Quantization of Time-dependent Singular Potential Systems in One-dimension by Using the Nikiforov-Uvarov Method

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The technique for quantizing simple static systems can be extended to more generalized systems that involve time-dependent parameters. In this work, a particle with linearly increasing mass that is bound by a time-dependent singular potential, which is composed of an inverse quadratic potential and a Coulomb-like potential, is quantized by using the Nikiforov-Uvarov method together with the invariant operator method and the unitary transformation method. The Nikiforov-Uvarov method is an alternative method for solving the Schrödinger equation on the basis of a particular mathematical technique that reduces second-order differential equations to generalized hypergeometric ones. The exact wave functions of the system are identified, and their properties are addressed in detail.

I. INTRODUCTION

The procedure of quantization is necessary for investigating the intrinsic nonclassical behavior of molecular systems. The mathematical manipulation for quantizing a simple static system can be extended to more generalized systems that involve time-dependent parameters. For several decades, active attention has been paid to the study of the quantum mechanical properties of time-dependent Hamiltonian systems (TDHSs). Time-dependent harmonic oscillators that are characterized by a time-dependent frequency and/or mass and harmonic oscillators driven by time-dependent forces may be the most typical types of TDHS. In most cases for finding quantum solutions of TDHSs, the conventional method of separation of variables may not hold because of the complexity of the given Hamiltonian. Thus, special mathematical techniques are necessary for investigating the quantum mechanical properties of such systems.

Theoretical investigations for various kinds of TDHS have been carried out up to now. The quantum properties of time-dependent coupled oscillators were studied on the basis of wave functions [1–4]. The research has been performed for the inverse quadratic potential system coupled to a time-dependent harmonic oscillator by using the space-time transformation approach [5]. A TDHS whose Hamiltonian involves a $(1/q)p + p(1/q)$ term, which gives the radial equation for a system obeying a Hydrogen-like force, was investigated [6,7]. Quantum solutions for other types of TDHSs have also become topics of active research in this context [8–12].

Stimulated by this trend of research, in this work, we investigate the exact wave functions for a system subjected to time-dependent singular potentials. The Coulomb potential, together with the inverse quadratic potential, will be considered as singular potentials. The singular potential systems can be applied to study many actual physical systems. The interaction of an electron with a polar molecule is described by using an inverse quadratic potential [13]. Indeed, the governing potential in polar molecules such as water can be successfully approximated by using $1/q^2$ [14]. Another example of this type of potential is the interaction of a cold neutral atom with a charged wire, which follows a pure attractive potential with a $1/q^2$ singularity [15]. A more generalized molecular potential of the form $V(t) = a(t) + b(t)/q + c(t)/q^2$ is also a topic of great interest for studying the radial equations of molecular interactions [14,16,17].

Due to the time-dependence of parameters, the mathematical procedure for unfolding the quantum theory of the system may not be an easy task. In order to overcome

such a difficulty, we will introduce an invariant operator of the system [18,19]. In fact, the eigenstates of an invariant operator of a TDHS are the same as the Schrödinger solutions (wave functions) of the given system provided that we neglect the phases of the wave functions. This is the reason we use the invariant operator method. From fundamental mechanics, we can derive the invariant operator of the system.

The original invariant operator may be somewhat complicated because it is a function of time. The unitary transformation is useful when treating such a complicated invariant operator. We perform a unitary transformation with an invariant operator so that it takes a simple form. Then, we can easily identify the eigenstates of the transformed invariant operator by using a particular mathematical procedure. We use the Nikiforov-Uvarov (NU) method [20–22] for that purpose. This method is an alternative method for solving Schrödinger equation on the basis of a particular mathematical technique that reduces the eigenvalue equations of the invariant operator, which are second-order differential equations, to generalized hypergeometric ones [20]. For the given system that involves a singular potential, the eigenvalue equation of the transformed invariant operator will be solved systematically by using the NU method. The eigenstates obtained in this way will be inversely transformed in order to obtain the eigenstates in the original system. Then, the full wave functions of the system can eventually be obtained. This is the strategy of our mathematical manipulation for finding the Schrödinger solutions of the system.

This paper is organized as follows: In section II, the Hamiltonian for time-dependent singular potentials will be introduced, and the properties of the corresponding invariant operator will be studied. The unitary transformation of the invariant operator will be done in section III so that it takes a simple form. Exact quantum solutions will be derived in section IV, by using the NU method [20–22]. Concluding remarks are given in the last section, which is section V.

