acta physica slovaca vol. 48 No. 1, 1 – 12 February 1998

COHERENT STATES OF THE PSEUDOHARMONICAL OSCILLATOR

Dušan Popov
University "Politehnica" of Timişoara, Department of Physics, Piaţa Horaţiu No. 1, 1900 Timişoara, ROMANIA

Received 2 June 1997, accepted 15 December 1997

For the pseudoharmonical oscillator we have built the creation and annihilation operators and the corresponding coherent states. After the deduction of the density operator expression in coherent-state representation in two ways (by their definition and by solving the Bloch equation), we have calculated the expected values of some characteristical physical observables.

1. Introduction

Although the molecular vibrations are anharmonical, in most cases the harmonic potential model is being used, due to its mathematical advantadges. But, an anharmonic potential which permits, also, an exact mathematical treatement is the so-called "pseudoharmonical potential". This potential is pointed out still in ref. [1], but just recently there has reappeared an interest for it [2], [3], [4].

The effective potential of the pseudoharmonical oscillator (PHO) is:

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

where r_0 is the equilibrium distance between the nuclei. As it admits the exact analytical solution of the Schrödinger equation, we consider the PHO , in a certain sense, an intermediate potential between the harmonic oscillator (HO) potential (an ideal potential) and the anharmonic potentials (such as the Morse potential, the more "realistic" potential). A comparative analysis of the three-dimensional harmonic potential (HO-3D) and the PHO is made in ref. [3].

Using the technics of Molski [5] (for the Morse potential), we can rewrite the PHO effective potential as:

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

where the changed equilibrium distance is:

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

and the new appearing rotational parameter α is defined as follows:

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

The obtained results (2) indicate that as a consequence of the action of centrifugal force, which operates in all systems with rotational degrees of freedom, the equilibrium distance increases $r_0 \to r_J$, that is, the equilibrium configuration changes [5]. Also, there appears the effective rotational energy:

$$E_{eff}^{Rot} = \frac{m\omega^2}{4}(r_J^2 - r_0^2), \tag{5}$$

which leads to the modification of the energy eigenvalues $E_{vJ}^{(p)}$ of the PHO.

On these considerations, the Schrödinger equation for the reduced radial function $u_v^\alpha(r)$ is:

$$\left[-\frac{\hbar^2}{2m}\frac{d^2}{dr^2} + \frac{m\omega^2}{8} r_J^2 \left(\frac{r}{r_J} - \frac{r_J}{r}\right)^2\right] u_v^\alpha(r) = (E_{vJ}^{(p)} - E_{eff}^{Rot}) u_v^\alpha(r). \tag{6}$$

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

The radial eigenfunctions and eigenvalues have been calculated in ref.[2] and we done here only the final expressions:

$$R_{vJ}^{(p)}(r) = \frac{1}{r} u_v^\alpha(r) = \left[\frac{B^3 v!}{2^\alpha \Gamma(\alpha + v + 1)}\right]^{\frac{1}{2}} (Br)^{\alpha - \frac{1}{2}} \exp\left(-\frac{B^2}{4} r^2\right) L_v^\alpha\left(\frac{B^2}{2} r^2\right), \tag{7}$$

$$E_{vJ}^{(p)} = \hbar\omega\left(v + \frac{1}{2}\right) + \frac{\hbar\omega}{2}\alpha - \frac{m\omega^2}{4} r_0^2, \tag{8}$$

where we have used the notation:

$$B = \left(\frac{m\omega}{\hbar}\right)^{\frac{1}{2}}. \tag{9}$$

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

The aim of this paper is to construct the coherent states (CS) of the PHO and to determine the expected values of some physical quantities by using the CS. This will be done by deducing the expression of the density operator ρ in the CS-representation in two ways: by their definition and by solving the Bloch equation for a quantum system which obeys the quantum canonical distribution.

