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# Analyzing Quantum Time-Dependent Singular Potential Systems in One Dimension

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#### **Abstract**

Quantum states of a particle subjected to time-dependent singular potentials in one-dimension are investigated using invariant operator method and the Nikiforov-Uvarov method. We consider the case that the system is governed by two singular potentials which are the Coulomb potential and the inverse quadratic potential. An invariant operator that is a function of time has been constructed via a fundamental mechanics. This invariant operator is transformed to a simple one using a unitary operator, which is a time-independent invariant operator. By solving the Schrödinger equation in the transformed system, analytical forms of exact eigenvalues and eigenfunctions of the invariant operator are evaluated in a simple elegant manner with the help of the Nikiforov-Uvarov method. Eventually, the full wave functions in the original system (untransformed system) are obtained through an inverse unitary transformation from the wave functions in the transformed system. Quantum characteristics of the system associated with the wave functions are addressed in detail.

**Keywords:** time-dependent Hamiltonian systems, singular potentials, unitary transformation, wave function, Schrödinger equation

#### 1. Introduction

After a seminal work of Lewis [1] for a quantum time-dependent harmonic oscillator, much attention has been paid to investigating quantum properties of time-dependent Hamiltonian systems (TDHSs). Any type of the time-dependent harmonic oscillator is a good example of TDHSs, and the study of its analytical quantum solutions requires particular mathematical techniques. The research topic of TDHSs has been gradually extended to more complicated systems beyond the one-dimensional time-dependent harmonic oscillators which are relatively



simple. The analytical forms of quantum wave functions of the time-dependent coupled oscillators have been reported by several researchers [2–4]. The system associated with a class of time-dependent singular potentials was investigated [5–10] and some of the corresponding results were applied to study the problem of a two-ion trap within a binding potential [7]. A TDHS that is described by a Hamiltonian that involves (1/x)p + p(1/x) term, which in fact is necessary for the description of radial equation for a central force system, was also studied [11–13].

In this chapter, quantum features of a time-dependent singular potential system [14] will be investigated. The singular potentials that will be considered here are the combination of the inverse quadratic potential and the Coulomb potential. Singular potentials not only can be applied for describing many actual physical systems but can also serve as mathematical models for quantum field theory and elementary particle theory. The research interest for singular potentials was first shown in a context of relativistic mechanics. Various applications of the singular potentials include interatomic or intermolecular descriptions of a molecular force, the scattering problem of elementary particles, and the interaction of relativistic particles such as quark-antiquark bound states [14–16].

It was reported by Plesset [17] that there is a difficulty in the derivation of a physically accepted solution for a relativistic Coulomb-like singular potential. To overcome such difficulty, the invariant operator method together with a unitary transformation method will be used in this chapter. These methods are useful for investigating the mechanics of TDHSs, like the case that will be represented here. For a TDHS, the eigenstates of the invariant operator are the same as the Schrödinger solutions of the system when we neglect the phase factors of the wave functions [18]. The unitary transformation with a suitable operator allows us to manage a certain complicated system in a transformed space that requires relatively simple mathematical treatments for the system.

## 2. Singular potential system

Let us consider a one-dimensional quantum system that is described by a time-dependent Hamiltonian of the form

$$H(t) = \frac{1}{2\mu(t)} \left( p^2 + \frac{f_0}{x^2} \right) - \frac{Z(t)}{x}, \tag{1}$$

where x is the position operator and  $p = -i\hbar \partial/\partial x$ ,  $\mu(t)$ , and Z(t) are time-dependent coefficients with Z(t) > 0, and  $f_0$  is a constant. This system is defined in the half space  $x \ge 0$ . The system described by Eq. (1) is different from that in Ref. [9], and a particular case of this type of Hamiltonian system can be found in Ref. [10]. The quantum problem of this Hamiltonian system is very difficult due to the explicit time dependence of parameters, and we are not

always possible to derive exact quantum solutions. We will find the condition for solvability of this quantum system in the subsequent development.

