

The construction of the Gilmore–Perelomov coherent states for the Kratzer–Fues anharmonic oscillator with the use of the algebraic approach

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Abstract By applying the algebraic approach and the displacement operator to the ground state, the unknown Gilmore–Perelomov coherent states for the rotating anharmonic Kratzer–Fues oscillator are constructed. In order to obtain the displacement operator the ladder operators have been applied. The deduced $SU(1, 1)$ dynamical symmetry group associated with these operators enables us to construct this important class of the coherent states. Several important properties of these states are discussed. It is shown that the coherent states introduced are not orthogonal and form complete basis set in the Hilbert space. We have found that any vector of Hilbert space of the oscillator studied can be expressed in the coherent states basis set. It has been established that the coherent states satisfy the completeness relation. Also, we have proved that these coherent states do not possess temporal stability. The approach presented can be used to construct the coherent states for other anharmonic oscillators. The coherent states proposed can find applications in laser-matter interactions, in particular with regards to laser chemical processing, laser techniques, in micro-machining and the patterning, coating and modification of chemical material surfaces.

Keywords Coherent states · Displacement operator · Hilbert space · Kratzer–Fues oscillator · Ladder operators

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1 Introduction

The coherent states introduced to quantum mechanics by Schrödinger in 1926 [1] are used in investigation of quantum optics problems, particles interactions, soliton formation and molecular systems. There are three definitions of the coherent states for harmonic and anharmonic oscillators:

- (1) They are eigenstates of the annihilation operator;
- (2) They minimize the Heisenberg position-momentum uncertainty relation;
- (3) They are the result of the action of unitary displacement operator on the ground state of the oscillator.

These three different techniques are generally not equivalent and only in the case of harmonic oscillator where the commutator of the raising and lowering operator is the unit operator, these three methods are equivalent.

The coherent states for anharmonic oscillators have been constructed and investigated by means of several algebraic procedures. For example, the supersymmetry quantum mechanics was widely used to study quantum coherent states. Recently, Pol'shin [2] constructed the generalized coherent states for the discrete spectra of the hydrogen atom. The author has proved that these states satisfy $SO(3, 2)$ and $SO(4, 2)$ dynamical symmetry groups. Furthermore, in this paper it was shown that these coherent states are invariant under $SO(4, 1)$ subgroups.

Moreover, Górska et al. [3] have studied asymptotic behaviour of coherent states for bounded discrete spectra. In this paper, the authors consider spectra of bound states for nonrelativistic motion in attractive potentials. For these potentials, the authors constructed collective quantum coherent states and asymptotic behaviour of these states has been studied. These coherent states in the sense of Klauder approach are normalizable and satisfy the resolution of unity in the Hilbert space.

Also, Chakrabarti [4] has investigated quantum anharmonic oscillator with the use of supersymmetry quantum mechanics. The author determined the eigenvalues for oscillators with quartic and sextic perturbed terms. The supersymmetry quantum mechanics approach has been employed to calculate restricted set of parameters. In this paper, the energy levels have been obtained algebraically. The results have been generalized to N dimensions.

The relationship between anharmonic oscillators and perturbed Coulomb potentials in N dimensions has been studied by Morales and Parra-Mejías [5]. These authors have demonstrated that supersymmetric partner potentials can allow to obtain approximate energy eigenvalues for the anharmonic oscillators considered. Furthermore, exact solutions of the Schrödinger equation have been obtained for the N -dimensional systems using supersymmetry formalism.

The Klauder–Perelomov and Gazeau–Klauder coherent states for some shape invariant potentials have been investigated by A. Chenaghloou and H. Fakhri. In this important paper, the solvability of quantum systems related to Eckart and Rosen–Morse potentials was explored. Two generalized types of the Klauder–Perelomov and Gazeau–Klauder coherent states were found and distribution function and poissonian statistics have been determined.

Recently, Tsereteli et al. [6] have developed the electron nuclear dynamics theory using generalization of the Hamiltonian via the coherent states. This method has been employed to the study of chemical reactions.

