COHERENT STATES FORMALISM FOR THE PSEUDOHARMONIC OSCILLATOR

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The Barut-Girardello, Klauder-Perelomov and Gazeau-Klauder coherent states for the pseudoharmonic oscillator are constructed and some of their properties are examined. The diagonal P-representation of the density operator is deduced and the thermal expectation values for a quantum canonical ideal gas of pseudoharmonic oscillators is calculated.

Keywords: Pseudoharmonic oscillator, Coherent states, Density matrix

1. Introduction

The pseudoharmonic oscillator (PHO) potential is one of the anharmonic potentials suitable for the treatment of diatomic molecular vibrations. The PHO effective potential [1] may be rewritten as follows [2]:

\[
V_J(r) = \frac{m\omega^2}{8} r_J^2 \left( \frac{r - r_J}{r} \right)^2 + \frac{m\omega^2}{4} (r_J^2 - r_0^2), \quad r_J = \frac{\sqrt{2m\omega}}{\omega} \sqrt{\alpha^2 - \frac{1}{4}}, \quad \alpha = \left( \frac{J + \frac{1}{2}}{2} \right) + \left( \frac{m\omega}{2\eta r_0^2} \right)^2 \tag{1}
\]

where \( m \) is the reduced mass, \( \omega \) - the angular frequency, \( r_0 \) - the equilibrium distance between the diatomic molecule nuclei and \( J = 0,1,2,... \) is the rotational quantum number. This procedure allows us to reduce the rotational case \( (J \neq 0) \) to the nonrotational one \( (J = 0) \). After the substitutions \( \omega = 2\omega_0 \) and \( y = Br / \sqrt{2} \), the corresponding rovibrational Schrödinger equation for the reduced radial function \( u_\nu^\alpha (r) \) [1] (where \( \nu = 0,1,2,... \) is the vibrational quantum number), becomes

\[
H^{(\text{red})}_\alpha (y) u_\nu^\alpha (y) = (2\nu + \alpha + 1) u_\nu^\alpha (y) \tag{2}
\]

where the dimensionless reduced PHO Hamiltonian and eigenvalues are:

\[
H^{(\text{red})}_\alpha (y) = -\frac{1}{2} \frac{d^2}{dy^2} + \frac{1}{2} y^2 + \frac{1}{2} \left( \alpha^2 - \frac{1}{4} \right) \frac{1}{y^2} = 2K_3, \quad e_\nu = 2\nu + \alpha + 1. \tag{3}
\]

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

The operator \( K_3 \), together with the operators

\[
K_\pm = \frac{1}{2} \left( \pm y \frac{d}{dy} \pm \frac{1}{2} - y^2 + 2\nu + \alpha + 1 \right) \tag{4}
\]
span the SU(1,1) Lie algebra:

\[
[K_+, K_+] = \pm K_\pm \\
[K_-, K_+] = 2K_3 \\
K^2 = K_3^2 - \frac{1}{2}(K_+ K_- + K_- K_+) = k(k-1).
\]  

So, the PHO quantum system possesses a SU(1,1) symmetry, with the Casimir operator \( K_3 \), where the Bargmann index \( k \) labels irreducible representations of the SU(1,1) group. We are interested only in the unitary irreducible representations with \( k > 0 \).

If we perform the substitution \( \alpha = 2k - 1 \), then the action of the operators \( K_\pm \) on the eigenfunctions \( u^\alpha (r) \) becomes exactly the same as the action on the eigenvectors \( |v,k> \), i.e.

\[
K_+ |v,k> = \sqrt{(v + 1)(v + 2k)} |v + 1,k> , \quad K_- |v,k> = \sqrt{v(v + 2k - 1)} |v - 1,k>.
\]  

This permits us to construct the CSs for the PHO.

3. Construction of the CSs for the PHO

The PHO quantum system admits the construction of three kinds of coherent states (CSs), each of them having specific properties, the most important of them being presented below.

