ORIGINAL PAPER

The supersymmetric quantum mechanics theory and Darboux transformation for the Morse oscillator with an approximate rotational term

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Abstract Anharmonic potentials with a rotational terms are widely used in quantum chemistry of diatomic systems, since they include the influence of centrifugal force on motions of atomic nuclei. For the first time the Taylor-expanded renormalized Morse oscillator is studied within the framework of supersymmetric quantum mechanics theory. The mathematical formalism of supersymmetric quantum mechanics and the Darboux transformation are used to determine the bound states for the Morse anharmonic oscillator with an approximate rotational term. The factorization method has been applied in order to obtain analytical forms of creation and annihilation operators as well as Witten superpotential and isospectral potentials. Moreover, the radial Schrödinger equation with the Darboux potential has been converted into an exactly solvable form of second-order Sturm–Liouville differential equation. To this aim the Darboux transformation has been used. The efficient algebraic approach proposed can be used to solve the Schrödinger equation for other anharmonic exponential potentials with rotational terms.

Keywords Factorization method · rotating Morse oscillator · Supersymmetric quantum mechanics · Darboux transformation · Pekeris transformation · Superpotential

1 Introduction

Analytical solution of the Schrödinger equation for anharmonic potentials with a rotational term, describing influence of centrifugal force on nuclei motions in diatomic

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systems, is of high importance in nonrelativistic quantum mechanics and quantum chemistry, since the wave function contains full information about a quantum system considered. The exact solutions of the one-dimensional Schrödinger equation for the Coulomb type of potential and for a three-dimensional harmonic potential plus Rosen-Morse non-central potential, derived with the use of the Laplace transform, represent two important examples in quantum mechanics [1,2]. There are only few anharmonic potentials for which exact energy levels and wave functions are determined. For example, some exactly solvable quantum systems such as: the Morse, Rosen-Morse, Kratzer, Wei-Hua and pseudoharmonic oscillator as well as Pöschl-Teller potential have attracted much attention [3].

In the last few years many quantum methods have been developed to solve the Schrödinger equation in the framework of an algebraic approach. One of the most important methods is to solve this second-order differential equation using its transformation into the same well known ordinary differential equations, whose exact solutions can be specified as the confluent hypergeometric functions, associated with the Kummer function, Laguerre polynomials and Whittaker function. Also, supersymmetric quantum mechanics (SUSY QM) method is strictly related with analytical solutions of eigenproblems for many anharmonic potentials [4–14]. Using the ideas of SUSY QM theory and an integrability condition called the shape invariance condition for a whole class of shape invariant potentials the exact (bound-state) spectrum of energy levels can be calculated [15–18]. It should be stressed that the concept of the shape invariant potentials within the SUSY QM method was introduced by Gendenshtein [19]. A potential is said to be shape invariant if its SUSY partner potential has the same spatial dependence as the original potential. The formalism of the SUSY QM and the factorization method have been mainly extended to anharmonic potentials and SUSY partner Hamiltonians for these potentials have been constructed and applied to determine exact solutions of the Schrödinger equation. Using this approach it has been proved that there exist an equivalence between the solution of the nonlinear Riccati equation and the related second-order linear differential equation. Also approximate methods based on SUSY QM approach have been introduced for quantum mechanics to solve many eigenproblems. Three of the notable ones are the $1/N$ expansion [20], δ-expansion of many classes of superpotentials [21] and SUSY-inspired WKB semi-quantum approximation [22,23].

The second method proposed to study the solutions of the Schrödinger equation is the Nikiforov–Uvarov method. This simple algebraic procedure was introduced for solution of the Schrödinger equation, and it is based on its transformation into hypergeometric type second-order differential equations [24,25]. Recently, Bayrak et al. [26] have determined analytical solutions of the radial Schrödinger equation for the Kratzer potential using the asymptotic iteration method (AIM). Energy eigenvalues can be determined using this method with applying of the quantization condition. This very efficient quantum method has been proposed to solve second-order differential equations, for which the Schrödinger equation with an exactly solvable potential can be converted [27–29]. It should be stressed that Al-Dossary [30] has obtained eigenenergies of the Schrödinger equation with the rotating Morse potential by means of the asymptotic iteration method. The approach proposed has been applied to several diatomic molecules. Moreover, Bayrak and Boztosun [31] have presented analytical