The main purpose of our paper was to derive the coherent state for the Kratzer–Fues oscillators with the use of the algebraic formalism of mathematical physics. The raising and lowering operators have been employed to construct the displacement operator. To verify the completeness of the basis set of the coherent states studied the resolution of the identity in the Hilbert space was proved.

2 Construction of the coherent states and their fundamental properties

In order to derive the coherent states for the rotating Kratzer–Fues oscillator we employ the algebraic approach. The Kratzer–Fues oscillator [7, 8] is the most important potential energy function employed in molecular quantum theory, theoretical spectroscopy of diatomic molecules and quantum optics. The Kratzer–Fues potential properly describes the rotational and vibrational motions of nuclei of diatomic molecules. The method developed starts with the rotational-vibrational Schrödinger equation including the Kratzer–Fues potential energy function [9].

$$\left[-\frac{\hbar^2}{2m} \frac{d^2}{dr^2} + B(r)J(J+1) + D_e \left(\frac{r-r_e}{r} \right)^2 - E_{vJ} \right] \Psi(r)_{vJ} = 0. \quad (1)$$

Employing the following quantity

$$r_J = r_e \left[1 + \frac{B_e J(J+1)}{D_e} \right] \quad (2)$$

we can rewrite the Eq. (1) in the following form:

$$\left[-\frac{\hbar^2}{2m} \frac{d^2}{dr^2} + D_J \left(\frac{r-r_J}{r} \right)^2 + V(r_J)_J - E_{vJ} \right] \Psi(r)_{vJ} = 0, \quad (3)$$

in which

$$D_J = \frac{D_e r_e}{r_J}, \quad V(r_J)_J = \frac{\hbar^2 J(J+1)}{2mr_J^2} + D_e \left(\frac{r_J - r_e}{r_J} \right)^2 = D_J \left(\frac{r_J - r_e}{r_J} \right). \quad (4)$$

Then, the Eq. (3) is transformed into dimensionless form [9]

$$\frac{1}{2} \left\{ -\frac{d^2}{d\xi^2} + \gamma_J^2 \left[\frac{(1-\xi)^2}{\xi^2} - 1 \right] + \beta_{vJ}^2 \right\} \Psi(\xi)_{vJ} = 0, \quad (5)$$

in which

$$\gamma_J^2 = \gamma^2 + J(J + 1), \quad \xi = \frac{r}{rJ} = \frac{x}{1 + \gamma^{-2}J(J + 1)}, \quad \beta_{vJ}^2 = \frac{2mr_J^2(D_e - E_{vJ})}{\hbar^2}. \tag{6}$$

The analytical solution of the Eq. (3) is given by [9]:

$$\Psi(\xi)_{vJ} = N_{vJ} \xi^{\lambda_J} \exp[-\beta_{vJ} \xi] F[-\nu, 2\lambda_J, 2\beta_{vJ} \xi], \tag{7}$$

in which

$$\lambda_J = \frac{1}{2} + \sqrt{\gamma_J^2 + \frac{1}{4}} = \frac{1}{2} + \sqrt{\gamma^2 + \left(J + \frac{1}{2}\right)^2}, \quad N_{vJ} = \left[\frac{\nu!}{2(\lambda_J + \nu)\Gamma(1 + \lambda_J + \nu)} \right]^{1/2}. \tag{8}$$

Using the well-known relationship between the hypergeometric confluent Kummer function and associated Laguerre polynomial, the wavefunction (7) takes the following form [9]:

$$\Psi(z)_{vJ} = C_{vJ} z^{\lambda_J} \exp\left[-\frac{z}{2}\right] L_{\nu}^{2\lambda_J - 1}(z) \tag{9}$$

