n^\alpha(z) + (\alpha + n)L_{n-1}^\alpha(z) = 0 \tag{12.20}$$

and the orthogonality relation of the generalized Laguerre polynomials (8.11), we have

$$N_{n'}^L = \sqrt{\frac{\alpha n_r!}{(n')^2 \Gamma(n' + L + 1)}}.$$

(12.21)

Thus, we may express the normalized radial wave functions as

$$u_{n'L}(\rho) = \sqrt{\frac{\alpha(n' - L - 1)!}{(n')^2 \Gamma(n' + L + 1)}} \rho^{L+1} e^{-\rho/2} L_{n'-L-1}^{2L+1}(\rho), \quad \rho = \frac{2\alpha r}{n'},$$

(12.22)

where L and n' are given in Eqs. (12.11) and (12.18), respectively.

3. Ladder operators

We now study the ladder operators for the wave functions with the factorization method. Generally speaking, we may use the creation and annihilation operators for the generalized Laguerre polynomials to obtain what appear to be the creation and annihilation operators for the radial wave functions $u_{n'L}(\rho)$, but what makes us discouraged is we find that the variable ρ depends on n' as shown in Eq. (12.22). In this case, we have to apply the creation operator to $u_{n'L}(\rho)$ to obtain

$$\hat{M}_{n'}^+ u_{n'L}(\rho_{n'}) = \hat{C}_{n'L} u_{(n'+1)L}(\rho_{n'}) \neq C_{n'L} u_{(n'+1)L}(\rho_{(n'+1)}),$$

(12.23)

which implies that we must apply a shift operator to change $\rho_{n'}$ to $\rho_{(n'+1)}$. Such a deep problem has been discussed by Aebersold *et al.* [494].

To this end, we begin by establishing the action of the differential operator $d/d\rho$ on the radial wave functions $u_{n'L}(\rho)$:

$$\frac{d}{d\rho} u_{n'L}(\rho) = \left(\frac{L+1}{\rho} - \frac{1}{2}\right) u_{n'L}(\rho) + N_{n'}^L \rho^{L+1} e^{-\rho/2} \frac{d}{d\rho} L_{n'-L-1}^{2L+1}(\rho).$$

(12.24)

If considering the derivative of the associated Laguerre functions (6.18) given in [263], then we may obtain the following result by substituting this into Eq. (12.24)

$$\left(-\frac{d}{d\rho} + \frac{L+1}{\rho} - \frac{n'}{2L+2}\right) u_{n'L}(\rho) = \frac{1}{2L+2} \frac{N_{n'}^L}{N_{n'}^{L+1}} u_{n'(L+1)}(\rho)$$

(12.25)

from which we may define

$$\hat{M}_L^+ = -\frac{d}{d\rho} + \frac{L+1}{\rho} - \frac{n'}{2L+2}$$

(12.26)

with the following effect over the radial wave functions

$$\hat{M}_L^+ u_{n'L}(\rho) = \frac{1}{2L+2}\sqrt{\frac{(n'-L-1)\Gamma(n'+L+2)}{\Gamma(n'+L+1)}}u_{n'(L+1)}(\rho). \quad (12.27)$$

We now proceed to find the corresponding annihilation operator. First, we need to obtain the relation between $(d/d\rho)L_n^\alpha(\rho)$ and $L_{n+1}^{\alpha-2}(\rho)$, which suggests the relation between $(d/d\rho)u_{n'L}(\rho)$ and the radial wave functions $u_{n'(L-1)}(\rho)$. The derivation procedure is similar to that of the Morse potential. Substituting Eq. (6.33) into Eq. (12.24), we have

$$\left(\frac{d}{d\rho} + \frac{L}{\rho} - \frac{n'}{2L}\right)u_{n'L}(\rho) = \frac{(n'-L)(n'+L)}{2L}\frac{N_{n'}^L}{N_{n'}^{L-1}}u_{n'(L-1)}(\rho), \quad (12.28)$$

from which we may define

$$\hat{M}_L^- = \frac{d}{d\rho} + \frac{L}{\rho} - \frac{n'}{2L} \quad (12.29)$$

with the following effect over the radial wave functions

$$\hat{M}_L^- u_{n'L}(\rho) = \frac{n'+L}{2L}\sqrt{\frac{(n'-L)\Gamma(n'+L)}{\Gamma(n'+L+1)}}u_{n'(L-1)}(\rho). \quad (12.30)$$

Let us study the limit of the potential parameters $\beta = 0$ and $\sigma = 0$. If so, we have $n' = n$ and $L = l$. Thus, we may obtain the following simple expressions

$$\hat{M}_l^+ = -\frac{d}{d\rho} + \frac{l+1}{\rho} - \frac{n}{2l+2}, \quad (12.31)$$

$$\hat{M}_l^+ u_{nl}(\rho) = \frac{1}{2l+2}\sqrt{(n-l-1)(n+l+1)}u_{n(l+1)}(\rho), \quad (12.32)$$

and

$$\hat{M}_l^- = \frac{d}{d\rho} + \frac{l}{\rho} - \frac{n}{2l}, \quad (12.33)$$

$$\hat{M}_l^- u_{nl}(\rho) = \frac{1}{2l}\sqrt{(n-l)(n+l)}u_{n(l-1)}(\rho). \quad (12.34)$$

Essentially, these results coincide with those given by Nieto [495].

4.   Mean values

In this section we study the mean values of r^k, which can be calculated directly from the wave functions (12.22), i.e.

$$\langle n'L|r^k|n'L\rangle = (N_{n'}^L)^2\left(\frac{n'}{2\alpha}\right)^{1+k}\int_0^\infty \rho^{2+2L+k}e^{-\rho}[L_{n'-L-1}^{2L+1}(\rho)]^2 d\rho. \quad (12.35)$$

Before proceeding to do so, we first recall an important Coulomb-like integral given by Nieto in 1979 [495]

$$
\begin{aligned}
J_{n,\alpha}^{\beta} &= \int_0^\infty x^{\alpha+\beta} e^{-x} [L_n^\alpha(x)]^2 dx \\
&= \frac{\Gamma(1+n+\alpha)}{\Gamma(n+1)} \sum_{k=0}^n (-1)^k \frac{\Gamma(n-k-\beta)}{\Gamma(-k-\beta)} \\
&\quad \times \frac{\Gamma(1+\alpha+k+\beta)}{\Gamma(1+k+\beta)} \frac{1}{k!\Gamma(1+n-k)}
\end{aligned}
\tag{12.36}
$$

with $\Re e(1+\alpha+\beta) > 0$. Substitution of this into Eq. (12.35) allows us to obtain

$$
\begin{aligned}
\langle n'L|r^k|n'L\rangle &= \left(\frac{n'}{2\alpha}\right)^{1+k} \frac{\alpha}{(n')^2} \sum_{j=0}^{n'-L-1} (-1)^j \frac{\Gamma(n'-L-j-k-2)}{\Gamma(-k-1-j)} \\
&\quad \times \frac{\Gamma(2L+k+3+j)}{\Gamma(2L+2+j)} \frac{1}{j!\Gamma(n'-L-j)}.
\end{aligned}
\tag{12.37}
$$

Nevertheless, we find that this formula is not practical to calculate the mean values of r^k. In this case we choose another approach to derive them analytically as shown in [487–489]. That is, based on the recurrence relations among the diagonal matrix elements, we may obtain the mean values of r^k analytically. Using the similar technique to Refs. [487–489], we only present two important recurrence relations and some explicit expressions of mean values $\langle n'L|r^k|n'L\rangle$. The two recurrence relations are given by

$$
\langle n'L|r^k|n'L\rangle = \frac{\Gamma(2L+k+3)}{\Gamma(2L-k)} \left(\frac{n'}{2\alpha}\right)^{2k+3} \langle n'L|r^{-k-3}|n'L\rangle, \tag{12.38}
$$

and

$$
\begin{aligned}
\left(\frac{\alpha}{n'}\right)^2 \langle n'L|r^k|n'L\rangle &= \frac{\alpha(1+2k)}{1+k} \langle n'L|r^{k-1}|n'L\rangle \\
&\quad - \frac{k[(1+2L)^2-k^2]}{4(1+k)} \langle n'L|r^{k-2}|n'L\rangle,
\end{aligned}
\tag{12.39}
$$

from which, together with normalization relation $\langle n'L|n'L\rangle = 1$, we may obtain all mean values of r^k. For example, we present some explicit results since these formulas are, sometimes, useful in various branches of physics such

as quantum mechanics and molecular physics, i.e.,

$$
\begin{aligned}
\langle n'L|r^6|n'L\rangle \; &= \frac{(n')^6}{16\alpha^6}\{429(n')^6 - 231[-10 + 3L(1 + L)](n')^4 \\
&\quad +[2121 + 315L(1 + L)(L^2 + L - 7)](n')^2 \\
&\quad +180 - 7L(1 + L)[126 + 5L(1 + L)(L^2 + L - 11)]\},
\end{aligned}
\tag{12.40}
$$

$$
\begin{aligned}
\langle n'L|r^5|n'L\rangle \; &= \frac{(n')^4}{16\alpha^5}\{231(n')^6 - 105[-7 + 3L(L + 1)](n')^4 \\
&\quad +21[14 + 5L(L + 1)(L^2 + L - 5)](n')^2 \\
&\quad -5(L - 2)(L - 1)L(L + 1)(L + 2)(L + 3)\},
\end{aligned}
\tag{12.41}
$$

$$
\begin{aligned}
\langle n'L|r^4|n'L\rangle \; &= \frac{(n')^4}{8\alpha^4}\{63(n')^4 + [105 - 70L(1 + L)](n')^2 \\
&\quad +12 + 5L(1 + L)(3L(L + 1) - 10)\},
\end{aligned}
\tag{12.42}
$$

$$
\begin{aligned}
\langle n'L|r^3|n'L\rangle \; &= \frac{(n')^2}{8\alpha^3}\{35(n')^4 - [30L(L + 1) - 25](n')^2 \\
&\quad +3(L - 1)L(L + 1)(L + 2)\},
\end{aligned}
\tag{12.43}
$$

$$
\langle n'L|r^2|n'L\rangle = \frac{(n')^2}{2\alpha^2}[5(n')^2 - 3L(L + 1) + 1],
\tag{12.44}
$$

$$
\langle n'L|r|n'L\rangle = \frac{3(n')^2 - L(L + 1)}{2\alpha},
\tag{12.45}
$$

$$
\langle n'L|r^{-1}|n'L\rangle = \frac{\alpha}{(n')^2},
\tag{12.46}
$$

$$
\langle n'L|r^{-2}|n'L\rangle = \frac{2\alpha^2}{(n')^3(1 + 2L)},
\tag{12.47}
$$

$$
\langle n'L|r^{-3}|n'L\rangle = \left(\frac{2\alpha}{n'}\right)^3 \frac{1}{2L(2L + 1)(2L + 2)},
\tag{12.48}
$$

$$
\langle n'L|r^{-4}|n'L\rangle = \frac{16\alpha^4}{(n')^5}\frac{\Gamma(2L - 1)}{\Gamma(2L + 4)}[3(n')^2 - L(L + 1)],
\tag{12.49}
$$

$$
\langle n'L|r^{-5}|n'L\rangle = \frac{64\alpha^5}{(n')^5}\frac{\Gamma(2L - 2)}{\Gamma(2L + 5)}[5(n')^2 - 3L(L + 1) + 1],
\tag{12.50}
$$

$$
\begin{aligned}
\langle n'L|r^{-6}|n'L\rangle \; &= \frac{64\alpha^6}{(n')^7}\frac{\Gamma(2L - 3)}{\Gamma(2L + 6)}\{35(n')^4 \\
&\quad -[30L(L + 1) - 25](n')^2 \\
&\quad +3(L - 1)L(L + 1)(L + 2)\},
\end{aligned}
\tag{12.51}
$$

$$\langle n'L|r^{-7}|n'L\rangle = \frac{256\alpha^7}{(n')^7}\frac{\Gamma(2L-4)}{\Gamma(2L+7)}[63(n')^4$$
$$+[105-70L(L+1)](n')^2 \qquad (12.52)$$
$$+12+5L(L+1)(-10+3L(L+1))],$$

$$\langle n'L|r^{-8}|n'L\rangle = \frac{512\alpha^8}{(n')^9}\frac{\Gamma(2L-5)}{\Gamma(2L+8)}[231(n')^6$$
$$-105[-7+3L(L+1)](n')^4 \qquad (12.53)$$
$$+21[14+5L(L+1)(L^2+L-5)](n')^2$$
$$-5(L-2)(L-1)L(L+1)(L+2)(L+3)\}.$$

In principle, we may obtain all mean values of r^k. However, the calculations for large k become very complicated. We do not show them for simplicity.

5. Continuum states

As we know, this new model potential is a non-central field, but it is independent of the angle ϕ. Therefore, the solutions of the Schrödinger equation for the continuum states must be axially symmetric about the z-axis, i.e. along with the direction of the incident particle. In other words, the continuum states can be discussed by the partial-wave method.

For continuum states $E > 0$, we take $k = \sqrt{2E} > 0$. Thus, we may modify Eq. (12.10) as

$$\frac{d^2u(r)}{dr^2} + \left(k^2 + \frac{2\alpha}{r} - \frac{L(L+1)}{r^2}\right)u(r) = 0, \qquad (12.54)$$

whose boundary condition is $u(0) = 0$. Substituting

$$u(r) = A(kr)^{L+1}e^{ikr}f(r) \qquad (12.55)$$

into Eq. (12.54), we have

$$r\frac{d^2f(r)}{dr^2} + (2L+2+2ikr)\frac{df(r)}{dr} + [2ik(L+1)+2\alpha]f(r) = 0. \quad (12.56)$$

Introducing a new variable $z = -2ikr$, we may rearrange above equation as

$$z\frac{d^2f(z)}{dz^2} + (2L+2-z)\frac{df(z)}{dz} - [L+1-\frac{i\alpha}{k}]f(z) = 0, \qquad (12.57)$$

whose analytical solutions are the confluent hypergeometric functions $f(r) = F(L+1-i\alpha/k, 2L+2, -2ikr)$ as $r \to 0$. Thus, the radial wave functions of the continuum states are expressed as

$$u(r) = A_{kL}(kr)^{L+1}e^{ikr}F(L+1-i\alpha/k, 2L+2; -2ikr). \qquad (12.58)$$

Let us study its asymptotic form for large r and calculate the normalization constant A_{kL} and the phase shifts δ'_l.

The asymptotic expression of the confluent hypergeometric functions is given by [263]

$$F(\lambda, \gamma; z) \to \frac{\Gamma(\gamma)}{\Gamma(\lambda)} e^z z^{\lambda-\gamma} + \frac{\Gamma(\gamma)}{\Gamma(\gamma - \lambda)} e^{\pm i\pi\lambda} z^{-\lambda}, \quad |z| \to \infty, \quad (12.59)$$

where "+" and "−" correspond to $-\pi/2 < \arg z < 3\pi/2$ and $-3\pi/2 < \arg z < \pi/2$, respectively. When $z = -2ikr = |z|e^{-i\pi/2}$, equation (12.59) is then reexpressed as

$$F(\lambda, \gamma; z) \to \frac{\Gamma(\gamma)}{\Gamma(\lambda)} e^z |z|^{\lambda-\gamma} e^{-i\pi(\lambda-\gamma)/2} + \frac{\Gamma(\gamma)}{\Gamma(\gamma - \lambda)} e^{-i\pi\lambda/2} |z|^{-\lambda}. \quad (12.60)$$

from which, we have for $r \to \infty$

$$\begin{aligned}
F(L + 1 - i\alpha/k, 2L + 2; -2ikr) \; &\to \; \frac{\Gamma(2L + 2)}{\Gamma(L + 1 - i\alpha/k)} e^{-2ikr} \\
&\quad (2kr)^{-(L+1+i\alpha/k)} e^{i\pi(L+1+i\alpha/k)/2} \\
&\quad + \frac{\Gamma(2L + 2)}{\Gamma(L + 1 + i\alpha/k)} e^{-i\pi(L+1-i\alpha/k)/2} \\
&\quad (2kr)^{-(L+1-i\alpha/k)}.
\end{aligned} \quad (12.61)$$

Let $\Gamma(L + 1 - i\alpha/k) = |\Gamma(L + 1 - i\alpha/k)|e^{i\delta_L}$, then $\Gamma(L + 1 + i\alpha/k) = |\Gamma(L + 1 - i\alpha/k)|e^{-i\delta_L}$, where δ_L is a real number. Thus, equation (12.61) becomes

$$\begin{aligned}
F(L + 1 - i\alpha/k, 2L + 2; -2ikr) \; &\to \; \frac{\Gamma(2L + 2)e^{-\pi\alpha/2k}e^{-ikr}}{|\Gamma(L + 1 - i\alpha/k)|(2kr)^{L+1}} \\
&\quad \times \Big[ie^{-i[kr+\delta_L-\pi L/2+\alpha(\ln 2kr)/k]} \\
&\quad - ie^{i[kr+\delta_L-\pi L/2+\alpha(\ln 2kr)/k]} \Big].
\end{aligned} \quad (12.62)$$

Substituting Eq. (12.62) into Eq. (12.58) leads to

$$u_{kL}(r) \to \frac{A_{kL}\Gamma(2L + 2)e^{-\pi\alpha/2k}}{|\Gamma(L + 1 - i\alpha/k)|2^{L+1}} 2\sin[kr + \delta_L - \pi L/2 + \alpha(\ln 2kr)/k]. \quad (12.63)$$

In contract, from the asymptotic behavior of the continuum states for the Coulomb potential

$$u_{kl}(r) \to 2\sin[kr + \delta_l - \pi l/2 + Z(\ln 2kr)/k], \qquad (12.64)$$

we know from Ref. [297] that these radial wave functions are normalized on the $k/2\pi$ scale. Because the new model potential (12.2) is the Coulomb potential surrounded by an inverse square potential plus a ring-shaped inverse square potential, which is a short range potential, the asymptotic expression of the wave functions for large r will not be affected by the additional contribution of the inverse square potential plus the ring-shaped inverse square potential. In other words, the asymptotic expression of the new model potential is equal to that of the Coulomb potential, i.e.

$$u_{kL}(r) \to 2\sin[kr + \delta'_l - \pi l/2 + \alpha(\ln 2kr)/k], \qquad (12.65)$$

where δ'_l represents the phase shifts. The wave functions of the continuum states for the new model potential are also normalized on the $k/2\pi$ scale. In comparison Eq. (12.63) with Eq. (12.65), we may obtain the normalization constant of the continuum states as

$$A_{kL} = \frac{2^{L+1}|\Gamma(L+1-i\alpha/k)|e^{\pi\alpha/2k}}{\Gamma(2L+2)}, \qquad (12.66)$$

and the phase shifts δ'_l as

$$\delta'_l = \delta_L + \pi(l-L)/2 = \arg\Gamma(L+1-i\alpha/k) + \pi(l-L)/2. \qquad (12.67)$$

If substituting Eq. (12.66) into (12.58), we obtain the normalized wave functions of the continuum states on the $k/2\pi$ scale as

$$\begin{aligned} u(r) \quad &= \frac{2^{L+1}|\Gamma(L+1-i\alpha/k)|e^{\pi\alpha/2k}}{\Gamma(2L+2)}(kr)^{L+1} \\ &\times e^{ikr}F(L+1-i\alpha/k, 2L+2; -2ikr). \end{aligned} \qquad (12.68)$$

Before ending this part, let us study the analytical properties of the scattering amplitude, i.e. we discuss the analytical properties of the scattering amplitude in the whole complex k plane by regarding the scattering amplitude as a function of the energy. From the general theory of the partial-wave method, the scattering amplitude is defined by

$$f(\theta) = \sum_{l=0}^{\infty}(2l+1)\left[\frac{e^{2i\delta'_l}-1}{2ik}\right]P_l(\cos(\theta)), \qquad (12.69)$$

where l is the angular quantum number. To this end, from Eqs. (12.67) and (12.69), we discuss the analytical properties of the $\Gamma(L + 1 - i\alpha/k)$. From the definition of the Gamma function

$$\Gamma(z) = \frac{\Gamma(z+1)}{z} = \frac{\Gamma(z+2)}{z(z+1)} = \cdots, \qquad (12.70)$$

we know that $z = 0, -1, -2, \ldots$, are the first order poles of the $\Gamma(z)$, namely, the first order poles of $\Gamma(L + 1 - i\alpha/k)$ are situated at

$$L + 1 - i\alpha/k = 0, -1, -2, \ldots = -n_r, \qquad n_r = 0, 1, 2, \ldots. \quad (12.71)$$

At the poles of scattering amplitude, the corresponding energy levels given by

$$E = \frac{k^2}{2} = -\frac{\alpha^2}{2(n_r + L + 1)^2} = -\frac{\alpha^2}{2(n')^2}, \quad n' = n_r + L + 1, \quad (12.72)$$

are nothing but the eigenvalues of the bound states. Similarly, the radial wave functions in the scattering states also reduce to those of the bound states.

6.   Concluding remarks

In this Chapter we have proposed a new exactly solvable non-central ring-shaped potential (12.2) and studied the quantum characteristics of bound and continuum states. For bound states, we have presented the normalized radial wave functions and energy eigenvalues explicitly. The shifted operators for the radial wave functions are derived. We have presented two useful recurrence relations and some explicit expressions of mean values of r^k. For the continuum states, however, we have derived the normalized radial wave functions on the $k/2\pi$ scale, the calculation formula of the phase shifts and the analytical properties of the scattering amplitude. Interestingly, we have found that the energy levels and the radial wave functions of the continuum states will reduce to those of the bound states at the poles of the scattering amplitude. Before ending this Chapter, we give some remarks here. First, it is possible to study the general calculation formula for the non-diagonal matrix elements and recurrence relation among them. Second, the recent contributions made by Kibler and co-workers are relevant to the present study since they have also considered the effect of the ring-shaped term. For example, they have investigated the generalized Aharonov-Bohm plus Coulomb and oscillator systems [496, 497], the generalized oscillator and Kepler-Coulomb systems [497–500] and the classical trajectories for two ring-shaped potentials [501]. Third, the formula (12.69) for the scattering amplitude in a potential dominated at large r by the Coulomb part is a non-trivial result. The derivation in spherical coordinates has been worked out by Lin and Mott [502, 503].

Chapter 13

PÖSCHL-TELLER LIKE POTENTIAL

1.   Introduction

As shown in several previous Chapters, we have used the factorization method to establish the ladder operators for some well-known physical potentials and constructed their suitable Lie algebras. With the same spirit, we want to study the PT like potential in this Chapter.

This Chapter is organized as follows. In Section 2 we study the exact solutions of this system. Section 3 is devoted to constructing the ladder operators directly from the eigenfunctions with the factorization method. The analytical matrix elements of the different functions $\sin \rho$ and $\cos \rho \frac{d}{d\rho}$ are obtained from these operators. The infinite square well and harmonic limits are to be studied in Section 4. The concluding remarks are given in Section 5.

2.   Exact solutions

In this section we study the exact solutions of the Schrödinger equation with the PT like potential. It should be mentioned that this PT-like potential is different from the traditional MPT potential $V(x) = -D/\cosh^2(\alpha x)$, which has been studied algebraically in our work [106]. However, the PT-like potential to be studied in this Chapter is taken as [504]

$$V(x) = V_0 \tan^2 \left(\frac{\pi x}{L} \right), \qquad x \in [-L/2, L/2], \qquad (13.1)$$

where V_0 and L are two constants.