As is well known, a useful method for a quantum mechanical treatment of the system in the situation where there exist time-dependent parameters is to use an invariant operator method [1, 18]. An invariant of the system that is described by a time-dependent Hamiltonian H(t) is constructed from the Liouville-von Neumann equation of the form

$$\frac{dI}{dt} = \frac{\partial I}{\partial t} + \frac{1}{i\hbar}[I, H] = 0.$$
 (2)

As represented in this equation, the whole time derivative of the invariant operator *I* should be zero because of its definition. Let us suppose that the exact invariant has the form

$$I(x,p,t) = \alpha(t)x^{2} + \gamma(t)\left(p^{2} + \frac{f_{0}}{x^{2}}\right) + \beta(t)(xp + px) - \frac{\eta(t)}{x},$$
(3)

where  $\alpha(t)$ ,  $\gamma(t)$ ,  $\beta(t)$ , and  $\eta(t)$  are time-dependent coefficients that will be derived afterward [see Eqs. (5)–(8)]. In the case of the counterpart classical system, x and p are no longer operators, and as a consequence the expression xp + px given in Eq. (3) can be reduced to 2xp.

The substitution of Eqs. (1) and (3) into the Liouville-von Neumann equation represented in Eq. (2) gives the following equations for the coefficients:

$$\dot{\alpha}(t) = 0, \quad \dot{\beta}(t) = -\alpha(t) / \mu(t), \quad \dot{\gamma}(t) = -2\beta(t) / \mu(t), 
\dot{\eta}(t) = -2\beta(t)Z(t), \quad \gamma(t)Z(t) = \eta(t) / [2\mu(t)].$$
(4)

By solving these equations, it is possible to determine the time-dependent coefficients. Hence, as a result of a minor evaluation, we have

$$\alpha(t) = \alpha_0 \,, \tag{5}$$

$$\beta(t) = \beta_0 - \alpha_0 \int_0^t \frac{1}{\mu(t')} dt', \qquad (6)$$

$$\gamma(t) = \gamma_0 - 2F(t), \tag{7}$$

$$\eta(t) = \frac{\eta_0}{\gamma_0^{1/2}} [\gamma_0 - 2F(t)]^{1/2} , \qquad (8)$$

where

$$F(t) = \beta_0 \int_0^t \frac{1}{\mu(t')} dt' - \alpha_0 \int_0^t \left[ \frac{1}{\mu(t')} \int_0^{t'} \frac{1}{\mu(t'')} dt'' \right] dt', \tag{9}$$

with an auxiliary condition for the solvability of the system, which is that the time dependence of Z(t) is chosen in a way that

$$Z(t) = \frac{\eta_0}{2\gamma_0^{1/2}\mu(t)} [\gamma_0 - 2F(t)]^{-1/2}.$$
 (10)

Now, notice that Eq. (3), with the coefficients given in Eqs. (5–8), is the exact invariant operator. If we express the eigenvalue equation of the invariant operator as  $I(t)\varphi_n(t) = E_n\varphi_n(t)$ , the eigenvalues  $E_n$  are time constants, due to the invariant operator not varying with time. Then we can specify the eigenstates  $\varphi_n(t)$  for the operators I(t) for overall range of time t.

By denoting the wave functions as  $\psi_n(t)$ , the Schrödinger equation is expressed in the form  $i\hbar\partial\psi_n(t)/\partial t=H(t)\psi_n(t)$ . For the TDHS, the wave functions are represented in terms of the eigenstates of the invariant operator, such that  $\psi_n(t)=\exp[i\theta_n(t)]\varphi_n(t)$  where  $\theta_n(t)$  are global phases.

Considering the Schrödinger equation, we can easily verify that  $\theta_n(t)$  satisfy the relation [18]:

$$\frac{d\theta_n(t)}{dt} = \langle \varphi_n(t) | \left( i \frac{\partial}{\partial t} - \frac{H}{\hbar} \right) | \varphi_n(t) \rangle. \tag{11}$$

Hence, if the eigenstates of the invariant operator,  $\varphi_n(t)$ , are completely known, the corresponding global phases  $\theta_n(t)$  are easily obtained by solving Eq. (11). Concerning this quantum formulation of the system based on the invariant operator, the solvability of  $\psi_n(t)$  for a TDHS is noticeable.