3.1 Barut-Girardello coherent states (BG-CSs) are defined as the eigenvalues of the lowering operator \( K_- \) [3]:

\[
K_- |z,k> = z |z,k>.
\]  

where \( z = |z| \exp(i\phi) \). The normalized BG-CSs of the PHO \( |z,k> \) can be written as [4]

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

The following resolution of the identity holds

\[
\int d\mu(z,k) |z,k> \otimes |z,k> = 1
\]  

with the positive integration measure \( (K_3(x) \) is the modified Bessel function of the second kind) [4]

\[
d\mu(z,k) = 2K_{2k-1}(2|z|)I_{2k-1}(2|z|) \frac{d\phi}{\pi}|z|d|z|.
\]  

3.2 Klauder-Perelomov coherent states (KP-CSs) are constructed by applying the generalized displacement operator \( \exp(\xi K_+ - \xi^* K_-) \) to the lowest state \( |v = 0,k> \):

\[
|z,k> = \exp(\xi K_+ - \xi^* K_-)|0,k> = e^{\xi K_1} e^{i\xi K_2} |0,k>.
\]  

where \( \xi = \frac{\theta}{2} \exp(-i\phi); z = \frac{\xi}{|\xi|} \text{tanh}\left|\frac{\theta}{2}\right|; \Gamma = \ln(1 - |z|^2); |z| < 1; -\infty < \theta < \infty; 0 \leq \phi \leq 2 \pi \).

Finally, we have found that the normalized KP-CSs of the PHO are

\[
|z,k> = (1 - |z|^2)^k \sum_{v=0}^{\infty} \frac{|z|^v}{\sqrt{\Gamma(v + 2k)}} |v,k>.
\]  

The resolution of the identity is accomplished for the following positive defined integration measure:

\[
d\mu(z,k) = (2k - 1) \frac{d\phi}{\pi} \frac{|z|d|z|}{(1 - |z|^2)^2}.
\]  

3.3 Gazeau-Klauder coherent states (GK-CSs) are connected with the reduced dimensionless Hamiltonian which admits the nondegenerate discrete energy spectrum: \( \epsilon_v = 2v + \alpha + 1 = 2(v + k) \). According to the general definition [5], the normalized GK-CSs for the PHO are characterized by a real two parameter set \( \{ J, \gamma | k >, J \geq 0, -\infty < \gamma < \infty \} \), so that
\[ |J, \gamma; k > = \frac{1}{\sqrt{1_iF_1(1; k + 1; J/2)}} \sum_{\nu=0}^{\infty} \frac{J^{\nu}}{\sqrt{\rho(\nu; k)}} e^{-i\nu \gamma}, \quad |v, k > \]  

(14)

where \( \rho(\nu; k) = e_\nu e_{k+1} \) \( e_{\nu} = 2^\nu \Gamma(\nu + k + 1)/\Gamma(\nu + 1) \), and \( _1F_1(1; k + 1; J/2) \) is the hypergeometric series.

The integration measure of the GK-CSs is

\[ d\mu(J, \gamma) = \frac{1}{4\Gamma(k+1)} |F_1(1; k + 1; J/2)| e^{-\frac{J}{2}} d\gamma dJ. \]  

(15)

We note that the convergence radius \( R \) [5] is infinite for the BG- and GK-CSs, while for the KP-CSs it is equal to unity. Sometimes, the weight function from the integration measure is unique for each kind of the above examined coherent states.

The Mandel parameter \( Q \), defined by means of the expectations of the number operator powers \( < N'^s > \), with \( s = 1, 2, \ldots \), as follows [5]

\[ Q = \frac{\langle \Delta N \rangle^2}{\langle N \rangle} - 1 = \frac{< N^2 > - < N >^2}{< N >} - 1 \]  

(16)

determine the nature of the weight distribution of the CSs. The distribution is super-Poissonian, Poissonian or sub-Poissonian for \( Q \) strictly positive, zero or strictly negative. The calculations for the CSs of the PHO show that the BG-CSs are sub-Poissonian for small \( |z| \) and Poissonian for large \( |z| \) while the KP-CSs and GK-CSs are supra-Poissonian for all \( |z| \), respectively all \( J \).