We now study the eigenfunctions and eigenvalues of this system, which are necessary for constructing the ladder operators. The Schrödinger equation

associated to the PT-like potential (13.1) can be expressed as

$$-\frac{\hbar^2}{2m}\frac{d^2\Psi(x)}{dx^2} + V_0 \tan^2\left(\frac{\pi x}{L}\right)\Psi(x) = E\Psi(x), \tag{13.2}$$

where m is the mass of the particle. Its solutions satisfy the boundary conditions

$$\Psi(\pm L/2) = 0. \tag{13.3}$$

Before proceeding further, it is convenient to introduce the following dimensionless variable and constants

$$\rho = \frac{\pi x}{L}, \quad V = \frac{2mL^2}{\pi^2\hbar^2}V_0, \quad \epsilon = \frac{2mL^2}{\pi^2\hbar^2}(E + V_0). \tag{13.4}$$

Substitution of them into Eq. (13.2) leads to

$$\frac{d^2\Psi(\rho)}{d\rho^2} + \left(\epsilon - \frac{V}{\cos^2(\rho)}\right)\Psi(\rho) = 0. \tag{13.5}$$

Let us take the following ansatz for the wave functions[1]

$$\Psi_n(\rho) = P_n(t)\cos^\lambda\rho, \quad \lambda > 0 \tag{13.6}$$

with the notation

$$t = \sin\rho. \tag{13.7}$$

Substitution of Eq. (13.6) into Eq. (13.5) allows us to write down

$$(1 - t^2)\frac{d^2P_n}{dt^2} - t(1 + 2\lambda)\frac{dP_n}{dt} + (\epsilon - \lambda^2)P_n = 0, \tag{13.8}$$

with

$$V = \lambda(\lambda - 1), \quad \lambda \neq 0, 1. \tag{13.9}$$

From the known differential equation for the Gegenbauer polynomials (see 8. 938 of Ref. [263])

$$\frac{d^2y}{dt^2} + \frac{t(1 + 2\lambda)}{t^2 - 1}\frac{dy}{dt} - \frac{n(2\lambda + n)}{t^2 - 1}y = 0, \tag{13.10}$$

it is found that the solutions of Eq. (13.8) are nothing but the Gegenbauer polynomials $C_n^\lambda(t)$. We can thus obtain the eigenfunctions as

$$\Psi_n(\rho) = N_n C_n^\lambda(\sin\rho)\cos^\lambda\rho, \tag{13.11}$$

where the normalization constant N_n to be determined below. On the other hand, it is shown from Eqs. (13.8) and (13.10) that the eigenvalues of this quantum system can be obtained as

$$\epsilon_n = (n + \lambda)^2, \qquad n = 0, 1, 2, 3, ..., \tag{13.12}$$

which can be reexpressed as

$$E_n = \frac{\pi^2 \hbar^2}{2mL^2}(n^2 + 2n\lambda + \lambda). \tag{13.13}$$

We now calculate the normalization factor N_n. From the normalization condition

$$\int_{-\frac{L}{2}}^{\frac{L}{2}} |\Psi_n(x)|^2 dx = 1, \tag{13.14}$$

we can obtain N_n. Before doing so, we recall an important formula (see 7. 313 of Ref. [263])

$$\int_{-1}^{1} (1-x^2)^{\nu-\frac{1}{2}} [C_n^\nu(x)]^2 dx = \frac{\pi 2^{(1-2\nu)} \Gamma(n+2\nu)}{n!(n+\nu)[\Gamma(\nu)]^2}, \quad [\Re e\, \nu > -\frac{1}{2}], \tag{13.15}$$

which is used to calculate the normalization constant N_n. In the calculation, we use the definition $t = \sin(\rho)$ and obtain finally

$$N_n = \sqrt{\frac{n!(n+\lambda)[\Gamma(\lambda)]^2}{L2^{(1-2\lambda)}\Gamma(n+2\lambda)}}. \tag{13.16}$$

3.   Ladder operators

We now construct the creation and annihilation operators for the wave functions (13.11) with the factorization method. In a similar way, we intend to find differential operators $\hat{\mathcal{L}}_\pm$ with the following property

$$\hat{\mathcal{L}}_\pm \Psi_n(\rho) = \ell_\pm \Psi_{n\pm 1}(\rho). \tag{13.17}$$

Specifically, we look for operators of the form

$$\hat{\mathcal{L}}_\pm = A_\pm(\rho)\frac{d}{d\rho} + B_\pm(\rho). \tag{13.18}$$

To this end we begin by applying the differential operator $\frac{d}{d\rho}$ on the wave functions (13.11)

$$\frac{d}{d\rho}\Psi_n(\rho) = N_n \left[\cos^\lambda \rho \frac{d}{d\rho}C_n^\lambda(\sin \rho) - \lambda \sin \rho C_n^\lambda(\sin \rho) \cos^{\lambda-1} \rho\right]. \tag{13.19}$$

One possible relation for the first derivative of the associated Laguerre functions is given by (see 8. 939 of Ref. [263])

$$(1 - t^2)\frac{d}{dt}C_n^\lambda(t) = (n + 2\lambda - 1)C_{n-1}^\lambda(t) - n\, t\, C_n^\lambda(t). \tag{13.20}$$

The substitution of this into (13.19) enables us to obtain the following relation

$$\left[\frac{d}{d\rho} + \frac{\sin\rho(n+\lambda)}{\cos\rho}\right]\Psi_n(\rho) = \frac{n + 2\lambda - 1}{\cos\rho}\frac{N_n}{N_{n-1}}\Psi_{n-1}(\rho). \tag{13.21}$$

Making use of Eq. (13.16) and introducing the number operator $\hat{n}$ with the property

$$\hat{n}\Psi_n(\rho) = n\Psi_n(\rho), \tag{13.22}$$

we can define the following operator

$$\hat{\mathcal{L}}_- = \left[\cos\rho\frac{d}{d\rho} + \sin\rho(\hat{n} + \lambda)\right]\sqrt{\frac{\hat{n} + \lambda - 1}{\hat{n} + 2\lambda - 1}}, \tag{13.23}$$

with the following effect over the wave functions

$$\hat{\mathcal{L}}_-\Psi_n(\rho) = \ell_-\Psi_{n-1}(\rho), \tag{13.24}$$

where

$$\ell_- = \sqrt{n(n+\lambda)}. \tag{13.25}$$

As we can see, this operator annihilates the ground state $\Psi_0(\rho)$, as expected from a step-down operator.

We now proceed to find the corresponding creation operator. Before proceeding to do so, we use another relation between the Gegenbauer polynomials (see 8. 939 of Ref. [263])

$$(1 - t^2)\frac{d}{dt}C_n^\lambda(t) = (n + 2\lambda)\, t\, C_n^\lambda(t) - (1 + n)C_{n+1}^\lambda(t). \tag{13.26}$$

Substitution of this expression into Eq. (13.19) allows us to obtain

$$\left[\frac{d}{d\rho} - \frac{\sin\rho(n+\lambda)}{\cos\rho}\right]\Psi_n(\rho) = -\frac{(n+1)}{\cos\rho}\frac{N_n}{N_{n+1}}\Psi_{n+1}(\rho). \tag{13.27}$$

Using Eq. (13.16) again, we can define the following operator

$$\hat{\mathcal{L}}_+ = \left[-\cos\rho\frac{d}{d\rho} + \sin\rho(\hat{n} + \lambda)\right]\frac{1 + \hat{n} + \lambda}{\sqrt{(\hat{n} + \lambda)(\hat{n} + 2\lambda)}}, \tag{13.28}$$

satisfying the relation

$$\hat{\mathcal{L}}_+\Psi_n(\rho) = \ell_+\Psi_{n+1}(\rho), \tag{13.29}$$

with

$$\ell_+ = \sqrt{(n+1)(n + \lambda + 1)}. \tag{13.30}$$

4.   Realization of dynamic group and matrix elements

We now study the algebra associated to the operators $\hat{\mathcal{L}}_+$ and $\hat{\mathcal{L}}_-$. Based on the results (13.24), (13.25), (13.29) and (13.30), we can calculate the commutator $[\hat{\mathcal{L}}_-, \hat{\mathcal{L}}_+]$:

$$[\hat{\mathcal{L}}_-, \hat{\mathcal{L}}_+]\Psi_n(\rho) = 2\ell_0\Psi_n(\rho), \tag{13.31}$$

where we have introduced the eigenvalue

$$\ell_0 = \left(n + \frac{\lambda + 1}{2}\right). \tag{13.32}$$

We can thus define the operator

$$\hat{\mathcal{L}}_0 = \left(\hat{n} + \frac{\lambda + 1}{2}\right). \tag{13.33}$$

The operators $\hat{\mathcal{L}}_\pm$ and $\hat{\mathcal{L}}_0$ thus satisfy the commutation relations

$$[\hat{\mathcal{L}}_-, \hat{\mathcal{L}}_+] = 2\hat{\mathcal{L}}_0, \qquad [\hat{\mathcal{L}}_0, \hat{\mathcal{L}}_\pm] = \pm\hat{\mathcal{L}}_\pm, \tag{13.34}$$

which correspond to an su(1, 1) algebra for the wave functions.

The Casimir operator can be calculated as

$$C\Psi_n(\rho) = [\hat{\mathcal{L}}_0(\hat{\mathcal{L}}_0 - 1) - \hat{\mathcal{L}}_+\hat{\mathcal{L}}_-]\Psi_n(\rho) = \frac{\lambda^2 - 1}{4}\Psi_n(\rho). \tag{13.35}$$

Likewise, it is known from Ref. [169] that the representation of the dynamic algebra su(1, 1) belongs to $D^+(j)$:

$$\begin{aligned}
I_0|j, \nu\rangle &= \nu|j, \nu\rangle, \\
I_-|j, \nu\rangle &= [(\nu + j)(\nu - j - 1)]^{\frac{1}{2}} |j, \nu - 1\rangle, \\
I_+|j, \nu - 1\rangle &= [(\nu + j)(\nu - j - 1)]^{\frac{1}{2}} |j, \nu\rangle, \\
\nu &= -j + n, \quad n = 0, 1, 2, \ldots, \quad j < 0.
\end{aligned} \tag{13.36}$$

In comparison with Eqs. (13.29), (13.30), (13.24), (13.25), (13.32) and (13.33), we have $j = -(\lambda + 1)/2$, $\nu = n + (\lambda + 1)/2$, and $\Psi_n(\rho) = |j, \nu\rangle$.

In addition, we find that the Hamiltonian can be written as

$$H = \frac{\pi^2\hbar^2}{2mL^2}\left(\hat{\mathcal{L}}_+\hat{\mathcal{L}}_- + \lambda\hat{\mathcal{L}}_0 - \frac{\lambda(\lambda - 1)}{2}\right). \tag{13.37}$$

On the other hand, the following expressions in terms of the creation and annihilation operators $\hat{\mathcal{L}}_{\pm}$ can be obtained

$$\sin\rho = \frac{1}{2(\hat{n}+\lambda)}\left[\hat{\mathcal{L}}_{-}\sqrt{\frac{\hat{n}+2\lambda-1}{\hat{n}+\lambda-1}}+\hat{\mathcal{L}}_{+}\sqrt{\frac{(\hat{n}+\lambda)(\hat{n}+2\lambda)}{(\hat{n}+\lambda+1)(\hat{n}+\lambda+1)}}\right],$$

$$\tag{13.38}$$

$$\cos\rho\frac{d}{d\rho} = \frac{1}{2}\left[\hat{\mathcal{L}}_{-}\sqrt{\frac{\hat{n}+2\lambda-1}{\hat{n}+\lambda-1}}-\hat{\mathcal{L}}_{+}\sqrt{\frac{(\hat{n}+\lambda)(\hat{n}+2\lambda)}{(\hat{n}+\lambda+1)(\hat{n}+\lambda+1)}}\right].$$

$$\tag{13.39}$$

Their matrix elements can be analytically obtained as follows:

$$\begin{aligned}\langle\Psi_m(\rho)|\sin\rho|\Psi_n(\rho)\rangle &= \frac{1}{2}\sqrt{\frac{n(n+2\lambda-1)}{(n+\lambda)(n+\lambda-1)}}\delta_{m,n-1}\\&+\frac{1}{2}\sqrt{\frac{(n+1)(n+2\lambda)}{(n+\lambda)(n+\lambda+1)}}\delta_{m,n+1},\end{aligned}\tag{13.40}$$

and

$$\begin{aligned}\left\langle\Psi_m(\rho)\left|\cos\rho\frac{d}{d\rho}\right|\Psi_n(\rho)\right\rangle &= \frac{1}{2}\sqrt{\frac{n(n+\lambda)(n+2\lambda-1)}{n+\lambda-1}}\delta_{m,n-1}\\&-\frac{1}{2}\sqrt{\frac{(n+1)(n+\lambda)(n+2\lambda)}{n+\lambda+1}}\delta_{m,n+1}.\end{aligned}\tag{13.41}$$

5. Infinitely square well and harmonic limits

In this section we want to study two limits of this potential. First, we investigate the infinitely square well limit. For $V_0 \to 0$, if leaving fixed L and the mass m, then we have $\lambda \simeq 0$. Thus, we obtain the eigenvalues as

$$E_n = \frac{\pi^2\hbar^2}{2mL^2}n^2, \quad n = 1, 2, \ldots.\tag{13.42}$$

On the other hand, it is shown from Eqs. (13.23), (13.28) and (13.33) that the operators $\hat{\mathcal{L}}_{\pm}$ and $\hat{\mathcal{L}}_0$ reduce to those of the infinitely symmetric square well potential (5.27), (5.28) and (5.29), respectively.

Now, let us study the harmonic limit of this potential. If performing a series expansion of the trigonometric function $\tan(\pi x/L)$ up to the first term, in the

harmonic limit $L \to \infty$ and $V \to \infty$ ($\lambda \to \infty$), but keeping the product $k = 2V_0\pi^2/L^2$ finite, then we have

$$\lim_{\lambda\to\infty} V(x) = \frac{1}{2}kx^2. \tag{13.43}$$

If introducing the renormalization operators [105]

$$b^\dagger = \frac{\hat{\mathcal{L}}_+}{\sqrt{\lambda}}, \quad b = \frac{\hat{\mathcal{L}}_-}{\sqrt{\lambda}}, \quad b_0 = \frac{2\hat{\mathcal{L}}_0}{\lambda}, \tag{13.44}$$

then we find that the operators $b^\dagger$ and b acting on the eigenstates Ψ_n have the following properties

$$
\begin{aligned}
b^\dagger\Psi_n(\rho) &= \sqrt{(n+1)\left(1 + \frac{n+1}{\lambda}\right)}\,\Psi_{n+1}(\rho), \\
b\Psi_n(\rho) &= \sqrt{n\left(1 + \frac{n}{\lambda}\right)}\,\Psi_{n-1}(\rho).
\end{aligned}
\tag{13.45}
$$

In order to obtain the energy levels in the harmonic limit, it is necessary to introduce the frequency of the harmonic oscillator

$$\omega = \sqrt{\frac{2\pi^2 V_0}{mL^2}}, \tag{13.46}$$

from which, together with Eqs. (13.4) and (13.9), we have

$$\lambda = \frac{1}{2} + \frac{m\omega L^2}{\hbar\pi^2}. \tag{13.47}$$

After tedious calculation, we can finally obtain the energy levels in this limit

$$E_n = \hbar\omega\left(n + \frac{1}{2}\right). \tag{13.48}$$

On the other hand, according to $L \to \infty$ ($\lambda \to \infty$) and the following expressions

$$\cos z = 1 - \frac{z^2}{2!} + \frac{z^4}{4!} + \mathcal{O}(z^6), \quad \sin z = z - \frac{z^3}{3!} + \mathcal{O}(z^5), \tag{13.49}$$

and

$$\frac{d}{d\rho} = \frac{L}{\pi}\frac{d}{dx}, \quad \sqrt{\lambda} \simeq \frac{L}{\pi}\sqrt{\frac{m\omega}{\hbar}}, \tag{13.50}$$

we have from Eqs. (13.28), (13.23) and (13.33)

$$\lim_{\lambda \to \infty} b^\dagger = \sqrt{\frac{m\omega}{2\hbar}}x - \sqrt{\frac{\hbar}{2m\omega}}\frac{d}{dx} = a^\dagger, \qquad (13.51)$$

$$\lim_{\lambda \to \infty} b = \sqrt{\frac{m\omega}{2\hbar}}x + \sqrt{\frac{\hbar}{2m\omega}}\frac{d}{dx} = a, \qquad (13.52)$$

$$\lim_{\lambda \to \infty} b_0 = 1. \qquad (13.53)$$

The operators $a^\dagger$ and a satisfy the bosonic commutation relations $[a, a^\dagger] = 1$; $[a, a] = [a^\dagger, a^\dagger] = 0$, as expected. On the other hand, it is found from Eq. (13.45) that the operators $b^\dagger$ and b are nothing but $a^\dagger$ and a when $\lambda \to \infty$.

6.   Concluding remarks

In this Chapter we have studied the eigenvalues and eigenfunctions for the PT-like potential and established the creation and annihilation operators directly from the eigenfunctions (13.11) with the factorization method. We have derived a realization of dynamic group only in terms of the physical variable ρ. It is shown that these operators satisfy an SU(1, 1) dynamic group. The representation of the bound states of this quantum system is described by the representation $D^+(j)$ with a spectrum bound below. The matrix elements of the different functions $\sin \rho$ and $\cos \rho \frac{d}{d\rho}$ are also analytically obtained from the ladder operators $\hat{\mathcal{L}}_\pm$. The infinitely square well and the harmonic oscillator limits are obtained. We find that the eigenvalues of this quantum system reduce to those of the infinitely deep square well potential and the harmonic oscillator.

Notes

1   It should be noted that the structure (13.6) ensures that the boundary conditions are satisfied and there are no zeros for $\rho \in [-\pi/2, \pi/2]$.

Chapter 14

POSITION-DEPENDENT MASS SCHRÖDINGER EQUATION FOR A SINGULAR OSCILLATOR

1. Introduction

It is well known that the effective mass is a constant in the traditional Schrödinger equation. Recently, the study of the Schrödinger equation with the position-dependent effective mass has attracted a lot of attention [275, 276, 388, 505–532]. This is because such systems have found wide applications in various fields like the study of electronic properties of the semiconductors [509], ^{3}He clusters [510], quantum wells, wires and dots [275, 276, 511], quantum liquids [513], the graded alloys and semiconductor heterostructures [514], etc.

On the other hand, the algebraic method has become the subject of the interest in physics. Systems displaying a dynamical symmetry can be treated by algebraic techniques. Up to now, this method has played an important role in the study of wave equations with a constant mass. Nevertheless, it has also been used to study the position-dependent effective mass Schrödinger equation [533, 534]. Motivated by recent work by Roy [534], we are going to explore the possibility of using Lie algebraic method [535] to study the position-dependent mass Schrödinger equation for a singular oscillator.

This Chapter is organized as follows. In Section 2 we study some basic properties of the Schrödinger equation with position-dependent effective mass. The harmonic oscillator case is briefly studied. Section 3 is devoted to constructing a singular oscillator hamiltonian and realizing the dynamic group SU(1, 1) for this system. The complete solutions of this system are obtained in Section 4. Finally, some concluding remarks are given in Section 5.

2.   Position-dependent effective mass Schrödinger equation for harmonic oscillator

Let us consider the position-dependent mass Schrödinger equation given by ($\hbar = 1$) [275, 276, 388, 523, 524, 527, 530]

$$\left[-\frac{d}{dx}\left(\frac{1}{2m(x)}\frac{d}{dx} \right) + V(x) \right]\phi(x) = E\phi(x), \tag{14.1}$$

which satisfies the following boundary condition

$$\frac{1}{m(x)}\frac{1}{\phi(x)}\frac{d\phi(x)}{dx}\bigg|_{-} = \frac{1}{m(x)}\frac{1}{\phi(x)}\frac{d\phi(x)}{dx}\bigg|_{+}. \tag{14.2}$$

This means that the boundary condition should be continuous at the mass discontinuity and at the interface.

In order to determine the effective-mass singular oscillator potential we begin by studying the harmonic oscillator within this formalism. For this purpose, we are able to factorize Eq. (14.1) as follows:

$$\begin{aligned} \mathcal{A}\phi(x) &= \frac{1}{\sqrt{2m(x)}}\frac{d}{dx}\phi(x) + W(x)\phi(x), \\ \mathcal{A}^{\dagger}\phi(x) &= -\frac{d}{dx}\left(\frac{1}{\sqrt{2m(x)}}\phi(x) \right) + W(x)\phi(x), \end{aligned} \tag{14.3}$$

where the $W(x)$ is to be determined below. From the point of view of SUSY, we may construct the following two isospectral Hamiltonians as

$$\hat{H}_1 = \mathcal{A}^{\dagger}\mathcal{A} = p(m) - \left(\frac{W(x)}{\sqrt{2m(x)}} \right)' + W(x)^2, \tag{14.4}$$

$$\begin{aligned} \hat{H}_2 &= \mathcal{A}\,\mathcal{A}^{\dagger} \\ &= p(m) - \left(\frac{W(x)}{\sqrt{2m(x)}} \right)' + W(x)^2 \\ &\quad + \frac{2W(x)'}{\sqrt{2m(x)}} - \frac{1}{\sqrt{2m(x)}}\left(\frac{1}{\sqrt{2m(x)}} \right)'', \end{aligned} \tag{14.5}$$

where

$$p(m) = -\frac{1}{2m(x)}\frac{d^2}{dx^2} - \left(\frac{1}{2m(x)} \right)'\frac{d}{dx} \tag{14.6}$$

and the prime denotes the first derivative with respect to variable x. It is shown from Eqs. (14.4) and (14.5) that

$$[\mathcal{A}, \mathcal{A}^{\dagger}] = \frac{2W(x)'}{\sqrt{2m(x)}} - \frac{1}{\sqrt{2m(x)}}\left(\frac{1}{2m(x)} \right)'', \tag{14.7}$$

from which, together with the commutation relation of harmonic oscillator $[\mathcal{A}, \mathcal{A}^\dagger] = 1$, we obtain the following equation

$$2W(x)' = \left(\frac{1}{\sqrt{2m(x)}}\right)'' + \sqrt{2m(x)}. \qquad (14.8)$$

This can be integrated to give $W(x)$

$$2W(x) = \left(\frac{1}{\sqrt{2m(x)}}\right)' + \int^x \sqrt{2m(y)}dy. \qquad (14.9)$$

Thus, the exact solutions of $\hat{H}_1$ and $\hat{H}_2$ are essentially those of the constant-mass harmonic oscillator.

3. Singular oscillator with a position-dependent effective mass

As shown above, it is clear that the effective-mass potentials depend on the mass function $m(x)$. In order to determine the explicit form of the singular oscillator potential we have to make a choice of effective mass. We take a modified position-dependent effective mass [536]

$$m(x) = \frac{1}{\tau^\alpha(x+a)^\alpha}, \qquad (14.10)$$

where τ, α and a are three constants. When $\alpha = 0$, the mass $m(x)$ becomes a constant. Thus, we may obtain $W(x)$ as

$$W(x) = \sqrt{\frac{1}{(a+x)^\alpha \tau^\alpha}} \frac{-8(a+x)^2 + (a+x)^\alpha (-2+\alpha) \alpha \tau^\alpha}{4\sqrt{2}(a+x)(-2+\alpha)}. \qquad (14.11)$$

In order to determine the form of the effective-mass singular oscillator we now consider the Hamiltonian

$$\hat{H} = \mathcal{A}^\dagger \mathcal{A} + R(x) + \frac{1}{2} \qquad (14.12)$$

and define two operators as

$$b = \mathcal{A}^2 - R(x), \quad b^\dagger = (\mathcal{A}^\dagger)^2 - R(x), \qquad (14.13)$$

where $R(x)$ is to be determined below.

If we consider the commutation relations of the su(1, 1) Lie algebra

$$[\hat{H}, b] = -2b, \quad [\hat{H}, b^\dagger] = 2b^\dagger, \quad [b, b^\dagger] = 4\hat{H}, \qquad (14.14)$$

then, by using Eqs. (4.26), (14.3) and (14.14) as well as the following useful results

$$[\mathcal{A}, R(x)] = \frac{1}{\sqrt{2m(x)}} R(x)', \quad [\mathcal{A}^\dagger, R(x)] = -\frac{1}{\sqrt{2m(x)}} R(x)', \quad (14.15)$$

$$\mathcal{A} + \mathcal{A}^\dagger = 2W(x) - \left(\frac{1}{\sqrt{2m(x)}}\right)' = \int^x \sqrt{2m(y)} dy, \quad (14.16)$$

we are able to obtain a unified differential equation for $R(x)$

$$2R(x) = -\frac{1}{\sqrt{2m(x)}} R(x)' \int^x \sqrt{2m(y)} dy, \quad (14.17)$$

from which, if considering Eq. (14.10), we have

$$R(x) = c(a + x)^{\alpha - 2}, \quad (14.18)$$

where c is an integral constant. Thus, the complete potential appearing in Eq. (14.1) can be calculated by using the following formula

$$V(x) = -\left(\frac{W(x)}{\sqrt{2m(x)}}\right)' + W(x)^2 + R(x) + \frac{1}{2} \quad (14.19)$$

as

$$V(x) = c(a + x)^{-2+\alpha} + \frac{2(a + x)^{2-\alpha}}{(-2 + \alpha)^2 \tau^\alpha} - \frac{(a + x)^{-2+\alpha} \alpha(-4 + 3\alpha) \tau^\alpha}{32}. \quad (14.20)$$

We make a few useful comments about this potential. For example, when $a = 0$ and $\alpha = 0$ it turns to an isotonic harmonic oscillator with a constant mass, i.e., $V(x) = c\frac{1}{x^2} + \frac{x^2}{2}$. If $a = 0$ and $\alpha = 4/3$, it yields an isotonic-like singular oscillator with a position-dependent mass, i.e., $V(x) = c\frac{1}{x^{2/3}} + \frac{x^{2/3}}{27\tau^{4/3}}$. When $c = 0$ and $\alpha = 0$, the potential $V(x)$ corresponds to a constant-mass harmonic oscillator.

