PHYSICAL REVIEW A **76**, 022107 (2007)

Coherent states of the Kratzer-Fues oscillator

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(Received 13 March 2007; revised manuscript received 18 June 2007; published 27 August 2007)

The coherent states for the Kratzer-Fues potential, which are eigenstates of the annihilation operator and minimize the generalized position-momentum uncertainty relation, are constructed using the algebraic approach. The method is extended to include the rotating Kratzer-Fues oscillator. Construction of such states is important in the theory of molecular interactions with coherent electromagnetic fields, for example, in calculation of the dynamic alternation of the refractive index due to the interactions of the laser pulse with the coherent vibration-rotational states of the diatomic molecule.

DOI: 10.1103/PhysRevA.76.022107 PACS number(s): 03.65.Fd

I. INTRODUCTION

In 1926 Schrödinger [1] discovered the coherent states of harmonic oscillator, which minimize the position-momentum uncertainty relation. The term *coherent* reflects the fact that such states are localized on the corresponding classical trajectory and do not change their functional form during propagation. The coherent states of the harmonic oscillator are defined as [2] (i) eigenstates of the annihilation operator, (ii) states that minimize the position-momentum uncertainty relation, and (iii) states that arise from the operation of a unitary displacement operator to the ground state of the oscillator.

Recently, much effort has been undertaken to generate coherent states for anharmonic potentials, particularly the Morse potential [3–10]. Such states are usually constructed using a transformation of the basic Hamiltonian to the form resembling that of a harmonic oscillator [3,4] or by making use of the irreducible representations of a Lie group which provides a spectrum generating algebra [11]. The generalized coherent states can also be constructed using an algebraic method [9,12] employing the supersymmetric quantum mechanics [10,13]. The algebraic approach is particularly useful as it straightforwardly leads to the construction of not only coherent but also squeezed states endowed with nonclassical features. Applying the above procedures the coherent states have been obtained for the Morse [3–9], Pöschl-Teller [14], hydrogen atom [15], Eckart and Rosen-Morse [16], double-well and linear (gravitational) potentials [17]. Unfortunately, such states have not been constructed so far [18] for the Kratzer-Fues (KF) potential [19],

$$V(r) = D_e\left[\left(\frac{r-r_e}{r}\right)^2 - 1\right], \tag{1}$$

widely used for description of anharmonic vibrations in diatomic systems [20]. Here, D_e denotes the dissociation energy of the system, whereas r_e is the equilibrium internuclear separation. The potential function (1) has four valuable properties: (i) it correctly behaves for united-atom ($r \to 0$) and dissociation ($r \to \infty$) limits, (ii) it takes into account the quasiharmonic behavior of the oscillator in the vicinity of the potential minimum, (iii) the Schrödinger equation with the KF potential can be exactly solved, and (iv) it can be easily generalized to include the rotating KF oscillator for which the exact analytical solutions are directly derived. Nowadays, the multiparametric generalization of Eq. (1) in the form of the Simons-Parr-Finlan potential [21]

$$V(r) = c_0\left(\frac{r-r_e}{r}\right)^2\left[1 + \sum_{n=1}^{N} c_n\left(\frac{r-r_e}{r}\right)^n\right] \tag{2}$$

has been widely applied in spectroscopy of rotation-vibrational diatomic systems as it contains the proper amount of potential parameters c_n indispensable to fit the spectral data [22]. In this work, we use the first term of the expansion (2), which differs from Eq. (1) by the additive term $D_e = c_0$.

The aim of this study is construction of the coherent states of the KF potential, which are eigenstates of the annihilation operator and minimize the position-momentum uncertainty principle. We shall also be concerned with their generalization to include the rotating KF oscillator and calculation of the dynamic alternation of the refractive index due to the interactions of the laser pulse with the coherent vibration-rotational states of the diatomic molecule.

