Barut–Girardello coherent states of the pseudoharmonic oscillator

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Abstract
In the paper we have investigated some properties of the Barut–Giraradello coherent states (BGCS) (the eigenstates of the $SU(1, 1)$ lowering generator K_-) for the Hamiltonian of the pseudoharmonic oscillator (PHO). By using these states, the diagonal P-representation of the density operator is constructed as a new result for this potential. In addition, we have calculated some thermal expectation values for the quantum canonical gas of the PHOs. The calculations using the BGCS representation seem to be much simpler and easier to program than the corresponding calculations in other representations (e.g. the position representation). At the end of the paper the time dependence of these states is presented.

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1. Introduction

It is well known that real molecular vibrations are anharmonic, but due to its mathematical advantages the harmonic oscillator (HO) model is used. An anharmonic potential, which also permits an exact mathematical treatment, is the so-called 'pseudoharmonic oscillator' (PHO) potential. This potential was pointed out in [1], but recently interest in it has reappeared [2–8].

The effective potential of the PHO is

$$V_J(r) = \frac{m\omega^2}{8} r_0^2 \left(\frac{r}{r_0} - \frac{r_0}{r} \right)^2 + \frac{\hbar^2}{2m} J(J+1) \frac{1}{r^2} \tag{1}$$

where r_0 is the equilibrium distance between the nuclei of the diatomic molecule, and $J = 0, 1, 2, \ldots$ is the rotational quantum number. This potential also admits the exact analytical solution of the rovibrational Schrödinger equation, being in a certain sense an intermediate potential between the HO potential (an ideal potential) and the anharmonic potentials (the more realistic potentials). A comparative analysis of three-dimensional HO potentials (HO-3D potentials) and the PHO is performed in [3].

Using Molski's techniques [9] (for the Morse oscillator) we have rewritten the PHO effective potential as follows [8]:

$$V_J(r) = \frac{m\omega^2}{8} r_J^2 \left(\frac{r}{r_J} - \frac{r_J}{r} \right)^2 + \frac{m\omega^2}{4} (r_J^2 - r_0^2) \tag{2}$$

where the changed equilibrium distance is

$$r_J = \left[\frac{2\hbar}{m\omega} \left(\alpha^2 - \frac{1}{4} \right)^{\frac{1}{2}} \right]^{\frac{1}{2}} \tag{3}$$

and the new rotational parameter, α, which appears is defined as

$$\alpha = \left[\left(J + \frac{1}{2} \right)^2 + \left(\frac{m\omega}{2\hbar} r_0^2 \right)^2 \right]^{\frac{1}{2}}. \tag{4}$$

Using this procedure, the rotational case ($J \neq 0$) is implicitly reduced to the non-rotational ($J = 0$) one and both cases can be examined together.

The corresponding rovibrational Schrödinger equation for the reduced radial function $u_v^\alpha(r)$ is

$$H_\alpha(r) u_v^\alpha(r) \equiv \left[-\frac{\hbar^2}{2m} \frac{d^2}{dr^2} + \frac{m\omega^2}{8} r_J^2 \left(\frac{r}{r_J} - \frac{r_J}{r} \right)^2 \right] u_v^\alpha(r) = (E_{vJ} - E_{\text{eff}}^{\text{rot}}) u_v^\alpha(r) \tag{5}$$

where v is the vibrational quantum number. In the right-hand side the effective rotational energy appears:

$$E_{\text{eff}}^{\text{rot}} = \frac{m\omega^2}{4} (r_J^2 - r_0^2). \tag{6}$$

It is evident that, from a mathematical point of view, equation (5) is similar to the reduced radial Schrödinger equation for the isotropic HO-3D. This similarity will be of further use in the construction of the corresponding lowering and raising operators for the PHO.

The HO-3D can be considered as a limit oscillator of the PHO. This limit is called *the harmonic limit of the PHO* and for a certain physical observable A is defined as (see [6])

$$\lim_{\substack{\omega \to 2\omega_0 \\ r_0 \to 0 \\ \alpha \to J + \frac{1}{2}}} A \equiv \lim_{\text{HO}} A = A^0 \tag{7}$$

where the quantities without any index corresponds to the PHO, while the same quantities with the index (0) corresponds to the HO-3D (with frequency ω_0).

The radial eigenfunctions and eigenvalues have been calculated in [2]:

$$u_v^\alpha(r) \equiv r R_{vJ}(r) = \frac{1}{B} \left[\frac{B^3 v!}{2^\alpha \Gamma(v + \alpha + 1)} \right]^{\frac{1}{2}} (Br)^{\alpha + \frac{1}{2}} \exp\left(-\frac{B^2}{4} r^2 \right) L_v^\alpha \left(\frac{B^2}{2} r^2 \right) \tag{8}$$

$$E_{vJ} = \hbar\omega \left(v + \frac{1}{2} \right) + \frac{\hbar\omega}{2} \alpha - \frac{m\omega^2}{4} r_0^2 \tag{9}$$

where we have used the notation

$$B = \left(\frac{m\omega}{\hbar} \right)^{\frac{1}{2}}. \tag{10}$$

Here $\Gamma(x)$ is Euler's gamma function and $L_v^\alpha(x)$ is the generalized Laguerre's polynomial.

The aim of this paper is to construct the coherent states (CS) of the PHO, particularly the Barut–Girardello coherent states (BGCS). These states will be obtained as the eigenstates of the lowering generator K_-. BGCS are of special importance due to their remarkable mathematical properties and interesting physical applications, especially in quantum optics.