II. HAMILTONIAN AND INVARIANT

We consider a generalized time-dependent singular potential system whose Hamiltonian is given in the form

$$
H(t) = \frac{1}{2m_0(1+\epsilon t)}\left(p^2 + \frac{f_0}{q^2}\right) \\
- \frac{Z_0}{(1+\epsilon t)\left[1-\ln(1+\epsilon t)\right]}\frac{1}{q}, \tag{1}
$$

where m_0, ϵ, and f_0 are constants. The range of q in this system is $q \geq 0$, and we impose the condition, $t \geq 0$ and $Z_0 > 0$, for convenience. Because we can put the time-dependence of the mass in this system as $m(t) = m_0(1+\epsilon t)$, the rate of mass increase is deter-

mined by the magnitude of ϵ. As you can see, the coupling parameter of the Coulomb potential in this Hamiltonian also depends on time. Note that the canonical variables obey the conventional commutation relation $[q,p] = i\hbar$.

For the TDHS, the use of the conventional method of separation of variables for solving Schrödinger equation is very difficult or sometimes impossible. For this reason, we need a special mathematical technique. The invariant operator method and the unitary transformation method are useful for this situation, and we will use such mathematical techniques.

According to the definition of the invariant operator I, it is obtained by solving the following equation:

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

which is known as the Liouville-von Neumann equation. From a little algebra after inserting Eq. (1) into the above equation, we have

$$
I(q,p,t) = \frac{\left[1-\ln(1+\epsilon t)\right]^2}{2m_0}\left(p^2 + \frac{f_0}{q^2}\right) + \frac{1}{2}m_0\epsilon^2 q^2 \\
+ \frac{\epsilon}{2}\left[1-\ln(1+\epsilon t)\right](qp+pq) - Z_0\left[1-\ln(1+\epsilon t)\right]\frac{1}{q}. \tag{3}
$$

The reason the invariant operator method is useful in the quantum problem of the TDHS is that the eigenstates of I are the same as the Schrödinger solutions (wave functions) of the system, provided that we do not consider the phase factors of the wave functions. Therefore, once the eigenstates of the invariant operator are derived, we can easily identify the wave functions. If we put the eigenvalue equation of I as

$$
I\phi_n = E_n\phi_n, \tag{4}
$$

the eigenvalues E_n do not depend on time. The Nikiforov-Uvarov method will later be used to solve this equation. In terms of the eigenstates ϕ_n, the wave functions are represented in the form

$$
\psi_n(t) = e^{i\theta_n(t)}\phi_n(t), \tag{5}
$$

where $\theta_n(t)$ are the global phases of the wave functions. By inserting this equation into the Schrödinger equation, such that

$$
i\hbar\frac{\partial}{\partial t}\psi_n(t) = H(t)\psi_n(t), \tag{6}
$$

we have the following equation for the phases $\theta_n(t)$:

$$
\hbar\frac{d}{dt}\theta_n(t) = \langle\phi_n(t) \mid i\hbar\frac{\partial}{\partial t} - H \mid \phi_n(t)\rangle. \tag{7}
$$

If we obtain the phases by solving this equation, the complete wave functions can be identified. This is the primary idea that will be used for investigating the quantum system in subsequent sections. In the next section, we will transform the invariant, Eq. (3), by using a suitable unitary operator.

III. UNITARY TRANSFORMATION

Let us consider the following unitary transformation for the eigenstates,

$$\Phi_n(q) = U(t)\phi_n(q,t), \tag{8}$$

where $U(t)$ is a unitary operator of the form

$$U(t) = \exp\left[\frac{i}{2\hbar}m_0\epsilon\left[1 - \ln(1+\epsilon t)\right]q^2\right]$$
$$\times \exp\left[\frac{-i}{2\hbar}\left[1 - \ln(1+\epsilon t)\right](qp + pq)\right]. \tag{9}$$

Then, by considering the transformation relations of canonical variables, which are

$$q \longrightarrow U(t)qU(t)^{-1} = \left[1 - \ln(1+\epsilon t)\right]q, \tag{10}$$

$$p \longrightarrow U(t)pU(t)^{-1} = \frac{1}{\left[1 - \ln(1+\epsilon t)\right]}p - m_0\epsilon q, \tag{11}$$

the original invariant operator is transformed to

$$I(t) \longrightarrow I_0 = UIU^{-1} = \frac{1}{2m_0}\left(p^2 + \frac{f_0}{q^2}\right) - \frac{Z_0}{q}. \tag{12}$$