II. COHERENT STATES OF THE KF OSCILLATOR

In order to construct the coherent states of KF oscillator, we employ the algebraic (or operator) method successfully applied by Cooper [9] to generate the coherent states of the anharmonic Morse oscillator. The starting point for this approach is the vibrational Schrödinger equation

$$\left[-\frac{\hbar^2}{2m}\frac{d^2}{dr^2} + D_e\left(\frac{r-r_e}{r}\right)^2 - E_v\right]\psi(r)_v = 0, \tag{3}$$

which can be transformed to the dimensionless form

$$\frac{1}{2}\left\{-\frac{d^2}{dx^2} + \gamma^2\left[\frac{(1-x)^2}{x^2} - 1\right] + \beta_v^2\right\}\psi(x)_v = 0, \tag{4}$$

in which

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$$\beta_v^2=\frac{2mr_e^2(D_e-E_v)}{\hbar^2}=\gamma^2-2\delta_v^2,\qquad \gamma^2=\frac{2mr_e^2D_e}{\hbar^2},\qquad x=\frac{r}{r_e}. \tag{5}$$

The solution of Eq. (4) in arbitrary normalization reads [23]

$$\psi(x)_v=x^{\lambda}\exp[-\beta_v x]F[\lambda-\gamma^2/\beta_v,2\lambda,2\beta_v x], \tag{6}$$

in which $\lambda=1/2+\sqrt{\gamma^2+1/4}$ is the positive solution of the parabolic relation $\lambda^2-\lambda-\gamma^2=0$, whereas $F(c,b;z)$ stands for the confluent hypergeometric function defined by the gamma function $\Gamma(c)$,

$$F(c,b;z)=\sum_{v=0}^{\infty}\frac{\Gamma(c+v)\Gamma(b)z^v}{\Gamma(b+v)\Gamma(c)v!}. \tag{7}$$

The eigenvalues of Eq. (4),

$$E_v=D_e\left[1-\frac{\gamma^2}{(v+1/2+\sqrt{\gamma^2+1/4})^2}\right],\qquad v=0,1,2\ldots, \tag{8}$$

are derived from the relation $\lambda-\gamma^2/\beta_v=-v$ for which the wave function (6) converges for $x\to\infty$.

A simple calculation reveals that Eq. (4) can be factorized to the form

$$\hat{A}^{\dagger}\hat{A}|v\rangle=(\delta_v^2-\delta_0^2)|v\rangle, \tag{9}$$

in which $\psi(x)_v=|v\rangle$ and

$$\hat{A}=\frac{1}{\sqrt{2}}\left(\frac{d}{dx}+\beta_0-\frac{\lambda}{x}\right),\qquad \hat{A}^{\dagger}=\frac{1}{\sqrt{2}}\left(-\frac{d}{dx}+\beta_0-\frac{\lambda}{x}\right), \tag{10}$$

whereas

$$\delta_v^2-\delta_0^2=(\beta_0^2-\beta_v^2)/2=\frac{mr_e^2(E_v-E_0)}{\hbar^2}. \tag{11}$$

The proof is starightforward if the relations $\lambda-\gamma^2/\beta_v=-v$ for $v=0$ and $\lambda^2-\lambda=\gamma^2$ are taken into considerations. Then

$$\begin{aligned}(\hat{A}^{\dagger}\hat{A}-\delta_v^2+\delta_0^2)|v\rangle &=\frac{1}{2}\left\{-\frac{d^2}{dx^2}+\left[\beta_0-\frac{\lambda}{x}\right]^2-\frac{\lambda}{x^2}+\beta_v^2-\beta_0^2\right\}|v\rangle\\ &=\frac{1}{2}\left\{-\frac{d^2}{dx^2}+\left[\frac{-2\beta_0\lambda x+\lambda^2-\lambda+\gamma^2x^2}{x^2}-\gamma^2\right]+\beta_v^2\right\}|v\rangle\\ &=\frac{1}{2}\left\{-\frac{d^2}{dx^2}+\gamma^2\left[\frac{(1-x)^2}{x^2}-1\right]+\beta_v^2\right\}|v\rangle=0.\end{aligned} \tag{12}$$