4. Thermal expectations

We have examined a quantum canonical ideal PHOs gas at the temperature \( T = (\beta k_B)^{-1} \). Their normalized density operator for a fixed \( k \) is

\[ \rho_k = \frac{1}{Z_k} \sum_{\nu=0}^{\infty} e^{-\beta E_\nu} \quad |v, k > < v, k | \]  

(17)

where \( Z_k \) is the partition function for a fixed rotational state. Their diagonal elements in the CSs representations (called the Husimi \( Q \)-function) for the BG-, KP- and GK-CSs are respectively

\[ < z, k | \rho_k | z, k > = \frac{1}{n+1} \left( \frac{\bar{n}}{n+1} \right)^{k-\frac{n}{2}} \sum_{\nu=0}^{\infty} \frac{J^{\nu}}{\sqrt{\rho(\nu; k)}} \frac{I_{2k-1} \left( 2 |z| \sqrt{\bar{n}/n+1} \right)}{I_{2k-1} \left( 2 |z| \right)} , \]  

(18)

\[ < z, k | \rho_k | z, k > = \frac{1}{n+1} \left( \frac{1-|z|^2}{1-|z|^2} \right)^{2k} \sum_{\nu=0}^{\infty} \frac{J^{\nu}}{\sqrt{\rho(\nu; k)}} \frac{I_{2k-1} \left( 2 |z|^2 \frac{n}{n+1} \right)}{I_{2k-1} \left( 2 |z|^2 \right)} , \]  

(19)

where \( \bar{n} = \left[ \exp(2\beta \eta \omega_b) - 1 \right]^{-1} \) is the well known bosonic distribution function.

We can perform the diagonal expansion of the density operator in the CSs – representations (where instead of the dots the variables which characterize the corresponding CS must be put):

\[ \rho K = \int d\mu(K) |K > P_k(K) < K | . \]  

(20)

The calculations of the \( P \)-function lead to the resolution of the Stieltjes (for the BG- and GK-CSs), respectively the Hausdorff (for the KP-CSs) – moment problems, using the properties of Meijer’s G – function and the Mellin inversion theorem [6]. The obtained results are (in the order: BG, KP and GK)
The diagonal expansion of the density operator, which is useful for calculating the thermal expectations,

\[
\langle A \rangle = \text{Tr}(\rho_A A) = \int d\mu(K) P_K(K) \langle K | A | K \rangle
\]

shows that the thermal expectations are the same for all three kinds of the above constructed CSs for the PHO. Using the total partition function \( Z \) (where the summation is performed also on the rotational quantum number), we have deduced the expressions for some physical observable of the PHO quantum canonical ideal gas (e.g. the internal energy, the entropy, the molar heat capacity at the constant volume) [4]. These results will not be repeated here anymore.

5. Concluding remarks

The PHO potential possesses a SU(1,1) group symmetry which permits us to construct the Barut-Girardello (BG-) and the Klauder-Perelomov coherent states (KP-CSs), using the generators of this group. Besides this, we have also constructed the Gazeau-Klauder coherent states (GK-CSs). These states accomplished all the conditions required to a CS. We have examined the thermal properties of a PHO quantum canonical ideal gas and we have deduced the Husimi's \( Q \)-function and, especially, the \( P \)-function from the diagonal expansion of the density operator for the BG-, KP- and GK-CSs – representations. With these functions one can calculate the thermal expectations of different physical observables concerning the PHO. By comparing to other representations (e.g. the position or the momentum [2]), the calculations in the CSs representations are very simple and this emphasizes one of the advantages of the CSs formalism.

5. References