2. Lowering and raising operators

In ref. [6] it is shown that a shape invariant potential Hamiltonian may be factorized until an aditive constant as follows:

$$H_J^{(p)} = \frac{p^2}{2m} + V_J^{(p)}(r) = \hbar\omega\, a_J^+ a_J + E_0, \tag{10}$$

where the operators (non Hermitian) are of the following kind:

$$a_J = i a_1 p - b_1 W, \tag{11}$$

$$a_J^+ = -i a_1 p - b_1 W. \tag{12}$$

The constants a_1 and b_1 must be determined, while the operator W is connected with the potential $V_J^{(p)}$ as follows [6]:

$$V_J^{(p)}(r) = \hbar\omega b_1 \left(b_1 W^2 - \sqrt{\frac{\hbar}{2m\omega}}\frac{\partial W}{\partial r}\right) + E_0. \tag{13}$$

In the case of PHO (1), after ordinary calculations, we obtain the following expressions:

$$a_J = -\frac{1}{2^{\frac{3}{2}}} B r + \frac{1}{2^{\frac{1}{2}}}\frac{1}{B}\left(\alpha + \frac{1}{2}\right)\frac{1}{r} - \frac{1}{2^{\frac{1}{2}}}\frac{1}{B}\frac{\partial}{\partial r}, \tag{14}$$

$$a_J^+ = -\frac{1}{2^{\frac{3}{2}}} B r + \frac{1}{2^{\frac{1}{2}}}\frac{1}{B}\left(\alpha + \frac{1}{2}\right)\frac{1}{r} + \frac{1}{2^{\frac{1}{2}}}\frac{1}{B}\frac{\partial}{\partial r}, \tag{15}$$

$$E_0 = \frac{\hbar\omega}{2}(\alpha + 1) - \frac{m\omega^2}{4} r_0^2. \tag{16}$$

We will demonstrate that the operators a_J and a_J^+, which act as lowering and raising operators on the vibrational quantum number v of the reduced radial eigenfunction $u_{vJ}^\alpha(r)$, are just the creation and annihilation operators of the vibrational quanta.

Using eq. (7) it is easy to demonstrate that the equations bellow are valid:

$$a_J\, u_v^\alpha(r) = \sqrt{v}\, u_{v-1}^{\alpha+1}(r), \tag{17}$$

$$a_J^+\, u_{v-1}^{\alpha+1}(r) = \sqrt{v}\, u_v^\alpha(r). \tag{18}$$

In the deduction of these equations we have using the following equations, involving the generalized Laguerre polynomials [7]:

$$\frac{d}{dx} L_v^\alpha(x) = -L_{v-1}^{\alpha+1}(x), \tag{19}$$

$$x\frac{d}{dx}L_{v-1}^{\alpha+1}(x) = vL_v^{\alpha}(x) - (\alpha+1-x)L_{v-1}^{\alpha+1}(x)\,. \tag{20}$$

After the elementary calculations, from eq. (17) and (18) we obtain:

$$a_J^+ a_J\, u_v^{\alpha}(r) = v\, u_v^{\alpha}(r) \tag{21}$$

and this equation shows that the operator

$$N_J = a_J^+ a_J \tag{22}$$

is just the number-particle operator in the vibrational state with the fixed rotational quantum number J, i.e. $|v,\alpha>$. On the other hand, eqs. (17) and (18) show that the operator a_J acts so that it decreases the vibrational quantum number v with the unity and increases the rotational parameter α with the unity, while the operator a_J^+ increases the vibrational quantum number v with the unity and decreases the rotational parameter α with the unity.

From eqs. (17), (18) and (21) we obtain that these operators satisfy the usual canonical algebra:

$$[a_J\,, a_J^+] = 1\,, \tag{23}$$

which was to expect.

In this manner we have constructed the annihilation and creation operators for the vibrational states of the PHO, with the fixed rotational quantum number J (which, in other words, play the role of a parameter).

3. Construction of the coherent states

The HO-3D can be considered as a limit oscillator of the PHO. This limit is called "the harmonic limit" and for a certain physical observable A is defined as [4]:

$$\lim_{\substack{r_0\to 0\\ \alpha\to J+\frac{1}{2}\\ \omega\to 2\omega_0}} A^{(p)} \equiv \lim_{HO} A^{(p)} = A^0\,, \tag{24}$$

where the index (p) reffers to the characteristical quantities of the PHO, while the index (0) reffers to the same quantities of the HO-3D (which has the frequency ω_0).

Then it is to be expected that the coherent states (CS) of the PHO are similar with the CS of the HO-3D.