The strategy of our manipulation for deriving exact quantum solutions of the system is that we transform the operator I(t) into a simple form  $I_0$  which is not a function of time. Then, it is easy to derive the eigenstates of  $I_0$  associated with the transformed system because  $I_0$  does not depend on time. The corresponding quantum results in the transformed system will be inversely transformed to the original system (untransformed system). This may lead to derive exact eigenfunctions in the original system.

For this purpose, let us first perform a unitary transformation of the eigenstates such that

$$\Phi_{n}(x) = U(x, p, t)\varphi_{n}(x, t), \tag{12}$$

where U is a time-dependent unitary operator given by [8]:

$$U(x,p,t) = \exp\left(\frac{i\beta(t)}{2\hbar\gamma_0}x^2\right) \exp\left[\frac{i}{2\hbar}\ln\left(\frac{\gamma(t)}{\gamma_0}\right)^{1/2}(xp+px)\right]. \tag{13}$$

The transformation of the invariant operator using this operator can be performed in a straightforward way with Eq. (3),  $I_0 = UIU^{-1}$ , leading to

$$I_0(x,p) = \gamma_0 \left( p^2 + \frac{f_0}{x^2} \right) + \frac{\alpha_0 \gamma_0 - \beta_0^2}{\gamma_0} x^2 - \frac{\eta_0}{x}.$$
 (14)

Here, the transformed invariant operator  $I_0$  does not depend on time as expected. Through this procedure, we can represent the eigenvalue equation for the transformed invariant operator as

$$\left[\gamma_0 \left(p^2 + \frac{f_0}{x^2}\right) + \frac{\alpha_0 \gamma_0 - \beta_0^2}{\gamma_0} x^2 - \frac{\eta_0}{x}\right] \Phi_n(x) = E_n \Phi_n(x).$$
 (15)

If we put  $\omega_0 = \alpha_0 \gamma_0 - \beta_0^2$ , it is possible to analyze the system in three cases which are  $\omega_0 > 0$ ,  $\omega_0 < 0$ , and  $\omega_0 = 0$ . Among them, the only solvable case is the third one. Hence, let us see the system with  $\omega_0 = 0$  from now on. In this case, the invariant quantity reduces to

$$I_0 = \gamma_0 \left( p^2 + \frac{f_0}{x^2} \right) - \frac{\eta_0}{x}. \tag{16}$$

Then, the eigenvalue equation given in Eq. (15) becomes

$$\frac{d^2\Phi_n(x)}{dx^2} - \left(\frac{-a^2x + \nu(\nu+1)}{x^2} + \kappa_n^2\right)\Phi_n(x) = 0,$$
(17)

where

$$\frac{E_n}{\gamma_0 \hbar^2} = -\kappa_n^2 \,, \quad \frac{\eta_0}{\gamma_0 \hbar^2} = a^2 \,, \quad \frac{f_0}{\hbar^2} = \nu(\nu + 1) \,, \tag{18}$$

with the condition that  $E_n < 0$ .

## 3. Spectrum of quantized solutions

In this section, we consider the solvable case that  $\omega_0 = 0$ . To evaluate the differential equation given in Eq. (17), we will use the Nikiforov-Uvarov (NU) method [19, 20] that is introduced in Appendix A. Using the transformation s = x, Eq. (17) can be transformed into

$$\frac{d^2\Phi_n(s)}{ds^2} - \left(\frac{-a^2s + \nu(\nu+1)}{s^2} + \kappa_n^2\right)\Phi_n(s) = 0.$$
 (19)

By comparing this equation with Eq. (A1) in the NU method of Appendix A, we get  $\tilde{\tau}(s) = 0$ ,  $\sigma(s) = s$ , and  $\tilde{\sigma}(s) = a^2 s - v(v+1) - \kappa_n^2 s^2$ .