Additionally, one may show that the operator $\hat{A}$ annihilates the ground state $\hat{A}|0\rangle=0$ hence the coherent states $|\alpha\rangle$ of the KF oscillator are eigenstates of the annihilation operator $\hat{A}$,

$$\hat{A}|\alpha\rangle=\alpha|\alpha\rangle,\qquad |\alpha\rangle=x^{\lambda}\exp[-\beta_0 x]\exp[\sqrt{2}\alpha x]. \tag{13}$$

It should be pointed out that Eq. (9) has the same form as that obtained for the anharmonic Morse oscillator by Cooper [9]. In particular, for the ground state it reduces to

$$\hat{A}^{\dagger}\hat{A}|0\rangle=0. \tag{14}$$

III. MINIMUM UNCERTAINTY COHERENT STATES

It is a straightforward matter to demonstrate that states $|\alpha\rangle$ minimize the generalized position-momentum uncertainty relation ($\hbar=1$) [9]

$$[\Delta y(x)]^2(\Delta p)^2\geqslant\frac{1}{4}\langle\alpha|g(x)|\alpha\rangle^2,\qquad [y(x),\hat{p}]=ig(x)=i\frac{dy(x)}{dx}, \tag{15}$$

in which $y(x)$ denotes an anharmonic coordinate, whose explicit form depends on the oscillator type, whereas $\hat{p}=-id/dx$ is the associate momentum operator. Adopting Eq. (15) to the KF oscillator we put

$$y(x)=\beta_0-\frac{\lambda}{x}, \tag{16}$$

which is, to within the constant β_0, the KF coordinate appearing in Eq. (10), whereas from Eqs. (15) and (16) one gets

$$g(x)=\frac{\lambda}{x^2}. \tag{17}$$

Now we can pass to calculate

$$\langle\alpha|y(x)|\alpha\rangle=\frac{1}{\sqrt{2}}\langle\alpha|\hat{A}+\hat{A}^{\dagger}|\alpha\rangle=\frac{1}{\sqrt{2}}(\alpha+\alpha^*), \tag{18}$$

$$\langle\alpha|\hat{p}|\alpha\rangle=-i\frac{1}{\sqrt{2}}\langle\alpha|\hat{A}-\hat{A}^{\dagger}|\alpha\rangle=-i\frac{1}{\sqrt{2}}(\alpha-\alpha^*), \tag{19}$$

$$\begin{aligned}2\langle\alpha|y(x)^2|\alpha\rangle&=\langle\alpha|\hat{A}\hat{A}+2\hat{A}^{\dagger}\hat{A}+\hat{A}^{\dagger}\hat{A}^{\dagger}-g(x)|\alpha\rangle=[(\alpha+\alpha^*)^2\\&\quad-\langle\alpha|g(x)|\alpha\rangle],\end{aligned} \tag{20}$$

$$\begin{aligned}-2\langle\alpha|\hat{p}^2|\alpha\rangle&=\langle\alpha|\hat{A}\hat{A}-2\hat{A}^{\dagger}\hat{A}+\hat{A}^{\dagger}\hat{A}^{\dagger}+g(x)|\alpha\rangle=[(\alpha-\alpha^*)^2\\&\quad+\langle\alpha|g(x)|\alpha\rangle],\end{aligned} \tag{21}$$

taking advantage of the operator relation

$$\hat{A}\hat{A}^{\dagger}=\hat{A}^{\dagger}\hat{A}-g(x). \tag{22}$$

Taking into account Eqs. (18)–(21) one may evaluate

$$[\Delta y(x)]^2=\langle\alpha|y(x)^2|\alpha\rangle-\langle\alpha|y(x)|\alpha\rangle^2=-\frac{1}{2}\langle\alpha|g(x)|\alpha\rangle, \tag{23}$$

$$(\Delta p)^2=\langle\alpha|\hat{p}^2|\alpha\rangle-\langle\alpha|\hat{p}|\alpha\rangle^2=-\frac{1}{2}\langle\alpha|g(x)|\alpha\rangle \tag{24}$$

providing that $\Delta y(x)=\Delta p$ and

$$[\Delta y(x)]^2(\Delta p)^2=\frac{1}{4}\langle\alpha|g(x)|\alpha\rangle^2=\frac{1}{4}\langle\alpha|\frac{\lambda}{x^2}|\alpha\rangle^2. \qquad (25)$$

