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Density Matrix Theory for the BDS-Hamiltonian

Dušan Popov[1]

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In the present paper, we have extended the usual uncertainty relations, as well as the entropic uncertainty relations to the mixed states, particularly to the thermal states, using the density matrix formalism. As quantum model we have choosen the quantum mechanical ideal gas with the harmonic oscillator-like Hamiltonian H_λ, introduced by Beckers, Debergh and Szafraniec, generically named BDS-Hamiltonian.

1. INTRODUCTION

Although much has been written about the harmonic oscillator coherent states, beginning from the fundamental papers of Glauber (1963), Klauder (1963), and Stoler (1970) and culminating by the well-known works about the applications of the coherent states (see, e.g., Klauder and Skagerstam, 1985; Perelomov, 1986; Zhang *et al.*, 1990), the interests for the coherent and, also, for the squeezed states actually remain.

Recently, Beckers *et al.* (1998) have proposed a new set of squeezed states where a new bosonic creation operator a_λ^+ is defined, which depends on a real continuos parameter λ, in the following way:

$$a_\lambda^+ \equiv a^+ + \lambda I, \tag{1}$$

where a^+ is the usual bosonic creation operator, which is Hermitic conjugate of the annihilation operator a. With these operators, a_λ^+, a^+, and a, it can be proved that the corresponding Heisenberg algebra is

$$\left[a,\ a_\lambda^+\right] = \left[a,\ a^+\right] = I. \tag{2}$$

Then, the following new operator can be constructed as the analogue of a Hamiltonian operator (Beckers *et al.*, 1998):

$$H_\lambda = \frac{\hbar\omega}{2}\left[a, a_\lambda^+\right]_+ = \frac{\hbar\omega}{2}\left[a, a^+\right]_+ + \lambda\hbar\omega a \equiv H^{(0)} + \lambda\hbar\omega a. \tag{3}$$

[1] Department of Physics, University "Politechnica" of Timişoara, Piaţa Regina Maria No. 1, Of. Postal 5, 1900 Timişoara, Romania; e-mail: dpopov@etv.utt.ro; dpopov@edison.et.utt.ro

Here $H^{(0)}$ is the Hamiltonian of the usual one-dimensional harmonic oscillator (HO-1D):

$$H^{(0)} = \frac{\hbar\omega}{2}\big[a, a^{+}\big]_{+} = \hbar\omega\left(a^{+}a + \frac{1}{2}\right). \tag{4}$$

By using the well-known relations of the bosonic annihilation and creation operators (Messiah, 1969):

$$a = \frac{1}{\sqrt{2}}\left(\sqrt{\frac{m\omega}{\hbar}}x + i\frac{1}{\sqrt{m\hbar\omega}}p\right) = \frac{1}{\sqrt{2}}\left(\sqrt{\frac{m\omega}{\hbar}}x + \sqrt{\frac{\hbar}{m\omega}}\frac{\partial}{\partial x}\right), \tag{5}$$

$$a^{+} = \frac{1}{\sqrt{2}}\left(\sqrt{\frac{m\omega}{\hbar}}x - i\frac{1}{\sqrt{m\hbar\omega}}p\right) = \frac{1}{\sqrt{2}}\left(\sqrt{\frac{m\omega}{\hbar}}x - \sqrt{\frac{\hbar}{m\omega}}\frac{\partial}{\partial x}\right), \tag{6}$$

the operator H_λ can be written with respect to the variable x, as follows:

$$H_\lambda(x) = -\frac{1}{2}\frac{\hbar^2}{m}\frac{\partial^2}{\partial x^2} + \frac{1}{2}m\omega^2x^2 + \frac{\lambda}{\sqrt{2}}\hbar\omega\sqrt{\frac{\hbar}{m\omega}}\frac{\partial}{\partial x} + \frac{\lambda}{\sqrt{2}}\hbar\omega\sqrt{\frac{m\omega}{\hbar}}x. \tag{7}$$