Let us briefly study special case $\alpha = 2$. If so, the present mass $m(x)$ reduces to the case of Ref. [536]. The corresponding $W(x)$, $R(x)$ and $V(x)$ are given by

$$W(x) = \frac{1}{2\sqrt{2\tau}}[\tau^2 + 2\ln(a + x)], \quad (14.21)$$

$$R(x) = c[\ln(a + x)]^{-2}, \quad (14.22)$$

$$V(x) = \frac{c}{\ln(a + x)^2} + \frac{1}{8}\left\{\frac{[\tau^2 + 2\ln(a + x)]^2}{\tau^2} - 2[\tau^2 + 2\ln(a + x)]\right\}, \quad (14.23)$$

with $a + x > 0$. It should be pointed out that the present potential $V(x)$, however, cannot reduce to the constant-mass harmonic oscillator since $m(x)$ for $\alpha = 2$ is not a constant.

4. Complete solutions

We now proceed to determine the energy levels of the singular oscillator $V(x)$ and the corresponding eigenfunctions using the su$(1, 1)$ algebra. For this purpose, we first note that if ϕ_0 denotes the ground state then

$$b\phi_0 = 0, \tag{14.24}$$

from which, together with Eq. (14.13), we have

$$
\begin{aligned}
& \left[-c\,(a + x)^{\alpha - 2} - \frac{1}{\alpha - 2} + \frac{2\,(a + x)^{2 - \alpha}}{(\alpha - 2)^2\,\tau^\alpha} \right] \phi(x) \\
& + \left[\frac{(a + x)^{\alpha - 2}\,\alpha\,(-4 + 3\,\alpha)\,\tau^\alpha}{32} \right] \phi(x) \\
& + \left[\frac{-2\,(a + x)}{\alpha - 2} + \frac{(a + x)^{\alpha - 1}\,\alpha\,\tau^\alpha}{2} \right] \phi'(x) + \frac{(a + x)^\alpha\,\tau^\alpha}{2}\phi''(x) = 0,
\end{aligned}
\tag{14.25}
$$

whose solution is exactly obtained as

$$
\phi_0(y) = N_0 e^{-\frac{2\,y^{2 - \alpha}}{(-2 + \alpha)^2\,\tau^\alpha}} y^{\frac{1}{4}\left[2 - 2\,\alpha + \tau^{-\frac{\alpha}{2}}\sqrt{32\,c + (-2 + \alpha)^2\,\tau^\alpha} \right]},
\tag{14.26}
$$

where $y = a + x$. The corresponding ground state energy can be obtained from the relation

$$\hat{H}\phi_0 = E_0\phi_0 \tag{14.27}$$

as

$$E_0 = \frac{1}{2} + \sigma, \tag{14.28}$$

with

$$\sigma = \frac{1}{2} + \frac{1}{2(2 - \alpha)}\tau^{-\alpha/2}\sqrt{32c + (\alpha - 2)^2\tau^\alpha}. \tag{14.29}$$

The Casimir operator as an important quantity can be calculated as

$$C = L_1^2 + L_2^2 - L_0^2 = \kappa(1 - \kappa) = \frac{3 - 4\sigma(\sigma - 1)}{16}, \tag{14.30}$$

where

$$L_0 = \frac{1}{2}\hat{H}, \quad L_1 = -\frac{1}{4}(b + b^\dagger), \quad L_2 = \frac{i}{4}(b - b^\dagger). \tag{14.31}$$

Consequently, the value $\kappa = \frac{1}{2}(\frac{1}{2} + \sigma)$ characterizes the discrete irreducible unitary representation $D^+(\kappa)$ of the group SU(1, 1).

We now study the eigenfunctions and eigenvalues of this system for the potential $V(y)$. Using the communication relations (14.14), we are able to obtain the following results

$$
\begin{aligned}
b^\dagger \phi_n &= 2\sqrt{(n+1)(n+\sigma+1/2)}\phi_{n+1}, \\
b\phi_n &= 2\sqrt{n(n+\sigma-1/2)}\phi_{n-1}.
\end{aligned}
\tag{14.32}
$$

The excited state eigenfunctions can be obtained by repeated application of the operator $b^\dagger$ on the ground state

$$
\phi_n = \sqrt{\frac{\Gamma(\sigma+1/2)}{2^{2n}n!\Gamma(\sigma+n+1/2)}}(b^\dagger)^n \phi_0,
\tag{14.33}
$$

while the corresponding eigenvalues are given by

$$
E_n = 2n + \sigma + 1/2, \quad n = 0, 1, 2, 3, \dots.
\tag{14.34}
$$

Before ending this part let us briefly consider the harmonic-oscillator potential. In this case, we take $c = 0$ and obtain from Eq. (14.20)

$$
V(x) = \frac{2(a+x)^{2-\alpha}}{(-2+\alpha)^2\tau^\alpha} - \frac{(a+x)^{-2+\alpha}\alpha(-4+3\alpha)\tau^\alpha}{32}.
\tag{14.35}
$$

Thus, the symmetry operators become $b = a^2$ and $b^\dagger = (a^\dagger)^2$. The corresponding Hamiltonian is $\hat{H} = a^\dagger a + 1/2$. Thus, the operators $b, b^\dagger$ and $\hat{H}$ also construct the same Lie algebra su(1, 1). In this case, due to Eq. (14.29) and $c = 0$ the admissible values of σ are taken as 0 and 1, and κ are given by $1/4$ and $3/4$. The ground state energies in these two sectors are given by

$$
E_0^+ = \frac{1}{2}, \quad E_0^- = \frac{3}{2},
\tag{14.36}
$$

while the corresponding eigenfunctions are given by

$$
\phi_0^+ \sim e^{-\dfrac{2y^{2-\alpha}}{(-2+\alpha)^2\tau^\alpha}}y^{-\alpha/4}, \quad \text{for } \sigma = 0,
\tag{14.37}
$$

$$
\phi_0^+ \sim e^{-\dfrac{2y^{2-\alpha}}{(-2+\alpha)^2\tau^\alpha}}y^{1-3\alpha/4} \quad \text{for } \sigma = 1.
\tag{14.38}
$$

5. Another position-dependent effective mass

In this section we briefly mention another position-dependent effective mass and its algebraic realization as shown by Roy [534]. For this effective mass, it is taken as

$$m(x) = \left(\frac{\beta + x^2}{1 + x^2}\right)^2, \tag{14.39}$$

so that $m(x)$ becomes a constant for $\beta = 1$.

By using the similar procedure to that studied above, we may obtain the corresponding $R(x)$ and $V(x)$[1] as follows:

$$R(x) = \frac{k^2}{f^2}, \tag{14.40}$$

$$V(x) = \frac{1}{2}f^2 - \frac{1-\beta}{2(\beta + x^2)^4}[2x^4 + 2(2-\beta)x^2 - \beta] + R(x),$$

where $k \in [0, \infty)$ is an integral constant and $f(x)$ is defined as

$$f \equiv f(x) = x + (\beta - 1)\arctan x. \tag{14.41}$$

Similarly, we may obtain the ground state as [534]

$$\psi_0(x) = \sqrt{\frac{2}{\Gamma(\tau + 1/2)}}\left(\frac{\beta + x^2}{1 + x^2}\right)f^\tau \exp[-\frac{1}{2}f^2], \tag{14.42}$$

where

$$\tau = \frac{1}{2} + \sqrt{1/4 + 2k^2}. \tag{14.43}$$

The corresponding $b^\dagger$ and b have the same properties as those (14.32), which are a little different from those given in Ref. [534] except for the sign "-" appearing in the front of the number 2.

On the other hand, by using the transformations of the operators, the exact solutions of the quantum system are given by [534]

$$\psi_n(x) = \sqrt{\frac{2n!}{\Gamma(n + \tau + 1/2)}}\sqrt{f'}f^\tau \exp[-\frac{1}{2}f^2]L_n^{\tau - 1/2}(f^2), \quad n = 1, 2, 3, \ldots, \tag{14.44}$$

where f' denotes differentiation with respect to x. The corresponding eigenvalues are given by

$$E_n = 2n + \tau + \frac{1}{2}. \tag{14.45}$$

6.   Concluding remarks

In this Chapter we have used Lie algebraic technique to study a singular-oscillator system within the framework of the effective-mass Schrödinger equation. We find that an su(1, 1) Lie algebra is the hidden symmetry of this quantum system. In particular, we have found that this dynamic group is independent of the position-dependent effective mass $m(x)$ that we choose. For the different mass $m(x)$ we shall obtain a potential isospectral with Eq. (14.20). Also, we have employed the properties of the Lie algebra su(1, 1) to obtain the eigenfunctions and eigenvalues completely. On the other hand, we have briefly studied another effective mass (14.39) and sketched their exact solutions. It should be noted that the exact solutions can also be obtained by acting the creation operator on the ground state as shown in Eq. (14.33).

Notes

1   In the calculation, the condition $\beta + x^2 \geq 0$ has to be used. Otherwise, $R(x)$ and $V(x)$ cannot be obtained correctly [534].

PART IV

APPLICATIONS IN RELATIVISTIC QUANTUM MECHANICS

Chapter 15

SUSYQM AND SWKB APPROACH TO THE DIRAC EQUATION WITH A COULOMB POTENTIAL IN 2+1 DIMENSIONS

1. Introduction

The exact solutions of quantum systems play an important role in quantum mechanics. For example, the exact solutions of the Schrödinger equation for a hydrogen atom and for a harmonic oscillator in three dimensions [11, 215, 297, 537] were important achievements at the beginning stage of quantum mechanics, which provided a strong evidence in favor of the theory being correct. In the comprehensive paper [538], Kolsrud fully exploited Hylleraas' approach [539–543] to propose two different methods to study the bound and continuous states of the Dirac equation with a Coulomb potential. On the other hand, Waldenstrøm [544, 545] directly solved the single second-order radial differential equation, which was derived by Dirac himself [546], where the same technique employed for solving the Schrödinger equation with a Coulomb potential was used. The relativistic Dirac-oscillator potential introduced in Refs. [547, 548] has been studied by adding an off-diagonal linear radial term to the Dirac operator.

Recently, the Schrödinger equation with the Coulomb and oscillator problems in arbitrary dimensions have been studied [549, 550]. On the other hand, due to recent interest in the lower-dimensional field theory and condensed matter physics, the two-dimensional case, which seems physically relevant, has been investigated. With this spirit, the study of quantum scattering theory of the relativistic particle by the Coulomb field has been discussed in two dimensions [551–556]. In addition, some papers are devoted to the studies of the non-relativistic equation with the Coulomb potential in one dimension [557–560] and in two dimensions [561–566] as well as those of the relativistic equation in one dimension [567]. The Dirac equation with the Coulomb potential in two dimensions was investigated by the series methods [568, 569]. The Dirac

equation with the Coulomb potential was solved in three dimensions [570–572]. On the other hand, we have studied the scattering theory of the Dirac equation with the Coulomb plus the scalar potential in two dimensions [573]. Similar problems have also been generalized to arbitrary dimensional case [453, 455, 456, 574]. In addition, the Klein-Gordon equation with the Coulomb-like potential has been studied in two dimensions [575]. It is worth pointing out that the Coulomb-like potential in almost all of contributions mentioned above and others [576, 577], including the present Chapter, takes the form "$1/r$". Even though the real Coulomb-like potential in two dimensions is taken as a logarithmic form "$\ln r$", its exact solutions have not been obtained yet except for the approximate solutions [578].

The purposes of this Chapter are as follows. First, we study the exact solutions of the Dirac equation with the Coulomb potential by power series expansion method. Second, we employ the SUSYQM and SWKB approaches to study this problem. Third, we choose an alternative method to derive the eigenfunctions of this system by using a recently proposed MATHEMATICA package INTEPFFLL.

The plan of this Chapter is organized as follows. Section 2 is devoted to the derivation of eigenfunctions and eigenvalues of the (2+1)-dimensional Dirac equation with the Coulomb potential. The study of this quantum system by the SUSYQM and SWKB approaches is carried out in Section 3. An alternative method to derive the eigenfunctions of this system is presented in Section 4. Some concluding remarks are given finally in Section 5.

2.   Dirac equation in 2 +1 dimensions

We now consider the $(2 + 1)$-dimensional Dirac equation

$$\sum_{\mu=0}^{2} i\gamma^{\mu}(\partial_{\mu} + ieA_{\mu})\Psi = M\Psi, \tag{15.1}$$

where M is the mass of the particle, and

$$\gamma^{0} = \sigma_3, \qquad \gamma^{1} = i\sigma_1, \qquad \gamma^{2} = i\sigma_2. \tag{15.2}$$

Let us consider the special case where only the zero component of A_{μ} is non-vanishing and cylindrically symmetric:

$$A_1 = A_2 = 0, \qquad eA_0 = V(r) = -\frac{Z\alpha}{r} = -\frac{\xi}{r}. \tag{15.3}$$

Let

$$\Psi_{jE}(t, \mathbf{r}) = \frac{1}{\sqrt{2\pi}} e^{-iEt} r^{-1/2} \begin{pmatrix} F_{jE}(r)e^{i(j-1/2)\varphi} \\ G_{jE}(r)e^{i(j+1/2)\varphi} \end{pmatrix}, \tag{15.4}$$

where j denotes the total angular momentum , $j = \pm 1/2, \pm 3/2, \ldots$. It is shown that the radial components $F_{jE}(r)$ and $G_{jE}(r)$ satisfy the following set of first-order coupled differential equations

$$\frac{d}{dr}G_{jE}(r) + \frac{j}{r}G_{jE}(r) = [E - V(r) - M]F_{jE}(r), \qquad (15.5)$$

$$-\frac{d}{dr}F_{jE}(r) + \frac{j}{r}F_{jE}(r) = [E - V(r) + M]G_{jE}(r). \qquad (15.6)$$

From the Sturm-Liouville theorem [579], for a small attractive potential a bound state may appear at the energy E less than and near M, and for a small repulsive potential, a bound state may appear at the energy E larger than and near $-M$. In fact, Eqs. (15.5) and (15.6) keep invariant in the transformations $j \leftrightarrow -j$, $E \leftrightarrow -E$, $V \leftrightarrow -V$, and $F_{jE}(r) \leftrightarrow G_{-j-E}(r)$. Therefore, we only need to discuss the attractive potential with $\xi > 0$.

3. Exact solutions

We now study the eigenvalues and eigenfunctions of this system. It is convenient to introduce a dimensionless variable ϱ in Eqs. (15.5) and (15.6) for bound states:

$$\varrho = 2M\sqrt{1 - \epsilon^2}r, \qquad \epsilon = \frac{E}{M} < 1. \qquad (15.7)$$

Solving $F_{jE}(\varrho)$ from Eqs. (15.5) and (15.6), we have

$$F_{jE}(\varrho) = \left(-\frac{\nu}{2} + \frac{\xi}{\varrho}\right)^{-1}\left[\frac{dG_{jE}(\varrho)}{d\varrho} + \frac{j}{\varrho}G_{jE}(\varrho)\right], \qquad (15.8)$$

where

$$\nu = \sqrt{\frac{1 - \epsilon}{1 + \epsilon}}. \qquad (15.9)$$

By substituting this into Eq. (15.6), we obtain a second-order differential equation of $G_{jE}(\varrho)$:

$$\frac{d^2}{d\varrho^2}G_{jE}(\varrho) + \left(-\frac{1}{4} - \frac{j^2 - \xi^2 + j}{\varrho^2} + \frac{\epsilon\xi}{\varrho\sqrt{1 - \epsilon^2}}\right)G_{jE}(\varrho)$$
$$+ \left(\varrho - \frac{\varrho^2}{2\xi}\nu\right)^{-1}\left(\frac{d}{d\varrho}G_{jE}(\varrho) + \frac{j}{\varrho}G_{jE}(\varrho)\right) = 0. \qquad (15.10)$$

From the behaviors of $G_{jE}(\varrho)$ at the origin and at infinity, we define

$$G_{jE}(\varrho) = \varrho^\gamma e^{-\frac{\varrho}{2}}R(\varrho), \qquad (15.11)$$

where

$$\gamma = \sqrt{j^2 - \xi^2} > 0, \quad \omega = \frac{\nu}{2\xi}, \quad \tau = \frac{\epsilon\xi}{\sqrt{1 - \epsilon^2}}. \tag{15.12}$$

Substitution of Eq. (15.11) into Eq. (15.10) allows us to obtain

$$\varrho(1 - \omega\varrho)\frac{d^2}{d\varrho^2}R(\varrho) + [\omega\varrho^2 - (2\gamma\omega + 1)\varrho + 2\gamma + 1]\frac{d}{d\varrho}R(\varrho)$$

$$+ [\omega(\gamma - \tau)\varrho + \omega(j + \gamma) + \tau - \gamma - \frac{1}{2}]R(\varrho) = 0. \tag{15.13}$$

It is worth noting that τ has the same sign as the energy E, and ω satisfies the identity

$$4\xi^2\omega^2 + 4\tau\omega = 1. \tag{15.14}$$

We now apply the power series expansion method, as used by Waldenstrøm in three-dimensional case [544] to solve Eq. (15.13).

If we take

$$R(\varrho) = \sum_{k=0}^{\infty} b_k \varrho^k, \tag{15.15}$$

then we can obtain the recursion relation by equating the coefficients of ϱ^{k-1} to zero

$$[\omega(j + \gamma) + \tau - \gamma - 1/2]b_0 + (2\gamma + 1)b_1 = 0,$$

$$A_k b_{k-2} + B_k b_{k-1} + C_k b_k = 0, \quad k \geq 2, \tag{15.16}$$

with

$$A_k = \omega(\gamma - \tau + k - 2),$$

$$B_k = \omega(j - \gamma) - \omega(k - 2)(2\gamma + k - 1) + \tau - \gamma - k + 1/2, \tag{15.17}$$

$$C_k = k(2\gamma + k).$$

The second equation is a three-term recursion relation. However, by using the first equation, it is not difficult to obtain the relation between b_k and b_0

$$\frac{b_k}{b_0} = \frac{\{2(\gamma - \tau) + k[1 - 2\omega(j + \gamma)]\} \prod_{t=1}^{k-1}(\gamma - \tau + t)}{2k! \prod_{s=1}^{k}(2\gamma + s)}, \tag{15.18}$$

where the identity (15.14) is used.

Before proceeding further, let us recall that the power series expansion of the confluent hypergeometric functions (Kummer functions) can be expressed as [263]:

$$F(\alpha, \beta; z) = 1 + \frac{\alpha}{\beta} \frac{z}{1!} + \frac{\alpha(\alpha+1)}{\beta(\beta+1)} \frac{z^2}{2!} + \frac{\alpha(\alpha+1)(\alpha+2)}{\beta(\beta+1)(\beta+2)} \frac{z^3}{3!} + \dots . \quad (15.19)$$

Therefore, $R(\varrho)$ can be written as a combination of two confluent hypergeometric functions:

$$R(\varrho) = b_0 \left[F(\gamma - \tau, 2\gamma + 1; \varrho) + \varrho \frac{1 - 2\omega(\gamma + j)}{2(2\gamma + 1)} F(\gamma - \tau + 1, 2\gamma + 2; \varrho) \right]. \quad (15.20)$$

Based on the recursion relation of the confluent hypergeometric functions [263]

$$\varrho \, F(1 + \alpha, 1 + \beta; \varrho) = \beta \, F(1 + \alpha, \beta; \varrho) - \beta \, F(\alpha, \beta; \varrho), \quad (15.21)$$

and the following identities derived from Eq. (15.14):

$$[1 - 2\omega(\gamma + j)][1 + 2\omega(j - \gamma)] = 4\omega(\tau - \gamma), \quad (15.22)$$

$$[1 + 2\omega(\gamma + j)][1 + 2\omega(j - \gamma)] = 4\omega(j + \frac{\tau}{\epsilon}), \quad (15.23)$$

we obtain

$$G_{jE}(\varrho) = c\varrho^\gamma e^{-\frac{\varrho}{2}} [(j + \tau/\epsilon) F(\gamma - \tau, 2\gamma + 1; \varrho) + (\tau - \gamma) F(\gamma - \tau + 1, 1 + 2\gamma; \varrho)], \quad (15.24)$$

where

$$c = \frac{2b_0 \omega}{1 + 2\omega(j - \gamma)}. \quad (15.25)$$

We now consider the eigenvalues. Considering the finiteness of the solutions at infinity, from Eq. (15.20) we may obtain the general quantum condition

$$\gamma - \tau = -n', \quad n' = 1, 2, \dots, \quad (15.26)$$

and $n' = 0$ where the second term vanishes, i.e., $2\omega(j + \gamma) = 1$. As a result, when $n' = 0$, we have $\gamma = \tau$. One obtains from Eqs. (15.7) and (15.12)

$$j^2 = \tau^2 + \xi^2 = \frac{\xi^2}{1 - \epsilon^2},$$
$$j = \pm \frac{\xi}{\sqrt{1 - \epsilon^2}} = \pm \left(-\tau + \frac{1}{2\omega} \right). \quad (15.27)$$

Thus, $2\omega(\gamma + j) = 1$ holds only for a positive j.

If introducing the principal quantum number

$$n = |j| + 1/2 + n' = |j| + 1/2 + \tau - \gamma, \tag{15.28}$$

we obtain the energy E_{nj} from Eqs. (15.12) and (15.28)

$$\epsilon = \frac{E_{nj}}{M} = \left[1 + \frac{\xi^2}{(\sqrt{j^2 - \xi^2} + n - |j| - 1/2)^2} \right]^{-1/2}. \tag{15.29}$$

Let us study the fine structure energy. This becomes evident by expanding Eq. (15.29) in powers of ξ^2:

$$E_{nj} \simeq M \left[1 - \frac{\xi^2}{2(n - 1/2)^2} - \frac{\xi^4}{2(n - 1/2)^4} \left(\frac{n - 1/2}{|j|} - \frac{3}{4} \right) \right], \tag{15.30}$$

where the first term on the right-hand side is the rest energy M ($c^2 = 1$ in our conventions), the second one coincides with the energy from the solutions to the Schrödinger equation, and the third one is the fine structure energy, which removes the degeneracy between the states of the same n. The principal quantum number n can be equal to 1 only for $j = 1/2$ and to other positive integers for both signs of j.

For completeness, we briefly derive the normalized wave functions. Substituting $G_{jE}(\varrho)$ given in Eq. (15.24) into Eq. (15.8), we obtain

$$F_{jE}(\varrho) = c\varrho^\gamma e^{-\frac{\varrho}{2}} \nu^{-1} [(j + \frac{\tau}{\epsilon}) F(-n', 2\gamma + 1; \varrho) - n' F(1 - n', 2\gamma + 1; \varrho)], \tag{15.31}$$

where c is given in Eq. (15.25). Before proceeding to do so, let us recall the following recursion relations [263]

$$\frac{d}{dz} F(\alpha, \gamma; z) = \frac{\alpha}{\gamma} F(1 + \alpha, 1 + \gamma; z),$$

$$zF(1 + \alpha, 1 + \gamma; z) = \gamma F(1 + \alpha, \gamma; z) - \gamma F(\alpha, \gamma; z),$$

$$\alpha F(1 + \alpha, \gamma; z) = (z + 2\alpha - \gamma) F(\alpha, \gamma; z) + (\gamma - \alpha) F(\alpha - 1, \gamma; z), \tag{15.32}$$

from which, together with the identities (15.14), (15.22), (15.23), Eqs. (8.10) and (8.11) as well as the normalization condition

$$\int_0^\infty (|F_{jE}(\varrho)|^2 + |G_{jE}(\varrho)|^2) dr = 1, \tag{15.33}$$

we have

$$
\left.\begin{array}{c} F_{jE}(\varrho) \\ G_{jE}(\varrho) \end{array}\right\} = \frac{(M^2 - E^2)^{1/4}}{\Gamma(2\gamma + 1)} \sqrt{\frac{(1 \pm \epsilon)\epsilon\Gamma(n' + 2\gamma + 1)}{2\tau(j + \frac{\tau}{\epsilon})n'!}} \varrho^\gamma e^{-\frac{\varrho}{2}}
$$
$$
\cdot [(j + \tfrac{\tau}{\epsilon})F(-n', 2\gamma + 1; \varrho) \mp n'F(1 - n', 2\gamma + 1; \varrho)].
$$
(15.34)

4. SUSYQM and SWKB approaches to Coulomb problem

As we know, the ideas of the SUSY and shape invariance are significant in quantum mechanics. With them the Dirac equation with a Coulomb potential was studied in three dimensions [100]. Recently, Qiang *et al.* have used the SUSYQM and shape invariance or SWKB methods to study the bound states of the (2+1)-dimensional Dirac equation with a Coulomb potential [580].