The plan of the paper is the following: we start in section 2 with the $SU(1, 1)$ algebraic treatment of the PHO, from which we discover the $SU(1, 1)$ generators for this oscillator potential. We have inserted a brief review of the properties which will be useful for the ensuing calculations. In section 3 we construct the CS for the PHO, as the eigenstates of the $SU(1, 1)$-generator K_-. These states are, as we had expected, just the BGCS. By using these states we have calculated, in section 4, some expectation values in the BGCS representation, while in section 5 we have examined the statistical properties of a quantum gas of PHOs which obeys the quantum canonical distribution. The discovery of the diagonal P-representation of the density operator, which is the main result of this paper, allows us to calculate the thermal expectation values of some physical observable concerning the PHO quantum canonical gas: the internal energy, the entropy and the molar heat capacity. All these formulae so obtained lead, in the harmonic limit, to the corresponding formulae for the HO-3D, because the HO-3D is a particular case of the PHO (in the conditions of the harmonic limit). The last section (section 6) is devoted to the time dependence of the BGCS. A brief discussion concludes the paper.

2. $SU(1, 1)$ algebraic treatment of the PHO

By using the substitution $\omega = 2\omega_0$, let us rewrite equation (5):

$$\left[-\frac{\hbar^2}{2m}\frac{d^2}{dr^2} + \frac{m\omega_0^2}{2}r^2 + \frac{m\omega_0^2}{2}r_J^4\frac{1}{r^2} - \hbar\omega_0(2v+\alpha+1) \right] u_v^\alpha(r) = 0. \tag{11}$$

Passing to the dimensionless variable $y = \left(\frac{m\omega_0}{\hbar}\right)^{\frac{1}{2}} r = \sqrt{2}Br$ allows us to rewrite this equation as follows:

$$\left[-\frac{1}{2}\frac{d^2}{dy^2} + \frac{1}{2}y^2 + \frac{1}{2}\left(\alpha^2 - \frac{1}{4}\right)\frac{1}{y^2} - (2v+\alpha+1) \right] u_v^\alpha(y) = 0 \tag{12}$$

where appears the dimensionless reduced Hamiltonian $H_\alpha^{(\text{red})}$ of the PHO:

$$H_\alpha^{(\text{red})}(y) = \frac{1}{\hbar\omega_0}\left[H_\alpha(y) + \frac{m\omega_0^2}{\hbar}r_0^2 \right] \equiv -\frac{1}{2}\frac{d^2}{dy^2} + \frac{1}{2}y^2 + \frac{1}{2}\left(\alpha^2 - \frac{1}{4}\right)\frac{1}{y^2}. \tag{13}$$

Following the procedure from [10] for HO-3D, we define the generators in a similar manner:

$$W_1 = \frac{1}{2}y^2 \tag{14}$$

$$W_2 = -\frac{i}{2}\left(y\frac{d}{dy} + \frac{1}{2} \right) \tag{15}$$

$$W_3 = -\frac{1}{2}\frac{d^2}{dy^2} + \frac{1}{2}\left(\alpha^2 - \frac{1}{4}\right)\frac{1}{y^2} \tag{16}$$

with the commutators

$$[W_1, W_2] = iW_1 \qquad [W_2, W_3] = iW_3 \qquad [W_1, W_3] = 2iW_2. \tag{17}$$

We define the operators K_i ($i = 1, 2, 3$) as follows:

$$K_1 = \frac{1}{2}(W_3 - W_1) = \frac{1}{2}\left[-\frac{1}{2}\frac{d^2}{dy^2} + \frac{1}{2}\left(\alpha^2 - \frac{1}{4}\right)\frac{1}{y^2} - \frac{1}{2}y^2 \right] \tag{18}$$

$$K_2 = W_2 = -\frac{i}{2}\left(y\frac{d}{dy} + \frac{1}{2}\right) \tag{19}$$

$$K_3 = \frac{1}{2}(W_3 + W_1) = \frac{1}{2}\left[-\frac{1}{2}\frac{d^2}{dy^2} + \frac{1}{2}\left(\alpha^2 - \frac{1}{4}\right)\frac{1}{y^2} + \frac{1}{2}y^2\right] = \frac{1}{2}H_\alpha^{(\text{red})}(y) \tag{20}$$

which have the characteristic commutation relation for the Lie algebra corresponding to the $SU(1,1)$ group:

$$[K_1, K_2] = -iK_3 \qquad [K_2, K_3] = iK_1 \qquad [K_3, K_1] = iK_2. \tag{21}$$

The $SU(1,1)$ group is the most elementary non-compact non-Abelian simple Lie group. It is customary to use the raising and lowering generators of this group:

$$K_\pm = K_1 \pm iK_2 \tag{22}$$

which satisfy the following commutation relations:

$$[K_3, K_\pm] = \pm K_\pm \qquad [K_-, K_+] = 2K_3. \tag{23}$$

The Casimir operator K^2 for any irreducible representation is the identity times a number:

$$K^2 = K_3^2 - K_1^2 - K_2^2 = k(k-1) \tag{24}$$

so, a representation of $SU(1,1)$ is determined by a single real number k (called the Bargmann index).