Moreover, by using the well-known relations

$$[x, p] = i\hbar, \qquad p = -i\hbar\frac{\partial}{\partial x}, \qquad x = i\hbar\frac{\partial}{\partial p}, \tag{8}$$

the same operator can be rewritten with respect to the variable p, as follows:

$$\begin{aligned} H_\lambda(p) = &-\frac{1}{2}\hbar^2m\omega^2\frac{\partial^2}{\partial p^2} + \frac{1}{2}\frac{1}{m}p^2 + \frac{\lambda}{\sqrt{2}}i\hbar\omega\sqrt{m\hbar\omega}\frac{\partial}{\partial p} \\ &+ \frac{\lambda}{\sqrt{2}}i\hbar\omega\sqrt{\frac{1}{m\hbar\omega}}p. \end{aligned} \tag{9}$$

Notice that, in both the representations (the position $\{x\}$ and the momentum $\{p\}$), the operator H_λ has the same mathematical expression:

$$H_\lambda(\xi) = -\frac{1}{2}a_1\frac{\partial^2}{\partial \xi^2} + \frac{1}{2}a_2\xi^2 + \frac{\lambda}{\sqrt{2}}a_3\frac{\partial}{\partial \xi} + \frac{\lambda}{\sqrt{2}}a_4\xi. \tag{10}$$

We refer in this paper the λ-dependent operator H_λ as the *BDS-Hamiltonian* and the Hamiltonian of the *harmonic λ-oscillator* as $HO(\lambda)$.

The variable ξ and the coefficients a_i can be carried out from Table I.

The aim of this paper is to find the explicit form of the density matrix that correspond to the BDS-Hamiltonian. After that, we intend to use this density matrix to calculate some thermal moments, the uncertainty product and the entropic uncertainty relations.

By writing the BDS-Hamiltonian as given in Eq. (10), we can solve this problem by finding the density matrix in both representations in a common manner.

Table I.

a_i	ξ: x	ξ: p
a_1	$\frac{\hbar^2}{m}$	$m\hbar^2\omega^2$
a_2	$m\omega^2$	$\frac{1}{m}$
a_3	$\hbar\omega\sqrt{\frac{\hbar}{m\omega}}$	$i\,\hbar\omega\sqrt{m\,\hbar\omega}$
a_4	$\hbar\omega\sqrt{\frac{m\omega}{\hbar}}$	$i\,\hbar\omega\frac{1}{\sqrt{m\,\hbar\omega}}$
$\lvert q\rvert$	1	1

2. DENSITY MATRIX FOR THE $HO(\lambda)$

Let us consider a quantum system of N identical noninteracting harmonic λ-oscillators, that is, $HO(\lambda)$, each with the BDS-Hamiltonian H_λ, in thermodynamical equilibrium with the reservoir (thermostat) at the temperature $T = (k_B\beta)^{-1}$, where k_B is the Boltzmann constant. This quantum system fullfil the conditions of the quantum canonical distribution. The basic function for the examination of the physical and chemical properties of such systems is the canonical density matrix. In the representation of the variable ξ, the density matrix $\rho_\lambda(\xi, \xi'; \beta)$ is defined as

$$\rho_\lambda(\xi, \xi'; \beta) = \sum_v e^{-\beta E_v}\Psi_{v,\lambda}(\xi)\Psi^*_{v,\lambda}(\xi'), \tag{11}$$

where v is the vibrational quantum number and $\Psi_v(\xi)$ and E_v are the eigenfunctions and the eigenvalues, respectively, of the Hamiltonian H_λ. In the position representation $\{x\}$, these expressions were carried out as (Beckers *et al.*, 1998)

$$\Psi_{v,\lambda}(x) = \left[\frac{\left(\frac{m\omega}{\pi\hbar}\right)^{1/2}}{2^v v! L_v^{(0)}(-\lambda^2)}\right]^{1/2} e^{-\frac{m\omega}{2\hbar}x^2} H_v\left(\sqrt{\frac{m\omega}{\hbar}}x + \frac{\lambda}{\sqrt{2}}\right), \tag{12}$$

