

**P-FUNCTION OF THE PSEUDOHARMONIC OSCILLATOR
IN TERMS OF KLAUDER-PERELOMOV COHERENT STATES**

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Using the Klauder-Perelomov coherent states of the pseudoharmonic oscillator Hamiltonian, corresponding diagonal P -representation for the density matrix of the gas of pseudoharmonic oscillators in thermal equilibrium is constructed. With a help of this new result, some corresponding characteristic thermal expectation values are obtained.

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1 Introduction

The pseudoharmonic oscillator (PHO) potential [1, 2] is an anharmonic potential, which, like the harmonic oscillator (HO) potential, also allows an exact mathematical treatment. This potential may be considered in a certain sense as an intermediate potential between the harmonic oscillator potential (an ideal model) and anharmonic potentials (which are more realistic). A comparative analysis of potentials HO-3D (3-dimensional harmonic oscillator potential) and PHO is performed in [2].

In the present work, we examine some properties of the Klauder-Perelomov coherent states of the pseudoharmonic oscillator. Using properties of these states we construct, in Section 3, the diagonal P -representation of the density operator for the PHO quantum canonical gas. This is the main new result of this work. Using it, we also derive expressions for some significant expectation values for this physical system.

2 Klauder-Perelomov coherent states for PHO

The effective potential of the PHO is

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

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where r_0 is the equilibrium distance between the diatomic molecule nuclei and $J = 0, 1, 2, \dots$ is the rotational quantum number.

This potential has been treated in detail previously so we will only recall some formulae that will be need.

Using Molski's techniques [3] (for the Morse oscillator) in our previous paper [4], we have rewritten the PHO effective potential as follows:

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

where

$$\lambda = \sqrt{\left(J + \frac{1}{2} \right)^2 + \left(\frac{m\omega}{2\hbar} r_0^2 \right)^2} \quad (3)$$

and

$$r_J = \sqrt{\frac{2\hbar}{m\omega} \left(\lambda^2 - \frac{1}{4} \right)^{\frac{1}{2}}}. \quad (4)$$

By using the substitution $\omega = 2\omega_0$ and the dimensionless variable $y = \left(\frac{m\omega_0}{\hbar} \right)^{\frac{1}{2}} r$, the corresponding rovibrational Schrödinger equation for the reduced radial function $u_v^\lambda(r)$ and the dimensionless Hamiltonian is [4]

$$\left[-\frac{1}{2} \frac{d^2}{dy^2} + \frac{1}{2} y^2 + \frac{1}{2} \left(\lambda^2 - \frac{1}{4} \right) \frac{1}{y^2} - (2v + \lambda + 1) \right] u_v^\lambda(y) = 0. \quad (5)$$

In the previous paper [4], we have demonstrated that the $SU(1, 1)$ is the natural dynamical group associated with the bounded states of the PHO. The discrete representations of the $SU(1, 1)$ group are given by

$$K^2 |v, k\rangle = k(k-1) |v, k\rangle, \quad (6)$$

$$K_+ |v, k\rangle = \sqrt{(v+1)(v+2k)} |v+1, k\rangle, \quad (7)$$

$$K_- |v, k\rangle = \sqrt{v(v+2k-1)} |v-1, k\rangle, \quad (8)$$

where v is the vibrational quantum number, $k = \frac{1}{2}(\lambda + 1) > \frac{1}{2}$ and the PHO realization of the raising and lowering operators K_\pm is

$$K_\pm = \frac{1}{2} \left(\pm y \frac{d}{dy} \pm \frac{1}{2} - y^2 + 2v + \lambda + 1 \right). \quad (9)$$