Using the new variable given in Eq. (15.7), we may obtain a set of modified first order-coupled differential equations

$$
\frac{d}{d\varrho}G_{jE}(\varrho) + \frac{j}{\varrho}G_{jE}(\varrho) + \left(\frac{1}{2}\nu - \frac{\xi}{\varrho}\right)F_{jE}(\varrho) = 0,
$$
(15.35)

$$
\frac{d}{d\varrho}F_{jE}(\varrho) - \frac{j}{\varrho}G_{jE}(\varrho) + \left(\frac{1}{2}\nu^{-1} + \frac{\xi}{\varrho}\right)G_{jE}(\varrho) = 0,
$$
(15.36)

which can be further rearranged in a matrix form

$$
\frac{d}{d\varrho}\Psi(\varrho) + \frac{t}{\varrho}\Psi(\varrho) + b\Psi(\varrho) = 0,
$$
(15.37)

with

$$
\Psi(\varrho) = \left(\begin{array}{c} G_{jE}(\varrho) \\ F_{jE}(\varrho) \end{array}\right), \quad t = \left(\begin{array}{cc} j & -\xi \\ \xi & -j \end{array}\right), \quad b = \frac{1}{2}\left(\begin{array}{cc} 0 & \nu \\ \nu^{-1} & 0 \end{array}\right).
$$
(15.38)

Following the work by Sukumar [74], we find that the matrix multiplying $1/\varrho$ can be diagonalized by multiplying it with a matrix $\mathcal{D}$ from the left and with $\mathcal{D}^{-1}$ from the right, where

$$
\mathcal{D} = \left(\begin{array}{cc} j + \gamma & -\xi \\ -\xi & j + \gamma \end{array}\right),
$$
(15.39)

where γ is given in Eq. (15.12).

Multiplying Eq. (15.37) from the left by the matrix $\mathcal{D}$ allows us to obtain

$$
\hat{B}\,f_{jE}(\varrho) = \frac{(j - \gamma)\nu - (j + \gamma)\nu^{-1}}{4\gamma}g_{jE}(\varrho),
$$
$$
\hat{B}^\dagger g_{jE}(\varrho) = \frac{(j + \gamma)\nu - (j - \gamma)\nu^{-1}}{4\gamma}f_{jE}(\varrho),
$$
(15.40)

with

$$\left(\begin{array}{c} g_{jE}(\varrho) \\ f_{jE}(\varrho) \end{array}\right) = \mathcal{D}\left(\begin{array}{c} G_{jE}(\varrho) \\ F_{jE}(\varrho) \end{array}\right), \tag{15.41}$$

$$\hat{B} = \frac{d}{d\varrho} - \frac{\gamma}{\varrho} + \frac{\tau}{2\gamma}, \qquad \hat{B}^\dagger = -\frac{d}{d\varrho} - \frac{\gamma}{\varrho} + \frac{\tau}{2\gamma}, \tag{15.42}$$

where τ is given in Eq. (15.12). If defining

$$H^- = \hat{B}^+\hat{B} = -\frac{d^2}{d\varrho^2} - \frac{\gamma}{\varrho^2} + \left(\frac{\gamma}{\varrho} - \frac{\tau}{2\gamma}\right)^2,$$

$$\tag{15.43}$$

$$H^+ = \hat{B}\hat{B}^+ = -\frac{d^2}{d\varrho^2} + \frac{\gamma}{\varrho^2} + \left(\frac{\gamma}{\varrho} - \frac{\tau}{2\gamma}\right)^2,$$

we can easily decouple Eq. (15.40) as follows:

$$H^- f_{jE}(\varrho) = -\frac{\gamma^2 - j^2\epsilon^2}{4\gamma^2(1 - \epsilon^2)} f_{jE}(\varrho),$$

$$\tag{15.44}$$

$$H^+ g_{jE}(\varrho) = -\frac{\gamma^2 - j^2\epsilon^2}{4\gamma^2(1 - \epsilon^2)} g_{jE}(\varrho),$$

which implies that $H^\pm$ are shape invariant supersymmetric partner potentials since

$$H^+(\gamma) = H^-(\gamma + 1) - \frac{\tau^2}{4}\left[\frac{1}{\gamma^2} - \frac{1}{(1 + \gamma)^2}\right]. \tag{15.45}$$

On the other hand, the eigenvalues of H^- can be obtained as

$$E_n^{(-)} = -\frac{\gamma^2 - j^2\epsilon^2}{4\gamma^2(1 - \epsilon^2)} = \sum_{k=1}^{n'} R(a_k) = \frac{(\gamma + n')^2}{4}\left[\frac{1}{\gamma^2} - \frac{1}{(\gamma + n')^2}\right], \tag{15.46}$$

where we have used the following results

$$a_0 = \gamma, \qquad a_k = \gamma + k, \qquad R(a_k) = \frac{\tau^2}{4}\left(\frac{1}{a_{k-1}^2} - \frac{1}{a_k^2}\right). \tag{15.47}$$

It is shown from Eqs. (15.45) and (15.46) that we can obtain eigenvalues (15.29).

In addition, it is worth pointing out that the eigenvalues can also be obtained by the SWKB method. To this end, we solve equation

$$\hat{B}\, g_{jE_0}(\varrho) = 0 \tag{15.48}$$

to obtain the eigenfunction of ground state of H^-

$$g_{jE_0}(\varrho) = e^{-\frac{\tau}{2\gamma}\varrho}\varrho^{\gamma}, \qquad (15.49)$$

from which we may obtain the corresponding superpotential

$$W(\varrho) = -\frac{1}{g_{jE_0}(\varrho)}\frac{dg_{jE_0}(\varrho)}{d\varrho} = -\frac{\gamma}{\varrho} + \frac{\tau}{2\gamma}. \qquad (15.50)$$

In fact, the $W(\varrho)$ can also be obtained from Eq. (15.42).

By substituting this equation into the SWKB quantization condition[1]

$$\int_{\varrho_L}^{\varrho_R} \sqrt{E_n^{(-)} - W^2(\varrho)}d\varrho = n'\pi, \qquad n' = 0, 1, 2, \ldots, \qquad (15.51)$$

where the two turning points ϱ_L and ϱ_R are given by $W(\varrho) = \pm\sqrt{E_n^{(-)}}$, we obtain

$$\gamma\pi\left[\left(1 - \frac{4\gamma^2 E_n^{(-)}}{\tau^2}\right)^{-\frac{1}{2}} - 1\right] = n'\pi. \qquad (15.52)$$

By substituting $E_n^{(-)}$ and τ given in Eqs. (15.46) and (15.12) into above equation and also considering the relation between n' and the principal quantum number n given in Eq. (15.28), we obtain Eq. (15.29) again.

5. Alternative method to derive exact eigenfunctions

Now, we want to review how to derive the eigenfunctions using an alternative approach [580]. Let us study Eq. (15.44) in order to obtain $f_{jE}(\varrho)$ and $g_{jE}(\varrho)$. From the behaviors of the radial wave functions $f_{jE}(\varrho)$ and $g_{jE}(\varrho)$ at the origin and at infinity, respectively, we take the following ansatz for them

$$f_{jE}(\varrho) = \varrho^{\gamma}e^{-\frac{\varrho}{2}}R_f(\varrho), \qquad g_{jE}(\varrho) = \varrho^{\gamma+1}e^{-\frac{\varrho}{2}}R_g(\varrho). \qquad (15.53)$$

Substitution of them into Eq. (15.44) allows us to obtain

$$\varrho\frac{d^2 R_f(\varrho)}{d\varrho^2} + (2\gamma - \varrho)\frac{dR_f(\varrho)}{d\varrho} + n'R_f(\varrho) = 0,$$

$$\varrho\frac{d^2 R_g(\varrho)}{d\varrho^2} + (2\gamma + 2 - \varrho)\frac{dR_g(\varrho)}{d\varrho} + (n' - 1)R_g(\varrho) = 0, \qquad (15.54)$$

whose solutions are nothing but the confluent hypergeometric functions [263]

$$R_f(\varrho) = C_1 F(-n', 2\gamma; \varrho), \qquad R_g(\varrho) = C_2 F(1 - n', 2\gamma + 2; \varrho). \qquad (15.55)$$

Thus, from Eq. (15.53) we may express the wave functions as

$$f_{jE}(\varrho) = C_1 \varrho^\gamma e^{-\frac{\varrho}{2}} F(-n', 2\gamma; \varrho),$$

$$g_{jE}(\varrho) = C_2 \varrho^{\gamma+1} e^{-\frac{\varrho}{2}} F(1 - n', 2\gamma + 2; \varrho).$$

(15.56)

If substituting Eq. (15.56) into Eq. (15.40), simplifying and removing the common factor $\varrho^\gamma e^{-\frac{\varrho}{2}}$, then setting $\varrho = 0$, we obtain

$$2C_1(n' + \gamma - \tau) = 0,$$

$$4C_2\gamma(1 + 2\gamma) + C_1 \left[j \left(\nu - \nu^{-1} \right) + \gamma \left(\nu + \nu^{-1} \right) \right] = 0.$$

(15.57)

Obviously, we see from Eq. (15.26) that the first formula is an identity.

Using the second recursion relation of the confluent hypergeometric function given in Eqs. (15.32) and the following formula [263]

$$(\gamma - \alpha)F(\alpha, 1 + \gamma; z) + \alpha F(1 + \alpha, 1 + \gamma; z) = \gamma F(\alpha, \gamma; z), \quad (15.58)$$

we can rewrite Eq. (15.56) as

$$f_{jE}(\varrho) = \frac{C_1}{2\gamma} e^{-\frac{\varrho}{2}} \varrho^\gamma [(2\gamma + n')F(-n', 1 + 2\gamma; \varrho) - n' F(1 - n', 1 + 2\gamma; \varrho)]$$

$$g_{jE}(\varrho) = C_2 e^{-\frac{\varrho}{2}} \varrho^\gamma (1 + 2\gamma)[F(1 - n', 1 + 2\gamma; \varrho) - F(-n', 1 + 2\gamma; \varrho)].$$

(15.59)

By using Eqs. (15.39), (15.40), (15.41), (15.57) and (15.59), we get [580]

$$
\begin{aligned}
F_{jE}(\varrho) &= \frac{C_1}{8\gamma^2} \varrho^\gamma e^{-\frac{\varrho}{2}} \sqrt{1 + \epsilon} \left\{ \left[\frac{2(n' + 2\gamma)}{\sqrt{1 + \epsilon}} \right. \right. \\
&\quad + \left. \left(\nu - \frac{j - \gamma}{(j + \gamma)\sqrt{1 - \epsilon}} \right) \xi \right] F(-n', 1 + 2\gamma; \varrho) \\
&\quad - \left[\frac{2n'}{\sqrt{1 + \epsilon}} + \left(\nu - \frac{j - \gamma}{(j + \gamma)\sqrt{1 - \epsilon}} \right) \xi \right] \\
&\quad \times F(1 - n', 1 + 2\gamma; \varrho) \left. \right\},
\end{aligned}
$$

(15.60)

$$
\begin{aligned}
G_{jE}(\varrho) \;=\; & \frac{C_1}{8\gamma^2}\varrho^\gamma e^{-\frac{\varrho}{2}}\sqrt{1-\epsilon}\Bigg\{\left[\frac{j+\gamma}{\sqrt{1+\epsilon}}\right.\\
& \left.-(j-\gamma)\nu^{-1}+\frac{2(n'+2\gamma)\xi}{(j+\gamma)\sqrt{1-\epsilon}}\right]F(-n',1+2\gamma;\varrho)\\
& -\left[\frac{j+\gamma}{\sqrt{1+\epsilon}}-(j-\gamma)\nu^{-1}+\frac{2n'\xi}{(j+\gamma)\sqrt{1-\epsilon}}\right]\\
& \times F(1-n',1+2\gamma;\varrho)\Bigg\}.
\end{aligned}
\tag{15.61}
$$

Based on Eqs. (15.9), (15.12), (15.22), (15.23) and (15.26), we can obtain the following relations

$$
\begin{aligned}
(j+\gamma)\nu-(j-\gamma)\nu^{-1}+\frac{2(n'+2\gamma)\xi}{j+\gamma} \;&=\; \frac{2\gamma\xi[1+2(j+\gamma)\omega]}{j+\gamma}\\
&=\; 2(n'+2\gamma)\nu\\
&\quad +\left(\nu^2-\frac{j-\gamma}{j+\gamma}\right)\xi,
\end{aligned}
\tag{15.62}
$$

and

$$
\begin{aligned}
-(j+\gamma)\nu+(j-\gamma)\nu^{-1}-\frac{2n'\xi}{j+\gamma} \;&=\; \frac{2\gamma\xi[1+2(j+\gamma)\omega]}{j+\gamma}\frac{n'}{j+\tau/\epsilon}\\
&=\; 2n'\nu+\left(\nu^2-\frac{j-\gamma}{j+\gamma}\right)\xi.
\end{aligned}
\tag{15.63}
$$

As a matter of fact, we are able to express the radial wave functions as follows:

$$
\begin{aligned}
\left.\begin{array}{c}F_{jE}(\varrho)\\[4pt]G_{jE}(\varrho)\end{array}\right\} \;=\; & \mathcal{N}\varrho^\gamma e^{-\frac{\varrho}{2}}\sqrt{1\pm\epsilon}\\
& \times[(j+\tfrac{\tau}{\epsilon})F(-n',1+2\gamma;\varrho)\mp n'F(1-n',1+2\gamma;\varrho)],
\end{aligned}
\tag{15.64}
$$

where the normalization factor $\mathcal{N}$ is to be determined below.

Generally speaking, we may use the normalization condition of the radial wave functions (15.33) to obtain the normalization factor. During the calculation, it is found that we have to use some useful integral formulas to derive it. Such a task can be performed by the recently developed MATHEMATICA package INTEPFFLL [581]. For example, we may calculate the following integral formulas systematically:

$$
I_{LL}(n,\triangle n,\beta,\triangle\beta,\lambda)=\int_0^\infty e^{-\rho}\,\rho^{\beta+\lambda}\,L_n^\beta(\rho)L_{n+\triangle n}^{\beta+\triangle\beta}(\rho)\,d\rho,
\tag{15.65}
$$

and

$$I_{FF}(n, \triangle n, \beta, \triangle \beta, \lambda) = \int_0^\infty e^{-\rho} \rho^{\beta+\lambda} F(-n, \beta; \rho) F(-n-\triangle n, \beta+\triangle \beta; \rho) \, d\rho,$$
(15.66)

where $\triangle n \geq 0$ and $\triangle n, \triangle \beta, \lambda$ are integers. We assume that n is a non-negative integer, and $\beta, \beta + \triangle \beta$ are not equal to zero or negative integers. For instance, we may easily obtain the following integrals often used in physics,

$$\int_0^\infty e^{-\rho} \rho^{\alpha-1} F(-n, \alpha; \rho)^2 d\rho = \frac{n! \Gamma(\alpha)^2}{\Gamma(\alpha + n)},$$
(15.67)

and the orthogonality relation

$$\int_0^\infty e^{-\rho} \rho^{\alpha-1} F(1-n, \alpha; \rho) F(-n, \alpha; \rho) d\rho = 0.$$
(15.68)

For given Δn, $\Delta \beta$ and λ, we can obtain the closed expressions of Eqs. (15.65) and (15.66). Making use of this package INTEPFFLL, thousands of integrals have been calculated. For simplicity, some formulas given in Table A.1 (see Appendix A) are used to calculate the mean values $\overline{r^k}$. In a similar way, we may obtain the normalization factor $\mathcal{N}$ as follows:

$$\mathcal{N} = \frac{(M^2 - E^2)^{1/4}}{\Gamma(2\gamma + 1)} \sqrt{\frac{(1 \pm \epsilon)\epsilon \Gamma(n' + 2\gamma + 1)}{2\tau(j + \tau/\epsilon) n'!}},$$
(15.69)

where the signs "+" and "-" correspond the radial wave functions $F_{jE}(\varrho)$ and $G_{jE}(\varrho)$, respectively. This coincides with the result given in Eq. (15.34).

6.   Concluding remarks

With the interest in the lower dimensional field theory and condensed matter physics, we have studied the (2 +1)-dimensional Dirac equation with a Coulomb potential. The eigenfunctions can be analytically obtained by power series expansion approach and expressed by the confluent hypergeometric functions. The eigenvalues and their fine structures are also studied. On the other hand, with the aid of the SUSYQM and shape invariance as well as the SWKB quantization condition, we have studied the same problem. The explicit eigenfunctions are also obtained with the help of the MATHEMATICA package INTEPFFLL. Before ending this Chapter, we make a few remarks. First, it should be noticed that the Dirac equation admits of solutions for which the particle has negative kinetic energy. From the Sturm-Liouville theorem [579], there are bound states with the energy less than and near M for the attractive Coulomb potential, and with the energy larger than and near $-M$ for the repulsive Coulomb potential, if the interaction is not too strong. Second, in

comparison with the case in three dimensions, the angular momentum quantum number j in two dimensions plays the role of the good quantum number κ in three dimensions (more strictly, $|j| + 1/2 \longleftrightarrow |\kappa|$). The ground state occurs for $j = 1/2$ in two dimensions, but for $j = 1/2$ and $l = 0$ in three dimensions. Note that Waldenstrøm has used the convention with the opposite sign for κ as usual (compare Eq. (4a) in [544, 545] with Eq. (53. 10) in [215]). Third, it should be noted that the matrix $\mathcal{D}$ used to diagonalize matrix t in Eqs. (15.37) and (15.38) and is not unique, its forms are different from each other by a similarity transformation. However, this does not affect the expression of the energy spectrum. Fourth, it is worth pointing out that when solving the Dirac equation with a central potential, one may apply a unitary transformation to obtain a modified Dirac equation so that the derivation procedure becomes rather simple.

Notes

1 Recently, quantum correction in exact quantization rules has been proposed by Ma and Xu [582]. They found that the correct expression of the quantization rule should be written as

$$\int_{x_A}^{x_B} k(x)dx = N\pi + \int_{x_A}^{x_B} \phi(x) \left[\frac{dk(x)}{dx}\right] \left[\frac{d\phi(x)}{dx}\right]^{-1} dx, \quad N = n + 1,$$

(15.70)

where $k(x) = \sqrt{2M[E - V(x)]}/\hbar$ and x_A, x_B are two turning points. $\phi(x) = \psi(x)^{-1}d\psi(x)/dx$ is the logarithmic derivative of the wave function $\psi(x)$. N is the number of nodes of $\phi(x)$, where n is the nodes of the wave function $\psi(x)$.

Chapter 16

REALIZATION OF DYNAMIC GROUP FOR THE DIRAC HYDROGEN-LIKE ATOM IN 2+1 DIMENSIONS

1.   Introduction

The algebraic method has been widely used in various fields of physics and chemistry. This powerful tool is especially demonstrated in the non-relativistic and relativistic Coulomb problem [583, 584]. Recently, Martínez-y-Romero *et al.* have introduced a novel realization of the classic SU(2) algebra for the Dirac hydrogen-like atom and non-unitary representations were used to explain the bound state energy spectrum [585, 586]. After that, Drăgănescu, Messina and Napoli have used the properties of the compact SU(2) group to study the radial coherent states for the Dirac hydrogen atom [587]. However, Li has shown that such a realization should be a non-compact Lie group SU(1, 1) after a careful analysis [588]. In fact, such a conclusion can be confirmed by the well-known fact that the harmonic oscillator, Coulomb and Morse potentials are equivalent under certain transformations and they are supersymmetric shape-invariant potentials, which are related to the su(1, 1) algebra [589, 590]. Recently, such a study has been carried out by Martínez *et al.* [591].

Due to the interest in the lower-dimensional field theory and condensed matter physics, we want to study this problem in two dimensions. In particular, we attempt to study the dynamic group for the radial wave functions of the Dirac equation with the Coulomb-like potential.

This Chapter is organized as follows. In Section 2 we construct the dynamic group for the radial wave functions by introducing an extra phase. The concluding remarks are given in Section 3.

2.   Realization of dynamic group SU(1, 1)

We begin by considering the radial wave functions (15.5) and (15.6) of the Dirac equation in two dimensions. As done before, we take the Coulomb-like

potential as

$$V(r) = -\frac{\xi}{r}. \tag{16.1}$$

By taking a new variable

$$\rho = M\sqrt{1 - \epsilon^2}\, r = \sqrt{M^2 - E^2}\, r, \quad \epsilon = \frac{E}{M}, \tag{16.2}$$

we may rearrange the radial wave functions as follows:

$$\frac{d}{d\rho}G(\rho) + \frac{j}{\rho}G(\rho) = \left[-v + \frac{\xi}{\rho}\right]F(\rho), \tag{16.3}$$

$$-\frac{d}{d\rho}F(\rho) + \frac{j}{\rho}F(\rho) = \left[v^{-1} + \frac{\xi}{\rho}\right]G(\rho), \tag{16.4}$$

where we introduced a new parameter

$$v = \sqrt{\frac{M - E}{M + E}} = \sqrt{\frac{1 - \epsilon}{1 + \epsilon}}. \tag{16.5}$$

As shown in Ref. [592, 593], introducing a new variable y through the relation $\varrho = e^y$ with $y \in (-\infty, \infty)$ and defining the following functions

$$F(\rho(y)) = \sqrt{M + E}[\Phi_+(y) - \Phi_-(y)],$$
$$G(\rho(y)) = \sqrt{M - E}[\Phi_+(y) + \Phi_-(y)]. \tag{16.6}$$

Substituting them into Eqs. (16.3) and (16.4) allows us to obtain

$$\frac{d\Phi_+(y)}{dy} + \frac{d\Phi_-(y)}{dy} + j[\Phi_+(y) + \Phi_-(y)] = [-e^y + v^{-1}\xi][\Phi_+(y) - \Phi_-(y)], \tag{16.7}$$

$$\frac{d\Phi_-(y)}{dy} - \frac{d\Phi_+(y)}{dy} + j[\Phi_+(y) - \Phi_-(y)] = [e^y + v\xi][\Phi_+(y) + \Phi_-(y)]. \tag{16.8}$$

Their addition and subtraction lead to

$$\frac{d\Phi_-(y)}{dy} - \left[e^y - \frac{\xi E}{\sqrt{M^2 - E^2}}\right]\Phi_-(y) = \left[\frac{\xi M}{\sqrt{M^2 - E^2}} - j\right]\Phi_+, \tag{16.9}$$

$$\frac{d\Phi_+(y)}{dy} - \left[-e^y + \frac{\xi E}{\sqrt{M^2 - E^2}} \right] \Phi_+(y) = - \left[\frac{\xi M}{\sqrt{M^2 - E^2}} + j \right] \Phi_-(y),$$

$$\text{(16.10)}$$

Introducing

$$\tau = \frac{\xi}{\sqrt{M^2 - E^2}}, \tag{16.11}$$

we have

$$\frac{d\Phi_-(y)}{dy} - \left[e^y - \tau E \right] \Phi_-(y) = \left[M\tau - j \right] \Phi_+(y), \tag{16.12}$$

$$\frac{d\Phi_+(y)}{dy} - \left[-e^y + \tau E \right] \Phi_+(y) = - \left[M\tau + j \right] \Phi_-(y), \tag{16.13}$$

which can be further modified as

$$\frac{d^2\Phi_-(y)}{dy^2} + \left[-e^{2y} + 2(\eta - 1)e^y - \frac{1}{4} \right] \Phi_-(y) = \left[j^2 - \xi^2 - \frac{1}{4} \right] \Phi_-(y),$$

$$\text{(16.14)}$$

$$\frac{d^2\Phi_+(y)}{dy^2} + \left[-e^{2y} + 2\eta e^y - \frac{1}{4} \right] \Phi_+(y) = \left[j^2 - \xi^2 - \frac{1}{4} \right] \Phi_+(y), \quad \text{(16.15)}$$

with

$$\eta = \tau E + 1/2. \tag{16.16}$$

It should be noted that equations (16.14) and (16.15) can be considered as the eigenfunctions with the known eigenvalue

$$\omega = j^2 - \xi^2 - \frac{1}{4}, \tag{16.17}$$

as follows from the radial symmetry of the hydrogen atom. Also, we find that these equations (16.14) and (16.15) are similar to those given in [591]. In order to construct the Lie algebra for this quantum system, let us introduce an extra variable θ through

$$\hat{L}_0 = -i \frac{\partial}{\partial \theta} \tag{16.18}$$

and then define [588]

$$\hat{L}_\pm = e^{\pm i\theta} \left(\pm \frac{\partial}{\partial y} - e^y - i \frac{\partial}{\partial \theta} \pm 1/2 \right), \tag{16.19}$$

or [591]

$$\hat{L}_{\pm} = i\, e^{\pm i\theta} \left(\frac{\partial}{\partial y} \mp e^y \mp i\frac{\partial}{\partial\theta} + 1/2 \right), \qquad (16.20)$$

which satisfy the commutation relations of the su(1, 1) group

$$[\hat{L}_0, \hat{L}_{\pm}] = \pm\hat{L}_{\pm}, \qquad [\hat{L}_-, \hat{L}_+] = 2\hat{L}_0. \qquad (16.21)$$

Furthermore, it is found that these operators satisfy

$$\hat{L}_{\pm}^{\dagger} = \hat{L}_{\mp}, \qquad \hat{L}_0^{\dagger} = \hat{L}_0, \qquad (16.22)$$

as we expect. Therefore, the suitable dynamic group for the Dirac hydrogen-like atom is the non-compact SU(1, 1) group. This is very similar to the SU(1, 1) realization for the Morse potential.