solution of the radial Schrödinger equation with the rotating Morse potential within the framework of the AIM method. Exact solutions of the D-dimensional Schrödinger equation with pseudoharmonic and modified Kratzer potentials have been obtained by applying an ansatz to the wavefunctions [32]. In this paper the authors have found that for $D = 3$ bound state eigensolutions recover their standard form, known from the literature. Recently, the analytical solution of radial Schrödinger equation in three dimensions has been derived for inverse-power potentials with the use of an ansatz for the eigenfunctions [33]. Khan [34] has solved the radial Schrödinger equation with fourth-order inverse-power potential in N-dimensional Hilbert space. In order to solve this equation power series method and a suitable ansatz for the wavefunction have been applied. Also, the analytical transfer matrix (ATM) method has been employed to determine the eigenvalues of the Schrödinger equation for the rotating Morse potential [35]. In this study a hierarchy of supersymmetric partner potentials has been obtained with the use of the Pekeris approximation [36]. The authors have computed the energies of rotational states of the dihydrogen molecule and compared the results with those obtained with the use of the hypervirial perturbation method. However, Nasser et al. [37] have studied the rotating Morse potential applying the tridiagonal J-matrix approach. The bound states for this potential have been computed using an infinite square integrable basis that supports a tridiagonal matrix representation for the reference Hamiltonian. Recently, Burkhardt and Leventhal [38] have studied three-dimensional problem including the Morse function with the centrifugal term. They proposed very efficient iterative method to solve the Schrödinger equation with the rotating Morse potential. This approach leads to the renormalized Morse oscillator and the energy eigenvalues of vibrational and rotational states.

The aim of this study is to determine the bound state eigensolutions for the Morse potential with rotational term using the SUSY QM approach and Darboux transformation. We apply the factorization procedure to derive analytical forms of superpotentials and isospectral potentials as well as annihilation and creation operators. Finally, by using Darboux transformation, we attempt to convert the Schrödinger equation with this potential into exactly solvable form of a Sturm–Liouville second-order differential equation.

2 Pekeris transformation

Let's consider the following radial Schrödinger equation for the Morse potential with rotational term:

$$\left\{ -\frac{\hbar^2}{2\mu}\frac{d^2}{dr^2} + \frac{\hbar^2 J(J+1)}{2\mu r^2} + D_e\left\{\exp\left[-2\alpha(r-r_e)\right] - 2\exp\left[-\alpha(r-r_e)\right]\right\}\right\} \Psi_{\upsilon J}(r)$$
$$= E_{\upsilon J}\Psi_{\upsilon J}(r),$$

(1)

where D_e stands for the dissociation energy of a diatomic molecule, r_e denotes the equilibrium internuclear distance, the parameter α is the range factor, J is the rotational quantum number, υ is the vibrational number and μ is the reduced mass of a system.

We apply the Pekeris transformation [36], $x = \exp[-\alpha(r - r_e)]$, and carry out a Taylor series expansion of the centrifugal potential, whence keeping just the terms through 2nd order we obtain from the Eq. (1)

$$V(r)_{eff} = D_e x^2 - 2D_e x + A \left(1 - \frac{3}{\alpha r_e} + \frac{3}{\alpha^2 r_e^2} \right) + A \left(\frac{4}{\alpha r_e} - \frac{6}{\alpha^2 r_e^2} \right) x$$

$$+ A \left(-\frac{1}{\alpha r_e} + \frac{3}{\alpha^2 r_e^2} \right) x^2, \tag{2}$$

where $x = \exp[-\alpha(r - r_e)]$ and $A = \frac{\hbar^2}{2\mu} \frac{J(J+1)}{r_e^2}$. In the next paper we will try to expand the effective potential including the centrifugal term about some other value of r than r_e. In particular, the expansion about the mean value of r seems to be appropriate.

We can also rewrite the Eq. (2) in a more transparent form:

$$V(r)_{eff} = B_0 - 2B_1 x + B_2 x^2, \tag{3}$$

where:

$$B_0 = A \left(1 - 3\gamma + 3\gamma^2 \right), \quad B_1 = D_e - A \left(2\gamma - 3\gamma^2 \right),$$

$$B_2 = D_e + A \left(-\gamma + 3\gamma^2 \right), \tag{4}$$

with $\gamma = \frac{1}{\alpha r_e}$.

After applying the following variables changes:

$$r'_e = r_e + \frac{1}{\alpha} \ln \left(\frac{B_2}{B_1} \right) \quad \text{and} \quad D'_e = \frac{B_1^2}{B_2} \tag{5}$$

we get the following form of the effective potential:

$$V(r)_{eff} = B_0 + D'_e \left\{ \exp \left[-2\alpha(r - r'_e) \right] - 2 \exp \left[-\alpha(r - r'_e) \right] \right\}. \tag{6}$$

The potential obtained above is congruent with the Morse potential with $J = 0$ (purely vibrational problem).