Here, we are only interested in the unitary irreducible representations known as positive discrete series, where $k > 0$. The corresponding state is spanned by the complete orthonormal basis of the number state $|v, k\rangle$ (where $v = 0, 1, 2, \ldots, \infty$ is the vibrational quantum number) of the PHO Hilbert space:

$$\langle v, k|v', k\rangle = \delta_{vv'} \qquad \sum_{v=0}^{\infty} |v, k\rangle\langle v, k| = 1. \tag{25}$$

The discrete representations of the $SU(1,1)$ group are given by

$$K^2|v, k\rangle = k(k-1)|v, k\rangle \tag{26}$$
$$K_+|v, k\rangle = \sqrt{(v+1)(v+2k)}|v+1, k\rangle \tag{27}$$
$$K_-|v, k\rangle = \sqrt{v(v+2k-1)}|v-1, k\rangle. \tag{28}$$

Let us now apply these general considerations concerning the $SU(1,1)$ group generators to our interesting problem, i.e. to the PHO operators (22) and (20). The PHO realization of the raising and lowering operators $K_\pm$ is

$$K_\pm = \frac{1}{2}(W_3 - W_1) = \frac{1}{2}\left[-\frac{1}{2}\frac{d^2}{dy^2} + \frac{1}{2}\left(\alpha^2 - \frac{1}{4}\right)\frac{1}{y^2} - \frac{1}{2}y^2\right] \pm \frac{1}{2}\left(y\frac{d}{dy} + \frac{1}{2}\right). \tag{29}$$

In order to eliminate the second-order derivative, we use the rovibrational Schrödinger equation (12) and we obtain

$$K_\pm = \frac{1}{2}\left(\pm y\frac{d}{dy} \pm \frac{1}{2} - y^2 + 2v + \alpha + 1\right). \tag{30}$$

The dimensionless radial reduced eigenfunction $u_v^\alpha(y)$ (see, equation (8)) is

$$u_v^\alpha(y) = C_v^\alpha 2^{\frac{1}{2}(\alpha+\frac{1}{2})} y^{\alpha+\frac{1}{2}} \exp\left(-\frac{1}{2}y^2\right) L_v^\alpha(y^2) \tag{31}$$

where we used the following notation:

$$C_v^\alpha = \frac{1}{B}\left[\frac{B^3 v!}{2^\alpha \Gamma(v+\alpha+1)}\right]^{\frac{1}{2}}. \tag{32}$$

Using the relation between the generalized Laguerre polynomials [11]:

$$x \frac{\mathrm{d}}{\mathrm{d}x} L_v^\alpha(x) = v L_v^\alpha(x) - (v + \alpha) L_{v-1}^\alpha(x) = (v + 1) L_{v+1}^\alpha(x) - (v + \alpha + 1 - x) L_v^\alpha(x) \tag{33}$$

we can easily demonstrate the equations

$$K_+ u_v^\alpha(y) = \sqrt{(v + 1)(v + \alpha + 1)} u_{v+1}^\alpha(y) \tag{34}$$

$$K_- u_v^\alpha(y) = \sqrt{v(v + \alpha)} u_{v-1}^\alpha(y). \tag{35}$$

Comparing these equations with the equations (27) and (28) we obtain the following useful connection:

$$\alpha = 2k - 1 \tag{36}$$

i.e. the rotational parameter α plays the role of the Bargmann index. Later in this paper, we will use the k-index instead of the α-index.

For the vibrational ground state ($v = 0$) we can demonstrate that the equation

$$K_- u_0^\alpha(y) = 0 \tag{37}$$

is also satisfied.

The properties of the $K_\pm$ and K_3 generators allow us to construct the CS corresponding to the PHO.

3. CS of PHO

Following the Barut and Girardello procedure [12], let us construct the eigenstates of the lowering generator K_-:

$$K_-|z, k\rangle = z|z, k\rangle \tag{38}$$

where z is an arbitrary complex number.

One can represent the eigenstates $|z, k\rangle$ as the superposition of the complete orthonormal basis $|v, k\rangle$ of the PHO Hilbert space:

$$|z, k\rangle = \sum_{v=0}^{\infty} \langle v, k|z, k\rangle |v, k\rangle. \tag{39}$$

Let the operator K_- act on equation (39). Then, using equations (38) and (28) and the orthonormality relation (25), we have the following result:

$$\langle v, k|z, k\rangle = \frac{z}{\sqrt{v(v + 2k - 1)}} \langle v - 1, k|z, k\rangle \tag{40}$$

which, after the recurrence procedure, becomes

$$\langle v, k|z, k\rangle = z^v \sqrt{\frac{\Gamma(2k)}{v! \Gamma(v + 2k)}} \langle 0, k|z, k\rangle. \tag{41}$$

By normalizing to unity the states $|z, k\rangle$ and using the relation (see [13])

$$\sum_{v=0}^{\infty} \frac{x^v}{v! \Gamma(v + v + 1)} = \frac{1}{x^v} I_v(2x) \tag{42}$$

where $I_v(x)$ is the modified Bessel function of order v, we have

$$\langle 0, k|z, k\rangle = \sqrt{\frac{|z|^{2k-1}}{I_{2k-1}(2|z|)\Gamma(2k)}} \tag{43}$$

i.e. finally, the eigenstates $|z, k\rangle$ become

$$|z, k\rangle = \sqrt{\frac{|z|^{2k-1}}{I_{2k-1}(2|z|)}} \sum_{v=0}^{\infty} \frac{z^v}{\sqrt{v! \Gamma(v + 2k)}} |v, k\rangle. \tag{44}$$

These states are, evidently, the BGCS [12, 14–16].