Here we want to show how to derive Eq. (16.21). Before proceeding to do so, we first define two new variables

$$A(y) = \frac{\partial}{\partial y} - e^y, \quad B(y) = -\frac{\partial}{\partial y} - e^y, \qquad (16.23)$$

then we are able to calculate $[\hat{L}_0, \hat{L}_+]$ as follows:

$$\begin{aligned}
(\hat{L}_0\hat{L}_+ - \hat{L}_+\hat{L}_0)\Phi &= \left(-i\frac{\partial}{\partial\theta} \right)(e^{i\theta})\left[A(y)\Phi - i\frac{\partial}{\partial\theta}\Phi + \frac{1}{2}\Phi \right] \\
&\quad - e^{i\theta}\left[A(y) - i\frac{\partial}{\partial\theta} + \frac{1}{2} \right]\left(-i\frac{\partial}{\partial\theta}\Phi \right) \\
&= e^{i\theta}\left[A(y)\Phi - i\frac{\partial}{\partial\theta}\Phi + \frac{1}{2}\Phi \right] \\
&\quad - e^{i\theta}\left[iA(y)\frac{\partial}{\partial\theta}\Phi + \frac{\partial^2}{\partial\theta^2}\Phi + \frac{i}{2}e^{i\theta}\Phi \right] \\
&\quad + e^{i\theta}\left[iA(y)\frac{\partial}{\partial\theta}\Phi + \frac{\partial^2}{\partial\theta^2}\Phi + \frac{i}{2}e^{i\theta}\Phi \right] \\
&= e^{i\theta}\left[A(y)\Phi - i\frac{\partial}{\partial\theta}\Phi + \frac{1}{2}\Phi \right] \\
&= \hat{L}_+\Phi,
\end{aligned} \qquad (16.24)$$

where Φ is an arbitrary wave function. In a similar way, we may obtain $[\hat{L}_0, \hat{L}_-] = -\hat{L}_-$.

On the other hand, we may calculate $[\hat{L}_-, \hat{L}_+]$ as follows:

$$
\begin{aligned}
(\hat{L}_-\hat{L}_+ - \hat{L}_+\hat{L}_-)\Phi \; &= e^{-i\theta}\left[B(y) - i\frac{\partial}{\partial\theta} - \frac{1}{2}\right] \\
&\quad \cdot e^{i\theta}\left[A(y) - i\frac{\partial}{\partial\theta} + \frac{1}{2}\right]\Phi \\
&\quad - e^{i\theta}\left[A(y) - i\frac{\partial}{\partial\theta} + \frac{1}{2}\right] \\
&\quad \cdot e^{-i\theta}\left[B(y) - i\frac{\partial}{\partial\theta} - \frac{1}{2}\right]\Phi \\
&= [B(y)A(y) - A(y)B(y)]\Phi \\
&\quad + \left[A(y) + B(y) - 2i\frac{\partial}{\partial\theta}\right]\Phi \\
&= -2i\frac{\partial}{\partial\theta}\Phi \\
&= 2\hat{L}_0\Phi,
\end{aligned}
\tag{16.25}
$$

where we used the relation

$$
[B(y), A(y)] = 2e^y.
\tag{16.26}
$$

Thus, we have proved the results (16.21).

The Casimir operator is calculated as

$$
\begin{aligned}
C \; &= -\hat{L}_+\hat{L}_- + \hat{L}_0^2 - \hat{L}_0 \\
&= \frac{\partial^2}{\partial y^2} - e^{2y} - 2ie^y\frac{\partial}{\partial\theta} - \frac{1}{4}.
\end{aligned}
\tag{16.27}
$$

As shown in [588], the eigenvalues of this system can be obtained by classifying the non-compact Lie algebra su(1, 1). The eigenvalues can be described by the discrete series D_k^+ with the parameter

$$
k = -\sqrt{\omega + \frac{1}{4}} - 1/2 = -\sqrt{j^2 - \xi^2} - 1/2
\tag{16.28}
$$

and $\eta = n' - k$, from which, together with (16.16), we are able to obtain the corresponding eigenvalues as

$$
E = M\left[1 + \frac{\xi^2}{(\eta - 1/2)^2}\right]^{-1/2},
\tag{16.29}
$$

where

$$
\eta - 1/2 = \sqrt{j^2 - \xi^2} + n', \quad n' = 0, 1, 2, 3, \ldots,
\tag{16.30}
$$

which coincides with that of Eq. (15.29) when introducing the principal quantum number n. The eigenfunctions of this system can be obtained as shown in Chapter 14.

3.   Concluding remarks

In this Chapter we have reviewed the dynamic group for the Dirac equation with the hydrogen-like atoms in three dimensions. After that, making use of some results given in the previous Chapter, we have studied the realization of the dynamic group for the Dirac equation in two dimensions. We have found that the dynamic group is a non-compact Lie group SU(1, 1) for the radial wave functions. Before ending this Chapter, we make a few remarks here. First, we know from our recent work [569] that the radial wave functions of the Dirac equation with the Coulomb potential can be expressed by the combination of the associated Laguerre functions. As mentioned in Chapter 11, it is known that generally the hidden symmetry of the quantum systems has the SU(1, 1) dynamic group if their eigenfunctions can be expressed by the associated Laguerre functions. Consequently, such a conclusion is not surprising. Second, as we know the su(1, 1) and su(2) algebras are both real forms of the complex Lie algebra sl(2). However, we prefer to regard the representations as a unitary representation for the non-compact Lie algebra su(1, 1) since the unitary representation of this group is fundamental in quantum physics. Third, it should be pointed out that the dynamic group of the relativistic harmonic oscillator was studied by the Infeld-Hull factorization method [594]. This is a useful applications of the factorization method to the relativistic equations.

Chapter 17

ALGEBRAIC APPROACH TO KLEIN-GORDON EQUATION WITH THE HYDROGEN-LIKE ATOM IN 2+1 DIMENSIONS

1.   Introduction

As we know, the Klein-Gordon equation can be used to describe relativistic particles with spin zero. The exact solutions of non-relativistic and relativistic equations with a Coulomb potential have become an important subject in quantum mechanics [11, 215, 297]. During the past several decades, the Klein-Gordon equation with the Coulomb potential has been investigated in three dimensions (e.g., the operator analysis [595] and the bound Klein-Gordon particle in an intense laser field [596]), in two dimensions [575] and in one dimension [558–560]. However, with the interest in the higher-dimensional field theory, the Schrödinger equation [495, 597–602] and the Dirac equation [603] with the Coulomb potential have been studied in $D + 1$ dimensions. The Klein-Gordon equation with the Coulomb potential in $D + 1$ dimensions has been discussed by the associated Laguerre equation approach [495] and the large-N expansion approximate method [449].

The purpose of this Chapter is to study the Klein-Gordon equation with the Coulomb potential in the two dimensional spaces with the algebraic method as used in Refs. [589, 604].

This Chapter is organized as follows. Section 2 is devoted to the derivation of the eigenfunctions and eigenvalues. The dynamical group SU(1, 1) is realized in Section 3. Some concluding remarks are given in Section 4.

2.   Exact solutions

For simplicity the atomic units $\hbar = c = 1$ are employed. Considering the motion of a particle in a spherically symmetric Coulomb potential $V(r)$, we

take the time-independent Klein-Gordon equation as [215]

$$\left\{ - \nabla^2 + M^2 \right\} \Psi(\mathbf{r}) = [E - V(r)]^2 \Psi(\mathbf{r}), \qquad (17.1)$$

where M and E denote the mass and the energy of the particle, respectively. The Coulomb potential is taken as $V(r) = -\xi/r \ (\xi = Z\alpha)$.

Let

$$\Psi(r, \varphi) = R_m(r) e^{\pm m\varphi}, \qquad m = 0, 1, 2, \ldots. \qquad (17.2)$$

Substitution of this into (17.1) allows us to obtain

$$\left[-\frac{1}{r}\frac{d}{dr}\left(r\frac{d}{dr}\right) + \frac{m^2}{r^2} \right] R_m(r) = \left[\left(E + \frac{\xi}{r}\right)^2 - M^2 \right]. \qquad (17.3)$$

Before proceeding further, it is convenient to introduce the following notations

$$\rho = \beta r, \quad \beta = 2\sqrt{M^2 - E^2}, \quad \lambda = \frac{2E\xi}{\beta} = \frac{E\xi}{\sqrt{M^2 - E^2}} = \frac{w}{4}. \qquad (17.4)$$

Substitution of these parameters into (17.3) leads to

$$\frac{d^2}{d\rho^2} R_m(\rho) + \frac{1}{\rho}\frac{d}{d\rho} R_m(\rho) - \frac{1}{\rho^2}(m^2 - \xi^2) R_m(\rho) + \frac{\lambda}{\rho} R_m(\rho) - \frac{1}{4} R_m(\rho) = 0. \qquad (17.5)$$

From the behaviors of the wave functions at the origin and at infinity, we take the wave functions of the form

$$R_m(\rho) = \rho^\kappa e^{-\rho/2} G_m(\rho), \quad \kappa = \sqrt{m^2 - \xi^2}. \qquad (17.6)$$

Substitution of this into (17.5) allows us to obtain

$$\frac{d^2}{d\rho^2} G_m(\rho) + \left(\frac{2\kappa + 1}{\rho} - 1\right)\frac{d}{d\rho} G_m(\rho) - \frac{\kappa - \lambda + 1/2}{\rho} G_m(\rho) = 0, \quad (17.7)$$

whose solutions are confluent hypergeometric functions $G_m(\rho) = cF(\kappa - \lambda + 1/2, 1 + 2\kappa; \rho)$ with a constant c. Thus, the eigenfunctions can be expressed as

$$R_m(\rho) = c\rho^\kappa e^{-\rho/2} F(\kappa - \lambda + 1/2, 1 + 2\kappa; \rho). \qquad (17.8)$$

From consideration of the finiteness of the solutions, it is shown from Eq. (17.8) that the general quantum condition is given by

$$\kappa - \lambda + 1/2 = -n', \quad n' = 0, 1, 2, \ldots. \qquad (17.9)$$

By introducing the principal quantum number

$$n = m + n' + 1, \qquad n = 1, 2, 3, \ldots, \tag{17.10}$$

from which, together with the results (17.4) and (17.9), we are able to obtain the eigenvalues as

$$E_{nm} = M \left[1 + \frac{\xi^2}{(\sqrt{m^2 - \xi^2} + n - m - 1/2)^2} \right]^{-1/2}. \tag{17.11}$$

Let us study the fine structure energy. This can be made evident by expanding this result in power of ξ^2. The corresponding result becomes

$$E_{nm} = M \left[1 - \frac{\xi^2}{2(n - 1/2)^2} - \frac{\xi^4}{2(n - 1/2)^4} \left(\frac{n - 1/2}{m} - \frac{3}{4} \right) \right], \tag{17.12}$$

where the first term on the right side is the rest energy $M(c^2 = 1$ in our conventions), the second one represents the energy from the solutions of the Schrödinger equation and the third one is the structure energy, which removes the degeneracy between the states with the same n.

On the other hand, using the normalization condition and Coulomb-like integral formula $J_{n,\alpha}^\beta$ (12.36), we may obtain the normalization constant c as

$$c = \frac{\alpha}{(2\kappa)! \Gamma(\lambda - \kappa + 1/2)} \sqrt{\frac{\Gamma(\lambda + \kappa + 1/2)(n - m - 1)!}{2\lambda}}. \tag{17.13}$$

By using the relation between associated Laguerre functions and the confluent hypergeometric functions (8.10), we can finally obtain the eigenfunctions as

$$R_m(\rho) = \alpha \left[\frac{(n - m - 1)!}{(2\lambda)\Gamma(\lambda + \kappa + 1/2)} \right]^{1/2} \rho^\kappa e^{-\rho/2} L_{n-m-1}^{2\kappa}(\rho). \tag{17.14}$$

3.   Realization of dynamic group SU(1, 1)

In general, we may use the recursion relations among the generalized Laguerre polynomials to obtain what appear to be the creation and annihilation operators for the radial wave functions $R_m(\rho)$, but we find that the variable ρ depends on n. Such a problem has been encountered in Chapter 12. The similar technique can be used to study the present problem, but we do not want to repeat it here for simplicity. In the following part, we are going to study the dynamic group of this system following Ref. [589].

As we know, the radial differential equation is actually a one-dimensional problem. Define new changes of the variables

$$\rho = x^2, \qquad R = x^{-1/2}Y. \tag{17.15}$$

Substituting them into (17.5) allows us to obtain

$$\frac{d^2R}{dx^2} + \frac{1}{x}\frac{dR}{dx} + \left[w - x^2 - \frac{4(m^2 - \xi^2)}{x^2}\right]R = 0, \tag{17.16}$$

which can be further modified to

$$-\frac{d^2Y}{dx^2} + \left(x^2 + \frac{s}{x^2}\right)Y = wY, \tag{17.17}$$

where

$$s = 4(m^2 - \xi^2) - \frac{1}{4}. \tag{17.18}$$

It is shown from [589] that the spectrum of such a second-order differential equation can be found by a noninvariance group SU(1, 1) of the two-dimensional Lorentz group.

Define

$$\hat{H} = p^2 + x^2 + \frac{s}{x^2} \tag{17.19}$$

where the momentum operator is defined by $p = -i\frac{d}{dx}$.

As shown in [589], we may define the following dynamic variables

$$\hat{L}_1 = \frac{1}{4}(\hat{H} - 2x^2), \quad \hat{L}_2 = \frac{1}{4}(x\,p + p\,x), \quad \hat{L}_3 = \frac{1}{4}\hat{H}, \tag{17.20}$$

from which we may derive the following commutation relations

$$[\hat{L}_1, \hat{L}_2] = -i\hat{L}_3, \quad [\hat{L}_2, \hat{L}_3] = i\hat{L}_1, \quad [\hat{L}_3, \hat{L}_1] = i\hat{L}_2, \tag{17.21}$$

which correspond to the commutation relations of the Lie algebra su(1, 1). In the calculation, we have used the relation

$$[x, p] = i. \tag{17.22}$$

The computation of the Casimir operator C leads to a constant

$$C = -\hat{L}_1^2 - \hat{L}_2^2 + \hat{L}_3^2 = \frac{1}{4}\left(s - \frac{3}{4}\right) = j(j+1), \tag{17.23}$$

where

$$j_\pm = -1/2 \pm \frac{1}{2}\sqrt{s + 1/4}. \tag{17.24}$$

For the present case, substitution of the s given in Eq. (17.18) into (17.24) allows us to obtain

$$j = -1/2 - \sqrt{m^2 - \xi^2}, \tag{17.25}$$

where we choose the negative value of the j as required by the su(1, 1) algebraic representation $D^+(j)$. The eigenvalues are determined by $\frac{1}{4}w = \lambda = -j + n'$. Essentially, it coincides with that of Eq. (17.11).

4. Concluding remarks

In this Chapter we have studied the exact solutions of the Klein-Gordon equation with the hydrogen-like atom in two dimensions and constructed the dynamic group SU(1, 1) for the radial wave functions. It should be noted that the present approach follows that of Ref. [589] not from the eigenfunctions.

Chapter 18

SUSYQM AND SWKB APPROACHES TO RELATIVISTIC DIRAC AND KLEIN-GORDON EQUATIONS WITH HYPERBOLIC POTENTIAL

1.   Introduction

It is known that the exactly solvable physical potentials have attracted much attention in quantum mechanics. The non-relativistic and relativistic equations have been solved for many physical potentials by using a variety of approaches such as the factorization method, group theoretical method, the SUSYQM and shape invariance and others. It should be noted that many of these approaches mentioned above could be formulated by rewriting them as some transformations to map the original wave equations into some second order ordinary differential equations, whose solutions are the special functions. On the other hand, it has been turned out that some well known solvable potentials with the shape invariance properties are exactly the same ones that can be obtained with the factorization method.

Up to now, the SWKB approximation has attracted some attention [100, 126–128, 605–616]. Following this method, many potentials have been solved exactly [88, 127, 128]. The Dirac equation with a Coulomb potential has been studied in three dimensions [100] by SUSY and shape invariance approaches. It should be pointed out that most of contributions mentioned above have been carried out in the framework of the Schrödinger equation with certain physical potentials.

With the recent interest in the relativistic equations with some physical potentials, many authors have solved the Klein-Gordon and Dirac equations with equal scalar and vector potentials, such as the Hulthén potential [617–619], the Morse potential [620], the Wood-Saxon potential [621], the $\tan^2(\pi\eta r)$ potential [622], the Pöschl-Teller, the reflection-less type potential [623, 624], the harmonic oscillator potential and others [625–629]. Recently, Chen [630]

has solved the Klein-Gordon and Dirac equations with the pseudoharmonic oscillator potential using SUSY and shape invariance approaches.

The purposes of this Chapter are the following. First, we solve the Klein-Gordon and Dirac equations with the hyperbolic potential $V_0 \tanh^2(r/d)$ [631] by SUSYQM and SWKB approaches and obtain the energy levels. Second, we apply the traditional approach, i.e. the hypergeometric differential equation approach to obtain the exact solutions of this system.

This Chapter is organized as follows. In Section 2 we study the Klein-Gordon and Dirac equations with potential $V_0 \tanh^2(r/d)$. Section 3 is devoted to obtaining the energy levels by using SUSYQM and SWKB approaches. In Section 4 we apply the traditional hypergeometric equation approach to obtain the eigenfunctions and energy levels simultaneously. We study the harmonic limit in Section 5. Some concluding remarks are given in Section 6.

2.   Relativistic Klein-Gordon and Dirac equations with hyperbolic potential $V_0 \tanh^2(r/d)$

The natural units $\hbar = c = 1$ are employed throughout this paper. We first recall the Klein-Gordon and Dirac equations with potential $V_0 \tanh^2(r/d)$. From Ref. [632], the Klein-Gordon equation with equal scalar and vector potentials can be expressed as

$$\left[-\nabla^2 - \left(E - \frac{V(r)}{2} \right)^2 \right] \psi(\mathbf{r}) = - \left(\mu + \frac{V(r)}{2} \right)^2 \psi(\mathbf{r}), \qquad (18.1)$$

with the potential

$$V(r) = V_0 \tanh^2(r/d), \qquad (18.2)$$

where V_0 is the depth of the well, d is related to the range of the potential and r gives the relative distance from the equilibrium position. Here E and μ represent the energy and rest mass of the particle, respectively.

Introduce

$$\rho = \frac{r}{d}, \qquad \psi(\mathbf{r}) = \frac{R(r)}{r} Y_{lm}(\theta, \varphi). \qquad (18.3)$$

Substitution of this into Eq. (18.1) allows us to obtain the following radial wave equation

$$\frac{d^2 R(\rho)}{d\rho^2} - \left[\frac{l(l+1)}{\rho^2} + d^2 \alpha_2 (\alpha_1 + V(\rho)) \right] R(\rho) = 0, \qquad (18.4)$$

where

$$\alpha_1 = \mu - E, \qquad \alpha_2 = \mu + E. \qquad (18.5)$$

We find that Eq. (18.4) cannot be solved exactly for the general angular momentum l except for S wave. For S wave ($l = 0$), however, we have

$$\frac{d^2 R(\rho)}{d\rho^2} - d^2 \alpha_2 (\alpha_1 + V(\rho)) R(\rho) = 0. \tag{18.6}$$

Before solving this equation, let us investigate the Dirac equation with scalar potential $s(r)$ and vector potential $v(r)$ described by

$$\{\alpha \cdot p + \beta[\mu + s(r)]\}\psi(\mathbf{r}) = [E - v(r)]\psi(\mathbf{r}), \tag{18.7}$$

where the wave function $\psi(\mathbf{r})$ is given by [633]

$$\psi(\mathbf{r}) = \begin{cases} \dfrac{1}{r}\begin{pmatrix} F(r)\phi_{jm_j}^A(\theta,\varphi) \\ iG(r)\phi_{jm_j}^B(\theta,\varphi) \end{pmatrix}, & \text{for } \kappa = j + \frac{1}{2}, \\[4mm] \dfrac{1}{r}\begin{pmatrix} F(r)\phi_{jm_j}^B(\theta,\varphi) \\ iG(r)\phi_{jm_j}^A(\theta,\varphi) \end{pmatrix}, & \text{for } \kappa = -(j + \frac{1}{2}), \end{cases} \tag{18.8}$$

where

$$\phi_{jm_j}^A(\theta,\varphi) = \frac{1}{\sqrt{2l+1}}\begin{pmatrix} \sqrt{l+m+1}\, Y_{lm} \\ \sqrt{l-m}\, Y_{l(m+1)} \end{pmatrix}, \tag{18.9}$$

$$\phi_{jm_j}^B(\theta,\varphi) = \frac{1}{\sqrt{2l+3}}\begin{pmatrix} -\sqrt{l-m+1}\, Y_{(l+1)m} \\ \sqrt{l+m+1}\, Y_{(l+1)(m+1)} \end{pmatrix}. \tag{18.10}$$

Substitution of Eq. (18.8) into Eq. (18.7) leads to a set of coupled radial wave equations

$$\frac{dF(r)}{dr} - \frac{\kappa}{r}F(r) = [\mu + E + s(r) - v(r)]\, G(r), \tag{18.11}$$

$$\frac{dG(r)}{dr} + \frac{\kappa}{r}G(r) = [\mu - E + s(r) + v(r)]\, F(r). \tag{18.12}$$

By taking

$$s(r) = v(r) = \frac{1}{2}V_0 \tanh^2(r/d) \tag{18.13}$$

and considering $\rho = r/d$, we have

$$\frac{dF(\rho)}{d\rho} - \frac{\kappa}{\rho}F(\rho) = d\,(\mu + E)\, G(\rho), \tag{18.14}$$

$$\frac{dG(\rho)}{d\rho} + \frac{\kappa}{\rho}G(\rho) = d\left(\mu - E + V_0 \tanh^2(\rho)\right) F(\rho). \tag{18.15}$$

Eliminating $G(\rho)$ from Eqs. (18.14) and (18.15) yields

$$\frac{d^2 F(\rho)}{d\rho^2} - \frac{\kappa \, (\kappa - 1)}{\rho^2} \, F(\rho) - d^2 \alpha_2 \, \left(\alpha_1 + V_0 \, \tanh^2(\rho) \right) \, F(\rho) = 0, \quad (18.16)$$

where α_1 and α_2 are given in Eq. (18.5). We find that Eq. (18.16) is the same as Eq. (18.6) essentially for S wave ($\kappa = 1$). We shall solve Eq. (18.6) by SUSYQM and SWKB methods below.

3.   SUSYQM and SWKB approaches to obtain eigenvalues

It is shown from Eq. (18.6) that this system has the following property

$$\hat{H} R(\rho) = \varepsilon R(\rho), \quad (18.17)$$

where

$$\hat{H} = -\frac{d^2}{d\rho^2} + v, \tanh^2(\rho), \quad \varepsilon = -d^2 \, \alpha_1 \, \alpha_2, \quad v = d^2 \, \alpha_2 \, V_0. \quad (18.18)$$

Following Ref. [634], introduce

$$\hat{A} = \frac{d}{d\rho} + w(\rho), \quad \hat{A}^+ = -\frac{d}{d\rho} + w(\rho), \quad \hat{H}_- = \hat{A}^+ \hat{A}, \quad (18.19)$$

where $w(\rho)$ is the superpotential. The identity $\hat{H} - \hat{H}_- = \epsilon_0$ allows us to obtain the following equation

$$\epsilon_0 - v \, \tanh^2(\rho) + w^2(\rho) - w'(\rho) = 0, \quad (18.20)$$

where ϵ_0 is the ground-state eigenvalue of the Hamiltonian $\hat{H}$. The solutions of this equation are

$$w(\rho) = b \tanh(\rho), \quad (18.21)$$

with the condition

$$\epsilon_0 = \frac{1}{2}(\sqrt{1 + 4\,v} - 1) = b. \quad (18.22)$$

The supersymmetric partner potentials can be obtained as

$$\begin{aligned} V_-(\rho) &= w(\rho)^2 - w'(\rho) = -b + b\,(b + 1)\,\tanh^2(\rho), \\ V_+(\rho) &= w(\rho)^2 + w'(\rho) = b + b\,(b - 1)\,\tanh^2(\rho). \end{aligned} \quad (18.23)$$

It is obvious to find that $V_-(\rho)$ and $V_+(\rho)$ are shape invariant,

$$\begin{aligned} V_+(\rho, b) &= b + (b - 1)\,b\,\tanh^2(\rho) \\ &= V_-(\rho, b - 1) + 2(b - 1) + 1 \\ &= V_-(\rho, b - 1) + R(\alpha_1), \end{aligned} \quad (18.24)$$

with

$$\alpha_0 = b, \quad \alpha_1 = b - 1, \quad \alpha_s = b - s,$$

$$R(\alpha_s) = 2\,\alpha_s + 1 = 2\,(b - s) + 1.$$

(18.25)

The eigenvalues of the Hamiltonian $\hat{H}_-$ are

$$E_n^{(-)} = \sum_{s=1}^{n} R(\alpha_s) = (2\,b - n)n,$$

(18.26)

which implies that the eigenvalues of the Hamiltonian $\hat{H}$ are given by

$$\varepsilon_n = E_n^{(-)} + \varepsilon_0 = 2\,b\,n - n^2 + b.$$

(18.27)

We now make use of the SWKB approach to obtain the eigenvalue ε_n by substituting $w(\rho)$ into SWKB quantization condition

$$\int_{\rho_L}^{\rho_R} \sqrt{E_n^{(-)} - (w(\rho))^2} d\rho = n\,\pi, \quad n = 0, 1, 2, \ldots,$$

(18.28)

where ρ_L and ρ_R are equal to $-\sqrt{E_n^{(-)}}$ and $\sqrt{E_n^{(-)}}$, respectively.