The calculations performed reveal that the states $|\alpha\rangle$ minimize the generalized position-momentum uncertainty relation for the KF anharmonic coordinate $y(x)$, and they are the eigenstates of the operator $\hat{A}$, which annihilates the ground state $\hat{A}|0\rangle=0$. Hence they satisfy the two fundamental requirements established for the coherent states of anharmonic oscillators [2]: they are eigenstates of the annihilation operator and they minimize the generalized position-momentum uncertainty principle.

The integral on the right-hand side of relation (25) can be easily calculated using the well-known formulas [24]

$$\int_0^\infty r^n e^{-\mu r}dr=n!\,\mu^{-(n+1)}, \quad \mathrm{Re}[\mu]>0 \qquad (26)$$

and the normalized form of $|\alpha\rangle$ [Eq. (13)],

$$|\alpha\rangle=N_\alpha x^\lambda \exp[-\beta_0 x]\exp[\sqrt{2}\alpha x], \qquad (27)$$

$$N_\alpha=\langle\alpha|\alpha\rangle^{-1/2}=\{r_e(2\lambda)![2\beta_0-\sqrt{2}(\alpha^*+\alpha)]^{-2\lambda-1}\}^{-1/2}. \qquad (28)$$

As the result one gets

$$\langle\alpha|\frac{\lambda}{x^2}|\alpha\rangle=\frac{\lambda[2(\lambda-1)]!}{(2\lambda)!}[2\beta_0-\sqrt{2}(\alpha^*+\alpha)]^2. \qquad (29)$$

The above expression has a mathematical and physical meaning only for the non-negative integer part of $\mathrm{Int}[2(\lambda-1)]$, $\mathrm{Int}[2\lambda]$, and $\beta_0>0$, which holds for the vibrational states below dissociation level ($E_v<D_e$).

Taking into account Eqs. (5) and (8) one gets

$$\Delta y(x)\Delta p=\frac{\lambda[2(\lambda-1)]!}{2(2\lambda)!}[2\gamma^2/\lambda-\sqrt{2}(\alpha^*+\alpha)]^2=f(\gamma,\alpha). \qquad (30)$$

Bearing in mind that $\lambda=1/2+\sqrt{\gamma^2+1/4}$, the right-hand side of the above equation can be calculated for specified values of α and γ parameters. The latter depends on the reduced mass of the diatomic molecule $m=m_1m_2/(m_1+m_2)$, internuclear separation r_e, and dissociation energy D_e. For example, in the case of dihydrogen $^1H_2$, we have $m=1.007\,825\,031\,9/2$ a.u., $r_e=0.741\,413\,01$ Å, and $D_e=36\,118.11\ \mathrm{cm}^{-1}$, hence $\gamma^2=593.45$ and $f(\gamma,0)=11.69$ for $\alpha=0$. This indicates that in the ground coherent state of the dihydrogen described in terms of the KF oscillator, both position and associated momentum uncertainties $\Delta y(x)=\Delta p=3.42$ are greater than those for the harmonic oscillator model yielding $f(\gamma,0)=0.5$ and $\Delta y(x)=\Delta p=0.7071$.

IV. COHERENT STATES OF THE ROTATING KF OSCILLATOR

Interactions of molecules with electromagnetic field in the microwave region excite their rotational degrees of freedom in the ground vibrational quantal state. If we use the infrared radiation, the vibrational degrees of freedom will be excited together with rotational ones. Then the rotating oscillator changes its characteristics, for example the potential parameters like dissociation energy and equilibrium distance are modified due to the deformational action of the centrifugal force generated by the rotation [25]. In such circumstances, the coherent states of the rotationless KF oscillator introduced in the previous section should be generalized to include the rotating oscillator.