Consequently, the CS which corresponds to the PHO are just the BGCS.

It is demonstrated (see, e.g. [12] or [14]) that these states are normalized but not orthogonal and that the following resolution of the identity holds:

$$\int d\mu(z, k) |z, k\rangle\langle z, k| = 1 \tag{45}$$

with the measure

$$d\mu(z, k) = \frac{2}{\pi} K_{2k-1}(2|z|) I_{2k-1}(2|z|) d^2z \qquad d^2z = d(\text{Re } z) d(\text{Im } z). \tag{46}$$

The function $K_v(x)$ is the v-order modified Bessel function of the second kind.

Here and below, all the integrals are performed over the whole complex z plane, where

$$z = r \exp(i\varphi) \qquad r \in [0, \infty) \qquad \varphi \in [0, 2\pi]. \tag{47}$$

The resolution of the identity is easy to demonstrate by using the following integral [11]:

$$\int_0^{\infty} dx\, x^{\mu} K_v(ax) = 2^{\mu-1} a^{-\mu-1} \Gamma\left(\frac{1 + \mu + v}{2}\right) \Gamma\left(\frac{1 + \mu - v}{2}\right) \tag{48}$$
$$[\text{Re}(\mu + 1 \pm v) > 0, \text{Re } a > 0].$$

As we see, the BGCS are not orthogonal:

$$\langle \sigma, k | z, k \rangle = \frac{I_{2k-1}(2\sqrt{\sigma^* z})}{\sqrt{I_{2k-1}(2|\sigma|) I_{2k-1}(2|z|)}} \tag{49}$$

where σ is also an arbitrary complex number.

4. Expectation values

Using equation (44), the expectation value of a physical observable A, which characterizes the PHO, with respect to the BGCS $|z, k\rangle$ is easy to obtain:

$$\langle z, k | A | z, k \rangle \equiv \langle A \rangle_{z,k} = \frac{|z|^{2k-1}}{I_{2k-1}(2|z|)} \sum_{v,n=0}^{\infty} \frac{(z^*)^n z^v}{\sqrt{v! \Gamma(v + 2k) n! \Gamma(n + 2k)}} \langle n, k | A | v, k \rangle. \tag{50}$$

In order to calculate different expectation values it is useful to evaluate the sum S_n, with $n = 0, 1, 2, \ldots$ (see the appendix):

$$S_n = \sum_{v=0}^{\infty} \frac{(x^2)^v}{v! \Gamma(v + v + 1)} v^n. \tag{51}$$

First, let us calculate the expectation values of the operators K_i ($i = 1, 2, 3$). Using the above equation, it is easy to prove that

$$\langle K_- \rangle_{z,k} = z \qquad \langle K_+ \rangle_{z,k} = z^* \tag{52}$$

$$\langle K_1 \rangle_{z,k} = \tfrac{1}{2} \langle K_- + K_+ \rangle_{z,k} = \tfrac{1}{2}(z + z^*) = \text{Re } z \tag{53}$$

$$\langle K_2 \rangle_{z,k} = \frac{i}{2} \langle K_- - K_+ \rangle_{z,k} = \frac{i}{2}(z - z^*) = -\text{Im } z. \tag{54}$$

For the generator K_3 and its second power K_3^2, by applying equation (50) and using equation (20), we obtain

$$\langle K_3 \rangle_{z,k} = \frac{|z|^{2k-1}}{I_{2k-1}(2|z|)} (S_1 + kS_0) = |z| \frac{I_{2k}(2|z|)}{I_{2k-1}(2|z|)} + k \tag{55}$$

$$\langle K_3^2 \rangle_{z,k} = \frac{|z|^{2k-1}}{I_{2k-1}(2|z|)} \left(S_2 + 2kS_1 + k^2 S_0 \right) = k^2 + (2k+1)|z| \frac{I_{2k}(2|z|)}{I_{2k-1}(2|z|)}$$
$$+ |z|^2 \frac{I_{2k+1}(2|z|)}{I_{2k-1}(2|z|)} \tag{56}$$

where we used the expressions for S_0, S_1 and S_2 from the appendix.

It is well known that the number operator N is defined as the operator which diagonalize the basis for the number states:

$$N|v, k\rangle = v|v, k\rangle. \tag{57}$$

Then, the expectation values for the number operator and its second power are

$$\langle N \rangle_{z,k} = \langle K_3 - k \rangle_{z,k} = |z| \frac{I_{2k}(2|z|)}{I_{2k-1}(2|z|)} \tag{58}$$

$$\langle N^2 \rangle_{z,k} = \langle K_3^2 - 2kN - k^2 \rangle_{z,k} = |z| \frac{I_{2k}(2|z|)}{I_{2k-1}(2|z|)} + |z|^2 \frac{I_{2k+1}(2|z|)}{I_{2k-1}(2|z|)}. \tag{59}$$

The intensity correlation function, defined as in [14], is

$$g_{z,k}^2 = \frac{\langle N^2 \rangle_{z,k} - \langle N \rangle_{z,k}}{\langle N \rangle_{z,k}^2} = \frac{I_{2k-1}(2|z|) I_{2k+1}(2|z|)}{[I_{2k}(2|z|)]^2}. \tag{60}$$

For two limiting cases of the $|z|$ variable, i.e. for $|z| \ll 1$ and $|z| \gg 1$, using the well known approximations for the modified Bessel function $I_v(x)$ (see [11])

$$I_v(x) \simeq \frac{1}{\Gamma(v+1)} \left(\frac{x}{2}\right)^v \qquad \text{respectively} \qquad I_v(x) = \frac{e^x}{\sqrt{2\pi x}} \left[1 + O\left(\frac{1}{x}\right) \right] \tag{61}$$

we obtain for the intensity correlation function the following expressions:

$$g_{z,k}^{(2)} \simeq \frac{2k}{2k+1} \qquad \text{respectively} \qquad g_{z,k}^{(2)} \simeq 1. \tag{62}$$

So, for small values of $|z|$, the intensity correlation function is smaller than unity, for all k values. The corresponding BG states have sub-Poissonian statistics, while for large $|z|$, these states tend to have Poissonian statistics [14].