$$E_v = \hbar\omega\left(v + \frac{1}{2}\right). \tag{13}$$

In comparison with the ordinary harmonic oscillator (HO), the $HO(\lambda)$ has the same eigenvalues, but the corresponding eigenfunctions are different: It appears as Hermite polynomials with the displaced argument and, more so as generalized Laguerre polynomials in the denominator of the normalization constant. As a consequence, the use of Eq. (12) in the definition (11) for building the density matrix is relatively difficult.

In order to avoid this difficulty, we propose another way to find the density matrix. Namely, it is well known that the canonical density matrix must satisfy the

Bloch equation (Feynman, 1972):

$$-\frac{\partial}{\partial\beta}\rho_\lambda(\xi,\xi';\,\beta) = H_\lambda(\xi)\rho_\lambda(\xi,\xi';\,\beta), \tag{14}$$

with the bounded condition

$$\lim_{\beta\to 0;\,\lambda\to 0}\rho_\lambda(\xi,\xi';\,\beta) = \delta(\xi-\xi'). \tag{15}$$

For the BDS-Hamiltonian H_λ, the Bloch equation is

$$-\frac{\partial}{\partial\beta}\rho_\lambda(\xi,\xi';\,\beta) = \left(-\frac{1}{2}a_1\frac{\partial^2}{\partial\xi^2} + \frac{1}{2}a_2\xi^2 + \frac{\lambda}{\sqrt{2}}a_3\frac{\partial}{\partial\xi} + \frac{\lambda}{\sqrt{2}}a_4\xi\right) \times \rho_\lambda(\xi,\xi';\,\beta). \tag{16}$$

This equation can be simplified by performing the following change of variables:

$$f = \beta\sqrt{a_1a_2}, \tag{17}$$

$$\eta = \sqrt[4]{\frac{a_2}{a_1}}\xi + \frac{\lambda}{\sqrt{2}}|q|. \tag{18}$$

Therfore, Eq. (16) becomes

$$-\frac{\partial}{\partial f}\rho_\lambda(\eta,\eta';\,f) = \left(-\frac{1}{2}\frac{\partial^2}{\partial\eta^2} + \frac{1}{2}\eta^2 + \frac{\lambda}{\sqrt{2}}|q|\frac{\partial}{\partial\eta} - \frac{\lambda^2}{4}|q|^2\right)\rho_\lambda(\eta,\eta';\,f). \tag{19}$$

In Eqs. (18) and (19), we have introduced the notation

$$|q| = \frac{a_3}{\sqrt{a_1a_2}}\sqrt[4]{\frac{a_2}{a_1}} = \frac{a_3}{a_1}\sqrt[4]{\frac{a_1}{a_2}}. \tag{20}$$

Let us try to solve this differential equation with partial derivatives by using Feynman's method for the Bloch equation of the usual HO (Feynman, 1972), that is, by requiring the solution of the following kind:

$$\rho_\lambda(\eta,\eta';\,f) = \exp[-A(f)\eta^2 + B(f)\eta + C(f)]. \tag{21}$$

After straighforward calculations (see the Appendix), the solution is

$$\rho_\lambda(\eta,\eta';\,f) = \frac{1}{\sqrt{\sinh f}}\ \exp\left[-\frac{1}{2}\ \coth f(\eta^2 + C_1) + \frac{1}{\sinh f}C_1\eta + \frac{\lambda}{\sqrt{2}}|q|\eta + C_0\right]. \tag{22}$$

Because the density matrix is a symmetrical function in the pair of variables η and η' and that, at the harmonic limit ($\lambda \to 0$), this density matrix must tend to the corresponding density matrix of the usual HO, the integration constants C_1 and C_0 must be particularized to the following values:

$$C_1 = \eta'; \qquad C_0 = \frac{\lambda}{\sqrt{2}}|q|\eta' + \ln\left(\frac{1}{\sqrt{2\pi}}\sqrt[4]{\frac{a_2}{a_1}}\right). \tag{23}$$