The starting point to realize this aim is the rotation-vibrational Schrödinger equation

$$\left[-\frac{\hbar^2}{2m}\frac{d^2}{dr^2}+B(r)J(J+1)+D_e\left(\frac{r-r_e}{r}\right)^2-E_{vJ}\right]\psi(r)_{vJ}=0, \qquad (31)$$

in which $B(r)=\hbar^2/(2mr^2)$ and $J=0,1,2\ldots$ is the rotational quantum number. The rotational term together with the KF potential form an effective KF potential $V(r)_J$, which attains a minimum for [25]

$$r_J=r_e\left[1+\frac{B_eJ(J+1)}{D_e}\right]=r_e[1+\gamma^{-2}J(J+1)], \qquad (32)$$

to be determined from the condition $dV(r)_J/dr=0$ [25]. Here $B_e=B(r=r_e)$ is the rotational constant. Employing the quantity r_J, Eq. (31) can be rewritten in the form [25]

$$\left[-\frac{\hbar^2}{2m}\frac{d^2}{dr^2}+D_J\left(\frac{r-r_J}{r}\right)^2+V(r_J)_J-E_{vJ}\right]\psi(r)_{vJ}=0, \qquad (33)$$

in which

$$D_J=\frac{D_er_e}{r_J},$$

$$V(r_J)_J=\frac{\hbar^2J(J+1)}{2mr_J^2}+D_e\left(\frac{r_J-r_e}{r_J}\right)^2=D_J\left(\frac{r_J-r_e}{r_J}\right). \qquad (34)$$

In the next step Eq. (33) is transformed to the dimensionless J-dependent variable ξ,

$$\frac{1}{2}\left\{-\frac{d^2}{d\xi^2}+\gamma_J^2\left[\frac{(1-\xi)^2}{\xi^2}-1\right]+\beta_{vJ}^2\right\}\psi(\xi)_{vJ}=0, \qquad (35)$$

in which

$$\gamma_J^2=\frac{2mr_J^2D_J}{\hbar^2}=\gamma^2+J(J+1), \qquad \xi=\frac{r}{r_J}=\frac{x}{1+\gamma^{-2}J(J+1)}, \qquad (36)$$

$$\beta_{vJ}^2=\frac{2mr_J^2[D_J+V(r_J)_J-E_{vJ}]}{\hbar^2}=\frac{2mr_J^2(D_e-E_{vJ})}{\hbar^2}. \qquad (37)$$

The solution of Eq. (35) in arbitrary normalization is the function

$$\psi(\xi)_{vJ} = \xi^{\lambda_J} \exp[-\beta_{vJ}\xi]F[\lambda_J - \gamma_J^2/\beta_{vJ}, 2\lambda_J, 2\beta_{vJ}\xi], \tag{38}$$

in which

$$\lambda_J = 1/2 + \sqrt{\gamma_J^2 + 1/4} = 1/2 + \sqrt{\gamma^2 + (J + 1/2)}, \tag{39}$$

whereas its eigenvalues

$$E_{vJ} = D_e\left\{1 - \frac{\gamma^2}{[v + 1/2 + \sqrt{\gamma^2 + (J + 1/2)^2}]^2}\right\} \tag{40}$$

can be determined from the relationship

$$\beta_{vJ}^2 = \frac{\gamma_J^4}{(v + \lambda_J)^2}. \tag{41}$$

Proceeding along the lines of the algebraic approach, Eq. (35) can be factorized

$$\hat{A}^\dagger\hat{A}|vJ\rangle = (\delta_{vJ}^2 - \delta_{0J}^2)|vJ\rangle, \tag{42}$$

$$\hat{A} = \frac{1}{\sqrt{2}}\left(\frac{d}{d\xi} + \beta_{0J} - \frac{\lambda_J}{\xi}\right), \quad \hat{A}^\dagger = \frac{1}{\sqrt{2}}\left(-\frac{d}{d\xi} + \beta_{0J} - \frac{\lambda_J}{\xi}\right), \tag{43}$$

in which

$$\delta_{vJ}^2 - \delta_{0J}^2 = (\beta_{0J}^2 - \beta_{vJ}^2)/2 = \frac{mr_J^2(E_{vJ} - E_{0J})}{\hbar^2}. \tag{44}$$