5. Statistical properties

In this section we will carry out a detailed discussion on the statistical properties of the BGCS for the PHO. We consider a quantum gas of the PHOs in thermodynamic equilibrium with the reservoir (the thermostat) at temperature T, which obeys the quantum canonical distribution [6]. The corresponding normalized density operator for a fixed rotational quantum number J (or, equivalently, for a fixed number k) is then

$$\rho_J \equiv \rho_k = \frac{1}{Z_k} \sum_{v=0}^{\infty} e^{-\beta E_{vJ}} |v, k\rangle \langle v, k| \tag{63}$$

where $Z_J = Z_k$ is the normalization constant, i.e. the partition function for a certain rotational state J.

The diagonal elements of the density operator in the BGCS representation are

$$\langle z, k | \rho_J | z, k \rangle \equiv \langle \rho_k \rangle_{z,k} = \frac{1}{Z_k} \frac{|z|^{2k-1}}{I_{2k-1}(2|z|)} \sum_{v=0}^{\infty} e^{-\beta E_{vJ}} \frac{\left(|z|^2\right)^v}{v! \Gamma(v+2k)} \tag{64}$$

where we have used equations (44) and (25).

Finally, using equations (9) and (42) we get

$$\langle z, k | \rho_k | z, k \rangle = \frac{1}{Z_k} e^{-\beta(\hbar\omega_0 - m\omega_0^2 r_0^2)} \frac{I_{2k-1}(2|z|e^{-\beta\hbar\omega_0})}{I_{2k-1}(2|z|)}. \tag{65}$$

By normalizing the density operator to unity, i.e.

$$\mathrm{Tr}\,\rho_k = \int \mathrm{d}\mu\,(z, k) \langle z, k | \rho_k | z, k \rangle = 1 \tag{66}$$

and using an integral of the following kind [11]:

$$\int_0^{\infty} \mathrm{d}x\, x^{-\lambda} K_\mu(ax) I_v(bx) = \frac{b^v \Gamma\left(\frac{1}{2} - \frac{1}{2}\lambda + \frac{1}{2}\mu + \frac{1}{2}v\right) \Gamma\left(\frac{1}{2} - \frac{1}{2}\lambda - \frac{1}{2}\mu + \frac{1}{2}v\right)}{2^{\lambda+1} \Gamma(v+1) a^{-\lambda+v+1}}$$

$$\times F\left(\frac{1}{2} - \frac{1}{2}\lambda + \frac{1}{2}\mu + \frac{1}{2}v, \frac{1}{2} - \frac{1}{2}\lambda - \frac{1}{2}\mu + \frac{1}{2}v; v+1; \frac{b^2}{a^2}\right)$$

$$[\mathrm{Re}\,(v+1-\lambda\pm\mu) > 0,\ a > b] \tag{67}$$

we obtain the expression for the partition function

$$Z_k = e^{-\beta(\hbar\omega_0 - m\omega_0^2 r_0^2) - \beta\hbar\omega_0(2k-1)} F\left(2k, 1; 2k; e^{-2\beta\hbar\omega_0}\right). \tag{68}$$

The degenerate hypergeometric function has the property (see [17])

$$F(\beta, \alpha; \beta; x) = F(\alpha, \beta; \beta; x) = (1-x)^{-\alpha} \tag{69}$$

and, finally, the partition function is

$$Z_k = e^{\beta m\omega_0^2 r_0^2 - \beta\hbar\omega_0(2k-1)} \frac{1}{2 \sinh \beta\hbar\omega_0}. \tag{70}$$

This is, of course, the same expression that was obtained in [8] (equation (41)), by using the trace of the PHO density matrix in the position representation.

Consequently, the diagonal elements of the density matrix (65) may be written as

$$\langle z, k | \rho_k | z, k \rangle = 2 e^{\beta\hbar\omega_0(2k-2)} \sinh \beta\hbar\omega_0 \frac{I_{2k-1}(2|z|e^{-\beta\hbar\omega_0})}{I_{2k-1}(2|z|)}. \tag{71}$$

Let us now perform the diagonal expansion of the density operator ρ_k in the BGCS:

$$\rho_k = \int \mathrm{d}\mu\,(z, k)\, P_k(z) |z, k\rangle \langle z, k|. \tag{72}$$

For the Glauber CS $|\alpha\rangle$ of the HO this expansion is called the Glauber–Sudarshan P-representation of the density operator [18]. In [14] it is shown that the diagonal representation of the density operator is well behaved for describing non-classical states of light.