For further development of the theory, we introduce a function  $\Pi(s)$  as [see Eq. (12) of Ref. [21]]

$$\Pi(s) = A(s) \pm \sqrt{A^2(s) - \tilde{\sigma}(s) + k\sigma(s)}, \qquad (20)$$

where  $A(s) = [\sigma'(s) - \tilde{\tau}(s)]/2$ . Here, k is determined from the fact that the discriminant associated with this equation should be zero so that the expression inside the square root in this equation can be rearranged as the square of a polynomial. From Eq. (20), we have four possible values of  $\Pi(s)$  as [10, 22]

$$\Pi(s) = \begin{cases} \kappa_n s + \nu, & \text{for } k = k_1 \\ -(\kappa_n s + \nu + 1), & \text{for } k = k_1 \\ \kappa_n s - \nu - 1, & \text{for } k = k_2 \\ -\kappa_n s + \nu, & \text{for } k = k_2, \end{cases}$$

$$(21)$$

where

$$k_1 = a^2 + 2\kappa_n(\nu + 1/2)$$
,  $k_2 = a^2 - 2\kappa_n(\nu + 1/2)$ . (22)

For the polynomial of  $\tau(s) = \tilde{\tau}(s) + 2\Pi(s)$ ,  $d\tau(s)/ds$  takes a negative value [23] and

$$\Pi(s) = -\kappa_{n} s + \nu, \tag{23}$$

with  $k = k_2$ . From the relation (see Appendix A)

$$\lambda = k + \Pi'(s), \tag{24}$$

 $\lambda$  can be expressed as

$$\lambda = a^2 - 2\kappa_n(\nu + 1). \tag{25}$$

For the case of  $k_2 = a^2 - 2\kappa_n(\nu + 1/2)$ , we have [23]

$$\lambda_{n} = 2n\kappa_{n}. \tag{26}$$

Now, let us equate Eq. (25) with Eq. (26) such that

$$2n\kappa_{n} = a^{2} - 2\kappa_{n}(\nu + 1). \tag{27}$$

Then, by inserting the first and the second relations in Eq. (18) into the above equation, we easily confirm that the eigenvalues are given in the form

$$E_n = -\frac{\eta_0^2}{4\gamma_0 \hbar^2} (n + \nu + 1)^{-2}, \tag{28}$$

where  $n=0, 1, 2, \cdots$ . These are bound-state eigenvalues satisfying the boundary conditions [24]. This consequence agrees well with the report of Ref. [8] performed without using the NU method. To find eigenfunctions, we first need to determine the weight function  $\rho(x)$  in Appendix A. Using Eq. (A5) in Appendix A and considering the condition in Eq. (23), we get  $\rho(x) = \exp(-2\kappa_n x)x^{2\nu+1}$ . Substituting this into Eq. (A6), we obtain the unnormalized values of  $z_n$  as  $[z_n]$  is defined in Eq. (A2).]:

$$z_{n}(x) = L_{n}^{2\nu+1}(2\kappa_{n}x), \qquad (29)$$

where  $L_n^{2\nu+1}$  is the associated Laguerre polynomials [25] and  $C_n$  is the normalization factor. Now, using Eq. (A7) in Appendix A, we find

$$u_n(x) = \exp(-\kappa_n x) x^{\nu}. \tag{30}$$

Finally, regarding Eq. (A2) in Appendix A for bound states, the eigenfunctions of the invariant  $I_{0}$ , that are finite for all x, have the form

$$\Phi_{n\nu}(x) = C_n \exp(-\kappa_n x) x^{\nu} L_n^{2\nu+1}(2\kappa_n x). \tag{31}$$

where  $\mathcal{C}_n$  is the normalization constant. By determining the exact formulae of  $\mathcal{C}_n$  from the well-known condition

$$\int_{0}^{\infty} \Phi_{n\nu}(x) \Phi_{n\nu}(x) dx = 1, \tag{32}$$

the corresponding normalized wave functions are found to be

$$\Phi_{n\nu}(x) = \left[ \frac{n!}{2\Gamma(n+2\nu+1)!} \right]^{1/2} \frac{1}{(n+\nu+1)^{\nu+2}} \left[ \frac{\eta_0}{\gamma_0 \hbar^2} \right]^{\nu+3/2} \\
\times x^{\nu} \exp \left[ \frac{-\eta_0}{2\gamma_0 \hbar^2 (n+\nu+1)} x \right] L_n^{2\nu+1} \left( \frac{\eta_0}{\gamma_0 \hbar^2 (n+\nu+1)} x \right).$$
(33)