Generally, the Klauder-Perelomov coherent states are obtained if the generalized displacement unitary operator $\exp(\alpha K_+ - \alpha^* K_-)$ on the lowest state of the quantum system $|v=0, k\rangle$ are applied [5–7]:

$$|z, k\rangle = \exp(\alpha K_+ - \alpha^* K_-) |0, k\rangle = e^{zK_+} e^{\Gamma K_3} e^{-z^* K_-} |0, k\rangle, \quad (10)$$

where $\alpha = -\frac{1}{2}\theta e^{-i\varphi}$, $z = \frac{\alpha}{|\alpha|} \tanh |\alpha| = -\tanh \frac{\theta}{2} e^{-i\varphi}$ and where the group generator K_3 is

$$K_3 = \frac{1}{2} [K_-, K_+], \quad \Gamma = \ln(1 - |z|^2). \quad (11)$$

The parameters $\theta \in (-\infty, \infty)$ and $\varphi \in [0, 2\pi]$ are group parameters similar to the Euler angles. The condition $|z| < 1$ shows that the $SU(1, 1)$ KP-CSs $|z, k\rangle$ are defined in the interior of the unit disc. In terms of the basis vectors $|v, k\rangle$, using the equations (7) and (8) and the equation

$$K_3|v, k\rangle = (k + v)|v, k\rangle, \quad (12)$$

the KP-CSs of the PHO may be expanded as

$$|z, k\rangle = \mathcal{N}(|z|^2) \sum_{v=0}^{\infty} \frac{z^v}{\sqrt{\rho(v; k)}} |v, k\rangle, \quad (13)$$

where

$$\rho(v; k) = \frac{\Gamma(v + 1)\Gamma(2k)}{\Gamma(v + 2k)} = (2k - 1)B(v + 1; 2k - 1) \quad (14)$$

and $B(a; b)$ is the Euler beta function.

We note here that in agreement with the choices of $\rho(v; k)$, there are many different families of coherent states, as illustrated in a series of recent works [8–11]. The normalization constant $\mathcal{N}(|z|^2)$ is obtained from the normalization condition $\langle z, k|z, k\rangle = 1$, so that

$$[\mathcal{N}(|z|^2)]^{-2} = \sum_{v=0}^{\infty} (2k)_v \frac{(|z|^2)^v}{v!} = {}_1F_0(2k; |z|^2) = \frac{1}{(1 - |z|^2)^{2k}}, \quad (15)$$

where ${}_pF_q(\dots)$ is the generalized hypergeometric function, while $(a)_v = \frac{\Gamma(a+v)}{\Gamma(a)}$ is the Pochhammer symbol [12]. Finally, the KP-CSs of the PHO are

$$|z, k\rangle = (1 - |z|^2)^k \sum_{v=0}^{\infty} \frac{z^v}{\sqrt{\rho(v; k)}} |v, k\rangle. \quad (16)$$

The overlap of two KP-CSs of the PHO (the scalar product) is

$$\langle \sigma, k|z, k\rangle = \frac{(1 - |\sigma|^2)^k (1 - |z|^2)^k}{(1 - \sigma^* z)^{2k}}, \quad (17)$$

where σ and z are the complex numbers.

We need to calculate the convergence radius R [9]

$$R = \lim_{v \rightarrow \infty} \sqrt[v]{\rho(v; k)}. \quad (18)$$

In view of the limit [12]

$$\lim_{x \rightarrow \infty} \frac{\Gamma(x + a)}{\Gamma(x)x^a} = 1 \quad (19)$$

it is not difficult to prove that, for the KP-CSs of the PHO, we have $R = 1$. Then

$$\int d\mu(z, k) |z, k\rangle \langle z, k| = I, \quad (20)$$

with the integration measure

$$d\mu(z, k) = \frac{d^2 z}{\pi} W_k(|z|^2), \quad d^2 z = d(\operatorname{Re} z) d(\operatorname{Im} z) = d\varphi dr r, \quad (21)$$

where $z = r \exp(i\varphi)$, $r \in [0, 1]$, $\varphi \in [0, 2\pi]$.