Let be z the complex variable involved in CS. Then, we define the CS as:

$$a_J\,|z,J> = z\,|z,J>\,, \tag{25}$$

where the quantum number J (or, equivalently, α) plays the role of an integer parameter.

By expanding the CS in terms of the basis set vectors $|v,J> = |v,\alpha(J)> \equiv |v,\alpha>$:

$$|z,J> = \sum_{v=0}^{\infty} <v,\alpha|z,J>\,|v,\alpha>\,. \tag{26}$$

we obtain:

$$a_J\,|z,J> = \sum_{v} <v,\alpha|z,J>\; a_J\,|v,\alpha>\,. \tag{27}$$

For the basis vectors $|v,\alpha>$, eq. (17) is:

$$a_J\,|v,\alpha> = \sqrt{v}\,|v-1,\alpha+1>\,. \tag{28}$$

Using eqs. (26) and (27) and the orthogonality relation of the eigenvectors, we obtain:

$$<v,\alpha|z,J> = \frac{z}{\sqrt{v}}\,<v-1,\alpha+1|z,J>\,. \tag{29}$$

This reccurence relation leads to:

$$<v,\alpha|z,J> = \frac{z^v}{(v!)^{\frac{1}{2}}}\,<0,\alpha+1|z,J>\,. \tag{30}$$

From eq. (26) and using the property that the CS are overcomplete but non- orthogonal:

$$<z',J|z,J> = \exp\left(z'^{*}z - \frac{1}{2}|z'|^2 - \frac{1}{2}|z|^2\right), \tag{31}$$

it is easy to demonstrate that:

$$<0,\alpha+1|z,J> = \exp\left(-\frac{1}{2}|z|^2\right) \tag{32}$$

and so, finally, the CS for PHO are:

$$|z,J> = \exp\left(-\frac{1}{2}|z|^2\right)\sum_{v=0}^{\infty}\frac{z^v}{(v!)^{\frac{1}{2}}}\,|v,\alpha>\,. \tag{33}$$

We observe that, formally, the CS for the PHO have the same form as the CS for the HO-3D, with the remark that, for each CS, the complex variable z is connected to the quantum rotational number J as a parameter. In other words, it exist an one-to-one correspondence between the coherent states $|z,J>$ and points in the complex z plane: $|z,J> \to z(J)$, but, due to the notation simplification reasons, we didn't write the complex variable $z(J)$, but only z.

The expected value of a physical observable A, which characterizes the PHO, with respect to the CS $|z,J>$ is, then:

$$<z,J|A|z,J> = \exp\left(-|z|^2\right)\sum_{v,v'}\frac{z^{*v'}z^{v}}{(v'!v!)^{\frac{1}{2}}}\,<v',\alpha|A|v,\alpha>\,, \tag{34}$$

which shows that in the diagonal elements in CS-representation contribute all elements (diagonal and non-diagonal) in $|v\alpha>$-representation.

If the operator A is just the normalized density operator of a quantum gas of the pseudoharmonical oscillators, in thermodynamical equilibrium with the reservoir (thermostat) at temperature T and into the rotational state with the quantum number J, i.e.:

$$\rho_J^{(p)} = \frac{1}{Z_J^{(p)}} \sum_{v=0}^{\infty} \exp\left(-\beta E_{vJ}^{(p)}\right) |v,\alpha><v,\alpha| , \tag{35}$$

which is diagonal with respect to the $|v,\alpha>$-basis, then eq. (34) becomes:

$$<z,J|\rho_J^{(p)}|z,J> = \frac{1}{Z_J^{(p)}} \exp\left(-|z|^2\right) \sum_{v=0}^{\infty} \frac{|z|^{2v}}{(v!)} \exp\left(-\beta E_{vJ}^{(p)}\right) . \tag{36}$$

Using eq. (8), we immediately obtain:

$$<z,J|\rho_J^{(p)}|z,J> = \frac{1}{Z_J^{(p)}} \exp\left[\beta\frac{m\omega^2}{4}r_0^2 - \beta\frac{\hbar\omega}{2}(\alpha+1) - |z|^2\left(1-\exp\left(-\beta\hbar\omega\right)\right)\right] . \tag{37}$$