Therefore, the final expression of the $HO(\lambda)$-density matrix, in terms of the variable η, is

$$\rho_\lambda(\eta, \eta'; \beta) = \frac{1}{\sqrt{2\pi}}\sqrt[4]{\frac{a_2}{a_1}}\frac{1}{\sqrt{\sinh\beta\sqrt{a_1 a_2}}}\ \exp\left\{-\frac{1}{2}\frac{1}{\sinh\beta\sqrt{a_1 a_2}}[(\eta^2 + \eta'^2)\right.$$
$$\left.\cosh\beta\sqrt{a_1 a_2} - 2\eta\eta'] + \frac{\lambda}{\sqrt{2}}\frac{a_3}{a_1}\sqrt[4]{\frac{a_1}{a_2}}(\eta + \eta')\right\} \tag{24}$$

The harmonic limit leads to the following expression for the density matrix of the usual harmonic oscillator HO (Feynman, 1972):

$$\begin{aligned}\lim_{HO}\rho_\lambda(\eta, \eta'; \beta) &\equiv \lim_{\lambda\to 0}\rho_\lambda(\eta, \eta'; \beta) = \rho_\lambda(\xi, \xi'; \beta)\\ &= \frac{1}{\sqrt{2\pi}}\sqrt[4]{\frac{a_2}{a_1}}\frac{1}{\sqrt{\sinh\beta\sqrt{a_1 a_2}}}\\ &\quad\times\ \exp\left\{-\frac{1}{2}\frac{1}{\sinh\beta\sqrt{a_1 a_2}}[(\xi^2 + \xi'^2)\cosh\beta\sqrt{a_1 a_2} - 2\xi\xi']\right\}.\end{aligned} \tag{25}$$

Like the density matrix of the usual HO, the density matrix for the $HO(\lambda)$ evidently satisfies the bounded condition (15)

$$\lim_{\beta\to 0;\,\lambda\to 0}\rho_\lambda(\eta, \eta'; \beta) = \lim_{\beta\to 0}\frac{1}{\sqrt{\pi}}\sqrt{\frac{1}{2\beta a_1}}\exp\left[-\frac{1}{2\beta a_1}(\xi - \xi')^2\right] \equiv \delta(\xi - \xi'). \tag{26}$$

Here we have used the "gaussian" representation of the Dirac δ-distribution

$$\delta(\xi - \xi') = \lim_{\gamma\to 0}\frac{1}{\sqrt{\pi}}\frac{1}{\gamma}\ \exp\left[-\frac{1}{\gamma^2}(\xi - \xi')^2\right]. \tag{27}$$

Using Table I, we can easily come back on the density matrix expressions for the position $\{x\}$ and momentum $\{p\}$-representations.

3. QUANTUM-STATISTICAL OR THERMAL AVERAGES

For calculating the quantum-statistical or thermal averages for an operator $A(\xi)$, which characterize the quantum-statistical system, that is, for calculating the average values in the mixed state described by the corresponding density matrix, it is necessary to normalize the density matrix $\rho_\lambda(\xi, \xi'; \beta)$. The trace of the density matrix is the partition function $Z_\lambda(\beta)$:

$$\int_{-\infty}^{+\infty} \rho_\lambda(\xi, \xi; \beta)\, d\xi = Z_\lambda(\beta). \tag{28}$$

The partition function $Z_\lambda(\beta)$ is very important because the quantum-statistical averages of all physical observables of the system are expressed by using this function. In addition, as we will see, the calculation of the entropy reduces to the problem of finding the explicit form of the density matrix.