In order to determine the unknown weight function, after the angular integration, we obtain

$$\sum_{v=0}^{\infty} \frac{|v, k\rangle \langle v, k|}{\rho(v; k)} \int_0^R dr r^{2v+1} W_k(r^2) (1-r^2)^{2k} = I, \quad (22)$$

from which the following infinite set of equations results:

$$\int_0^R dr r^{2v+1} W_k(r^2) (1-r^2)^{2k} = \rho(v; k), \quad v = 0, 1, 2, \dots, \quad 0 \leq R < \infty. \quad (23)$$

The quantities $\rho(v; k) > 0$ are then the power moments of the new unknown function

$$h_k(r^2) = \frac{1}{(1-r^2)^{2k}} W_k(r^2) \quad (24)$$

and the problem stated in (23) is the Hausdorff ($R < \infty$) moment problem [9]. After the variable change $x = r^2$, we have

$$\int_0^R dx x^v h_k(x) = \Gamma(2k) \frac{\Gamma(v+1)}{\Gamma(v+2k)}. \quad (25)$$

In the above Hausdorff moment problem we extend the integer values of v to the complex values s , so that $v \rightarrow s - 1$ and rewrite it as

$$\int_0^R dx x^{s-1} h_k(x) = \Gamma(2k) \frac{\Gamma(s)}{\Gamma(2k-1+s)}. \quad (26)$$

As is usual in such a problem [8, 10], it is convenient to define

$$g_k(x) = \begin{cases} h_k(x), & 0 \leq x \leq R \\ 0, & R < x < \infty \end{cases} \quad (27)$$

and to interpret (26) as the Mellin transform $g_k^*(s)$ of $g_k(x^2)$:

$$\int_0^{\infty} dx x^{s-1} g_k(x) \equiv g_k^*(s) \stackrel{def}{=} \mathcal{M}[g_k(x); s] = \Gamma(2k) \frac{\Gamma(s)}{\Gamma(2k-1+s)}. \quad (28)$$

The explicit formula for obtaining $g_k(x)$ from $g_k^*(s)$ is given by

$$g_k(x) = \frac{1}{2\pi i} \int_{c-i\infty}^{c+i\infty} ds x^{-s} g_k^*(s) \stackrel{def}{=} \mathcal{M}^{-1}[g_k^*(s); x], \quad (29)$$

which denotes the inverse Mellin transform.

Using the definition of the Meijer's G-function and Mellin inversion theorem it follows that [13]:

$$\int_0^\infty dx x^{s-1} G_{p,q}^{m,n} \left(\alpha x \left| \begin{matrix} a_1, & \dots, & a_n, & a_{n+1}, & \dots, & a_p \\ b_1, & \dots, & b_m, & b_{m+1}, & \dots, & b_q \end{matrix} \right. \right) = \tag{30}$$

$$= \frac{1}{\alpha^s} \frac{\prod_{j=1}^m \Gamma(b_j + s) \prod_{j=1}^n \Gamma(1 - a_j - s)}{\prod_{j=m+1}^q \Gamma(1 - b_j - s) \prod_{j=n+1}^p \Gamma(a_j + s)}.$$

Comparing equations (26) and (30), we obtain that [13]

$$h_k(x) = \Gamma(2k) G_{1,1}^{1,0} \left(x \left| \begin{matrix} 2k-1 \\ 0 \end{matrix} \right. \right) = (2k-1)(1-x)^{2k-2}, \tag{31}$$

so that the weight function $W_k(|z|^2)$ becomes

$$W_k(|z|^2) = (2k-1) \frac{1}{(1-|z|^2)^2}. \tag{32}$$

This is a positive function for $|z| < 1$ and $k > \frac{1}{2}$. Therefore, the integration measure (21) finally is

$$d\mu(z, k) = \frac{2k-1}{\pi} \frac{d^2z}{(1-|z|^2)^2}. \tag{33}$$

The sufficient condition for the solution (32) to be unique is given by the Carleman condition [7, 8]: if the solution of the problem (26) exists then

$$S \stackrel{def}{=} \sum_{v=1}^\infty [\rho(v; k)]^{-\frac{1}{2v}} = \begin{cases} \infty, & \text{the solution is unique} \\ < \infty, & \text{non-unique solutions exist} \end{cases}. \tag{34}$$