The quantity $Z_J^{(p)}$ is called the vibrational statistical sum for a certain rotational state pointed out by J. Its expression is obtained as follows:

$$Z_J^{(p)} = Tr\rho_J^{(p)} = \int_0^{\infty} dr\, r^2 \rho_J^{(p)}(r,r;\beta) , \tag{38}$$

where the radial density matrix for the PHO was deduced in ref. [4]:

$$\rho_J^{(p)}(r,r';\beta) = \exp\left(\beta\frac{m\omega^2}{4}r_0^2\right) \frac{1}{\sinh\beta\frac{\hbar\omega}{2}} \frac{\frac{m\omega}{2\hbar}}{(rr')^{\frac{1}{2}}}$$
$$\times \exp\left[-\frac{m\omega}{4\hbar}\left(r^2+r'^2\right)\coth\beta\frac{\hbar\omega}{2}\right] I_\alpha\left(\frac{\frac{m\omega}{2\hbar}rr'}{\sinh\beta\frac{\hbar\omega}{2}}\right) . \tag{39}$$

We use the following integral involving the modified Bessel functions I_α [7]:

$$\int_0^{\infty} dx \exp(-ax) I_\alpha(bx) = \frac{b^\alpha}{\left(a^2-b^2\right)^{\frac{1}{2}}\left[a+\left(a^2-b^2\right)^{\frac{1}{2}}\right]^{\alpha}} \tag{40}$$

and finally, we obtain the expression for the statistical sum:

$$Z_J^{(p)} = \exp\left(\beta\frac{m\omega^2}{4}r_0^2 - \beta\frac{\hbar\omega}{2}\alpha\right)\frac{1}{2\sinh\beta\frac{\hbar\omega}{2}} . \tag{41}$$

On the other hand, it is demonstrated that the diagonal CS-representation of the density operator (called the Glauber-Sudarshan representation) is [8]:

$$\rho_J^{(p)} = \int \frac{d^2 z'}{\pi} \rho_J^{(p)}(z') |z',J><z',J| , \tag{42}$$

so that, we have:

$$<z,J|\rho_J^{(p)}|z,J> = \int \frac{d^2 z'}{\pi} \rho_J^{(p)}(z') \exp\left[-|z|^2 - |z'|^2 + z^* z' + z z'^*\right] . \tag{43}$$

We shall determine, in a simple manner, the diagonal elements $\rho_J^{(p)}(z)$ of the density operator (42) for the PHO. Evidently, the r.h.s. of the eqs. (37) and (43) must be equal. We suppose that the function $\rho_J^{(p)}(z)$ must be a gaussian distribution function. This , because the gaussian distribution appears wheneaver there exist a lot of identical sources which emit independently one of another [9]:

$$\rho_J^{(p)}(z') = C_N \exp\left(-s|z'|^2\right) , \tag{44}$$

where C_N is the normalization constant and s is a positive constant, which must be determined.

We consider that the complex variable z' is:

$$z' = r\exp(i\varphi) \tag{45}$$

and so, the integral from eq.(43) becomes:

$$I^{(r,\varphi)} = \int_0^{\infty} dr\, r \exp\left[-(s+1)r^2\right] \int_0^{2\pi} \frac{d\varphi}{\pi} \exp\left(a\cos\varphi + b\sin\varphi\right) , \tag{46}$$

where the constants are:

$$a = 2r\,Re\,z ; \qquad b = 2r\,Im\,z . \tag{47}$$

The integral with respect to φ is of the kind [7]:

$$\int_0^{2\pi} d\varphi \cos\left(p\cos\varphi + q\sin\varphi + n\varphi\right)\exp\left(a\cos\varphi + b\sin\varphi\right) =$$
$$= \pi\frac{(A+iB)^{\frac{n}{2}} I_n\left(\sqrt{C-iD}\right) + (A-iB)^{\frac{n}{2}} I_n\left(\sqrt{C+iD}\right)}{\left[(p-b)^2+(q+a)^2\right]^{\frac{n}{2}}} , \tag{48}$$

where the following notations have been used:

$$A = a^2 - b^2 + p^2 - q^2 ; \qquad B = 2(ab+pq) ;$$
$$C = a^2 + b^2 - p^2 - q^2 ; \qquad D = 2(ap+bq) . \tag{49}$$