Hence, we can rewrite the eigenvalue equation given in Eq. (4), in the transformed system, as

$$\left[\frac{1}{2m_0}\left(p^2 + \frac{f_0}{q^2}\right) - \frac{Z_0}{q}\right]\Phi_n(q) = E_n\Phi_n(q). \tag{13}$$

Notice that this does not depend on time while the original eigenvalue equation, Eq. (4) explicitly depends on it. After a little rearrangement using $p = -i\hbar\partial/\partial q$, this equation becomes

$$\Phi_n''(q) + \left(\frac{-\kappa_n^2 q^2 - \varepsilon^2 q - \nu(\nu+1)}{q^2}\right)\Phi_n(q) = 0, \tag{14}$$

where

$$\frac{2m_0 E_n}{\hbar^2} = -\kappa_n^2, \ \frac{2m_0 Z_0}{\hbar^2} = -\varepsilon^2, \ f_0/\hbar^2 = \nu(\nu+1). \tag{15}$$

From the first relation of Eq. (15), obviously $E_n < 0$. This means that the system is bound in a potential well. The differential equation, Eq. (14), will be solved and the eigenstates will be identified in the next section.

IV. EXACT QUANTUM SOLUTIONS

To solve the equation given in Eq. (14), we will use the NU method [20,21], which is described in Appendix A. A large class of second-order linear differential equations relevant to the Schrödinger equation or the eigenvalue equation of I_0 can be solved by using this method and,

as a consequence, the solutions are represented in terms of special orthogonal functions.

Considering the notation in Appendix A, let us change the variable q as $q \rightarrow s$. Then, Eq (14) can be rewritten as

$$\Phi_n''(s) + \left(\frac{-\kappa_n^2 s^2 - \varepsilon^2 s - \nu(\nu+1)}{s^2}\right)\Phi_n(s) = 0. \tag{16}$$

The comparison of this equation with Eq. (A1) in Appendix A yields

$$\tilde{\tau}(s) = 0, \ \sigma(s) = s, \ \tilde{\sigma}(s) = -\kappa_n^2 s^2 - \varepsilon^2 s - \nu(\nu+1). \tag{17}$$

To develop the NU theory of the system, we also need the function $\Pi(s)$ introduced in Eq. (A8) of Appendix A. The possible values of $\Pi(s)$ are known to be [23]

$$\Pi(s) = $$
$$\begin{cases} \kappa_n s + \nu, & \text{for } k_1 = -\varepsilon^2 + 2\kappa_n(\nu+1/2), \\ -(\kappa_n s + \nu + 1), & \text{for } k_1 = -\varepsilon^2 + 2\kappa_n(\nu+1/2), \\ \kappa_n s - \nu - 1, & \text{for } k_2 = -\varepsilon^2 - 2\kappa_n(\nu+1/2), \\ -\kappa_n s + \nu, & \text{for } k_2 = -\varepsilon^2 - 2\kappa_n(\nu+1/2), \end{cases}$$
$$\tag{18}$$

where $k_{(1,2)}$ are parameters introduced in Eq. (A9) in Appendix A. Regarding the polynomial $\tau(s) = \tilde{\tau}(s) + 2\Pi(s)$ given in Eq. (A4) in Appendix A, negative value for $\Pi(s)$, which corresponds the fourth value of $\Pi(s)$ in Eq. (18), is suitable:

$$k_2 = -\varepsilon^2 - 2\kappa_n(\nu+1/2) \quad \text{and} \quad \Pi(s) = -\kappa_n s + \nu. \tag{19}$$

Then, for λ introduced in Eq. (A5) in Appendix A, we use the relation $\lambda = k + \Pi'(s)$ given in Eq. (A9). Hence, we have

$$\lambda = -\varepsilon^2 - 2\kappa_n(\nu+1). \tag{20}$$

After a little algebra, λ can be rewritten as

$$\lambda_n = 2n\kappa_n. \tag{21}$$

Then, with the use of this formula, the eigenvalues of I are found to be

$$E_n = -\frac{m_0 Z_0^2}{2\hbar^2}\frac{1}{(n+\nu+1)^2}, \ n = 0,1,2,\cdots. \tag{22}$$

These correspond to the bound-state energies [24].