It is not difficult to prove using the mathematical analysis test methods (e.g. the logarithmic or d'Alembert test), for the function $\rho(v; k)$ defined by (14), that the sum S diverges. So, the weight function for the KP-CSs of the PHO is unique.

3 *P*-representation for PHO canonical gas density matrix

We consider a quantum canonical gas of PHOs in thermodynamical equilibrium with a thermostat at temperature $T = (k_B\beta)^{-1}$, where k_B is the Boltzmann's constant and β -the well-known temperature parameter.

By using the equation (3) and taking into account that the Bargmann index is $k = \frac{1}{2}(\lambda + 1)$, the corresponding normalized canonical density operator for a fixed rotational quantum number J (or, equivalently, for a fixed number k), is

$$\rho_J \equiv \rho_k = \frac{1}{Z_k} \sum_{v=0}^\infty e^{-\beta E_{vJ}} |v, k\rangle \langle v, k|, \tag{35}$$

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

$$E_{v,J} = \hbar\omega_0 2k - m\omega_0^2 r_0^2 + 2\hbar\omega_0 v \equiv E_{0,J} + 2\hbar\omega_0 v. \quad (36)$$

The average value of normalized canonical density operator in the KP-CS representation, i.e. the Husimi's distribution function, is

$$\langle z, k | \rho_k | z', k \rangle = \frac{1}{Z_k} e^{-\beta E_{0,J}} \left(\frac{\sqrt{(1-|z|^2)^k (1-|z'|^2)^k}}{1 - z^* z' e^{-\beta \hbar \omega_0}} \right)^{2k}. \quad (37)$$

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

$$\text{Tr} \rho_k = \int d\mu(z, k) \langle z, k | \rho_k | z, k \rangle = 1 \quad (38)$$

we obtain the expression for the partition function of the PHO (for the fixed rotational state J):

$$Z_k = e^{\beta m \omega_0^2 r_0^2 - \beta \hbar \omega_0 (2k-1)} \frac{1}{2 \sinh \beta \hbar \omega_0}, \quad (39)$$

where the exponential represents the contribution of the anharmonicity.

Using these results, we can write the Husimi distribution function as follows:

$$\langle z, k | \rho_J | z, k \rangle \equiv \langle \rho_k \rangle_{z,k} = (1 - e^{-\beta \hbar \omega_0}) \left(\frac{1 - |z|^2}{1 - |z|^2 e^{-\beta \hbar \omega_0}} \right)^{2k}. \quad (40)$$

Let us now perform the diagonal expansion of the density operator in the KP-CSs:

$$\rho_k = \int d\mu(z, k) |z, k\rangle P_k(|z|^2) \langle z, k|. \quad (41)$$

In order to find the quasi-probability distribution function $P_k(|z|^2)$ let us note that the equation

$$\langle f | \rho_k | g \rangle = \int d\mu(z, k) \langle f | z, k \rangle P_k(|z|^2) \langle z, k | g \rangle \quad (42)$$

must be fulfilled for any arbitrary vectors $\langle f |$ and $|g\rangle$ from the Hilbert space. Using equation (35), the left-hand side of (42) becomes

$$LHS \equiv \frac{1}{Z_k} \sum_{v=0}^{\infty} e^{-\beta E_{v,J}} \langle f | v, k \rangle \langle v, k | g \rangle, \quad (43)$$

while, after the angular integration and the variable change $x = r^2$, the right-hand side may be represented in the form

$$RHS \equiv (2k-1) \sum_{v=0}^{\infty} \frac{\langle f | v, k \rangle \langle v, k | g \rangle}{\rho(v; k)} \int_0^1 dx x^v (1-x)^{2k-2} P_k(x). \quad (44)$$