In our case $n = p = q = 0; B = D = 0; C = 4|z|^2 r^2$ and finally, we obtain:

$$I^{(r,\varphi)} = 2\int_0^\infty dr\, r\, \exp\left[-(s+1)r^2\right] I_0(2|z|r)\,, \tag{50}$$

where I_n are the Bessel functions of the second kind. By passing to the Bessel functions of the first kind:

$$I_0(x) = J_0(ix)\,, \tag{51}$$

we are dealing with the integral of the following kind [7]:

$$\int_0^\infty dx\, x^{\nu+1} \exp\left(-a^2x^2\right) J_\nu(bx) = \frac{b^\nu}{(2a^2)^{\nu+1}} \exp\left(-\frac{b^2}{4a^2}\right). \tag{52}$$

After these calculations, we obtain the checking expression, via eqs. (37), (41), (43) and (44):

$$\rho_J^{(p)}(z') = \left[\exp(\beta\hbar\omega) - 1\right] \exp\left[-|z'|^2(\exp(\beta\hbar\omega) - 1)\right] \tag{53}$$

and, then, the density operator $\rho_J^{(p)}$ of the PHO can be written in the diagonal representation in respect to the CS:

$$\rho_J^{(p)} = \left[\exp(\beta\hbar\omega) - 1\right] \int \frac{d^2z'}{\pi} \exp\left[-|z|^2(\exp(\beta\hbar\omega) - 1)\right] |z', J><z', J|\,. \tag{54}$$

We must observe that this expression has the same form as the corresponding expression for the HO-3D [8], which was to be expected, as a consequence of the same form of corresponding CS.

4. The Bloch equation

In the CS-representation, the Bloch equation (which is an alternative way of finding the density operator), for a noninteracting PHO can be brought to the following form [10]:

$$-\frac{\partial}{\partial\beta}\rho_J^{(p)}(z^*, z'; \beta) = H_J^{(p)}\left(z^*, \frac{\partial}{\partial z^*}\right) \rho_J^{(p)}(z^*, z'; \beta)\,, \tag{55}$$

$$\lim_{\beta\to 0} \rho_J^{(p)}(z^*, z'; \beta) = exp(z^*z')\,, \tag{56}$$

where $\rho_J^{(p)}(z^*, z'; \beta)$ is an analytical non-normalized function in variables z' and z^*, defined as follows:

$$\rho_J^{(p)}(z^*, z'; \beta) = <z, J|\rho_J^{(p)}|z', J> \exp\left(\frac{1}{2}|z|^2 + \frac{1}{2}|z'|^2\right). \tag{57}$$

Due to the canonical algebra of the operators a_J and a_J^+ (23), in the Hamiltonian (10) we must replace the creation operator a_J^+ by z^* and the annihilation operator a_J

by $\frac{\partial}{\partial z^*}$ (this fact is valid only when the Hamiltonian is built from the normal-ordered operators) [10].

We try to find the solution of eq. (55) as an exponential:

$$\rho_J^{(p)}(z^*, z'; \beta) = \exp\left[G_J^{(p)}(z^*, z'; \beta)\right], \tag{58}$$

which leads to the solving of a new equation of the Hamilton-Jakobi kind from the analytical mechanics:

$$-\frac{\partial}{\partial\beta}G_J^{(p)}(z^*, z'; \beta) = H_J^{(p)}\left(z^*, \frac{\partial G_J^{(p)}}{\partial z^*}\right), \tag{59}$$

$$\lim_{\beta\to 0} G_J^{(p)}(z^*, z'; \beta) = z^*z'\,. \tag{60}$$

For the PHO rotational Hamiltonian (10) (with J as a parameter !), eq. (59) becomes:

$$-\frac{\partial}{\partial\beta}G_J^{(p)} = \hbar\omega\, z^* \frac{\partial}{\partial z^*}G_J^{(p)} + \frac{\hbar\omega}{2}(\alpha + 1) - \frac{m\omega^2}{4}r_0^2\,. \tag{61}$$

The solution is a sum of the general solution of the homogeneous equation (that is an equation with the separable variables) and a particular solution (like a free term). It is easy to prove that the solution is:

$$G_J^{(p)}(z^*, z'; \beta) = -\beta\frac{\hbar\omega}{2}(\alpha + 1) + \beta\frac{m\omega^2}{4}r_0^2 + z^*z' \exp(-\beta\hbar\omega)\,. \tag{62}$$