3 The rotational-vibrational Morse isospectral potential (Darboux potential). Application of the SUSY QM theory

We assume the following form of the Witten superpotential, from which we will obtain the analitycal form of the Morse potential with a rotational term:

$$W_{0J}(r) = C \exp \left[-\alpha(r - r'_e) \right] - D - E. \tag{7}$$

The C, D and E constants that can be seen in the equation above will be determined with the use of the Riccati equation:

$$V(r)_{eff} = \frac{\hbar^2}{2\mu}\left[W_{0J}^2(r) + W_{0J}'\right] + E_{0J}. \tag{8}$$

After substituting (7) to the Eq. (8) we receive:

$$V(r)_{eff} = \frac{\hbar^2}{2\mu}C^2\left\{-\frac{[\alpha + 2(D+E)]}{C}\exp\left[-\alpha(r-r_e)\right] + \exp\left[-2\alpha(r-r_e)\right]\right\}$$
$$+ \frac{\hbar^2}{2\mu}\left(D^2 + 2DE + E^2\right). \tag{9}$$

Notice that the potential (9) is only congruent with the potential (6) when following conditions are fulfilled:

$$C = \left(\frac{2\mu D_e'}{\hbar^2}\right)^{1/2}, \quad D = \frac{4B_0\mu}{\hbar^2(2C-\alpha)}, \quad E = \frac{2C-\alpha}{2} - \frac{4B_0\mu}{\hbar^2(2C-\alpha)}. \tag{10}$$

We see that the Witten superpotential allows to reconstruct the Morse potential considered if only we use appropriate constants, with whom the Eq. (8) is true. The energy of the vibrational ground state for a given rotational quantum number J takes the following form:

$$E_{0J} = -\frac{\hbar^2}{2\mu}E^2 = -\frac{\hbar^2}{2\mu}\left[\frac{2C-\alpha}{2} - \frac{4B_0\mu}{\hbar^2(2C-\alpha)}\right]^2 \tag{11}$$

and the vibrational ground state wave function for a given rotational quantum number J can be expressed as:

$$\Psi_{0J}(r) = \exp\left[\int W_0(r)dr\right] = \exp\left[-(D+E)r\right]\exp\left\{-\frac{C}{\alpha}\exp\left[-\alpha\left(r-r_e'\right)\right]\right\}. \tag{12}$$

Hence, according to the SUSY QM theory [39–43], the creation and annihilation operators, that factorize the Hamiltonian $\hat{H}^\pm$, take the following forms:

$$\hat{a} = \frac{\hbar}{\sqrt{2\mu}}\left\{C\exp\left[-\alpha(r-r_e')\right] - (D+E) + \frac{d}{dr}\right\}$$
$$\hat{a}^\dagger = \frac{\hbar}{\sqrt{2\mu}}\left\{C\exp\left[-\alpha(r-r_e')\right] - (D+E) - \frac{d}{dr}\right\} \tag{13}$$

and fulfill the following relationship:

$$\hat{a}^\dagger\hat{a} = \hat{H}^\pm - E_{0J}, \tag{14}$$

where $\hat{H}^{\pm} = -\frac{\hbar^2}{2\mu}\frac{d^2}{dr^2} + V^{\pm}(r)$. $V^{+}(r)$ denotes the analytical form of (6), whilst $V^{-}(r)$ stands for, isospectral with (6), Darboux potential. Within the SUSY QM theory $\overset{\wedge}{H^{+}}$ and $\overset{\wedge}{H^{-}}$ denote two partner Hamiltonians. Applying the Darboux transformation [44] we obtain the following form of the Darboux potential, isospectral with (6):

$$V_D(r) = V_{eff}(r) - \frac{\hbar^2}{\mu}\left[\frac{dW_0(r)}{dr}\right] = V_{eff}(r) - \frac{\hbar^2 C\alpha}{\mu}\exp\left[-\alpha(r - r'_e)\right], \quad (15)$$

which corresponds to the following rotational-vibrational wave function of a vibrational ground state:

$$\varphi_{0J}(r) = \exp\left[-\int W_0(r)dr\right] = \exp\left[(D+E)\,r\right]\exp\left\{\frac{C}{\alpha}\exp\left[-\alpha\left(r - r'_e\right)\right]\right\}. \quad (16)$$

In general we can write the solution of Riccati equation in a following manner:

$$W_g(r) = W_0(r) + \frac{b}{\lambda(r)}, \quad (17)$$

where b is an integration constant and $\lambda(r)$ can be expressed in a following way:

$$\lambda(r) = \exp\left[2\int W_0(r)dr\right]\left\{\gamma + b\int\exp\left[-2\int W_0(r)dr\right]dr\right\}, \quad (18)$$

where γ plays a role of an integration constant.