In order to find the function $P_k(z)$ let us begin with the diagonal elements of the density operator ρ_k in the basis of the number states $|v, k\rangle$:

$$\langle v, k | \rho_k | v, k \rangle = \int 2 \frac{\mathrm{d}^2 z}{\pi} K_{2k-1}(2|z|) I_{2k-1}(2|z|) P_k(z) \langle v, k | z, k \rangle \langle z, k | v, k \rangle \tag{73}$$

where these diagonal elements are well known (see, equations (63) and (70)):

$$\langle v, k | \rho_k | v, k \rangle = \frac{1}{Z_k} e^{-\beta E_{vJ}} = (1 - e^{-2\beta\hbar\omega_0})[(e^{\beta\hbar\omega_0})^2]^v \tag{74}$$

as well as the functions

$$\langle v, k | z, k \rangle = \sqrt{\frac{|z|^{2k-1}}{I_{2k-1}(2|z|)}} \frac{z^v}{\sqrt{v!\Gamma(v+2k)}}. \tag{75}$$

Then, equation (73) becomes

$$(1 - e^{-2\beta\hbar\omega_0})[(e^{-\beta\hbar\omega_0})^2]^v = \frac{2}{v!\Gamma(v+2k)} \int 2\frac{d^2z}{\pi} K_{2k-1}(2|z|) P_k(z)|z|^{2k-1+2v}. \tag{76}$$

It is possible to choose intuitively an expression for $P_k(z)$, as is performed in [14]. But, we will choose the function $P_k(z)$ to have a similar expression as the diagonal elements of the density operator in BGCS (see, equation (71)):

$$P_k(z) = C \frac{K_{2k-1}(2|z|A)}{K_{2k-1}(2|z|)} \tag{77}$$

where the normalization constant C and the constant A must be determined.

Using the integral (see, equation (48)) we easily find the required expression:

$$P_k(z) = \left(e^{2\beta\hbar\omega_0} - 1\right)e^{\beta\hbar\omega_0(2k-1)} \frac{K_{2k-1}(2|z|e^{\beta\hbar\omega_0})}{K_{2k-1}(2|z|)}. \tag{78}$$

Of course, this function satisfies the normalization condition

$$\int d\mu\,(z, k)\, P_k(z) = 1 \tag{79}$$

which is not difficult to prove.

In this manner, the diagonal representation of the normalized density operator of the PHO in BGCS is

$$\rho_k = (e^{2\beta\hbar\omega_0} - 1)e^{\beta\hbar\omega_0(2k-1)} \int d\mu\,(z, k)\, \frac{K_{2k-1}(2|z|e^{\beta\hbar\omega_0})}{K_{2k-1}(2|z|)} |z, k\rangle\langle z, k|. \tag{80}$$

Then the thermal expectation value (the thermal average) of an observable A concerning the PHO is given by

$$\langle A \rangle_k = \text{Tr}(\rho_k A) = \int d\mu\,(z, k)\, P_k(z)\langle z, k|A|z, k\rangle. \tag{81}$$

For example, the thermal expectation value of the number operator, N, is

$$\langle N \rangle_k = \int d\mu\,(z, k)\, P_k(z)\langle z, k|N|z, k\rangle. \tag{82}$$

By using the equations (58), (68) and (69) we find that it is independent of the Bargmann index k:

$$\langle N \rangle_k = \frac{1}{e^{2\beta\hbar\omega_0} - 1} \equiv \langle N \rangle. \tag{83}$$

This is the same expression as the Bose–Einstein thermal distribution and, consequently, the PHO is suitable for association with a boson (e.g. a photon).

Similarly, using equations (59), (68) and (69), the thermal expectation value of the square of the number operator becomes

$$\langle N^2 \rangle_k = \frac{1}{e^{2\beta\hbar\omega_0} - 1} + 2\frac{1}{\left(e^{2\beta\hbar\omega_0} - 1\right)^2} \equiv \langle N^2 \rangle \tag{84}$$

also independent of the index k.

We can now define the thermal intensity correlation function, which, after the calculations above, is also independent of the index k:

$$\langle g^2 \rangle_k \equiv \frac{\langle N^2 \rangle - \langle N \rangle}{\langle N \rangle^2} = \langle g^2 \rangle = 2. \tag{85}$$

The normalized density operator characterizes the quantum gas of PHOs, regarded as the whole quantum system, is

$$\rho = \frac{1}{Z} \sum_J (2J + 1) Z_J \rho_J \tag{86}$$

where $\rho_J \equiv \rho_k$ is the diagonal representation of the density operator for (see, equation (80)) the rotational state J.

Consequently, the total thermal expectation value of an observable A is

$$\langle A \rangle = \operatorname{Tr} A\rho = \frac{1}{Z} \sum_J (2J + 1) Z_J \operatorname{Tr} A\rho_J \tag{87}$$

where $\operatorname{Tr} A\rho_J = \langle A \rangle_J = \langle A \rangle_k$ is the expectation value for the rotational state J (see, equation (81)).