Because the eigenstates of I(x, p, t) are given by  $\varphi_{nv}(x, t) = U^{-1} \Phi_{nv}(x)$ , the normalized wave functions are evaluated as

$$\psi_{n\nu}(x,t) = U^{-1}\Phi_{n\nu}(x) \exp[i\theta_{n\nu}(t)]$$

$$= \left[\frac{n!\eta_0}{2\gamma_0\hbar^2(n+2\nu+1)!}\right]^{1/2} \frac{1}{(n+\nu+1)^{\nu+2}} \left[\frac{\eta(t)}{\gamma(t)\hbar^2}\right]^{\nu+1}$$

$$\times x^{\nu} \exp\left[\frac{-i\beta(t)}{2\hbar\gamma(t)}x^2\right] \exp\left[\frac{-\eta(t)}{2\gamma(t)\hbar^2(n+\nu+1)}x\right]$$

$$\times L_n^{2\nu+1} \left(\frac{\eta(t)}{\gamma(t)\hbar^2(n+\nu+1)}x\right) \exp[i\theta_{n\nu}(t)].$$
(34)

There still remains the problem of finding the phases  $\theta_{nv}(t)$  which satisfy Eq. (11). By carrying out the unitary transformation by means of U(t), Eq. (11) becomes

$$\frac{d\theta_{n\nu}(t)}{dt} = -\frac{1}{2\hbar\mu(t)\gamma(t)} \langle \Phi_{n\nu}(x) | I_0(x,p) | \Phi_{n\nu}(x) \rangle. \tag{35}$$

Then, with the help of Eq. (28), this equation can be easily evaluated and, consequently, we obtain the phase factors in the form

$$e^{i\theta_{m'}(t)} = \exp\left[\frac{i\eta_0^2}{8\gamma_0\hbar^3(n+\nu+1)^2} \int_0^t \frac{1}{\mu(t')\gamma(t')} dt'\right].$$
 (36)

Now, by substituting Eq. (36) into Eq. (34), we find the exact nth-order solutions of the Schrödinger equation associated to the Hamiltonian H(x, p, t). Eq. (34) is the full wave functions in the original system and agrees with the results of the report given in Ref. [8], which is performed for a little different system using another method. The wave functions are interpreted as probability amplitudes for finding the particle in the potential. These functions are defined everywhere and possess general properties for physical meaning such as continuousness and infinite differentiability. On the basis of the wave functions, various quantum properties of the system, such as expectation values of physical observables, energy eigen spectrum, and the uncertainty relation, can be investigated.

Let us see for a particular case that  $\mu(t)$  is given by [10]

$$\mu(t) = m_0 (1 + \varepsilon t) \tag{37}$$

where  $m_0$  and  $\varepsilon$  are positive real constants. In this case, Eq. (9) can be evaluated to be

$$F(t) = \frac{\beta_0 \ln(1 + \varepsilon t)}{m_0 \varepsilon} \left( 1 - \frac{\beta_0}{2m_0 \varepsilon \gamma_0} \ln(1 + \varepsilon t) \right). \tag{38}$$

In this formula, we have used  $\alpha_0 = \beta_0^2/\gamma_0$  according to the condition  $\omega_0 = 0$  (see Section 2). If we substitute Eq. (38) in Eqs. (7) and (8), we have full expressions of  $\gamma(t)$  and  $\eta(t)$ . By using  $\gamma(t)$  obtained in such a way, the integration given in Eq. (36) can be fulfilled, and this results in

$$\int_0^t \frac{1}{\mu(t')\gamma(t')} dt' = \frac{\ln(1+\varepsilon t)}{m_0 \varepsilon \gamma_0 - \beta_0 \ln(1+\varepsilon t)}.$$
(39)