Hence, we obtain the general formula of the Darboux potential:

$$V_{GD}(r) = V_D(r) - \frac{\hbar^2}{\mu}\frac{d}{dr}\left[\frac{b}{\lambda(r)}\right], \quad (19)$$

which is correlated with the following vibrational ground state function:

$$\vartheta_{g0J}(r) = \exp\left\{-\int\left[W_0(r) + \frac{b}{\lambda(r)}\right]dr\right\} = \frac{\varphi_{0J}(r)}{\gamma + b\int\varphi_{0J}^2(r)dr}. \quad (20)$$

Moreover, we can factorize the general Hamiltonian operator $\hat{H}_g^{\pm}$ with the use of the following operators:

$$\hat{A} = \frac{\hbar}{\sqrt{2\mu}}\left\{C\exp\left[-\alpha(r - r'_e)\right] - (D+E) + \frac{b}{\lambda(r)} + \frac{d}{dr}\right\}$$

$$\hat{A}^{\dagger} = \frac{\hbar}{\sqrt{2\mu}}\left\{C\exp\left[-\alpha(r - r'_e)\right] - (D+E) + \frac{b}{\lambda(r)} - \frac{d}{dr}\right\}. \quad (21)$$

These operators satisfy the following relations:

$$\hat{A}^{\dagger}\hat{A} = \hat{H}_g^{\pm} - E_{0J}, \quad (22)$$

4 Analytical determination of the $\Psi_{\upsilon J}(r)$ wave function with the use of the SUSY approach

4.1 Basic formalism of SUSY QM

In general eigenproblem for a given potential takes the following form:

$$-\frac{\hbar^2}{2\mu}\Psi_\upsilon''(x) + V(x)\Psi_\upsilon(x) = E_\upsilon\Psi_\upsilon(x) \tag{23}$$

and we can transform it into the well-known nonlinear Riccati equation:

$$\frac{\hbar^2}{2\mu}\left[W_\upsilon^2(x) + W_\upsilon'(x)\right] + E_\upsilon = V(x), \tag{24}$$

where

$$W_\upsilon(x) = \frac{d}{dx}\ln\Psi_\upsilon(x). \tag{25}$$

In the Eq. (24) $W_\upsilon'(x)$ is the first-order derivative of the superpotential with respect to x. The Eq. (24) is valid for every υ. In particular for $\upsilon = 0$ we obtain

$$\frac{\hbar^2}{2\mu}\left[W_0^2(x) + W_0'(x)\right] + E_0 = V(x). \tag{26}$$

The Eq. (26) has a crucial meaning, since it allows to determine potentials analytically, when one knows the Witten superpotential $W_0(x)$. With the knowledge of the Witten superpotential we can immediately find the analytical form of the ground state wave function by the use of the following Darboux transformation:

$$\Psi_0(x) = \exp\left[\int W_0(x)dx\right]. \tag{27}$$

To solve the Eq. (23) analytically we presume the following form of the wave function:

$$\Psi_\upsilon(x) = \Psi_0(x)f_\upsilon(x), \tag{28}$$

where $f_\upsilon(x)$ is the function that we need to determine. This function fulfills the condition $f_0(x) = 1$ for $\upsilon = 0$. Hence we can rewrite Eq. (25) in the following manner:

$$W_v(x) = \frac{f'_v(x)}{f_v(x)} + W_0(x). \tag{29}$$

In this way we obtain the following equation:

$$\frac{\hbar^2}{2\mu}\left[W_v^2(x) + W'_v(x)\right] = \frac{\hbar^2}{2\mu}\left[W'_0(x) + W_0^2(x) + \frac{f''_v(x) + 2W_0 f'_v(x)}{f_v(x)}\right]. \tag{30}$$

Therefore, the Eq. (30) yields

$$V(x) = \frac{\hbar^2}{2\mu}\left[W_0^2(x) + W'_0(x) + \frac{f''_v(x) + 2W_0 f'_v(x)}{f_v(x)}\right] + E_0. \tag{31}$$

Finally, on the basis of Eqs. (24) and (26), we get the following second-order Sturm–Liouville differential equation, allowing us to determine the function $f_v(x)$ for a particular form of Witten superpotential:

$$f''_v(x) + 2W_0(x) f'_v(x) + \frac{2\mu}{\hbar^2}(E_v - E_0) f_v(x) = 0. \tag{32}$$

It should be stressed that in all the above equations variable x does not correspond to the variable x used in the Eq. (2).