The non-diagonal elements of $\rho_J^{(p)}$ in CS-representation are obtained from eq. (57):

$$<z, J|\rho_J^{(p)}|z', J> = \exp\left[-\beta\frac{\hbar\omega}{2}(\alpha + 1) + \beta\frac{m\omega^2}{4}r_0^2 - \frac{1}{2}|z|^2 - \frac{1}{2}|z'|^2 + z^*z' \exp(-\beta\hbar\omega)\right]. \tag{63}$$

We must remark here that this density operator , which satisfies the Bloch equation, is a non-normalized operator. By considering eqs. (37) and (41), we obtain the same operator. So, we have obtained the density operator expression into two alternative manners.

5. A short application

As an example of using the creation and annihilation operators (17) and (18) we present a short application by making the calculation first of the expected value of the ordered products $(a_J^+)^m a_J^n$ and, later, of the internal energy of a PHO quantum gas, $U^{(p)}$. Let us consider the system of N identical pseudoharmonical oscillators (the quantum gas), without interactions, in thermodynamical equilibrium at temperature T with the reservoir, which is characterized by the density operator [4]:

$$\rho_J^{(p)} = \frac{1}{Z^{(p)}} \sum_{vJM} \exp\left(-\beta E_{vJ}^{(p)}\right) |vJM><vJM| \quad (64)$$

and, due to the decoupling of the vibrational and rotational degrees of freedom of the PHO (see, eq. (8)), because of the absence of interaction between two motions, but only with a certain parametrical influence, we can write:

$$|vJM> = |v> |J> |M> . \quad (65)$$

Due to the M-degeneration (where M is the quantum number of the z-axis projection of the angular momentum), we obtain:

$$\rho_J^{(p)} = \frac{1}{Z^{(p)}} \sum_J (2J+1)\, Z_J^{(p)} \rho_J^{(p)} , \quad (66)$$

where $\rho_J^{(p)}$ is given by eq. (35). Then, the expected value of a certain physical observable A of the system will be:

$$<A> = Tr\, \rho^{(p)} A = \frac{1}{Z^{(p)}} \sum_J (2J+1)\, Z_J^{(p)} <A>_J \quad (67)$$

and, when in the operator A the normally ordered creation and annihilation operators are involved, then the expected value $<A>_J$ with respect to the CS is:

$$<A>_J = \int \frac{d^2 z}{\pi} \rho_J^{(p)}(z)\, A(z^*, z) , \quad (68)$$

i.e. the expected value is formally calculated by substituting the operators a_J^+ and a_J (from the operator A) with their eigenvalues z^*, respectively, z.

The expected values of the normal ordered products (moments) , using eq. (53), are:

$$<\left(a_J^+\right)^m a_J^n> = [\exp(\beta\hbar\omega) - 1] \int \frac{d^2 z}{\pi} \exp\left[-|z|^2 (\exp(\beta\hbar\omega) - 1)\right] (z^*)^m z^n . \quad (69)$$

Using eq. (45), the complex integral splits into the two real integrals:

$$<\left(a_J^+\right)^m a_J^n> =$$

$$= [\exp(\beta\hbar\omega) - 1] \int_0^{2\pi} \frac{d\varphi}{\pi} \exp[i(n-m)\varphi] \int_0^{\infty} dr\, r^{m+n+1} \exp\left[-r^2 (\exp(\beta\hbar\omega) - 1)\right] , \quad (70)$$

which, after two simple integrations, leads to:

$$<(a_{J+})^m a_J^n> = \frac{\Gamma\left(\frac{m+n}{2} + 1\right)}{[\exp(\beta\hbar\omega) - 1]^{\frac{m+n}{2}}} \delta_{n-m;0} , \quad (71)$$

For $m = n = 1$, we obtain:

$$<a_J^+ a_J> = \frac{1}{\exp(\beta\hbar\omega) - 1} . \quad (72)$$

This results is useful for calculating the internal energy of a PHO gas of N oscillators:

$$U^{(p)} = N <H^{(p)}> = N\, Tr \rho^{(p)} H^{(p)} = N \frac{1}{Z^{(p)}} \sum_J (2J+1)\, Z_J^{(p)} <H^{(p)}>_J . \quad (73)$$