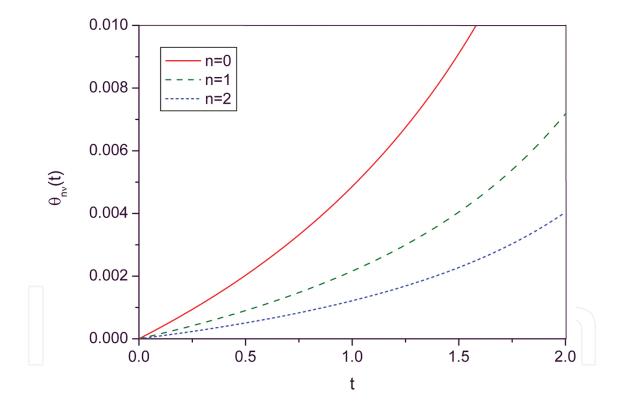
Besides, Eq. (10) becomes

$$Z(t) = \frac{\eta_0}{2\gamma_0 m_0 (1 + \varepsilon t)} \left[ 1 - 2 \frac{\beta_0 \ln(1 + \varepsilon t)}{m_0 \varepsilon \gamma_0} \left( 1 - \frac{\beta_0}{2m_0 \varepsilon \gamma_0} \ln(1 + \varepsilon t) \right) \right]^{-1/2}.$$
(40)

If we choose  $\beta_0=m_0\gamma_0\varepsilon$  and  $\eta_0=2m_0\gamma_0Z_0$  where  $Z_0$  is a real constant, Eq. (40) reduces to

$$Z(t) = \frac{Z_0}{(1+\varepsilon t)[1-\ln(1+\varepsilon t)]'}$$
(41)

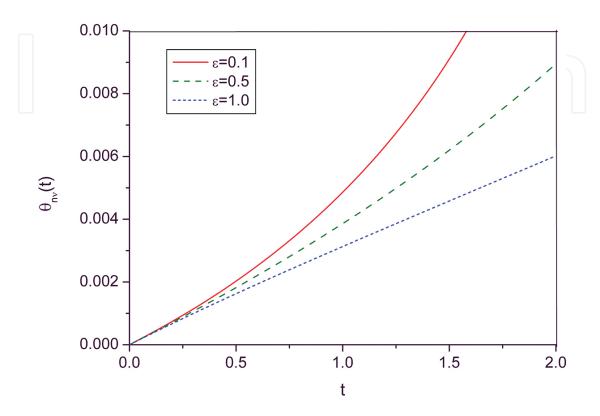
within the time interval  $0 \le t < (e-1)/\varepsilon$ . Notice that Eq. (1) with Eqs. (37) and (41) is the same as Eq. (1) of Ref. [10]. Hence, we can confirm that the system treated in Ref. [10] is a particular case of a more general system that is studied in this chapter.



**Figure 1.** Time evolution of the phase  $\theta_{n\nu}(t)$  for several different values of n. This is the case when  $\mu(t)$  is given by Eq. (37). We have used  $\beta_0=1$ ,  $\gamma_0=3$ ,  $\eta_0=1$ ,  $m_0=1$ ,  $\nu=1$ ,  $\hbar=1$ , and  $\varepsilon=0.1$ .

Considering the relation given in Eq. (39), we have plotted the phase given in Eq. (36) in **Figures 1** and **2** as a function of time. From **Figure 1**, the increment of  $\theta_{nv}(t)$  in time becomes

smaller as the quantum number n increases. We can confirm from **Figure 2** that the increment of  $\theta_{nv}(t)$  also becomes smaller as  $\varepsilon$  increases.



**Figure 2.** Time evolution of the phase  $\theta_{n\nu}(t)$  for several different values of  $\varepsilon$ , where  $\mu(t)$  is given by Eq. (37). We have used  $\beta_0=1$ ,  $\gamma_0=3$ ,  $\eta_0=1$ ,  $m_0=1$ ,  $\nu=1$ ,  $\hbar=1$ , and n=0.

## 4. Conclusion

The invariant operator method and unitary transformation method were used in order to derive the quantum solutions of a time-dependent singular potential system that is described by the Hamiltonian given in Eq. (1). The quadratic invariant operator of the system has been determined from the use of its definition as shown in Eq. (3). The wave functions that satisfy the Schrödinger equation are given by multiplying the eigenstates  $\varphi_n(t)$  of the invariant

operator and the phase factors  $e^{i\theta_n(t)}$  [see Eq. (34) with Eq. (12)]. By using the unitary operator, the original invariant operator I(t) which is a time function was transformed to a simple form  $I_0$  that is not a function of time. The NU method was used to derive the eigenstates of  $I_0$ . The eigenstates of I were derived from the inverse transformation of the eigenstates of  $I_0$ . The phases of the system were also derived from a fundamental relation in the framework of the

invariant operator theory. Through these procedures, the whole wave functions of the system as well as the eigenvalues of the invariant operator were obtained as shown in Eq. (34).