The J-dependent operator $\hat{A}$ annihilates the vibrational ground state $\hat{A}|0J\rangle=0$ in an arbitrary rotational quantum J state hence the coherent states $|\alpha J\rangle$ of the rotating KF oscillator are eigenstates of the annihilation operator $\hat{A}$,

$$\hat{A}|\alpha J\rangle = \alpha|\alpha J\rangle, \quad |\alpha J\rangle = \xi^{\lambda_J}\exp[-\beta_{0J}\xi]\exp[\sqrt{2}\alpha\xi]. \tag{45}$$

It is easy to demonstrate that the states $|\alpha J\rangle$ minimize the generalized position-momentum uncertainty relation (15) yielding

$$[\Delta y(\xi)]^2(\Delta p)^2 = \frac{1}{4}\langle\alpha J|\frac{\lambda_J}{\xi^2}|\alpha J\rangle^2 \tag{46}$$

in which

$$y(\xi) = \beta_{0J} - \frac{\lambda_J}{\xi} \tag{47}$$

is, to within the constant β_{0J}, the J-dependent KF coordinate, whereas $\lambda_J/\xi^2 = g(\xi)$.

Proceeding along the lines of the previous section one may calculate the integral on the right-hand side of uncertainty relation (46) yielding

$$\Delta y(\xi)\Delta p = \frac{\lambda_J[2(\lambda_J - 1)]!}{2(2\lambda_J)!}[2\beta_{0J} - \sqrt{2}(\alpha^* + \alpha)]^2 = f(\gamma, \alpha, J). \tag{48}$$

It has a mathematical and physical meaning only for the non-negative integer part of $\text{Int}[2(\lambda_J - 1)]$, $\text{Int}[2\lambda_J]$, and $\beta_{0J} > 0$, which holds for the rotation-vibrational states below dissociation limit $(E_{vJ} < D_e)$. Remembering that $\beta_{0J} = \gamma_J^2/\lambda_J$ and $\lambda_J = 1/2 + \sqrt{\gamma^2 + (J + 1/2)^2}$, the right-hand side of Eq. (48) can be calculated for specified values of α and γ parameters in an arbitrary rotational state J. We have performed the symbolic calculations for dihydrogen $^1H_2$, using the Maple vs 7 processor, which revealed that for $\alpha=0$, $f(\gamma,\alpha,J)$ increases (approximately) parabolically with J and takes the exemplary values $f(\gamma,0,0)=11.69$, $f(\gamma,0,10)=12.77$, $f(\gamma,0,25)=17.14$, $f(\gamma,0,50)=27.54$. They indicate that in the ground coherent state of the dihydrogen described in terms of the rotating KF oscillator, both position and associated momentum uncertainties increase with J.

V. THE TIME EVOLUTION OF THE KF COHERENT STATES

In the absence of external fields the time evolution of the coherent states of the KF oscillator is governed by the equation [2]

$$|\alpha(t)\rangle = |\alpha J\rangle e^{-iEt/\hbar} \tag{49}$$

in which

$$\alpha(t) = \frac{1}{\sqrt{2}}[y(t) + ip(t)] = \frac{1}{\sqrt{2}}[y(0) + ip(0)]e^{-iEt/\hbar}, \tag{50}$$

$$y(t) = \langle\alpha(t)|\hat{y}|\alpha(t)\rangle, \quad p(t) = \langle\alpha(t)|\hat{p}|\alpha(t)\rangle. \tag{51}$$

Here $y(t)$ is the J-dependent KF coordinate (47), which includes the time-dependent radial variable $\xi(t)$, whereas p is the associated momentum.