Now, let us look at the wave functions starting from the weight function $\rho(q)$ given in Appendix A. The use of Eq. (A7) in Appendix A, together with Eq. (19), leads to

$$\rho(q) = e^{-2\kappa_n q}q^{2\nu+1}. \tag{23}$$

The substitution of this into Eq. (A6) in Appendix A gives

$$y_n(q) = C_n L_n^{2\nu+1}(2\kappa_n q), \tag{24}$$

where C_n are normalization constants and $L_n^{2\nu+1}$ are the associated Laguerre polynomials defined in Ref. [25]. Using the condition given in Eq. (A10), we have

$$\phi_n(q) = q^\nu e^{-\kappa_n q}. \qquad (25)$$

Now the bound eigenstates of the transformed invari-

ant operator I_0 are obtained as

$$\Phi_{n\nu}(s) = N_n q^\nu e^{-\kappa_n q} L_n^{2\nu+1}(2\kappa_n q), \qquad (26)$$

where N_n are normalization factors. From the condition $\int_0^\infty \Phi_{n\nu}^*(q)\Phi_{n\nu}(q) = 1$, we easily identify the value of N_n; hence, the full eigenstates become

$$
\begin{aligned}
\Phi_{n\nu}(q) \;=\; & \left(\frac{\Gamma(n+1)}{2(n+\nu+1)\,\Gamma(n+2\nu+2)}\right)^{1/2} \left(\frac{2m_0 Z_0}{\hbar^2(n+\nu+1)}\right)^{3/2} \\
& \times \left(\frac{2m_0 Z_0 q}{\hbar^2(n+\nu+1)}\right)^\nu \exp\left(\frac{-m_0 Z_0}{\hbar^2(n+\nu+1)}q\right) L_n^{2\nu+1}\left(\frac{2m_0 Z_0}{\hbar^2(n+\nu+1)}q\right).
\end{aligned} \qquad (27)
$$

Then, from the use of the inverse transformation relation, which is $\phi_{n\nu}(q,t) = U^{-1}\Phi_{n\nu}(q)$, we obtain the eigenstates of I as

$$
\begin{aligned}
\phi_{n\nu}(q,t) \;=\; & \left(\frac{\Gamma(n+1)}{2(n+\nu+1)\,\Gamma(n+2\nu+2)}\right)^{1/2} \left(\frac{2m_0 Z_0}{\hbar^2(n+\nu+1)}\right)^{1/2} \\
& \times \left(\frac{2m_0 Z_0}{\hbar^2[1-\ln(1+\epsilon t)](n+\nu+1)}\right)^{\nu+1} q^\nu \exp\left(\frac{im_0\epsilon}{2\hbar[1-\ln(1+\epsilon t)]}q^2\right) \\
& \times \exp\left(\frac{-m_0 Z_0}{\hbar^2[1-\ln(1+\epsilon t)](n+\nu+1)}q\right) L_n^{2\nu+1}\left(\frac{2m_0 Z_0}{\hbar^2[1-\ln(1+\epsilon t)](n+\nu+1)}q\right).
\end{aligned} \qquad (28)
$$

To derive the phase of the wave functions, we use the expression of Eq. (7) in the transformed system, which is

$$\hbar\frac{d}{dt}\theta_{n\nu}(t) =$$
$$\langle\Phi_{n\nu}(q)\mid -\frac{1}{(1+\epsilon t)\,[1-\ln(1+\epsilon t)]^2}I_0\mid\Phi_{n\nu}(q)\rangle. \quad (29)$$

Now, considering that the eigenvalue of I_0 given by Eq. (22), the global phases are found to be

$$\theta_{n\nu}(t) = \frac{m_0 Z_0^2}{4\hbar^3\epsilon\,[1-\ln(1+\epsilon t)](n+\nu+1)^2}. \qquad (30)$$

From the substitution of Eqs. (28) and (30) in Eq. (5), we easily have

$$\psi_{n\nu}(q,t) = \phi_{n\nu}(q,t)\exp(i\theta_{n\nu}(t)). \qquad (31)$$

This equation with Eqs. (28) and (30) is the full wave functions in the original system, which are the central results of this research. Although these are somewhat complicated forms, they can be usefully applied when we investigate the quantum characteristics of the system. The wave functions are the most basic and crucial tools for investigating the quantum behaviors of systems. The expectation values, fluctuations, and uncertainties of various quantum observables can be evaluated through the

use of the wave functions. In addition, the time behaviors of the quantized energy, probability densities, density operator, and Wigner function of the system can be clarified by means of this wave functions.