Similarly, the total partition function is

$$Z = \sum_J (2J + 1) \sum_v \mathrm{e}^{-\beta E_{vJ}} = \sum_J (2J + 1) Z_J. \tag{88}$$

Using equation (70), the total partition function becomes

$$Z = \mathrm{e}^{\beta m \omega_0^2 r_0^2} Z_1^{(0)} T_\alpha(x) \tag{89}$$

where we have used the notation

$$T_\alpha(x) = \sum_{J=0}^{\infty} (2J + 1) \mathrm{e}^{-x\alpha} \qquad x = \beta \hbar \omega_0 \tag{90}$$

and, also, the notation for the one-dimensional HO (HO-3D) partition function:

$$Z_1^{(0)} = \frac{1}{2 \sinh \beta \hbar \omega_0} = \frac{1}{2 \sinh x}. \tag{91}$$

By applying the harmonic limit (7) to equation (90), we obtain

$$\lim_{\mathrm{HO}} T_\alpha = T_{J+\frac{1}{2}} = 2 \sum_J \left(J + \frac{1}{2} \right) \mathrm{e}^{-x(J+\frac{1}{2})} = \frac{1}{2} \frac{1}{\sinh^2 \frac{x}{2}} \cosh \frac{x}{2}. \tag{92}$$

Then, the harmonic limit of the total partition function (89) is

$$\lim_{\mathrm{HO}} Z = \frac{1}{2 \sinh x} T_{J+\frac{1}{2}} = \left(\frac{1}{2 \sinh \beta \frac{\hbar \omega_0}{2}} \right)^3 \equiv \left(Z_1^{(0)} \right)^3 \tag{93}$$

i.e. we obtain the partition function for the HO-3D, as we expected [6].

The internal energy of the whole quantum gas of the N_{tot} PHOs is

$$U = N_{\mathrm{tot}} \langle H \rangle = N_{\mathrm{tot}} \frac{1}{Z} \sum_J (2J + 1) Z_J \langle H \rangle_J \tag{94}$$

and using equations (13), (20) and (55), after integration, we obtain

$$U = -N_{\mathrm{tot}} m \omega_0^2 r_0^2 + N_{\mathrm{tot}} \hbar \omega_0 \left[\coth \beta \hbar \omega_0 - \frac{\partial}{\partial x} \ln T_\alpha \right] \tag{95}$$

where N_{tot} is the total number of the PHO in the quantum gas. This result is the same as the one in [8], where we have used the position representation of the PHO density matrix.

The entropy of the whole quantum gas is

$$S = -k_{\text{B}} \langle \ln \rho \rangle = k_{\text{B}} (\ln Z + \beta \langle H \rangle) \tag{96}$$

where we have taken into account that the quantum distribution is canonical and, consequently, the density operator is proportional to $\exp(-\beta H)$. After the calculations, we obtain the following expression:

$$S = k_{\text{B}} (\beta \hbar \omega_0 \coth \beta \hbar \omega_0 - \ln 2 \sinh \beta \hbar \omega_0) + k_{\text{B}} \left(\ln T_\alpha - \beta \hbar \omega_0 \frac{\partial}{\partial x} \ln T_\alpha \right). \tag{97}$$

Finally, the molar heat capacity at the constant volume

$$C_V = \frac{1}{\nu} \frac{\partial U}{\partial T} = -\frac{1}{\nu} k_{\text{B}} \beta^2 \frac{\partial U}{\partial \beta} \tag{98}$$

is easily obtained:

$$\frac{C_V}{R} = \left[\left(\frac{x}{\sinh x} \right)^2 + x^2 \frac{\partial^2}{\partial x^2} (\ln T_\alpha) \right]. \tag{99}$$

In order to verify the above-obtained formulae for the thermal expectation values of the PHO observables, let us apply the harmonic limit (7) to these formulae. In order to calculate the harmonic limit we need to calculate the expression

$$\frac{\partial}{\partial x} \ln T_{J+\frac{1}{2}} = -\coth \frac{x}{2} + \frac{1}{2} \frac{1}{\coth \frac{x}{2}}. \tag{100}$$

After straightforward calculations, we successively obtain

$$\lim_{\text{HO}} U = 3N_{\text{tot}} \frac{\hbar \omega_0}{2} \coth \beta \frac{\hbar \omega_0}{2} = 3N_{\text{tot}} \left[\frac{\hbar \omega_0}{2} + \frac{\hbar \omega_0}{e^{\beta \hbar \omega_0} - 1} \right] \equiv 3U_1^{(0)} \tag{101}$$

$$\lim_{\text{HO}} S = 3k_{\text{B}} \left[\beta \left(\frac{\hbar \omega_0}{2} + \frac{\hbar \omega_0}{e^{\beta \hbar \omega_0} - 1} \right) - \ln 2 \sinh \beta \frac{\hbar \omega_0}{2} \right] \equiv 3S_1^{(0)} \tag{102}$$

$$\lim_{\text{HO}} \frac{C_V}{R} = 3 \left(\frac{\beta \frac{\hbar \omega_0}{2}}{\sinh \beta \frac{\hbar \omega_0}{2}} \right)^2 \equiv 3 \frac{C_{V;1}^{(0)}}{R} \tag{103}$$

where the notation $A_1^{(0)}$ represents the corresponding quantity for the HO-1D.

We will point out here that these formulae are the same as those derived from the use of the position representation of the PHO density matrix (see, [6]). This fact demonstrates that the BGCS for the PHO are correct, as well as our obtained formula for the diagonal representation of the density operator in these states (80).

6. The time dependence of the BGCS

At the end of this paper we will refer to the time dependence of the BGCS. Using equation (44) and the radial Schrödinger equation for the PHO,

$$H_k |v.k\rangle = [\hbar \omega_0 (2v + 2k) - m\omega_0^2 r_0^2] |v, k\rangle \tag{104}$$

we obtain the time dependence of the BGCS as follows:

$$|z, k; t\rangle = e^{-\frac{i}{\hbar} H_k t} |z, k; 0\rangle \tag{105}$$

where we have

$$H_k \equiv H_\alpha = \hbar\omega_0 H_\alpha^{(\text{red})}(y) = \hbar\omega_0 \left(2K_3 - \frac{m\omega_0}{\hbar}r_0^2\right) \tag{106}$$

and $|z, k; 0\rangle \equiv |z, k\rangle$.