Using the wavefunction (9), we construct the ladder operators which fulfill the following relations:

$$\hat{K}_+ \Psi(z)_{vJ} = K_+ \Psi(z)_{v+1,J} \tag{10}$$

$$\hat{K}_- \Psi(z)_{vJ} = K_- \Psi(z)_{v-1,J} \tag{11}$$

After several simple calculations, the ladder operators take the following forms [9]:

$$\hat{K}_+ = \left[z \frac{d}{dz} - \frac{1}{2}z + \nu + \lambda_J \right] \tag{12}$$

$$\hat{K}_- = \left[-z \frac{d}{dz} - \frac{1}{2}z + \nu + \lambda_J \right], \tag{13}$$

whereas coefficients associated with these operators are [9]

$$K_+ = (\nu + 1) \frac{C_{vJ}}{C_{v+1,J}}, \quad K_- = (\nu + 1) \frac{C_{vJ}}{C_{v-1,J}}. \tag{14}$$

Therefore, the operators \hat{K}_+ and \hat{K}_- can be considered as linear operators in a separable Hilbert space \mathbb{B} (Fock space) spanned by eigenvectors.

We now study the dynamical Lie group associated with \hat{K}_+ and \hat{K}_- operators. It is easy to check that the ladder operators satisfy the following commutator relation [9]:

$$\left[\hat{K}_-, \hat{K}_+ \right] \Psi(z)_{\nu J} = m_{\nu J} \Psi(z)_{\nu J}, \quad (15)$$

in which

$$m_{\nu J} = 2(\nu + \lambda_J + 1). \quad (16)$$

Using the following operator definition [9]:

$$\hat{M}_{\nu J} = 2(\hat{\nu} + \lambda_J + 1) \quad (17)$$

simple calculations provide the algebraic relations [9]:

$$\left[\hat{K}_-, \hat{K}_+ \right] = 2\hat{M}_{\nu J}, \quad \left[\hat{M}_{\nu J}, \hat{K}_{\pm} \right] = \pm \hat{K}_{\pm}. \quad (18)$$

According to this result we have justified that the ladder operators correspond to $SU(1, 1)$ Lie algebra. Referring to the generators of this symmetry algebra we are able to assume the displacement operator in the general form:

$$\hat{D} = \exp \left[\alpha \hat{K}_+ - \alpha^* \hat{K}_- \right], \quad (19)$$

in which $\alpha = |\alpha|e^{i\varphi} \in \mathbb{C}$ is a complex number corresponding to the complex wave amplitude in classical optics. This operator generates the Gilmore–Perelomov type of the coherent states [10–13] which act on the ground vibrational J -dependent state in the following way:

$$\hat{D}\Psi_{0J}(z) = \Psi_{\alpha J}(z) \hat{D}|0, J\rangle = |\alpha, J\rangle \quad (20)$$

In order to demonstrate how the method works, let's determine the analytical form of the coherent states. Expanding the exponentials of operators into the Taylor series

$$\exp(\alpha \hat{K}_+) = \sum_{n=0}^{\infty} \frac{\alpha^n}{n!} (\hat{K}_+)^n, \quad \exp(-\alpha^* \hat{K}_-) = \sum_{n=0}^{\infty} \frac{(-\alpha^*)^n}{n!} (\hat{K}_-)^n \quad (21)$$

we get

$$\hat{D}|0, J\rangle = \sum_{n=0}^{\infty} \frac{\alpha^n}{n!} \hat{K}_+^n |\Psi_{0J}\rangle. \quad (22)$$

Hence, employing the Eqs. (10) and (11), one may generate the explicit form of the coherent states:

$$|\alpha, J\rangle = \sum_n \left(\frac{\alpha^n}{n!} \prod_{k=0}^n k_{kJ} \right) |n, J\rangle, \quad (23)$$

in which k_{kJ} are the coefficients arising from Eq. (14). This result proves that the space of the coherent state vectors constructed is the space spanned by the set $|n, J\rangle$. Therefore, the coherent states studied can be written in terms of an exact expansion in Fock space.