Introducing $z = \tanh(\rho)$, we may transform Eq. (18.28) to

$$\int_{z_L}^{z_R} \frac{1}{1 - z^2} \sqrt{(z - z_L)(z_R - z)} dz = n\,\pi,$$

(18.29)

where

$$z_L = -\frac{\sqrt{E_n^{(-)}}}{b}, \quad z_R = \frac{\sqrt{E_n^{(-)}}}{b}.$$

(18.30)

The integration of Eq. (18.29) gives

$$b\,\pi\left[1 - \sqrt{(1 - z_L)(1 - z_R)}\right] = n\,\pi,$$

(18.31)

from which we find that $E_n^{(-)}$ obtained from Eq. (18.31) is the same as Eq. (18.26).

4. Complete solutions by traditional method

As discussed above, we have obtained the energy levels by the SUSYQM and SWKB approaches. In this section we want to obtain both the energy levels and eigenfunctions simultaneously in terms of the traditional hypergeometric differential equation approach. It should be pointed out that one may obtain the exact solutions of this system by using the SUSYQM approach, but the calculation is tedious. More detailed discussions are shown in Ref. [73].

Let us reexpress Eq. (18.17) ($F(\rho) = R(\rho)$) as

$$\frac{d^2}{d\rho^2}F(\rho) + \frac{v}{\cosh^2(\rho)}F(\rho) + (\varepsilon - v)F(\rho) = 0. \qquad (18.32)$$

Introducing

$$\epsilon = \sqrt{-(\varepsilon - v)}, \quad v = b(b+1), \quad z = \tanh(\rho), \qquad (18.33)$$

equation (18.17) becomes

$$\frac{d}{dz}\left[(1-z^2)\frac{d}{dz}F(z)\right] + \left[b(b+1) - \frac{\epsilon^2}{1-z^2}\right]F(z) = 0, \qquad (18.34)$$

whose exact solutions have been obtained in Chapter 7 as

$$F(z) = \mathcal{N}(1-z^2)^{\epsilon/2}F[\epsilon - b, \epsilon + b + 1; \epsilon + 1; \frac{1}{2}(1 - z)], \qquad (18.35)$$

where the normalization constant $\mathcal{N}$ is to be determined below.

For $F(z)$ to remain finite for $u = 0$, we find the quantum condition

$$\epsilon - b = -n, \quad n = 0, 1, 2, \ldots, \qquad (18.36)$$

then $F[\epsilon - b, \epsilon + b + 1; \epsilon + 1; \frac{1}{2}(1 - z)]$ is the hypergeometric polynomials of degree n. In this case, the eigenvalues can be determined by the constraint condition $b - \epsilon = n$, from which, together with Eq. (18.33), we obtain the eigenvalues as

$$\varepsilon_n = 2nb - n^2 + b, \qquad (18.37)$$

which is the same as Eq. (18.27). The vibrational quantum number n taking odd or even values is determined by the properties of the wave functions as shown below [see Eq. (18.46)].

To calculate $\mathcal{N}$, using the relation between the hypergeometric functions and the associated Legendre polynomials (7.22) and substitution of it into (18.35) allows us to write the solutions in the form

$$F(z) = (-1)^{(n-b)}N_n^b P_b^{b-n}(z), \qquad (18.38)$$

where N_n^b is a normalization constant to be determined from the associated Legendre polynomials $P_b^{b-n}(z)$. Taking into account the orthogonality relation (7.24) with a weight factor $(1 - x^2)^{-1}$, we obtain

$$N_n^b = \sqrt{\frac{2n!(b-n)}{d(2b-n)!}}. \qquad (18.39)$$

The wave functions for this potential acquire the final form in terms of the associated Legendre polynomials

$$F(z) = \mathcal{N}_n^b P_b^{b-n}(z), \tag{18.40}$$

where

$$\mathcal{N}_n^b = (-1)^{(n-b)} \sqrt{\frac{2n!(b-n)}{d(2b-n)!}}. \tag{18.41}$$

On the other hand, in terms of Eq. (7.22) we may reexpress the wave functions as follows:

$$F(z) = \mathcal{N}(1-z^2)^{(b-n)/2} F(-n, 1+2b-n; 1+b-n; \frac{1-z}{2}), \tag{18.42}$$

with

$$\mathcal{N} = \frac{1}{2^{b-n}n!(b-n)!} \sqrt{\frac{2n!(b-n)(2b-n)!}{d}}. \tag{18.43}$$

We find that Eq. (18.42) is same as Eq. (18.35) essentially since $\epsilon = b - n$.

In order to determine whether the vibrational quantum number n appearing in Eq. (18.27) is odd or even, we may use the relation between the Gegenbauer polynomials and the hypergeometric functions (18.35) to express the wave functions Eq. (18.35) as

$$F(z) = \mathcal{C}(1-z^2)^{(b-n)/2} C_n^{b+\frac{1}{2}-n}(z), \tag{18.44}$$

where $\mathcal{C}$ is the normalization constant to be determined. In terms of Eqs. (18.42) - (18.44) and the formula (7.35), we are able to obtain

$$\mathcal{C} = \frac{2^{b-n}(b-n-\frac{1}{2})!}{\pi^{\frac{1}{2}}} \sqrt{\frac{2n!(b-n)}{d(2b-n)!}}. \tag{18.45}$$

Let us analyze Eq. (18.44) in order to determine whether the vibrational quantum number n is odd or even. Before proceeding further, let us first review the following properties of the Gegenbauer polynomials [635]

$$C_n^\nu(0) = \begin{cases} 0, & n \text{ odd} \\ (-1)^m \frac{\Gamma(\nu+m)}{\Gamma(\nu)\Gamma(m+1)}, & n \text{ even } (n = 2m), \end{cases} \tag{18.46}$$

which implies that the vibrational quantum number n must be taken to have *odd* integer value since the wave functions $F(z)$ have to satisfy the boundary condition $F(0) = 0$ at $z = 0$ ($\rho = 0$ or $r = 0$). Therefore, the integer n appearing in all of the above equations must be replaced by $2n + 1$.

Introducing

$$\gamma = \sqrt{\alpha_2(\alpha_1 + V_0)} \equiv \frac{b-n}{d}, \qquad (18.47)$$

from Eqs. (18.3), (18.11), (18.35) and (18.47), we are able to reexpress the radial wave functions as

$$
\begin{aligned}
R(r) \;&=\; \frac{1}{r}\,[\cosh(r/d)]^{-d\gamma/2} \\
&\times F\!\left(-(2\,n+1),2\,(n+1+d\,\gamma);1+d\,\gamma;\tfrac{1-\tanh(r/d)}{2}\right) \\
&=\; \frac{\Gamma(1+2\,d\,\gamma)(2\,n+1)!}{\Gamma[2(n+1+d\gamma)]}\frac{1}{r}[\cosh(r/d)]^{-d\gamma/2} \\
&\times C_{2\,n+1}^{\frac{1}{2}+d\gamma}(\tanh(r/d))
\end{aligned}
\qquad (18.48)
$$

for the Klein-Gordon equation, and

$$
\begin{aligned}
F(r) \;&=\; [\cosh(r/d)]^{-d\,\gamma/2} \\
&\times F\!\left[-(2\,n+1),2\,(n+1+d\,\gamma);1+d\,\gamma;\tfrac{1-\tanh(r/d)}{2}\right] \\
&=\; \frac{\Gamma(1+2\,d\,\gamma)(2n+1)!}{\Gamma[2(n+1+d\gamma)]}\,[\cosh(r/d)]^{-d\,\gamma/2} \\
&\times\, C_{2n+1}^{\frac{1}{2}+d\,\gamma}[\tanh(r/d)],
\end{aligned}
\qquad (18.49)
$$

$$
\begin{aligned}
G(r) \;&=\; -\frac{1}{\alpha_2}[\cosh(r/d)]^{-d\gamma/2}\Big\{\frac{1}{r} \\
&\times F\!\left[-(2\,n+1),2\,(n+1+d\,\gamma);1+d\,\gamma;\tfrac{1-\tanh(r/d)}{2}\right] \\
&-\frac{(1+2n)(1+n+d\,\gamma)}{d(1+d\,\gamma)\cosh^2(r/d)} \\
&\times F\!\left[-2\,n,2\,n+3+2\,d\,\gamma;2+d\,\gamma;\tfrac{1-\tanh(r/d)}{2}\right] \\
&+\gamma\,\tanh(r/d) \\
&\times F\!\left[-(2\,n+1),2\,(n+1+d\,\gamma);1+d\,\gamma;\tfrac{1-\tanh(r/d)}{2}\right]\Big\} \\
&=\; \frac{\Gamma(1+2\,d\,\gamma)\,(2n+1)!}{d\,\alpha_2\,\Gamma[2(n+1+d\gamma)]}[\cosh(r/d)]^{-(2+d\,\gamma/2)} \\
&\times\Big\{(1+2\,d\,\gamma)C_{2\,n}^{3/2+d\,\gamma}(\tanh(r/d)) - d\,\cosh(r/d) \\
&\quad\left[\frac{1}{r}\,\cosh(r/d)+\gamma\sinh(r/d)\right]C_{2\,n+1}^{\frac{1}{2}+d\,\gamma}(\tanh(r/d))\Big\}
\end{aligned}
\qquad (18.50)
$$

for the Dirac equation.

On the other hand, replacing n by $2n + 1$ in Eq. (18.47) and considering Eqs. (18.5) and (18.22), we are able to obtain the following energy equation

$$4n + 3 + 2\, d\sqrt{(\mu + E)(\mu - E + V_0)} = \sqrt{1 + 4\, d^2\, V_0(\mu + E)}. \quad (18.51)$$

5. Harmonic limit

Generally speaking, we can solve Eq. (18.51) exactly for E, but the expression of E is too complicated to reveal its physical meaning. In the following part, we discuss the energy equation in the harmonic limit.

For this purpose, we expand the potential $V_0\, \tanh^2(r/d)$ as the power series of r as follows

$$V(r) = \frac{V_0\, r^2}{d^2} - \frac{2\, V_0\, r^4}{3\, d^4} + \mathcal{O}(r)^6. \quad (18.52)$$

As we know, for a particle moving at the bottom of the potential well, we have $r \ll d$. By only taking the first term of Eq. (18.52), i.e. identifying it as a harmonic oscillator, we obtain the relations between the proper frequency or elastic coefficient of the harmonic oscillator and the maximum V_0 of the potential as follows

$$V_0 = \frac{1}{2}\mu\, d^2\, \omega^2 = \frac{1}{2}\, d^2\, k. \quad (18.53)$$

Moreover, for the kinetic energy of the particle moving in the potential well, we have $E_k = E - \mu \ll V_0$. As discussed above, we know that V_0 and d are infinitely large in comparison with the variable r.

In order to further investigate the relation between $V_0\, \tanh^2(r/d)$ and the harmonic oscillator potential, let us review the main results given in Ref. [605]. The energy equations of a relativistic harmonic oscillator are given by

$$(4\, n + 2\, l + 3)\sqrt{k} - (E - \mu)\, \sqrt{2\, (\mu + E)} = 0, \quad \text{for Klein} - \text{Gordon},$$
$$(4\, n + 2\, \kappa + 1)\sqrt{k} - (E - \mu)\, \sqrt{2\, (\mu + E)} = 0, \quad \text{for Dirac},$$
$$(18.54)$$

where $n = 0, 1, 2, \ldots$. For S wave, i.e. $l = 0$ or $\kappa = 1$, we find that Eq. (18.54) can be unified as the form

$$(4\, n + 3)\, \sqrt{k} + (\mu - E)\, \sqrt{2\, (\mu + E)} = 0, \quad (18.55)$$

from which we are able to obtain

$$E = \frac{1}{12}\left[4\mu + \frac{16\, \sqrt[3]{4}\mu^2}{\xi} + \sqrt[3]{16}\xi\right], \quad (18.56)$$

with

$$\xi = \left\{ 27k(3+4n)^2 - 32\mu^3 + \sqrt{27k(3+4n)^2[27k(3+4n)^2 - 64\mu^3]} \right\}^{1/3}.$$

(18.57)

On the other hand, we may obtain Eq. (18.55) in terms of Eq. (18.51) by assuming that the parameters V_0 and d are very large. To this end, we may modify Eq. (18.51) as

$$4n + 3 + \sqrt{2}\, d\, \sqrt{2\,\alpha_2} \left(\sqrt{\alpha_1 + V_0} - \sqrt{V_0 + \frac{1}{4\,d^2\,(2\,\mu - \alpha_1)}} \right) = 0, \quad (18.58)$$

which can be rewritten as

$$4n + 3 + d\sqrt{2}\,\sqrt{2\,\alpha_2}\, f(\alpha_1) = 0, \tag{18.59}$$

with

$$f(\alpha_1) = \sqrt{V_0 + \alpha_1} - \sqrt{V_0 + \frac{1}{4\,d^2\,(2\,\mu - \alpha_1)}} \approx \sqrt{V_0 + \alpha_1} - \sqrt{V_0}. \quad (18.60)$$

By expanding $f(\alpha_1)$ as the power series of α_1 and only taking the first term, we have

$$f(\alpha_1) \approx \frac{1}{2\sqrt{V_0}}\,\alpha_1. \tag{18.61}$$

Substitution of Eqs. (18.5), (18.53) and (18.61) into Eq. (18.59) allows us to obtain Eq. (18.55) again.

6.   Concluding remarks

In this Chapter we have studied the properties of the Klein-Gordon and Dirac equations with the hyperbolic potential $V_0 \tanh^2(r/d)$. It is interesting to find that the master equations for the Klein-Gordon and Dirac equations with this potential for the S wave are unified by same second order differential equation. We have obtained the energy levels by SUSYQM and SWKB approaches. On the other hand, we have applied the traditional hypergeometric differential equation approach to solve the master equation and obtained the energy levels and eigenfunctions simultaneously. We have found that the vibrational quantum number n for the energy levels is restricted to have odd values only by studying the properties of the eigenfunctions expressed by the Gegenbauer polynomials at the origin. Also, we have discussed the harmonic limit of this system in the case of the large V_0 and d and found that the energy equation becomes that of the Klein-Gordon and Dirac equations with the harmonic oscillator potential [625–628].

PART V

QUANTUM CONTROL

Chapter 19

CONTROLLABILITY OF QUANTUM SYSTEMS FOR THE MORSE AND PT POTENTIALS WITH DYNAMIC GROUP SU(2)

1. Introduction

With the revolution of the microelectronic processing power, the study of the quantum control theory for the manipulation of a quantum system state has been the subject of interest [636]. Since the pioneering work on the quantum computation by DiVincenzo [637], the investigation of quantum control has attracted much attention of many authors [636–676]. Almost all of these studies are motivated by the recent advances in the field of the nuclear magnetic resonance and laser spectroscopy, e.g., the quantum control by laser pulse can now be realized experimentally [638]. Recently, Ramakrishna and Rabitz have shown how sequences of short laser pulses can be applied to control the state of a molecule with a given Hamiltonian through a unitary operator representing quantum evolution [639]. In addition, the nondegenerate quantum control problem has been solved analytically by [640]. The quantum state control via tunnelling in a double-well optical potential has been reported [641]. It is shown by these works that the quantum control has been widely applied to molecular and atomic physical problems and that much attention has been paid to the problem of a quantum system with nondegenerate eigenstates.

The reasons why the great efforts have been made in this field are the following. First, it is possible to understand the basic physics associated with the quantum structures such as the quantum fluctuation and other quantum effects and to explore their controllability and design new species of useful devices. Therefore, the investigation in this recently sprung up field becomes exciting and potential. Second, the quantum control is a kind of underlying technology which makes quantum computation possible. In turn, the quantum information processing may provide the quantum control with many novel techniques for performing feedback and state estimation with possible applications to

algorithmics, quantum cryptographic protocols, quantum interrogation or potential applications in nanotechnology and nanoscience, etc. Third, the study along this line is possibly used to investigate the problem of controlling a two-level quantum system in implementations of quantum computer.

As we know, one of its objects is to drive an initial state of a given quantum system to a selected target state at any chosen time under the guidance of the laser pulses. In quantum control problems, some mathematical tools including the algebraic, group theoretical and topological methods are necessary and useful. The reason originates from the fact that the system's quantum Hamiltonian, sometimes, is associated to the Lie algebra. That a quantum system is completely controllable or not depends on the knowledge of the Lie algebra generated by the system's quantum Hamiltonian and the corresponding properties of the Lie group structure [642]. In addition, it is well known that the system displaying a dynamic symmetry can be solved with algebraic techniques [117, 677]. Moreover, the controllability of the quantum system with the dynamic group could be realized [636, 639, 642–649, 654, 656]. We can thus establish the relation between a given quantum system and its controllability through the hidden dynamic symmetry.

Motivated by the recent work on the controllability of the quantum system for the PT potential with the Lie group SU(1, 1) [678] and our approach with the Lie group SU(2) [158], we want to investigate the controllability of a quantum system for the Morse potential due to its importance in molecular physics.

This Chapter is organized as follows. In Section 2 the preliminaries on control theory are reviewed. In Section 3 we analyze the controllability of this quantum system with the SU(2) group. The concluding remarks are given in Section 4.

2. Preliminaries on control theory

Generally speaking, the quantum system whose state $\psi(t)$ evolves from the initial state $\psi(t = 0) = \psi_0$ can be described by the time-dependent Schrödinger equation as

$$i\hbar \frac{d}{dt}\psi(t) = H\psi(t), \tag{19.1}$$

where H is the Hamiltonian operator with the form

$$H = H_0 + \sum_{i=1}^{m} H_i u_i(t), \tag{19.2}$$

where $u_i(t)$ are control functions of the quantum system. The H_0 describes the Hamiltonian of free evolution for the given quantum system, while the H_i can be interpreted as the effect of the external perturbations which are sufficiently weak in comparison with that of the H_0. The energy levels thus are

not changed significantly by the perturbations. Additionally, from the point of view of quantum theory, imposing unit norm at the initial time $t = 0$, we have $\langle \psi(t)|\psi(t)\rangle = 1 \; \forall t$, which means that the system evolves on the unit sphere $S_{\mathcal{H}}$ in the Hilbert space $\mathcal{H}$. On the other hand, it should be pointed out that the control system (19.1) divided by $i\hbar$ was denoted by Jurdjevic and Sussmann as (X, U) in their classic work [654], where X denotes the right-invariant vector field on the Lie group and U the control functions. Such a slight deformation, in principle, can not change the essence of the control system. To address the existence issue systematically, it is necessary to precise the reachable sets and controllability . For simplicity, we recall some most fundamental and necessary definitions and theorems, which are useful for analyzing the controllability of the Morse quantum system with the SU(2) group. For more information, we strongly refer the reader to Refs. [636, 654].

Definition: For the initial state ψ_0 and the final state ψ_f with the properties $\psi_0, \psi_f \in M$, where M represents the finite or infinite-dimensional differential manifold. We say that the state ψ_f is reachable from the initial state ψ_0 at time t_f if there exists a control $U(t)$ such that $\psi(t = t_f|u, \psi_0) = \psi_f$. The corresponding states are denoted as $R_{t_f}(\psi_0)$. The set of states reachable from the initial one ψ_0 at some positive time t are $R(\psi_0) = \cup_{t>0} R_t(\psi_0)$.

This concept has become one of the cornerstones of mathematical systems theory. It has also become a discipline widely accepted in classical dynamics.

Definition: We say that the studied control system is strongly completely controllable if $R_t(\psi_0) = M, \forall t > 0, \forall \psi_0 \in M$. The system is completely controllable if $R_t(\psi_0) = M, \forall \psi_0 \in M$.

Theorem 1 (see [679]): If $dim \; \mathcal{L}_s(m) = d$ holds for all $m \in M$, then the quantum system (1) is strongly completely controllable, where $\mathcal{L}_s$ is the Lie algebra and it is assumed $dim \; M = d < \infty$.

This theorem was given by Kunita [679] and applied by Huang, Tarn, Clark [636] and others. This theorem means that the dimensions d of the Lie algebra generated by the studied quantum system is finite not infinite.

Theorem 2 (see [654]): A necessary condition for (X, U) to be controllable is that the Lie group G is connected and that the Lie algebra $L = L(G)$. If G is compact, or if the system is homogeneous, the condition is also sufficient.

Theorem 3 (see [654]): Let G be compact, and let (X, U) be controllable. Then there exists $t > 0$ such that, for every $g \in G, g' \in G$, there is a control that steers g into g' in less than t units of time. If G is semisimple, then there exists $t > 0$ such that, for every $g \in G, g' \in G$, there is a control that steers g into g' in exactly t units of time.

3. Analysis of the controllability

We now analyze the controllability of this quantum system. It is shown from Eq. (6.6) and (6.45) that, for a given quantum number ν, the E will change

with the quantum number $m(m \leq |j|)$. The quantum number j is related with the parameter V_0 of the Morse potential as shown in Eq. (6.6). It is shown from Eq. (6.44) that the Casimir operator C keeps invariant for a given j. The Hamiltonian $H_0 \propto -m^2$ with the constraint $m \leq |j|$ as shown in Eq. (6.47). As addressed in Ref. [678], if the free evolution is driven by a Casimir invariant, the control Hamiltonian can be physically realized by the group generators $\hat{K}_{\pm,0}$, the quantum system can be guaranteed to be strongly analytically controllable. In physical language, this quantum system can be solved from the combination of the ladder operators as shown in Eq. (6.47). More importantly, it is found from Eq. (6.49) that the eigenfunctions of this system can be obtained directly by acting the $\hat{K}_+$ on the ground state $\Psi_0^\nu(u)$. The transition from the initial state to the selected target can be realized theoretically and experimentally [638, 639]. Therefore, the controllability of this quantum system will confirm powerfully that such a combination exist.

We now construct the control system

$$\frac{d\psi(t)}{dt} = [H_0 + u_1(t)(\hat{K}_+ - \hat{K}_-) + i\, u_2(t)(\hat{K}_+ + \hat{K}_-)]\psi(t), \quad \psi(0) = \psi_0, \tag{19.3}$$

where the quantities $\psi(t)$ and ψ_0 should be interpreted as abstract state vectors rather than wave functions since the eigenfunctions of the quantum system can form finite-dimensional Hilbert spaces, which construct the compact Lie group SU(2), namely, the quantum system evolves in the finite-dimensional state spaces with the dimensions $2j + 1$. On the other hand, it is shown from Eq. (19.3) that $H_1 = \hat{K}_+ - \hat{K}_-$ and $H_2 = i(\hat{K}_+ + \hat{K}_-)$ as done in [678]. Accordingly, it is shown from **Theorems 1, 2** and **3** that this quantum system is strongly completely controllable since su(2) algebra generated by H_0, H_1 and H_2 is connected, compact and finite-dimensional Hilbert space with the dimensions $2j + 1$.

On the other hand, since the PT quantum system has the same dynamic structure as that of the Morse potential, we may draw the conclusion that the PT potential quantum system is also strongly controllable.

4.   Concluding remarks

The controllability of the Morse system with a compact Lie group SU(2) is investigated. Based on those well known theorems for the control theory, we have found that this quantum system with the nondegenerate discrete bound states can, in principle, be strongly completely controlled. That is to say, the system eigenfunction can be guided by the external field to approach an arbitrarily selected target state at any chosen time, which can be realized by acting the ladder operators on the ground state.