The action of the operator K_3 on the states $|z, k; 0\rangle$ reduces to the action of the same operator on the number states $|v, k\rangle$ (see, equation (26)). After the calculations we obtain

$$|z, k; t\rangle = \exp\left[\frac{\mathrm{i}}{\hbar}(m\omega_0^2 r_0^2 - \hbar\omega_0\, 2k)t\right]\sqrt{\frac{|z|^{2k-1}}{I_{2k-1}(2|z|)}}\sum_{v=0}^{\infty}\frac{\left(z\mathrm{e}^{-2\mathrm{i}\omega_0 t}\right)^v}{\sqrt{v!\Gamma(v+2k)}}|v, k\rangle. \tag{107}$$

When we use the notation

$$z(t) = z\mathrm{e}^{-2\mathrm{i}\omega_0 t} \tag{108}$$

we obtain

$$|z(t), k\rangle = \sqrt{\frac{|z(t)|^{2k-1}}{I_{2k-1}(2|z(t)|)}}\sum_{v=0}^{\infty}\frac{[z(t)]^v}{\sqrt{v!\Gamma(v+2k)}}|v, k\rangle. \tag{109}$$

By inserting $v = 0$ into equation (9), we obtain the energy for the ground vibrational state

$$E_{0J} = \hbar\omega_0\, 2k - m\omega_0^2 r_0^2. \tag{110}$$

In this manner, we obtain the following time dependence of the BGCS:

$$|z, k; t\rangle = \mathrm{e}^{-\frac{\mathrm{i}}{\hbar}E_{0J}t}|z(t), k\rangle. \tag{111}$$

The properties and applications of the time-dependent BGCS will be the subject matter of a forthcoming paper.

7. Conclusion remarks

The PHO is an interesting oscillator model not only for its spectral properties, in good agreement with the experimental data, but also due to the fact that as the limiting case of the PHO we obtain the HO-3D. In other words, by applying the harmonic limit to an equation or formula concerning the PHO (7) we obtain the corresponding equation or formula for the HO-3D. This is a suitable method for verifying the correctness of the equations or formulae for the PHO thus obtained, and at the same time for testing new methods, procedures and concepts.

In this paper we achieved the implementation of the BGCS in the case of the PHO Hamiltonian. We have shown that the symmetry group which corresponds to the pseudoharmon oscillator Hamiltonian is the $SU(1, 1)$ group. As a consequence, we constructed the CS as the eigenstates of the group generator K_-, i.e. the BGCS for the PHO. By using these CS we calculated some expectation values in the BGCS representation for a few observables concern for the PHO. As a result we obtained that, for small $|z|$, the corresponding statistic distribution is sub-Poissonian, while for $|z|$ large it is Poissonian.

In section 5 of the paper we examined the statistical properties of the PHO; i.e., we have constructed the density matrix in the BGCS representation and, especially, its diagonal representation. In our opinion this seems to be a new result, because, to our knowledge, this result has not yet appeared in the literature. In order to prove the correctness of the expression we obtained for the diagonal representation of the density operator ρ, we calculated some thermal expectation values (thermal averages) for few observables of concern for the PHO (i.e. the number operator, internal energy, entropy and C_V). By applying the harmonic limit (7) to these averages we obtained the corresponding averages for the HO-3D. It was to be expected. It

seems that one of the advantages of the use of the BGCS representation consists in the relative simplicity of the mathematical calculations, versus the corresponding calculations using the position representation of the density operator [8].

Acknowledgments

Appendix

We consider the general sum

$$S_n \equiv \sum_{v=0}^{\infty} \frac{(x^2)^v}{v!\Gamma(v+\nu+1)} v^n \tag{A.1}$$

which, in the particular case $n = 0$, according to equation (42), is

$$S_0 = \frac{1}{x^\nu} I_\nu(2x). \tag{A.2}$$

On the other hand, from the well known relation [13]

$$\frac{\mathrm{d}}{\mathrm{d}x}\left[\frac{1}{x} I_\nu(x)\right] = \frac{1}{x^\nu} I_{\nu+1}(x) \tag{A.3}$$

we obtain

$$S_1 = x^2 \frac{\mathrm{d}}{\mathrm{d}(x^2)} S_0 = \frac{1}{2}(2x)\frac{\mathrm{d}}{\mathrm{d}(2x)} S_0 = x\frac{1}{x^\nu} I_{\nu+1}(2x). \tag{A.4}$$

To calculate the sum S_2 it is useful to write the power v^2 as $v^2 = v(v-1)+v$. Consequently, the result becomes

$$S_2 = \sum_{v=0}^{\infty} \frac{(x^2)^v}{v!\Gamma(v+\nu+1)} v^2 = (x^2)^2 \left(\frac{\mathrm{d}}{\mathrm{d}(x^2)}\right)^2 S_0 + x^2 \frac{\mathrm{d}}{\mathrm{d}(x^2)} S_0. \tag{A.5}$$

After straightforward calculation, we obtain

$$S_2 = x\frac{1}{x^\nu} I_{\nu+1}(2x) + x^2 \frac{1}{x^\nu} I_{\nu+2}(2x). \tag{A.6}$$

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