The fundamental mathematical property of the coherent states introduced is non-orthogonality

$$\langle \alpha, J | \beta, J \rangle \neq 0 \text{ for } \alpha \neq \beta \tag{24}$$

Employing the following forms of two different coherent states:

$$|\alpha, J\rangle = \sum_n \left(\frac{\alpha^n}{n!} \prod_{k=0}^n k_{kJ} \right) |n, J\rangle \tag{25}$$

$$|\beta, J\rangle = \sum_m \left(\frac{\beta^m}{m!} \prod_{k=0}^m k_{kJ} \right) |m, J\rangle \tag{26}$$

after simple calculations, we obtain the result:

$$\langle \alpha, J | \beta, J \rangle = \sum_n \sum_m \frac{\alpha^{*n} \beta^m}{n! m!} \prod_{k=0}^n k_{kJ} \prod_{k=0}^m k_{kJ} \langle n, J | m, J \rangle. \tag{27}$$

From this, it evidently follows that

$$\langle \alpha, J | \beta, J \rangle \neq 0 \text{ for } \alpha \neq \beta. \tag{28}$$

This finding is the consequence of orthonormality of the Kratzer–Fues basis set. This property can be specified by the general formula

$$\langle n, J | m, J \rangle = \delta_{nm}. \tag{29}$$

The vectors $|\alpha, J\rangle$ are the elements of the Hilbert space, therefore the proper coherent states must be normalized. To normalize these quantum states, the following calculation has been adopted:

$$1 = \frac{1}{N^2(\alpha, J)} \sum_{n=0}^{\infty} \left(\frac{\alpha^n}{n!} \right)^2 \left(\prod_{k=0}^n k_{kJ} \right)^2 \tag{30}$$

$$N(\alpha, J) = \sqrt{\sum_{n=0}^{\infty} \left(\frac{\alpha^n}{n!} \prod_{k=0}^n k_{kJ} \right)^2}; \quad -\infty < J < \infty; \quad J \geq 0; \quad 0 \leq \alpha < R. \tag{31}$$

Using this expression for normalization constant, the coherent states satisfy the relation

$$\langle \alpha, J | \alpha, J \rangle = 1 \tag{32}$$

The coherent states basis set is complete in the Hilbert space. This indicates that these coherent states should fulfill the resolution of the identity which is defined as follows

$$\int |\alpha, J\rangle\langle\alpha, J|d\mu(\alpha, J) = \mathbb{1}, \quad (33)$$

where $\mu(\alpha, J)$ is a positive Lebesgue measure that we try to search. To verify this statement for the constructed coherent states, we performed the following calculations:

$$\begin{aligned} & \int |\alpha, J\rangle\langle\alpha, J|d\mu(\alpha, J) \\ &= \lim_{\Gamma \rightarrow \infty} \frac{1}{2\Gamma} \int_{-\Gamma}^{\Gamma} \frac{1}{N(\alpha, J)^2} \sum_{n,m} \frac{\alpha^{n+m}}{n!m!} \prod_{k=0}^n k_{kJ} \prod_{k=0}^m |m, J\rangle\langle n, J|d\alpha \\ &= \frac{1}{N(\alpha, J)^2} \sum_{n=0}^{\infty} \frac{\alpha^{2n}}{(n!)^2} \left(\prod_{k=0}^n k_{kJ} \right)^2 |n, J\rangle\langle n, J| \\ &= \frac{1}{N(\alpha)^2} \sum_{n=0}^{\infty} \frac{\alpha^{2n}}{\rho_n} |n, J\rangle\langle n, J|, \end{aligned} \quad (34)$$

in which

$$\rho_n = \frac{(n!)^2}{\left(\prod_{k=0}^n k_{kJ} \right)^2}. \quad (35)$$

Defining the following relations:

$$\rho_n = \int_0^R \alpha^{2n} \rho(\alpha) d\alpha; \quad 0 \leq \alpha < R; \quad \rho(\alpha) \geq 0 \quad (36)$$

$$K(\alpha) \equiv N(\alpha)^2 \rho(\alpha) d\alpha \geq 0; \quad 0 \leq \alpha < R \quad (37)$$

$$K(\alpha) \equiv \rho(\alpha) \equiv 0; \quad \alpha > R \quad (38)$$

we obtain

$$\frac{1}{\rho_n} \int_0^R N(\alpha)^{-2} \alpha^{2n} K(\alpha) d\alpha = 1. \quad (39)$$