During the derivation of quantum solutions of the system, no approximation or perturbation methods were used. In fact, the merit of the invariant operator method for investigating quantization problem of TDHSs is that the corresponding quantum results are exact [3, 4]. Several methods for numerical treatment of time-dependent Schrödinger equations are known. If we enumerate some of them, they are the finite difference time domain (FDTD) method [26–31], the discretization method that takes advantage of the asymptotic behavior correspondence (ABC) [32, 33], and the discrete local discontinuous Galerkin method [34]. In particular, the FDTD method has been widely applied to obtain numerical solutions of mechanical problems of dynamical systems including Maxwell-Schrödinger equations for electromagnetic fields [30, 31]. If the methods for deriving numerical solutions of the Schrödinger equation for singular potential systems would be known in the future, it will be possible to compare our results developed in this chapter with them, leading to deepen the knowledge on quantum characteristics of relevant systems.

## **Appendices**

## Appendix A: Summary of the Nikiforov-Uvarov method

In this appendix, we introduce a useful method for solving Eq. (17) in the text, which is known as the NU method. This is useful for deriving the solutions of the Schrödinger-like second-order differential equations that play central roles in studying many important problems of theoretical physics. We first start from an appropriate coordinate transformation s = s(x) for an arbitrary function g that satisfies the differential equation [19]:

$$g''(s) + \frac{\tilde{\tau}(s)}{\sigma(s)}g'(s) + \frac{\tilde{\sigma}(s)}{\sigma^2(s)}g(s) = 0,$$
(A1)

where  $\sigma(s)$  and  $\tilde{\sigma}(s)$  are some polynomials which at most are the second degree, and  $\tilde{\tau}(s)$  is a polynomial of the first degree. A large part of special orthogonal polynomials [19] necessary in developing physics can be represented in the form of Eq. (A1). By expressing

$$g_{n}(s) = u_{n}(s)z_{n}(s), \tag{A2}$$

where  $u_n(s)$  are appropriate functions that will be chosen depending on the system. Eq. (A1) can be reduced into an equation of the following hypergeometric type [21]:

$$\sigma(s)z_n'' + \tau(s)z_n' + \lambda_n z_n = 0, \tag{A3}$$

where  $\tau(s) = \tilde{\tau}(s) + 2\Pi(s)$  and  $\lambda_n$  are constants given in the form [23]

$$\lambda_n = -n\tau'(s) - n(n-1)\sigma''(s) / 2. \tag{A4}$$

Notice that the derivative of  $\tau(s)$  should be negative, while  $\lambda_n$  is obtained from a particular solution of the form  $z(s) = z_n(s)$  which is a polynomial of degree n.

In terms of the weight function  $\rho(s)$  that satisfies the condition [19]

$$\frac{d[\sigma(s)\rho(s)]}{ds} - \tau(s)\rho(s) = 0, \tag{A5}$$

the hypergeometric-type function  $y_n(s)$  is given by [21]:

$$z_{n}(s) = C_{n} \rho^{-1}(s) \frac{d^{n}[\sigma^{n}(s)\rho(s)]}{ds^{n}},$$
(A6)

where  $C_n$  is the normalization constant. This is known as the Rodrigues relation. Notice that Eq. (A5) is obtained from Eq. (20).

The relationship between  $\lambda$  and k introduced in the expression of Eq. (20) is  $k = \lambda - \Pi'(s)$ . Regarding this point, an appropriate formula for  $u_n$  can be evaluated from the condition [21]

$$u'(s) - \Omega(s)u(s) = 0, \tag{A7}$$

where  $\Omega(s) = \Pi(s)/\sigma(s)$ . For more details of the NU method, see Refs. [10, 19–23].

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