The states (49) minimize the position-momentum uncertainty relation (15) and follow the classical motion of the KF oscillator,

$$y(t) = \sqrt{2}\,\text{Re}[\alpha(t)] = y(0)e^{-iEt/\hbar}, \tag{52}$$

$$p(t) = \sqrt{2}\,\text{Im}[\alpha(t)] = p(0)e^{-iEt/\hbar}. \tag{53}$$

Such states evolve coherently in time, remaining localized on the corresponding classical space trajectory; being coherent for $t=0$, they remain coherent at an arbitrary moment of time [2]. This property makes the coherent states a convenient tool to interpret the micro-macro or quantum-classical correspondences [26]. For example, using the Husimi Q representation [27], one finds precise patterns of classical trajectories corresponding to the wave function of the system. The Q distribution follows the classical periodic orbits [28], whereas the classical unstable periodic orbits are endowed with "scars" in the Q distribution [29].

VI. INTERACTION OF THE ROTATING KF OSCILLATOR WITH LASER PULSE

The resonant interaction of the laser beam with molecules produces the coherent effects such as self-induced transparency, soliton formation [30], excitation of a coherent superposition of rotational states [31], periodic alternations of the refractive index in both nuclear [32] and molecular systems [31,33,34]. In the latter case the variation of the refractive index appears due to interaction of the coherent radiation with the coherent rotational states of the molecules. The same effect has been theoretically predicted by Avram *et al.* [35] for vibrating diatomic systems described in terms of the coherent states of the Morse oscillator. Here, we extend the research area onto the interaction of the rotating KF oscillator with monochromatic, polarized, and coherent radiation $|\beta\rangle$ satisfying the Glauber relation [36]

$$\hat{b}_{k,\sigma}|\beta\rangle = \beta|\beta\rangle \tag{54}$$

in which $\hat{b}_{k,\sigma}$ denotes the annihilation operator whereas k is the wave vector of the radiation quanta endowed with the spin σ.

The refractive index of a material interacting with the radiation can be expressed in the form [35]

$$n = n_0 + n_{int}(t)I \tag{55}$$

in which n_0 stands for the refractive index in the absence of radiation, whereas n_{int} represents the variation of the refractive index due to the interaction of a material with the radiation of intensity I. The term $n_{int}(t)$ can be calculated using the following relationship [35]:

$$n_{int}(t) = \frac{qi}{\sqrt{V}}\sqrt{\frac{k}{2}}\langle\phi|\vec{\epsilon}_{k,\sigma}\cdot\vec{r}\hat{b}_{k,\sigma}e^{i\vec{k}\cdot\vec{r}}|\phi\rangle e^{-i\omega t} \tag{56}$$

in which V stands for the normalization volume, $\vec{\epsilon}_{k,\sigma}$ is the polarization vector of the radiation characterized by the angular frequency ω; q is an effective electric charge generating a dipolar moment $\vec{d}=q\vec{r}$ of a molecule, whereas

$$|\phi\rangle = |\beta\rangle|\alpha J\rangle \tag{57}$$

represents the molecule in the coherent state $|\alpha J\rangle$ interacting with laser beam in the state $|\beta\rangle$.

The crucial for determining $n_{int}(t)$ is the vector product $\vec{\epsilon}_{k,\sigma}\cdot\vec{r}$. It can be easily calculated for purely vibrational systems and static orientation of molecules with respect to laser pulse polarization [37]. In the case of rotation-vibrational systems, $\vec{r}$ changes both its length due to vibration and orientation due to rotation. In such circumstances the term $\vec{\epsilon}_{k,\sigma}\cdot\vec{r}$ changes its value and for the molecule bond orientation orthogonal to the laser pulse polarization, it can vanish. Hence the coherent excitation leading to the dynamic alternation of $n_{int}(t)$ is impossible. To overcome this difficulty Hornung and de Vivie-Riedle [38] introduced a technique, which employes suitably shaped pulses to restore a high laser control of the rotational degrees of freedom. In this approach it is assumed that $\vec{\epsilon}_{k,\sigma}\cdot\vec{r}=r\cos(\theta)$ in which θ is the angle between $\vec{\epsilon}_{k,\sigma}$ and $\vec{r}$, which alters due to rotation.