Comparing the LHS and the RHS, we conclude that

$$\int_0^1 dx x^v (1-x)^{2k-2} P_k(x) = \frac{1}{2k-1} \frac{1}{Z_k} e^{-\beta E_{0,J}} \rho(v; k) e^{-2\beta \hbar \omega_0 v}, \quad (45)$$

which, after the function change,

$$P_k(x) = \frac{1}{Z_k} e^{-\beta E_{0,J}} \frac{1}{(1-x)^{2k-2}} g_k(x), \quad (46)$$

leads to the integral equation

$$\begin{aligned} \int_0^1 dx x^v g_k(x) &= (e^{-2\beta\hbar\omega_0})^v B(v+1; 2k-1) \\ &= \Gamma(2k-1) \frac{1}{(e^{2\beta\hbar\omega_0})^v} \frac{\Gamma(v+1)}{\Gamma(v+2k)}. \end{aligned} \quad (47)$$

The method of solving this equation is the same as the one for obtaining the weight function $W_k(|z|^2)$ (32), i.e. the solving of the Hausdorff moment problem. Using equation (30) and the tables of the Meijer's G-functions [13], we obtain

$$g_k(x) = e^{2\beta\hbar\omega_0} \Gamma(2k-1) G_{1,1}^{1,0} \left(x \left| \begin{matrix} 2k-1 \\ 0 \end{matrix} \right. \right) = e^{2\beta\hbar\omega_0} (1 - e^{2\beta\hbar\omega_0} x)^{2k-2}. \quad (48)$$

We can finally write for the P-distribution function

$$P_k(|z|^2) = (e^{2\beta\hbar\omega_0} - 1) \left(\frac{1 - e^{2\beta\hbar\omega_0} |z|^2}{1 - |z|^2} \right)^{2k-2}. \quad (49)$$

Using the tabular integrals it is not difficult to prove that this function satisfies the normalization condition

$$\int d\mu(z, k) P_k(z) = 1. \quad (50)$$

In this way, the diagonal representation of the normalized density operator of the PHO in KS-CSs is

$$\rho_k = (2k-1) (e^{2\beta\hbar\omega_0} - 1) \int \frac{d^2 z}{\pi} \frac{1}{(1 - |z|^2)^2} \left(\frac{1 - e^{2\beta\hbar\omega_0} |z|^2}{1 - |z|^2} \right)^{2k-2} |z, k\rangle \langle z, k|, \quad (51)$$

which fulfills the normalization condition (38).

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

$$\begin{aligned} \langle A \rangle_k &= Tr(\rho_k A) = (2k-1) (e^{2\beta\hbar\omega_0} - 1) \times \\ &\times \int \frac{d^2 z}{\pi} \frac{1}{(1 - |z|^2)^2} \left(\frac{1 - e^{2\beta\hbar\omega_0} |z|^2}{1 - |z|^2} \right)^{2k-2} \langle z, k | A | z, k \rangle. \end{aligned} \quad (52)$$

In many cases (e.g. with the aim of calculating the thermal averages of the powers of the number operator N) it is necessary to solve the integrals of the following kind [12]:

$$\begin{aligned} I_{lm} &\equiv \int_0^1 x^l (1-x)^{-2k-m} (1-Ax)^{2-2k} \\ &= \frac{\Gamma(l+1)\Gamma(1-2k-m)}{\Gamma(2-2k+l-m)} {}_2F_1(2-2k, l+1; 2-2k+l-m; A) \end{aligned} \quad (53)$$

and, besides that, to use the following property of the hypergeometric function ${}_2F_1(\dots)$ [14]

$${}_2F_1(a, b; b - n; z) = \frac{1}{(1 - z)^{a+n}} \sum_{k=0}^n \frac{(-n)_k (b - a - n)_k}{(b - n)_k} \frac{z^k}{k!}. \quad (54)$$