V. CONCLUSION

Quantum mechanical solutions of a TDHS that consists of an inverse quadratic potential and a Coulomb potential have been investigated. Because the Hamiltonian is represented in terms of time-dependent parameters, finding quantum solutions on the basis of conventional methods is very difficult. For this reason, other methods, which are the invariant operator method, the unitary transformation method, and the NU method, were used. The invariant operator that we have introduced has a quadratic form and is somewhat complicated. Through a unitary transformation, this invariant operator is transformed to a simple form that does not involve time functions. Consequently, the mathematical manipulation with the transformed invariant operator is easier than that with the original one. To solve the eigenvalue equation of the transformed invariant operator, we used a special mathematical technique, which is the NU method. This method enabled us to identify the solutions to the eigenvalue equation of I_0 in an elegant and direct way. The eigenstates of the invariant

operator obtained in this way in the transformed system are inversely transformed to those of the original system, as shown in Eq. (28). Then, by determining the time-dependent phases $\theta_{n\nu}(t)$ by using Eq. (29), we derived the full wave functions of the system.

The wave functions we have obtained in this work belong to Fock states, which are the most basic ones in quantum mechanics. Indeed, the derivation of the wave functions of the system is very important for the study of the quantum features of the system. Noticeably no approximation or perturbation methods were used during our derivation of the analytical wave functions. Hence, the quantum solutions given in this work are exact. In general, the invariant operator technique in quantum mechanics does not require any approximation so long as a closed form of the invariant operator of the system exists.

The complete wave functions represented in Eq. (31) enable us to discover useful informations for the quantum characteristics, such as fluctuations of canonical variables, the uncertainty relation, the time evolution of the Hamiltonian, and the quantum behavior of wave packets, of the system. The study of the propagator, the Wigner distribution, and the geometric phase of the system may be good topics for further research task, that can be done on the basis of the wave functions derived in this work. In addition, the quantum properties of the system in coherent states and squeezed states may also be important research topics available to study with the results of this research.

APPENDIX A: THE NIKIFOROV-UVAROV METHOD

Let us consider a differential equation of the form

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

where $\tilde{\tau}(s)$, $\sigma(s)$, and $\tilde{\sigma}(s)$ are arbitrary polynomials of s while $\tilde{\tau}(s)$ is allowed up to first degree and $\sigma(s)$ and $\tilde{\sigma}(s)$ are allowed up to at most second degree. Let us represent $\varphi_n(s)$ in terms of appropriate functions $v_n(s)$, which are chosen considering the type of Eq. (A1), as

$$\varphi_n(s) = v_n(s)y_n(s), \tag{A2}$$

Then, Eq. (A1) can be rewritten in the form [22]

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

where $\tau(s)$ and λ are given by

$$\tau(s) = \tilde{\tau}(s) + 2\Pi(s), \tag{A4}$$

$$\lambda = \lambda_n = -n\tau' - \frac{n(n-1)}{2}\sigma''. \tag{A5}$$

Notice that λ is a constant whereas $\tau(s)$ is not. Let us consider the case in which the derivative of $\tau(s)$ is negative. Then, we can identify λ_n from the particular solutions which are given by $y(s) = y_n(s)$, i.e., given in terms of an nth degree polynomial. Here, $y_n(s)$ are hypergeometric functions known as Rodrigues formula [22]:

$$y_n(s) = \frac{B_n}{\rho(s)}\frac{d^n}{ds^n}[\sigma^n(s)\rho(s)], \tag{A6}$$

where B_n are normalization factors and $\rho(s)$ is a weight function that yields [20]

$$[\sigma(s)\rho(s)]' = \tau(s)\rho(s). \tag{A7}$$

In order to obtain the exact form of $\rho(s)$, we consider a polynomial of the form (see Eq. (12) of Ref. [22])

$$\Pi(s) = \frac{\sigma'(s) - \tilde{\tau}(s)}{2} \pm \sqrt{\left(\frac{\sigma'(s) - \tilde{\tau}(s)}{2}\right)^2 - \tilde{\sigma}(s) + k\sigma(s)}. \tag{A8}$$

When the discriminant of the formula given in the square root of Eq. (A8) is zero, that formula can be represented as a square of a polynomial. Then, we can obtain a simple form for k, and k can be expressed as

$$k = \lambda - \Pi'(s). \tag{A9}$$

Now, the formula for $v_n(s)$ can be found from [22]

$$v_n'(s)/v_n(s) = \Pi(s)/\sigma(s). \tag{A10}$$

For a more detailed description of the NU method and its applications, one can refer to Refs. [20–22].

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