Another possibility is to use the circularly polarized radiation, which excites the rotational degrees of freedom due to the transfer of spin angular momentum of a laser mode to molecule [39]. If the polarization vector is parallel to the rotating molecule bond then

$$\vec{\epsilon}_{k,\sigma}\cdot\vec{r} = r, \quad \vec{k}\cdot\vec{r} = 0 \tag{58}$$

and the relation (56) reduces to the simple form

$$n_{int}(t) = \frac{qi\beta}{\sqrt{V}}\sqrt{\frac{k}{2}}\langle\alpha J|\xi|\alpha J\rangle r_J e^{-i\omega t}. \tag{59}$$

The integral on the right-hand side of Eq. (59) can be easily calculated using Eq. (26) and the normalized form of $|\alpha J\rangle$ (31), yielding

$$n_{int}(t) = \frac{qi\beta}{\sqrt{V}}\sqrt{\frac{k}{2}}\frac{(2\lambda_J+1)!}{(2\lambda_J)!}[2\beta_{0J} - \sqrt{2}(\alpha^* + \alpha)]^{-1}r_J^2 e^{-i\omega t}. \tag{60}$$

The derived formulas have a mathematical and physical meaning only for the non-negative integer part of $\mathrm{Int}[2\lambda_J+1]$ and $\beta_{0J}>0$, which holds for the states below dissociation level ($E_{vJ}<D_e$). Equation (60) contains the time-dependent exponential term responsible for the periodic change of the refractive index due to the interaction of circularly polarized coherent radiation of frequency ω with diatomic molecule in the coherent rotation-vibrational state $|\alpha J\rangle$. Such an effect has been reported in [31,33,34].

VII. CONCLUSIONS

The KF potential is a realistic zero-order model useful for a description of the anharmonic rotation-vibrational motion in diatomic molecules. Although the function (1) provides only a crude approximation to the true molecular potential it has many valuable advantages which make it a powerful tool for investigation of the rotation-vibrational diatomic systems. In particular, it allows the system to dissociate, which is forbidden for a harmonic oscillator and the rotation-vibrational Schrödinger equation can be exactly solved.

Studies of the rotating anharmonic oscillators are of interest in respect to their interactions with intense electromagnetic radiation [40]. The theoretical models describing such interactions employ mainly the Morse potential as a reliable representation of the anharmonic vibrations in molecules [41]. The problem appears when we try to generalize the problem of the Morse oscillator to include rotation. Then only the approximate parabolic expansion of the rotational term in the rotation-vibrational Schrödinger equation can be taken into consideration to obtain the analytical solutions [23]. In the case of the KF oscillator, the exact analytical solutions can be obtained without any approximations. Hence this model seems to be a better physical representation of the internal rotation-vibrational motion in diatomic systems than the Morse one. In particular it permits construction of the coherent states of the rotating and rotationless KF oscillator. In this work the coherent states of the KF oscillator have been constructed by a simple algebraic procedure applied by Cooper [9] to the Morse oscillator. The method can be generalized to include the rotating KF oscillator. To this aim the basic rotation-vibrational Schrödinger equation is expressed in the J-dependent parameter r_J, which permits mapping of the J-dependent problem onto the purely vibrational one. The resultant effective Schrödinger equation can be factorized to obtain the operator, which annihilates the ground vibrational state $|0J\rangle$ for an arbitrary rotational quantum number J. The constructed states represent both minimum uncertainty coherent states and annihilation operator eigenstates, where the annihilation operator is chosen to annihilate the ground state of the KF oscillator. In view of this, from the three fundamental requirements established for the coherent states of the harmonic oscillator [2], namely the (i) states which minimize the uncertainty relation, (ii) eigenstates of the annihilation operator, and (iii) states which are produced by the action of the displacement operator, only the first two can be applied directly to the KF oscillator since the third one relies on the form of the displacement operator, which is specific to harmonic oscillator [9]. In this case, only approximate KF coherent states can be derived using Nieto and Simons [3] or Kais and Levine [8] approaches. In the former, the vibrational Hamiltonian is expressed in terms of transformed position and momentum variables which permit formulation of the problem in terms of the harmonic oscillator, whereas the latter uses the Perelomov [11] method of the construction of generalized coherent states via the Lie group algebra.

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