By using these results, we obtain the thermal expectation values of the number operator N and the square of the number operator N^2 respectively

$$\langle N \rangle_k = 2k(2k - 1) (e^{2\beta\hbar\omega_0} - 1) I_{11} = \frac{1}{e^{2\beta\hbar\omega_0} - 1} \equiv \langle N \rangle = \bar{n} \quad (55)$$

$$\begin{aligned} \langle N^2 \rangle_k &= 2k(2k - 1) (e^{2\beta\hbar\omega_0} - 1) (I_{12} + 2kI_{22}) = \\ &= \frac{1}{e^{2\beta\hbar\omega_0} - 1} + 2 \frac{1}{(e^{2\beta\hbar\omega_0} - 1)^2} \equiv \langle N^2 \rangle = \bar{n}(1 + 2\bar{n}). \end{aligned} \quad (56)$$

These expectation values are independent of the index k . The thermal expectation of the number operator N is the same as the expression of the Bose-Einstein thermal distribution (thermal mean occupancy \bar{n})

$$\bar{n} = \frac{1}{e^{2\beta\hbar\omega_0} - 1}, \quad (57)$$

which shows that the PHO is suitable for associating it with a boson (e.g. a photon or phonon).

We can now calculate the thermal second-order correlation function $(g^2)_k$.

$$(g^2)_k \equiv \frac{\langle N^2 \rangle - \langle N \rangle^2}{\langle N \rangle^2} = (g^2) = 2 \quad (58)$$

and the thermal analogue of the Mandel parameter also Q_k [15, 16]:

$$Q_k \equiv \langle N \rangle [(g^2) - 1] = \langle N \rangle = \bar{n}. \quad (59)$$

The total normalized density operator which characterizes the quantum gas of pseudoharmonic oscillators is

$$\rho = \frac{1}{Z} \sum_J (2J + 1) Z_J \rho_J, \quad (60)$$

where $\rho_J \equiv \rho_k$ is the diagonal representation of the density operator for the rotational state J (see equation (51)).

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

$$\langle A \rangle = Tr A \rho = \frac{1}{Z} \sum_J (2J + 1) Z_J Tr A \rho_J, \quad (61)$$

where $Tr A \rho_J = \langle A \rangle_J = \langle A \rangle_k$ is the expectation value for the rotational state J . Similarly, the total partition function is

$$Z = \sum_J (2J + 1) \sum_v e^{-\beta E_{vJ}} = \sum_J (2J + 1) Z_J, \quad (62)$$

where $Z_J = Z_k$ is the partition function for the rotational state J (see equation (39)).

Let us note here that the HO-3D can be considered as an appropriate limit of the PHO. This limit is called *the harmonic limit of the PHO* and for a certain physical observable A is defined as [17]

$$\lim_{\substack{\omega \rightarrow 2\omega_0 \\ r_0 \rightarrow 0 \\ \alpha \rightarrow J + \frac{1}{2}}} \mathcal{F}^{(PHO)} \equiv \lim_{HO} \mathcal{F}^{(PHO)} = \mathcal{F}^{(HO-3D)}, \quad (63)$$

where the quantities with the superscript (PHO) corresponds to the PHO with the angular frequency ω , while the same quantities with the superscript $(HO-3D)$ corresponds to the HO-3D (with the frequency ω_0).

By applying to the harmonic limit (63), all results and equations obtained in the present paper for PHO lead to the corresponding results and equations for the HO-3D. This fact may be considered as a good check of the correctness of our results.

To conclude, our new results for PHO obtained in terms of Klauder-Perelomov coherent states are encouraging, and we believe that these results may contribute to a better understanding of the behaviour and properties of the PHO.

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