Chapter 20

CONTROLLABILITY OF QUANTUM SYSTEM FOR THE PT-LIKE POTENTIAL WITH DYNAMIC GROUP SU(1, 1)

1.   Introduction

As we know, most of contributions to quantum control are primarily focused on investigating the controllability of pure states for some quantum systems. Due to the importance of some general mixed states in the control of temperature distribution in systems and the need to include dissipative effects, however, the controllability of the mixed states has been studied by Schirmer *et al.* [680–683], in which they have investigated the criteria for reachability of quantum states and the constructive control of quantum systems using factorization of unitary operators. In this work, however, we restrict ourselves to study the controllability of pure states with the group theoretical method [157, 158, 678, 684], in which the controllability of quantum systems with dynamic groups SU(2) and SU(1, 1) has been investigated.

Up to now, the quantum control theory has been developed well for the closed quantum systems governed by the time-dependent Schrödinger equation [157, 158, 636, 639, 642–649, 656, 684, 685], in which the state $\Psi(t)$ evolving from the initial state can be described by the Schrödinger equation $i\hbar \, d\Psi(t)/dt = H\Psi(t)$. The state $\Psi(t)$ can be realized by acting a unitary time-evolution operator $U(t) = e^{-iHt/\hbar}$ on the initial state Ψ_0, i.e., $\Psi(t) = U(t)\Psi_0$.

In general, we restrict our attention to the closed quantum systems and not to the open quantum systems, since it is possible to find a dynamic Lie algebra for pure states of the closed quantum systems. Once a suitable dynamic Lie algebra could be found in the studied quantum system, we might use some well known theorems on the control theory to investigate the controllability of quantum system. Consequently, this will force us to employ some necessary and useful mathematical tools including the algebraic, group theoretical and topological methods for studying the quantum control problem since the sys-

tem's quantum Hamiltonian, sometimes, is associated to the Lie algebras such as the compact Lie algebra su(2) or noncompact su(1, 1) Lie algebra for one-dimensional quantum system. For many quantum systems, however, the Lie algebra is not known. The determination of the Lie algebra has become one of main questions in quantum control for quantum systems. Generally speaking, it is possible to realize the dynamic Lie algebra for the studied quantum system by factorization method, the SUSYQM and others.

Recently, the controllability of quantum system with the dynamic Lie algebra has been studied [157, 158, 636, 639, 642–649, 654, 656, 678, 684–690]. The conditions on the quantum control depend on the quantum system being closed or open, the quantum states being pure or mixed, the dynamic Lie algebra being compact or noncompact. With this spirit, for example, Tarn *et al.* have studied the controllability of the quantum system for the MPT potential based on the non-compact Lie algebra su(1, 1) [678]. Recently, the controllability of the quantum system for the Morse potential has been studied by the non-compact dynamic group SU(1, 1) [684] and the compact group SU(2) [157]. For the MPT potential, we have used the compact dynamic group SU(2) to study the controllability of the MPT quantum system with the discrete nondegenerate bound states [158]. The study of the controllability of the Morse and MPT systems has been investigated in previous Chapter.

The purposes of this Chapter are the following. First, we review basic control theory in order to study the controllability of the PT-like quantum system. Second, we employ some well known theorems of the control theory about the SU(1, 1) group to investigate the controllability of this quantum system following the similar approaches used in Refs. [678, 684].

This Chapter is organized as follows. Section 2 is devoted to reviewing some fundamental control theories. In Section 3 we analyze the controllability of this quantum system with the noncompact SU(1, 1) group. Some concluding remarks are given in Section 4.

2.   **Preliminaries on the control theory**

Generally speaking, the quantum system whose state $\Psi(t)$ evolves from the initial state Ψ_0 can be described by the time-dependent Schrödinger equation as

$$i\hbar\frac{d}{dt}\Psi(t) = H\Psi(t) = \left(H_0 + \sum_{i=1}^{m} H_i u_i(t)\right)\Psi(t), \qquad (20.1)$$

where $u_i(t)$ are control functions of the quantum system. Through adjusting these control functions, it is possible to guide the time development of the state $\Psi(t)$ so as to attain a specified target. In general, the state vector $\Psi(t)$ could be expressed by a unitary transformation $U(t)\exp[-iHt/\hbar] = \exp[\hat{H}t]$ ($\hbar =$

1) acting on the initial state Ψ_0, where we have denoted the skew-Hermitian counterpart $-iH$ of H by $\hat{H}$ as done by Clark *et al.*[685] [1].

Before proceeding further, let us recall some most fundamental and necessary definitions and theorems in order to study the PT-like quantum system. The more information and a rigorous treatment on the subject can be found in references [636, 678, 684, 685].

Definition 1: For the initial state Ψ_0 and the final state Ψ_f with the properties $\Psi_0, \Psi_f \in M$, where M represents the finite or infinite-dimensional differential manifold. We say that the state Ψ_f is reachable from the initial state Ψ_0 at time t_f if there exists a control $u(t)$ such that $\Psi(t = t_f | u, \Psi_0) = \Psi_f$. The corresponding states are denoted as $R_{t_f}(\Psi_0)$. The set of states reachable from the initial one Ψ_0 at some positive time t are $R(\Psi_0) = \cup_{t>0} R_t(\Psi_0)$.

This concept has become one of the cornerstones of mathematical system theory. It has also become a discipline widely accepted both in classical dynamics and in quantum control theory . What this definition is concerned with is that the final state Ψ_f can be obtained from the initial state Ψ_0 at time t_f through a control $u(t)$.

Definition 2 (see Refs. [636, 678, 685]): We say that the studied control system is strongly completely controllable if $R_t(\psi_0) = M$ holds for all times $t > 0$ and all $\psi_0 \in M$. The system is completely controllable if $R(\psi_0) = M$ holds for all $\psi_0 \in M$.

Generally speaking, the controllability for the pure states is a weaker concept than that for the mixed states [680–683]. The concept of the complete controllability has also been defined by Schirmer *et al.*[680–683], which need not be repeated here since our present work is restricted to the controllability of the pure states. We find, from this definition, that there exists the difference between the strongly complete controllability and the complete controllability since the latter has nothing with the time $t > 0$.

On the other hand, it should be noted that the M can form a differential manifold, finite or infinite-dimensional [687, 688]. If the initial and target states are restricted to a subset of manifold M and an analytical domain D_ω, we can introduce a modified definition of controllability as given by Tarn *et al.* [636, 678, 685]:

Definition 3: Let ψ_0 be an analytical vector belonging to an analytical domain D_ω that is dense in the state space. Then the control system (1) is strongly analytically controllable on $M \subseteq S_{\mathcal{H}}$ if $R_t(\psi_0) = M \bigcap D_\omega$ holds for all $t > 0$ and all $\psi_0 \in M \bigcap D_\omega$.

Definition 4 (see Refs. [636, 678]): An element ω of $\mathcal{H}$ is called an analytical vector of the operator A in $\mathcal{H}$ if the series expansion of $e^{sA}\omega$ in the real parameter

s has a positive radius of absolute convergence,

$$\sum_{n=0}^{\infty} ||A^n \omega|| \frac{s^n}{n!} < \infty. \tag{20.2}$$

Note: If the operator A is bounded, all vectors of $\mathcal{H}$ are trivially analytical vectors.

Definition 5 (see Refs. [636, 678]): An element ω of $\mathcal{H}$ is called an analytical vector for the Lie algebra $\mathcal{L}$ if the series

$$\sum_{n=0}^{\infty} \sum_{\substack{0 \leq n_1, n_2, \ldots, n_d \leq \infty \\ n_1 + \ldots + n_d = n}} \sum_{1 \leq i_1 < \ldots < i_d \leq d} ||\hat{H}_{i_1}^{n_1} \ldots \hat{H}_{i_d}^{n_d} \omega|| \frac{s^n}{n!} \tag{20.3}$$

is absolutely convergent for some $s > 0$ and some linear basis $\hat{H}_{(1)}, \ldots, \hat{H}_{(d)}$ of Lie algebra $\mathcal{L}$.

We now recall some preliminary results as follows.

HTC Corollary(see Refs. [636, 678, 685]): Let $C = \{ad_{\hat{H}_0}^j \hat{H}_l | l = 1, 2, \ldots, m; j = 0, 1, \ldots\}_{LA}$ be the ideal in the Lie Algebra $\mathcal{A} = \{\hat{H}_0, \hat{H}_1, \ldots, \hat{H}_m\}_{LA}$ generated by $\hat{H}_1, \ldots, \hat{H}_m$. The system, with piecewise constant controls, is strongly analytically controllable on M provided that (i) $[\mathcal{C}, \mathcal{B}] \subset \mathcal{B}$ and (ii) $dim\, \mathcal{C}(\phi) = d < \infty$ for all $\phi \in M \cap D_\omega$.

The first condition of this Corollary means that $X \in \mathcal{C}, Y \in \mathcal{B}$ implies that $[X, Y] \in \mathcal{B}$; namely, the Lie algebra $\mathcal{B}$ must be an ideal in $\mathcal{C}$. The second one means that the tangent space associated with $\mathcal{C}$ at all points ϕ have constant, finite dimension d for all $\phi \in M \bigcap D_\omega$.

It should be pointed out that the analytical domain D_ω is a set of state vectors with three properties [636, 678, 685]: (i) D_ω is dense in the Hilbert space $\mathcal{H}$, (ii) D_ω keeps invariant under the given operators $\hat{H}_i$ (with $i = 0, 1, 2, \ldots, m$) and (iii) the solutions of the Schrödinger equation (1) could be expressed in exponential form on the domain D_ω, which allows us to write the unitary time-evolution operator $U(t)$ with the form (20.2) in the context of piecewise-constant controls.

More important, the existence of an analytical domain D_ω is guaranteed by Nelson's Theorem [687, 688]:

Nelson Theorem : Let $\mathcal{L}$ be a Lie algebra of skew-Hermitian operators in a Hilbert space $\mathcal{H}$, the operator basis $\hat{H}_1, \ldots, \hat{H}_d$, $d < \infty$, of $\mathcal{L}$ having a common invariant dense domain. If the operator $T = \hat{H}_1^2 + \ldots + \hat{H}_d^2$ is essentially self-adjoint, then there exists a unitary group Γ on $\mathcal{H}$ with Lie algebra $\mathcal{L}$. Let $\bar{T}$ denote the unique self-adjoint extension of T, then it furthermore follows that the analytical vectors of $\bar{T}$ (i) are analytical vectors for the whole Lie algebra $\mathcal{L}$ and (ii) form a set invariant under Γ and dense in $\mathcal{H}$.

This theorem essentially establishes the existence of a dense domain D_ω of analytical vectors that provide a foothold for the extension of the some results

of the controllability for the finite-dimensional spaces of the classic dynamics to the given quantum system. For the limited space, the reader is strongly advised to consult the original work by Nelson or Barut *et al.* for the underlying motivation and the detailed development of the concepts of the analytical vector and analytical domain D_ω [687, 688].

Assuming the existence of an analytical domain D_ω, Huang, Tarn, and Clark in their classical work [636] could derive sufficient conditions for controllability of a studied quantum system in order to characterize the reachable sets $R_t(\psi_0)$ and $R(\psi_0)$ by three Lie algebras

$$\mathcal{A} = \{\hat{H}_0, \hat{H}_1, ..., \hat{H}_m\}_{LA},$$
$$\mathcal{B} = \{\hat{H}_1, \hat{H}_2, ..., \hat{H}_m\}_{LA}, \qquad (20.4)$$
$$\mathcal{C} = \{ad_{\hat{H}_0}^j \hat{H}_i | i = 1, ..., m; j = 0, 1, ...\}_{LA},$$

where $ad_X^j Y = [X, ad_X^{j-1}Y], j \geq 1$ with $ad_X^0 Y = Y$.

These definitions and theorem, particularly the **HTC Corollary**, are useful for analyzing the controllability of the quantum system for the PT-like potential with the discrete nondegenerate bound states.

3. Analysis of controllability

We now analyze the controllability of this quantum system with the dynamic group SU(1, 1). It is shown from Eq. (13.35) that the Casimir operator C keeps invariant for the given potential. As addressed in Ref. [678], if the Hamiltonian $\hat{H}_0$ of the free or autonomous evolution is driven by a Casimir invariant (a dynamic symmetry, the SU(1, 1) group here), the control Hamiltonian can be physically realized by the group generators $\hat{\mathcal{L}}_{\pm,0}$ and the quantum system can be guaranteed to be strongly completely controllable. For the present case, the Hamiltonian $\hat{H}_0$ can be realized by the combination of the ladder operators as shown by Eq. (13.37). Following Ref. [678] by Tarn *et al.* , we can construct the control system as

$$\frac{d\psi(t)}{dt} = [-\hat{H}_0 + u_1(t)(\hat{\mathcal{L}}_+ - \hat{\mathcal{L}}_-) + i\, u_2(t)(\hat{\mathcal{L}}_+ + \hat{\mathcal{L}}_-)]\psi(t), \quad \psi(0) = \psi_0,$$
$$(20.5)$$

where the quantities $\psi(t)$ and ψ_0 should be interpreted as the abstract state vectors rather than wave functions. A set of analytical vectors constructs the representations of the su(1, 1) algebra. On the other hand, it is shown from Eq. (20.5) that we take $\hat{H}_1 = \hat{\mathcal{L}}_+ - \hat{\mathcal{L}}_-$ and $\hat{H}_2 = i(\hat{\mathcal{L}}_+ + \hat{\mathcal{L}}_-)$ as done by Tarn *et al.* in Ref. [678]. This means that the $\hat{H}_0, \hat{H}_1, \hat{H}_2$ are a set of generators of SU(1, 1) group, i.e. the principal Hamiltonian $\hat{H}_0$ of this quantum system is connected to the non-compact group SU(1, 1) as shown by Eq. (13.37). The external perturbations $\hat{H}_1$ and $\hat{H}_2$ can also be expressed by the combinations

of the ladder operators $\hat{\mathcal{L}}_{\pm}$ as shown above. Therefore, the $\hat{H}_0$, $\hat{H}_1$ and $\hat{H}_2$ can be expressed by the combinations of the operators $\hat{\mathcal{L}}_{\pm,0}$, which are nothing but the generators of the SU(1, 1) group as proved and shown by Eq. (13.37). The controllability analysis then is based on the properties of the following three Lie algebras

$$
\begin{aligned}
\mathcal{A} &= \{\hat{H}_0, \hat{\mathcal{L}}_+ - \hat{\mathcal{L}}_-, i(\hat{\mathcal{L}}_+ + \hat{\mathcal{L}}_-)\}_{LA}, \\
\mathcal{B} &= \{\hat{\mathcal{L}}_+ - \hat{\mathcal{L}}_-, i(\hat{\mathcal{L}}_+ + \hat{\mathcal{L}}_-)\}_{LA}, \\
\mathcal{C} &= \{ad^j_{\hat{H}_0} \hat{H}_i | i = 1, j = 0, 1, \ldots\}_{LA},
\end{aligned}
\tag{20.6}
$$

which implies that $ad^j_{\hat{H}_0} \hat{\mathcal{L}}_\pm = 0$ for $j > 0$ since the Casimir operator C commutes with the generators $\hat{\mathcal{L}}_\pm$. The ideal generated by $\mathcal{C}$ in $\mathcal{A}$ coincides with $\mathcal{B}$. Accordingly $[\mathcal{C}, \mathcal{B}] \in \mathcal{B}$. Therefore, from the **HTC Corollary**, we draw a conclusion that this quantum system is strongly completely controllable.

4.   Concluding remarks

We have reviewed the basic knowledge about the quantum control and studied the controllability of a quantum system for the PT like potential with the symmetry SU(1, 1). We have shown from the **HTC Corollary** that this quantum system with the dynamic group SU(1, 1) for the nondegenerate discrete bound states can, in principle, be strongly completely controlled, i.e. the system eigenfunctions with the invariant Casimir operator can be guided by the external field to approach arbitrarily closely a selected target state at any chosen time, which can be theoretically realized by the actions of the transition operators on the ground state.

Notes

1   It should be mentioned that the control system (20.1) divided by $i\hbar$ ($\hbar = 1$) was first studied by Jurdjevic and Sussmann in their classic work [686], where the system (20.1) was denoted by (X, U), i.e. $\frac{dx(t)}{dt} = X_0(x(t)) + \sum_{i=1}^{m} u_i(t) X_i(x(t))$ where $X_0, ..., X_m$ are the right-invariant vector fields on the Lie group G. Likewise, the $u_i(t)$ are the control functions. To our understanding, the so-called right-invariant vector fields on the Lie group G are nothing but the state space $\mathcal{H}$ of the studied system.

PART VI

CONCLUSIONS AND OUTLOOKS

Chapter 21

CONCLUSIONS AND OUTLOOKS

1.   Conclusions

We are now in the position to draw some conclusions for this work. First, we have given some historic review of the factorization method. It should be noted that the lists of references in this direction are far from complete even though we have mentioned almost all important contributions. After that we have proposed our new factorization method to study some important quantum systems. It should be pointed out that the procedure of our present method is converse to that of the Infeld-Hull method. The latter approach can be used to obtain the exact solutions of quantum systems from a given Hamiltonian. However, we assume that the exact solutions of the studied quantum system are known or can be obtained from the traditional quantum mechanics method and then act the first differential operator $d/d\xi$ on the obtained wave functions. It is worth noting that the ladder operators only depend on the physical variable ξ. By using the recurrence relations of the some special functions, we are able to obtain the ladder operators and realize a suitable Lie algebra and so on. Once the hidden symmetry of the studied quantum system is known, we may study other properties of the quantum systems such as the coherent states and the controllability of the system, etc. Based on this method, we have studied some interesting quantum systems such as the infinitely deep square well potential, the Morse potential, the PT potential, the pseudoharmonic oscillator, the ring-shaped potential, the PT-like potential and so on. In addition, we have proposed some new anharmonic potentials such as the noncentral ring-shaped molecular potentials. The advantages of the present method are the following. First, we can construct a suitable Lie algebra for a given quantum system with exact solutions. Second, we may calculate the analytical expressions of the related physical functions.

On the other hand, we have addressed the applications of the factorization method in the relativistic equations. For example, we have employed the SUSYQM and SWKB approaches to study the symmetrical potential well and the Coulomb potential since these two approaches are closely related to the factorization method. In addition, we have systematically studied the integral formulas of the product of the associated Laguerre functions and the Confluent hypergeometric functions, which are used to derive the eigenfunctions of the Dirac equation with the Coulomb-like potential.

Finally, due to the importance of quantum control we have studied the controllability of some quantum systems by analyzing the properties of the dynamic groups since the controllability of the quantum systems is closely related to the hidden symmetries of the studied systems. For example, we have investigated the controllability of the Morse and PT quantum systems and found that these two systems can be strongly controllable since the dynamic groups for the bound states of these systems are the compact Lie group SU(2). On the other hand, we have also studied the controllability of the PT-like potential whose bound states can be described by the non-compact Lie group SU(1, 1). Such a system can also be strongly controllable.

2.   Outlooks

The investigations of dynamic groups for some quantum systems would be investigated only if their exact solutions could be obtained. On the other hand, one may study the controllability of those quantum systems if the Lie algebras are known. It should be noted that not all of solvable quantum systems could be performed by our present approach to study their hidden dynamic groups. This is because the normalization factor or the recursion relations among the special functions for the studied quantum system are not available. In this case, we may study the dynamic group of the quantum system based on the SUSYQM approach or traditional factorization method. On the other hand, with the recent interest in the algebraic method to the position-dependent mass Schrödinger equation, it is possible to carry out some interesting investigations on this topic using factorization method, in particular following the SUSYQM approach.

Appendix A
Integral formulas of the confluent hypergeometric functions

In this Appendix let us study the integral of the product of the associated Laguerre functions and the confluent hypergeometric functions with the MATHEMATICA package INTEPFFLL [691] due to their wide applications in various fields of physics.

We now derive the integral formula of the confluent hypergeometric functions, which can be found in many references [216, 297, 692–695],

$$J(\alpha, \gamma, \alpha', \gamma', \rho) = \int_0^\infty e^{-\rho} \rho^\nu F(\alpha, \gamma; \rho) F(\alpha', \gamma'; \rho) d\rho, \quad \nu > -1. \qquad (A.1)$$

To obtain the normalization factor and matrix elements of some physical functions we have to derive the exact expressions of Eq. (A.1). For simplicity, we study the following integrals

$$I_{LL}(n, \triangle n, \beta, \triangle\beta, \lambda) = \int_0^\infty e^{-\rho} \rho^{\beta+\lambda} L_n^\beta(\rho) L_{n+\triangle n}^{\beta+\triangle\beta}(\rho) \, d\rho, \qquad (A.2)$$

$$I_{FF}(n, \triangle n, \beta, \triangle\beta, \lambda) = \int_0^\infty e^{-\rho} \rho^{\beta+\lambda} F(-n, \beta; \rho) F(-n - \triangle n, \beta + \triangle\beta; \rho) \, d\rho, \qquad (A.3)$$

where $\triangle n \geq 0$ and $\triangle n, \triangle\beta, \lambda$ are integers. We assume that n is a non-negative integer, and $\beta, \beta + \triangle\beta$ are not equal to zero or negative integers.

We first consider integral (A.2). It can be further expressed as [430]

$$\begin{aligned}
\int_0^\infty e^{-\rho} \rho^{\beta+\lambda} L_n^\beta(\rho) L_{n+\triangle n}^{\beta+\triangle\beta}(\rho) d\rho \quad &= (-1)^{\triangle n} \Gamma(1 + \beta + \lambda) \\
&\times \sum_k \binom{\lambda}{n-k} \binom{\lambda-\triangle\beta}{n+\triangle n-k} \binom{\beta+\lambda+k}{k}.
\end{aligned} \qquad (A.4)$$

It is found that $k_{\max} = n$, but $k_{\min} \geq 0$, i.e.,

$$
k_{\min} = \begin{cases}
0, & \text{for } \lambda < 0 \text{ and } \lambda - \triangle\beta < 0; \\
\min(n, n + \triangle n - \lambda + \triangle\beta), & \text{for } \lambda < 0 \text{ and } \lambda - \triangle\beta \geq 0; \\
\min(n, n - \lambda), & \text{for } \lambda \geq 0 \text{ and } \lambda - \triangle\beta < 0; \\
n, & \text{for } \lambda \geq 0 \text{ and } \lambda - \triangle\beta \geq 0 \text{ and} \\
& \max(n - \lambda, n + \triangle n - \lambda + \triangle\beta) \geq n; \\
\max(n - \lambda, n + \triangle n - \lambda + \triangle\beta), & \text{for } \lambda \geq 0 \text{ and } \lambda - \triangle\beta \geq 0 \text{ and} \\
& \max(n - \lambda, n + \triangle n - \lambda + \triangle\beta) < n,
\end{cases}
$$

$$(A.5)$$

where we have assumed that $\max(n - \lambda, n + \triangle n - \lambda + \triangle\beta) \geq 0$. For given $\triangle n, \triangle\beta$ and λ, we can obtain various closed expressions of integral (A.2).

Now, let us consider integral (A.3). Using Eq. (8.10), we can reexpress Eq. (A.3) as

$$
\begin{aligned}
I_{FF}(n, \Delta n, \beta, \Delta\beta, \lambda) &= \int_0^\infty e^{-\rho} \rho^{\beta+\lambda} F(-n, \beta; \rho) \, F(-(n + \Delta n), \beta + \Delta\beta; \rho) \, d\rho \\
&= \frac{n!(n + \Delta n)!\Gamma(\beta)\Gamma(\beta + \Delta\beta)}{\Gamma(n + \beta)\Gamma(n + \Delta n + \beta + \Delta\beta)} I_{LL}(n, \Delta n, \beta - 1, \Delta\beta, \lambda + 1).
\end{aligned}
$$

$$(A.6)$$

For given $\Delta n, \Delta\beta$ and λ, we can obtain the closed expressions of Eq. (3) as shown in Table A.1.

Table A.1. Some exact expressions of the integral (A.3).