By the use of specified calculating procedure, we can pass to evaluate:

$$\begin{aligned}
 \int_0^R K(\alpha) d\alpha \int |\alpha, J\rangle \langle \alpha, J| d\mu(\alpha, J) &= \int_0^R K(\alpha) d\alpha \frac{1}{N(\alpha)^2} \sum_n \frac{\alpha^{2n}}{\rho_n} |n, J\rangle \langle n, J| \\
 &= \sum_n \int_0^R K(\alpha) \frac{1}{N(\alpha)^2} \frac{\alpha^{2n}}{\rho_n} |n, J\rangle \langle n, J| \\
 &= \sum_n \frac{1}{\rho_n} \int_0^R K(\alpha) N(\alpha)^{-2} \alpha^{2n} |n, J\rangle \langle n, J|
 \end{aligned}
 \tag{40}$$

Based on the fact that for the rotating Kratzer–Fues oscillator eigenstates the following resolution of unity holds:

$$\sum_n |n, J\rangle \langle n, J| = \mathbb{1}
 \tag{41}$$

the algebraic calculations performed prove the completeness as fundamental requirement for the coherent states has been established.

From the quantum mechanics theory, it is obvious that the coherent states for harmonic oscillator are characterized by temporal stability during the time of their evolution in the space. The temporal stability is described by the following relation:

$$e^{\frac{-i\hat{H}t}{\hbar}} |\alpha, J\rangle = |\alpha + \omega t, J\rangle,
 \tag{42}$$

in which $e^{\frac{-i\hat{H}t}{\hbar}}$ stands for the unitary hermitian operator of the time evolution. In the next part we will check whether the coherent states introduced satisfy this requirement.

To this purpose, with the use of the general formula of the constructed coherent states, we proceed with the following algebraic manipulations:

$$\begin{aligned}
 e^{\frac{-i\hat{H}t}{\hbar}} \frac{1}{N(\alpha, J)} \sum_{n=0}^{\infty} \frac{\alpha^n}{n!} \prod_{k=0}^n k_{kJ} |n, J\rangle &= \sum_{n=0}^{\infty} \frac{1}{N(\alpha, J)} \frac{\alpha^n}{n!} e^{\frac{-i\hat{H}t}{\hbar}} \prod_{k=0}^n k_{kJ} |n, J\rangle \\
 &= \sum_{n=0}^{\infty} \frac{1}{N(\alpha, J)} \frac{\alpha^n}{n!} e^{-iE_n J t} |n, J\rangle \prod_{k=0}^n k_{kJ} \\
 &= \sum_{n=0}^{\infty} \frac{1}{N(\alpha, J)} \frac{\alpha^n}{n!} \prod_{k=0}^n k_{kJ} e^{-iE_n J t} |n, J\rangle.
 \end{aligned}
 \tag{43}$$

The above calculations reveal that in comparison with other coherent states, the coherent states introduced in this paper do not remain coherent under the time evolution. Only in the Gazeau-Klauder formalism these states should satisfy this criterion.

The number state $|n, J\rangle$ represents the rovibrational state with exactly n photons in vibrational state. Hence, the probability that the coherent state has n photons can be calculated from the following relation:

$$P = |\langle n, J | \alpha, J \rangle|^2 \quad (44)$$

It is easily verified that this relation is a Poisson distribution with average number of photons. To calculate this probability, we have made use of the following form of the coherent state:

$$|\alpha, J\rangle = \frac{1}{N(\alpha, J)} \sum_{n=0}^{\infty} \frac{\alpha^n}{n!} \prod_{k=0}^n k_{kJ} |n, J\rangle \quad (45)$$

and the normalization relation

$$\langle n, J | n, J \rangle = 1 \quad (46)$$

Taking into account the calculations:

$$\begin{aligned} \langle n, J | \alpha, J \rangle &= \frac{1}{N(\alpha, J)} \sum_{n=0}^{\infty} \frac{\alpha^n}{n!} \prod_{k=0}^n k_{kJ} \langle n, J | n, J \rangle \\ &= \frac{1}{N(\alpha, J)} \sum_{n=0}^{\infty} \frac{\alpha^n}{n!} \prod_{k=0}^n k_{kJ}, \end{aligned} \quad (47)$$

one yields

$$|\langle n, J | \alpha, J \rangle|^2 = \frac{1}{N^2(\alpha, J)} \frac{\alpha^{2n}}{(n!)^2} \left(\prod_{k=0}^n k_{kJ} \right)^2. \quad (48)$$

Any vector $|\Psi\rangle$ in the Hilbert space of the Kratzer–Fues basis set can be expressed in the coherent state basis, by using the relation

$$|\Psi\rangle = \int |\alpha, J\rangle \langle \alpha, J | \Psi \rangle d^2\alpha, \quad (49)$$

in which $\langle \alpha, J | \Psi \rangle$ is the representation of the vector $\langle \alpha, J |$ in the quantum state $|\Psi\rangle$. In particular, any of the coherent states, for example $|\beta, J\rangle$ can be expressed in the following manner:

$$|\beta, J\rangle = \int |\alpha, J\rangle \langle \alpha, J | \beta, J \rangle d^2\alpha \quad (50)$$

This expression shows the linear dependence of the infinite basis set of the coherent states. Adopting to calculations the following representation of the eigenstate of the Kratzer–Fues oscillator:

$$|n, J\rangle = \int \frac{1}{N(\alpha, J)} \frac{\alpha^{*n}}{n!} \prod_{k=0}^n k_{kJ} |\alpha, J\rangle d^2\alpha \tag{51}$$

we can express the expansion coefficients in Eq. (49) as

$$\langle \alpha, J | \Psi \rangle = \sum_n \langle \alpha, J | n, J \rangle \langle n, J | \Psi \rangle. \tag{52}$$

Taking into account the advantage of the following relation:

$$\langle \Psi | \Psi \rangle = \sum_n |\langle n, J | \Psi \rangle|^2 = 1 \tag{53}$$

these coefficients can be simplified to the closed formula

$$\langle \alpha, J | \Psi \rangle = \sum_n \langle n, J | \Psi \rangle \frac{\alpha^{*n}}{n!} \frac{1}{N(\alpha, J)} \prod_{k=0}^n k_{kJ}. \tag{54}$$

Introducing the analytical form of the entire function

$$f_\Psi(\alpha^*) = \sum_n \langle n, J | \Psi \rangle \frac{\alpha^{*n}}{n!} \frac{1}{N(\alpha, J)} \prod_{k=0}^n k_{kJ} \tag{55}$$

we can see that the series in the right hand side of Eq. (54) is absolutely convergent in any finite region of the complex plane. This function connects the representation of the coherent state $\langle \alpha, J | \Psi \rangle$ in the Hilbert space and the Segal-Bargmann space of entire functions. Hence, we can easily verify that the coherent state vectors are the elements of the space \mathbb{B} which is closely related to classical Bargmann’s space.

3 Conclusions

In this paper for the rotating Kratzer–Fues oscillator the unknown displacement coherent states have been constructed. We have explored that the quantum system considered has a symmetrical realisation of the $SU(1, 1)$ Lie algebra. Thus, we have generated the explicit form of these coherent states from the displacement operator. Their several fundamental properties have been established using algebraic approach. The results obtained reveal that those states are the vectors in the Hilbert space. The resolution of the identity has been established analytically and, as a consequence, the over-completeness relation for these states is demonstrated. We have proved that the coherent states proposed can be expanded in the convergent series of the Kratzer–Fues basis set. The ladder operators have been applied to derive these states. We hope that

the constructed coherent states will be used to study the optical properties of molecular systems.

Conflict of interest The authors have no financial disclosures and conflict of interest.

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