The function $H_J^{(p)}(z^*, z)$ which corresponds to the Hamiltonian (10) is:

$$H_J^{(p)}(z^*, z) = \hbar\omega |z|^2 + \frac{\hbar\omega}{2}(\alpha + 1) - \frac{m\omega^2}{4} r_0^2 . \quad (74)$$

By substituting this equation in eq. (68) and after integrations, we obtain the expression of the internal energy of the PHO gas [4]:

$$U^{(p)} = -N \frac{m\omega^2}{4} r_0^2 + N \frac{\hbar\omega}{2} \left[\coth \beta \frac{\hbar\omega}{2} - \frac{\partial}{\partial y} (\ln T_\alpha)\right] , \quad (75)$$

where we have used the notations:

$$T_\alpha = \sum_{J=0}^{\infty} (2J+1) \exp(-y\alpha) , \quad (76)$$

$$y = \beta \frac{\hbar\omega}{2} . \quad (77)$$

The first and last terms of eq.(75) may be considered as the contribution of the anharmonicity.

From this expression, using the harmonic limit defined by eq. (24), we obtain the expression of the internal energy for the HO-3D [4]:

$$\lim_{HO} U^{(p)} = U^{(0)} \doteq 3N \frac{\hbar\omega_0}{2} \coth \beta \frac{\hbar\omega_0}{2} = 3N \left[\frac{\hbar\omega_0}{2} + \frac{\hbar\omega_0}{\exp(\beta\hbar\omega_0) - 1}\right] , \quad (78)$$

which demonstrate the correctness of the expression (75).

In a similar way we can obtain the expressions of the other physical observables of the PHO and, at the harmonic limit, the corresponding expressions of the HO-3D.

This illustrates the utility and the simplicity of the using of CS-representation.

6. Conclusions

The pseudoharmonical potential is a more realistic potential in comparation with the harmonic potential. Due to the mathematical facilities in the approach of the PHO (it admits an exact solution of the Schrödinger equation and the exact calculations of the expected values), the PHO is useful for the examination of the molecular vibrations.

We are building the creation and annihilation operators for the PHO and, consequently, the coherent states, which, to our knowledge, have not appeared in the literature to this point.

Also, we are building the density operator in CS-representation for the PHO, in two ways, directly by their definition and by solving the Bloch equation. This second way seems to be more efficient and elegant.

As we can see, the use of the CS-representation is more efficient rather than other representations in the case of the quantum gas of the pseudoharmonical oscillators in thermodynamical equilibrium with the reservoir [4].

In the short application in Sec. 5, we are showing how one can use the CS-representation in calculating the expected values of some physical observables of the PHO. The results lead, at the harmonic limit, to the corresponding results for the HO-3D, which represent a good test of the validity of ours obtained results.

Acknowledgments The author gratefully acknowledges Professor *Oliviu GHERMAN* for discussions and for encouraging him to carry out researches in this field.

References

[1] I. I. Gol'dman, V. D. Krivchenkov, V. I. Kogan, V. M. Galitskii: *Problems in Quantum Mechanics*, Ed. D. ter Haar, Infosearch, London 1960.

[2] M. Sage: *Chem. Phys.* **87** (1984) 431

[3] M. Sage, J. Goodisman: *Am. J. Phys* **53** (1985) 350

[4] D. Popov: *Acta Phys. Slovaca* **45** (1995) 557

[5] M. Molski: *Acta Phys. Polonica A* **83** (1993) 417

[6] A. Das, W. J. Huang: *Phys. Rev. D* **41** (1990) 3241

[7] I. S. Gradshtein, I. M. Ryzhik: *Table of Integrals, Series and Products*, Academic Press, London, New York 1980.

[8] A. I. Ahiezer, B. V. Berestetskyi: *Quantum Electrodynamics*, Nauka, Moskow 1981 (in Russian).

[9] A. Messiah: *Mécanique quantique*, Tome I, Dunod, Paris 1969.

[10] I. A. Vakarchuk: *Teoreticeskaya i Matematiceskaya Fizika (TMF)* **35** (1978) 76