λ	Δ n	$\Delta\,\beta$	I_{FF}
1	1	1	$-\dfrac{(1+n)!\,\Gamma(\beta)\Gamma(1+\beta)}{\Gamma(n+\beta)}$
0	0	0	$\dfrac{(2n+\beta)n!\,\Gamma(\beta)^2}{\Gamma(n+\beta)}$
1	1	0	$-\dfrac{2(1+2n+\beta)(1+n)!\,\Gamma(\beta)^2}{\Gamma(n+\beta)}$
1	0	1	$\dfrac{(1+3n+\beta)n!\,\Gamma(\beta)\Gamma(1+\beta)}{\Gamma(n+\beta)}$
0	1	1	0
1	0	0	$\dfrac{(6n^2+\beta+6n\beta+\beta^2)n!\,\Gamma(\beta)^2}{\Gamma(n+\beta)}$
0	0	1	$\dfrac{n!\,\Gamma(\beta)\Gamma(1+\beta)}{\Gamma(n+\beta)}$
0	1	0	$-\dfrac{(1+n)!\,\Gamma(\beta)^2}{\Gamma(n+\beta)}$
-1	1	0	0
1	0	-1	$\dfrac{\left[2n(-1+5n)+\beta+8n\beta+\beta^2\right]n!\,\Gamma(-1+\beta)\Gamma(\beta)}{\Gamma(-1+n+\beta)}$
-1	0	1	$\dfrac{n!\,\Gamma(\beta)\Gamma(1+\beta)}{\Gamma(1+n+\beta)}$
0	1	-1	$-\dfrac{(3n+2\beta)(1+n)!\,\Gamma(-1+\beta)\Gamma(\beta)}{\Gamma(n+\beta)}$
-1	0	0	$\dfrac{n!\,\Gamma(\beta)^2}{\Gamma(n+\beta)}$
0	0	-1	$\dfrac{n!\,(3n+\beta)\Gamma(-1+\beta)\Gamma(\beta)}{\Gamma(-1+n+\beta)}$
1	1	-1	$-\dfrac{\left[10n^2+3\beta(1+\beta)+2n(1+6\beta)\right](1+n)!\,\Gamma(-1+\beta)\Gamma(\beta)}{\Gamma(n+\beta)}$
-1	1	1	$\dfrac{(1+n)!\,\Gamma(\beta)\Gamma(1+\beta)}{\Gamma(2+n+\beta)}$
-1	1	-1	$-\dfrac{(1+n)!\,\Gamma(-1+\beta)\Gamma(\beta)}{\Gamma(n+\beta)}$
-1	0	-1	$\dfrac{n!\,\Gamma(-1+\beta)\Gamma(\beta)}{\Gamma(-1+n+\beta)}$

Appendix B
Mean values $\overline{r^k}$ for hydrogen-like atom

In this Appendix we study the mean values $\overline{r^k}$ for hydrogen-like atom using the MATHEMATICA package INTEPFFLL [691]. For a Coulomb field $V = -\xi/r$ with $\xi = Z\alpha$ ($\alpha \simeq 1/137$), Using the Coulomb units we express the exact solutions of radial Schrödinger equation as [297]

$$R_{nl} = N_{nl}(2\,r)^l e^{-r/n}\, F(-n+l+1, 2\,l+2; 2r/n), \qquad (B.1)$$

where N_{nl} is the normalization constant to be determined by the normalization condition

$$
\begin{aligned}
\int_0^\infty R_{nl}(r)^2\, r^2\, dr &= \int_0^\infty N_{nl}^2 2^{2l} r^{2l+2}\, e^{-2\,r/n} F(-n+l+1, 2l+2; 2r/n)^2\, dr \\
&= N_{nl}^2 \left(\frac{n}{2}\right)^{2l+3} 2^{2l} I_{FF}(n-l-1, 0, 2l+2, 0, 0) = 1,
\end{aligned}
\qquad (B.2)
$$

which implies that $\Delta n = 0$, $\Delta\beta = 0$ and $\lambda = 0$. From Table A.1, it is easy to obtain

$$N_{nl} = \frac{2}{n^{l+2}(2l+1)!}\sqrt{\frac{(n+l)!}{(n-l-1)!}}. \qquad (B.3)$$

We now study the mean value $\overline{r^k}$

$$
\begin{aligned}
\overline{r^k} &= \int_0^\infty R_{nl}(r)^2\, r^{2+k}\, dr \\
&= \int_0^\infty N_{nl}^2\, 2^{2l} r^{2l+2+k}\, e^{-2\,r/n} F(-n+l+1, 2l+2; 2r/n)^2\, dr \\
&= N_{nl}^2 \left(\frac{n}{2}\right)^{2l+3+k} 2^{2l} I_{FF}(n-l-1, 0, 2\,l+2, 0, k).
\end{aligned}
\qquad (B.4)
$$

Using the results of $I_{FF}(n, 0, \beta, 0, k)$ obtained by package INTEPFFLL, we may easily obtain the mean values $\overline{r^k}$ ($|k| \leq 4$) as given in [581]

$$\bar{r} = \frac{1}{2}[3n^2 - l(l+1)], \qquad (B.5)$$

$$\overline{r^2} = \frac{n^2}{2}[5n^2 + 1 - 3l(l+1)], \qquad (B.6)$$

$$\overline{r^3} = \frac{n^2}{8} \{3(l-1)l(l+1)(l+2) - 5[6l(l+1) - 5]n^2 + 35n^4\}, \qquad \text{(B.7)}$$

$$\overline{r^4} = \frac{n^4}{8} \{5l(l+1)[3l(l+1) - 10] - 70l(l+1)n^2 + 63n^4 + 3(4+35n^2)\}, \qquad \text{(B.8)}$$

and

$$\overline{r^{-1}} = \frac{1}{n^2}, \qquad \text{(B.9)}$$

$$\overline{r^{-2}} = \frac{1}{n^3(l+1/2)}, \qquad \text{(B.10)}$$

$$\overline{r^{-3}} = -\frac{2}{l(1+l)(1+2l)n^3}, \qquad \text{(B.11)}$$

$$\overline{r^{-4}} = -\frac{4(l+l^2 - 3n^2)}{l(1+l)(-1+2l)(1+2l)(3+2l)n^5}. \qquad \text{(B.12)}$$

It is found that these results coincide with those given in [297, 692].

Due to their possible applications in atomic physics, Van Vleck has studied the $\overline{r^{-5}}$ and $\overline{r^{-6}}$ [696], but they were not expressed explicitly by quantum numbers n and l. By making use of the MATHEMATICA package, however, we can obtain the analytical expressions of the mean values $\overline{r^k}$ ($|k| \in [5, 8]$) as follows:

$$\begin{aligned}
\overline{r^5} &= \frac{n^4}{16}\{-5(l-2)(l-1)l(l+1)(l+2)(l+3) \\
&\quad + 21[14 + 5l(1+l)(l^2 + l - 5)]n^2 \\
&\quad - 105[3l(l+1) - 7]n^4 + 231n^6\},
\end{aligned} \qquad \text{(B.13)}$$

$$\begin{aligned}
\overline{r^6} &= \frac{n^6}{16}\{180 - 7l(l+1)[126 + 5l(l+1)(l^2 + l - 11)] \\
&\quad + [2121 + 315l(l+1)(l^2 + l - 7)]n^2 \\
&\quad - 231[3l(l+1) - 10]n^4 + 429n^6\},
\end{aligned} \qquad \text{(B.14)}$$

$$\begin{aligned}
\overline{r^7} &= \frac{n^6 \Gamma(n-l)}{256(n+l)!}\left[\frac{(n+l)!}{\Gamma(-8-l+n)} + \frac{64(7+l+n)!}{\Gamma(-1-l+n)} + \frac{64\Gamma(2+l+n)}{\Gamma(-7-l+n)}\right. \\
&\quad + \frac{784\Gamma(3+l+n)}{\Gamma(-6-l+n)} + \frac{3136\Gamma(4+l+n)}{\Gamma(-5-l+n)} + \frac{4900\Gamma(5+l+n)}{\Gamma(-4-l+n)} \\
&\quad \left. + \frac{3136\Gamma(6+l+n)}{\Gamma(-3-l+n)} + \frac{784\Gamma(7+l+n)}{\Gamma(-2-l+n)} + \frac{\Gamma(9+l+n)}{\Gamma(-l+n)}\right],
\end{aligned} \qquad \text{(B.15)}$$

$$\begin{aligned}
\overline{r^8} &= \frac{n^7 \Gamma(-l+n)}{512(l+n)!}\left[\frac{(l+n)!}{\Gamma(-9-l+n)} + \frac{1296(7+l+n)!}{\Gamma(-2-l+n)}\right. \\
&\quad + \frac{81\Gamma(2+l+n)}{\Gamma(-8-l+n)} + \frac{1296\Gamma(3+l+n)}{\Gamma(-7-l+n)} + \frac{7056\Gamma(4+l+n)}{\Gamma(-6-l+n)} \\
&\quad + \frac{15876\Gamma(5+l+n)}{\Gamma(-5-l+n)} + \frac{15876\Gamma(6+l+n)}{\Gamma(-4-l+n)} + \frac{7056\Gamma(7+l+n)}{\Gamma(-3-l+n)} \\
&\quad \left. + \frac{81\Gamma(9+l+n)}{\Gamma(-1-l+n)} + \frac{\Gamma(10+l+n)}{\Gamma(-l+n)}\right],
\end{aligned} \qquad \text{(B.16)}$$

and

$$\overline{r^{-5}} = -\frac{4\left[3l(l+1) - 1 - 5n^2\right]}{(l-1)l(l+1)(l+2)(2l-1)(2l+1)(2l+3)n^5}, \qquad \text{(B.17)}$$

$$\overline{r^{-6}} = \frac{4\left\{3(l-1)l(l+1)(l+2) - 5\left[6l(l+1)-5\right]n^2 + 35n^4\right\}}{(l-1)l(l+1)(l+2)(2l-3)(2l-1)(2l+1)(2l+3)(2l+5)n^7}, \quad \text{(B.18)}$$

$$\overline{r^{-7}} = \frac{4}{(l-2)_6}\,\frac{12 + 5l(l+1)[3l(l+1)-10] + [105 - 70l(l+1)]n^2 + 63n^4}{(2l-3)(2l-1)(2l+1)(2l+3)(2l+5)n^7}, \quad \text{(B.19)}$$

$$\overline{r^{-8}} = -\frac{8}{(l-2)_6}$$
$$\frac{5(-2+l)_6 - 21[14 + 5l(l+1)(l^2+l-5)]n^2 + 105[3l(l+1)-7]n^4 - 231n^6}{(2l-5)(2l-3)(2l-1)(2l+1)(2l+3)(2l+5)(2l+7)n^9},$$
$$\text{(B.20)}$$

where the Pochhammer symbol is defined as $(x)_n = \Gamma(x+n)/\Gamma(x)$. For any k, we can, in principle, obtain all mean values $\overline{r^k}$ with this MATHEMATICA package. However, the calculations of the mean values $\overline{r^k}$ for large $|k|$ ($|k| \geq 9$) become rather complicated.

Appendix C
Commutator identities

In this Appendix we review a few useful commutator identities to simplify the commutation relations, which often occur in the determination of realizations of a Lie algebra. As we know, we often use the following well-known relations

$$[AB, C] = A[B, C] + [A, C]B, \quad [A, BC] = B[A, C] + [A, B]C \tag{C.1}$$

to simplify the commutators involving the products of the operators. On the other hand, it is shown that for arbitrary polynomial functions r, t of the indicated operators,

$$r(A)[t(A), B] = [t(A), r(A)B], \quad [A, t(B)]r(B) = [Ar(B), t(B)] \tag{C.2}$$

can be effectively used to move the operators in and out of the commutators. In particular, we find that the following formula is very useful

$$[A, B^m] = \sum_{i=0}^{m-1} B^i [A, B] B^{m-i-1} \tag{C.3}$$

which can be proved by induction on m.

In addition, we have to calculate the operator transformations of the $e^{-B} A e^{B}$ in scaling transformations. For this purpose, let us define

$$g(\alpha) = e^{-\alpha B} A e^{\alpha B}. \tag{C.4}$$

By differentiating, we have

$$g(\alpha)' = e^{-\alpha B}[A, B]e^{\alpha B}, \qquad g(\alpha)'' = e^{-\alpha B}[[A, B], B]e^{\alpha B} \tag{C.5}$$

and in general
$$g^m(\alpha) = e^{-\alpha B}[\dots[[A, B], B], \dots, B]e^{\alpha B}, \tag{C.6}$$

where the multiple commutator contains B exactly m times. Let us expand the $g(\alpha)$ in Taylor series

$$g(\alpha) = \sum_{m=0}^{\infty} \frac{1}{m!} g^m(0)\alpha^m. \tag{C.7}$$

If setting $\alpha = 1$, we have the following identity

$$e^{-B} A e^{B} = A + [A, B] + \frac{1}{2!}[[A, B], B] + \frac{1}{3!}[[[A, B], B], B] + \dots, \qquad \text{(C.8)}$$

which can be used to obtain some scaling transformations.

Appendix D
Angular momentum operators in spherical coordinates

In this Appendix we give a brief review of the angular momentum operators in spherical coordinates [697, 698] due to its wide applications in quantum mechanics.

It is well known that the expressions for the components of the angular momentum operator **L** in Cartesian coordinates can be easily obtained as

$$L_x = yp_z - zp_y = -i\hbar \left(y\frac{\partial}{\partial z} - z\frac{\partial}{\partial y} \right), \tag{D.1}$$

$$L_y = zp_x - xp_z = -i\hbar \left(z\frac{\partial}{\partial x} - x\frac{\partial}{\partial z} \right), \tag{D.2}$$

$$L_z = xp_y - yp_x = -i\hbar \left(x\frac{\partial}{\partial y} - y\frac{\partial}{\partial x} \right), \tag{D.3}$$

from which we can obtain the following commutation relation

$$[L_i, L_j] = i\hbar\epsilon_{ijk}L_k, \tag{D.4}$$

where the indices i, j, k can be x, y, or z, and the coefficient ϵ_{ijk} is unity if i, j, k form a cyclic permutation of x, y, z and -1 for a reverse cyclic permutation.

We now want to find the form of these operators in spherical coordinates. By using the following transformation equations

$$x = r\sin\theta\cos\phi, \quad y = r\sin\theta\sin\phi, \quad z = r\cos\theta, \tag{D.5}$$

then we have

$$r = \sqrt{x^2 + y^2 + z^2}, \quad \cos\theta = \frac{z}{r}, \quad \tan\phi = \frac{y}{x}. \tag{D.6}$$

Consequently, we have

$$\frac{\partial r}{\partial x} = \sin\theta\cos\phi, \quad \frac{\partial r}{\partial y} = \sin\theta\sin\phi, \quad \frac{\partial r}{\partial z} = \cos\theta,$$

$$\frac{\partial\theta}{\partial x} = \frac{\cos\theta\cos\phi}{r}, \quad \frac{\partial\theta}{\partial y} = \frac{\cos\theta\sin\phi}{r}, \quad \frac{\partial\theta}{\partial z} = -\frac{\sin\theta}{r}, \qquad\text{(D.7)}$$

$$\frac{\partial\phi}{\partial x} = -\frac{\sin\phi}{r\sin\theta}, \quad \frac{\partial\phi}{\partial y} = \frac{\cos\phi}{r\sin\theta}, \quad \frac{\partial\phi}{\partial z} = 0.$$

Making use of these relations we are able to obtain the following expressions

$$L_x = i\hbar\left(\sin\phi\frac{\partial}{\partial\theta} + \frac{\cos\theta}{\sin\theta}\cos\phi\frac{\partial}{\partial\phi}\right),$$

$$L_y = -i\hbar\left(\cos\phi\frac{\partial}{\partial\theta} - \frac{\cos\theta}{\sin\theta}\sin\phi\frac{\partial}{\partial\phi}\right), \qquad\text{(D.8)}$$

$$L_z = -i\hbar\frac{\partial}{\partial\phi},$$

from which we have

$$L^2 = L_x^2 + L_y^2 + L_z^2 = -\hbar^2\left\{\frac{1}{\sin\theta}\frac{\partial}{\partial\theta}\left(\sin\theta\frac{\partial}{\partial\theta}\right) + \frac{1}{\sin^2\theta}\frac{\partial^2}{\partial\phi^2}\right\}, \qquad\text{(D.9)}$$

with the following properties

$$[L^2, L_i] = 0, \quad i = x, y, z. \qquad\text{(D.10)}$$

Instead of the operators L_x and L_y, we often use the linear combinations of the operators L_x and L_y as

$$L_\pm = L_x \pm iL_y = \hbar e^{\pm i\phi}\left[\pm\frac{\partial}{\partial\theta} + i\frac{\cos\theta}{\sin\theta}\frac{\partial}{\partial\phi}\right], \qquad\text{(D.11)}$$

from which, together with the operator L_z we have the following commutation relations

$$[L_z, L_\pm] = \pm L_\pm, \quad [L_+, L_-] = 2L_z, \qquad\text{(D.12)}$$

which correspond to the SU(2) group. On the other hand, it is not difficult to see that

$$\begin{aligned} L^2 &= L_+L_- + L_z^2 - L_z \\ &= L_-L_+ + L_z^2 + L_z, \end{aligned} \qquad\text{(D.13)}$$

with the property

$$L^2 Y_{lm} = l(l+1)Y_{lm}, \qquad\text{(D.14)}$$

where Y_{lm} is the spherical function.

Appendix E
Confluent hypergeometric function

In this appendix we shall give some basic properties of the confluent hypergeometric function for the sake of easy reference. It is well known that the confluent hypergeometric function is defined by the series

$$F(\alpha, \beta; z) = 1 + \frac{\alpha}{\beta}\frac{z}{1!} + \frac{\alpha(\alpha+1)}{\beta(\beta+1)}\frac{z^2}{2!} + \frac{\alpha(\alpha+1)(\alpha+2)}{\beta(\beta+1)(\beta+2)}\frac{z^3}{3!} + \cdots, \tag{E.1}$$

where the parameter α is arbitrary, but the parameter β is supposed not zero or a negative integer.

The confluent hypergeometric function $F(\alpha, \beta; z)$ satisfies the differential equation

$$z\frac{d^2\phi}{dz^2} + (\beta - z)\frac{d\phi}{dz} - \alpha\phi = 0. \tag{E.2}$$

Substitution of $\phi = z^{1-\beta}\phi_1$ into (E.2) leads to

$$z\frac{d^2\phi_1}{dz^2} + (2 - \beta - z)\frac{d\phi_1}{dz} - (\alpha - \beta + 1)\phi_1 = 0. \tag{E.3}$$

Therefore, the general solution of Eq. (E.2) can be expressed as

$$\phi = a_1 F(\alpha, \beta; z) + a_2 z^{1-\beta} F(\alpha - \beta + 1, 2 - \beta; z), \tag{E.4}$$

which implies that the second term, unlike the first, has a singular point at $z = 0$. It should be noted that Eq. (E.2) is of Laplace's type and its solutions can be represented as contour integrals as shown by Landau *et al.*[297]. The function $F(\alpha, \beta; z)$ is regular at $z = 0$ and has the value 1 there; it satisfies the following relationship

$$F(\alpha, \beta; z) = e^z F(\beta - \alpha, \beta; -z), \tag{E.5}$$

which is called the Kummer transformation. On the other hand, this function $F(\alpha, \beta; z)$ also satisfies the following recursion relations [698]

$$(\beta - \alpha)F(\alpha - 1, \beta; z) + (2\alpha - \beta + z)F(\alpha, \beta; z) = \alpha F(\alpha + 1, \beta; z),$$

$$(\alpha - \beta + 1)F(\alpha, \beta; z) + (\beta - 1)F(\alpha, \beta - 1; z) = \alpha F(\alpha + 1, \beta; z), \tag{E.6}$$

$$\frac{d}{dz}F(\alpha, \beta; z) = \frac{\alpha}{\beta}F(\alpha + 1, \beta + 1; z).$$

By successive applications of (E.6), we have

$$\frac{d^n}{dz^n}F(\alpha,\beta;z) = \frac{\Gamma(\beta)\Gamma(\alpha+n)}{\Gamma(\alpha)\Gamma(\beta+n)}F(\alpha+n,\beta+n;z), \tag{E.7}$$

where $\Gamma(x)$ is the Gamma function.

On the other hand, the polynomials $F(-n,m;z)(m \in [0,n])$ are associated with the generalized Laguerre polynomials defined by

$$\begin{aligned}
L_n^m(z) &= (-1)^m \frac{(n!)^2}{m!(n-m)!}F(-[n-m],m+1;z) \\
&= \frac{n!}{(n-m)!}e^z \frac{d^n}{dz^n}(e^{-z}z^{n-m}) \\
&= (-1)^m \frac{n!}{(n-m)!}e^z z^{-m} \frac{d^{n-m}}{dz^{n-m}}(e^{-z}z^n),
\end{aligned} \tag{E.8}$$

from which we may obtain the following relation [263]

$$L_n^m(z) = \frac{\Gamma(n+m+1)}{\Gamma(n+m)}F(-n,m+1;z). \tag{E.9}$$

When $m = 0$, the polynomials $L_n^m(z)$ are called simply Laguerre polynomials

$$L_n(z) = e^z \frac{d^n}{dz^n}(e^{-z}z^n). \tag{E.10}$$

Based on Eqs. (E.9) and (E.10), we have

$$L_n(z) = \frac{\Gamma(n+1)}{\Gamma(n)}F(-n,1;z). \tag{E.11}$$

We are now in the position to indicate the asymptotic behavior of the confluent hypergeometric function. For small values of z, the asymptotic value of the function $F(\alpha,\beta;z)$ is given immediately by the first terms of the series (E.1). For large values of the $|z|$, we have

$$\begin{aligned}
F(\alpha,\beta;z) &= \frac{\Gamma(\beta)}{\Gamma(\alpha)}z^{\alpha-\beta}e^z[1+\mathcal{O}(|z|^{-1})], &\Re z \to \infty, \\
F(\alpha,\beta,z) &= \frac{\Gamma(\beta)}{\Gamma(\beta-\alpha)}(-z)^{-\alpha}[1+\mathcal{O}(|z|^{-1})], &\Re z \to -\infty.
\end{aligned} \tag{E.12}$$

On the other hand, for bounded values of z and infinitely large values of one of the parameters we have more asymptotic values of the confluent hypergeometric function $F(\alpha,\beta;z)$

$$\begin{aligned}
F(\alpha,\beta;z) &= 1+\mathcal{O}(|\beta|^{-1}), &\text{if } z \text{ and } \alpha \text{ are bounded,} &\quad \beta \to \infty, \\
F(\alpha,\beta;z) &= e^z(1+\mathcal{O}(|\beta|^{-1})), &\text{if } \beta-\alpha \text{ and } z \text{ are bounded,} &\quad \beta \to \infty.
\end{aligned} \tag{E.13}$$

It should be noted that the great significance of the confluent hypergeometric function in physics is connected with the fact that the solutions of many homogeneous differential equations

can be expressed in terms of this function. For example, consider the following second-order differential equation

$$(\alpha_0 y + \beta_0)\frac{d^2\phi}{dy^2} + (\alpha_1 y + \beta_1)\frac{d\phi}{dy} + (\alpha_2 y + \beta_2)\phi = 0. \tag{E.14}$$

By taking the following substitution

$$\phi = e^{\nu y}\psi, \quad y = \lambda z + \eta, \tag{E.15}$$

we may transform Eq. (E.14) into the form

$$(a_0 z + b_0)\frac{d^2\psi}{dz^2} + (a_1 z + b_1)\frac{d\psi}{dz} + (a_2 z + b_2)\psi = 0, \tag{E.16}$$

where

$$\begin{aligned}
&a_0 = \frac{\alpha_0}{\lambda}, \quad a_1 = A_1, \quad a_2 = \lambda A_2, \\
&b_0 = \frac{\alpha_0 \eta + \beta_0}{\lambda^2}, \quad b_1 = \frac{\eta A_1 + B_1}{\lambda}, \quad b_2 = \eta A_2 + B_2, \\
&A_1 = 2\alpha_0 \nu + \alpha_1, \quad A_2 = \alpha_0 \nu^2 + \alpha_1 \nu + \alpha_2, \\
&B_1 = \beta_1 + 2\beta_0 \nu, \quad B_2 = \beta_0 \nu^2 + b_1 \nu + b_2.
\end{aligned} \tag{E.17}$$

If we define the parameters ν, η and λ so that

$$\alpha_0 \eta + \beta_0 = 0, \quad \alpha_0 = -\lambda A_1, \quad A_2 = 0, \tag{E.18}$$

then Eq. (E.16) coincides with Eq. (E.2). Therefore, if we select values of the parameters ν, η and λ, which satisfy the constraint condition (E.18), and then use the transformation (E.15), then we find that an arbitrary equation of the type (E.14) reduces to the equation for the confluent hypergeometric function (E.2).

By substituting

$$\psi = z^{-\beta/2} e^{z/2} w, \quad \alpha = \frac{1}{2} - k + \eta, \quad \beta = 1 + 2\eta, \tag{E.19}$$

we may transform Eq. (E.2) into the Whittaker equation

$$\frac{d^2 w}{dz^2} + \left(-\frac{1}{4} + \frac{k}{z} + \frac{\frac{1}{4} - \eta^2}{z^2}\right)w = 0, \tag{E.20}$$

whose solution is denoted by $W_{k,\eta}$. The connection between the confluent hypergeometric function $F(\alpha, \beta; z)$ and the Whittaker function $W_{k,\eta}$ is defined by the relationships (E.19). Many mathematical functions which are used in physics can be expressed in terms of the Whittaker function. The asymptotic value of the Whittaker functions for large values of z and $|\arg z| < \pi$ is given by the formula

$$W_{k,\eta} = e^{-z/2} z^k (1 + \mathcal{O}(z^{-1})). \tag{E.21}$$

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