4.2 SUSY QM approach towards the rotational-vibrational Morse oscillator

Applying the algebraic approach developed by Peña et al. [43] and after substituting superpotential (7) to the differential Eq. (32) we obtain:

$$f''_{vJ}(r) + 2\left\{C\exp\left[-\alpha(r-r'_e)\right] - \delta\right\} f'_{vJ}(r) + \frac{2\mu}{\hbar^2}(E_{vJ} - E_{0J}) f_{vJ}(r) = 0, \tag{33}$$

where $\delta = D + E$.
After applying the following variable changes:

$$x = r - r'_e \quad \text{and} \quad y = 2\gamma\exp(-\alpha x), \quad \text{where} \quad \gamma = \frac{C}{\alpha} \tag{34}$$

we get:

$$y f''_{vJ}(y) + (2\gamma - 1 - y) f'_{vJ}(y) + \left(\omega_{0J}^2 - \omega_{vJ}^2\right)\frac{1}{y} f_{vJ}(y) = 0, \tag{35}$$

where $\omega_{vJ}^2 = -\frac{2\mu}{\hbar^2\alpha^2}E_{vJ}, \quad \omega_{0J}^2 = -\frac{2\mu}{\hbar^2\alpha^2}E_{0J}$.

Then, assuming that $f_{\upsilon J}(y) = y^\zeta \Phi_{\upsilon J}(y)$, we can transform the Eq. (35) to the following form:

$$y\Phi''_{\upsilon J}(y) + (2\zeta + 2\gamma - 1 - y)\,\Phi'_{\upsilon J}(y) + \left(\frac{\Omega}{y} - \xi\right)\Phi_{\upsilon J}(y) = 0, \qquad (36)$$

where $\Omega = \zeta^2 - 2\zeta + 2\zeta\gamma + (\omega_{0J}^2 - \omega_{\upsilon J}^2)$. The function $f_{\upsilon J}(y)$ fulfills the condition of regularity for $y = 0$.

We can transform the Eq. (36) to a hypergeometrical equation, demanding that $\Omega = 0$. For each ζ that satisfies this condition we obtain the following Kummer equation:

$$y\Phi''_{\upsilon J}(y) + (2\zeta + 2\gamma - 1 - y)\,\Phi'_{\upsilon J}(y) - \zeta\Phi_{\upsilon J}(y) = 0, \qquad (37)$$

where $\zeta = 1 - \gamma + \sqrt{1 - 2\gamma + \gamma^2 + \omega_{0J}^2 - \omega_{\upsilon J}^2}$.

The solution of the Eq. (37) is the following confluent hypergeometric function:

$$\Phi_{\upsilon J}(y) = F(\zeta, 2\zeta + 2\gamma - 1, y). \qquad (38)$$

Hence, the wave function which is the solution of the Eq. (1) takes the following form:

$$\Psi_{\upsilon J}(r) = N_{\upsilon J}\Psi_{oJ}(r)\left\{2\gamma\exp\left[-\alpha(r - r'_e)\right]\right\}^\zeta$$
$$F\left(\zeta, 2\zeta + 2\gamma - 1, \left\{2\gamma\exp\left[-\alpha(r - r'_e)\right]\right\}^\zeta\right), \qquad (39)$$

where $N_{\upsilon J}$ denotes a normalization constant.

We can obtain energy levels from the condition for the confluent hypergeometric function to be a υ-degree polynomial:

$$\xi = -\upsilon. \qquad (40)$$

The stipulation mentioned leads us to the following equation for energy levels:

$$E_{\upsilon J} = -\frac{\upsilon^2 - \omega_{0J}^2 - 2\upsilon + 2\gamma\upsilon}{k}, \qquad (41)$$

where $k = -\frac{2\mu}{\hbar^2\alpha^2}$.

5 Concluding remarks

In this paper the Schrödinger equation with Morse potential with rotational term has been solved applying SUSY QM approach. Isospectral Darboux potentials, associated with the considered potential have been constructed, using the algebraic approach. To derive annihilation and creation operators the Darboux transformation has been

employed. These operators have been constructed directly from the analytical eigen-functions of the Schrödinger equation for the Darboux anharmonic potential. The procedure developed can be used to solve other eigenvalue problems with diverse anharmonic potentials, extended with rotational terms. We hope that this method will be applied to compute energy level spacings in theoretical molecular spectroscopy and perturbation theory method. Furthermore, the approach presented can be applied to approximate solution of the Schrödinger equation with other anharmonic potentials including rotational term.

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