The integrals in Eq. (28) and in the following Equations are of the "gaussian" kind (Gradshteyn and Ryzhik, 1980):

$$\int_{-\infty}^{+\infty} x^n e^{-bx^2+sx}\, dx = \sqrt{\frac{\pi}{b}} \frac{\partial^n}{\partial s^n} \exp\left(\frac{s^2}{4b}\right). \tag{29}$$

After straighforward calculations, the partition function $Z_\lambda(\beta)$ is given as

$$Z_\lambda(\beta) = Z^{(0)}(\beta)\ \exp\left(\frac{\lambda^2}{2}|q|^2\ \coth \frac{\beta}{2}\sqrt{a_1 a_2}\right), \tag{30}$$

with the harmonic limit:

$$\lim_{\lambda\to 0} Z_\lambda(\beta) = Z^{(0)}(\beta) = \frac{1}{2\ \sinh\frac{\beta}{2}\sqrt{a_1 a_2}}. \tag{31}$$

Therefore, the quantum-statistical average of the operator $A(\xi)$ must be calculated in the following manner:

$$\langle A\rangle = \frac{1}{Z_\lambda(\beta)} \int_{-\infty}^{+\infty} A(\xi')\rho_\lambda(\xi, \xi'; \beta)|_{\xi=\xi'}\, d\xi, \tag{32}$$

where the following successive operations must be performed: (1) The operator A acts on the density function $\rho_\lambda(\xi, \xi'; \beta)$, acting only on the primed variables, that is, ξ'; (2) the prime is deleted; (3) the integration is performed over the variables without the prime.

When the operator A has a multiplicative character, diagonal elements of the density matrix will appear directly in the last formula.

So, the nth order moments of the variable ξ are defined as the quantum-statistical averages of the nth power of the variable ξ:

$$\begin{aligned}\langle \xi^n\rangle &= \frac{1}{Z_\lambda(\beta)} \int_{-\infty}^{+\infty} \xi^n \rho_\lambda(\xi, \xi; \beta)\, d\xi \\ &= \left(\sqrt[4]{\frac{a_1}{a_2}}\right)^{n+1} \sum_{k=0}^{n} (-1)^{n-k} \binom{n}{k} \left(\frac{\lambda}{\sqrt{2}}|q|\right)^{n-k} \quad \langle \eta^k\rangle,\end{aligned} \tag{33}$$

where, for simplicity reasons, we have introduced the k-order moment of the variable η:

$$\begin{aligned}\langle \eta^k \rangle &= \frac{1}{Z_\lambda(\beta)} \int_{-\infty}^{+\infty} \eta^k \rho_\lambda(\eta, \eta; \beta)\, d\eta \\ &= \frac{1}{\sqrt{2\pi}} \sqrt[4]{\frac{a_2}{a_1}} \frac{1}{\sqrt{\sinh \beta \sqrt{a_1 a_2}}} \frac{1}{Z_\lambda(\beta)} \\ &\quad \times \int_{-\infty}^{+\infty} \eta^k \exp\left(-\tanh \frac{\beta}{2} \sqrt{a_1 a_2} \eta^2 + s\eta \right) d\eta. \end{aligned} \tag{34}$$

Here, we have used the notation

$$s = 2 \frac{\lambda}{\sqrt{2}} |q|. \tag{35}$$

After straighforward calculations, we obtain

$$\langle \eta^k \rangle = \sqrt[4]{\frac{a_2}{a_1}} \exp\left(-\frac{\lambda^2}{2} |q|^2 \coth \frac{\beta}{2} \sqrt{a_1 a_2} \right) \frac{\partial^k}{\partial s^k} \exp\left(\frac{s^2}{4} \coth \frac{\beta}{2} \sqrt{a_1 a_2} \right). \tag{36}$$

The most important are the first two moments of the variable η:

$$\langle \eta \rangle = \sqrt[4]{\frac{a_2}{a_1}} \frac{\lambda}{\sqrt{2}} |q| \coth \frac{\beta}{2} \sqrt{a_1 a_2}, \tag{37}$$

$$\langle \eta^2 \rangle = \sqrt[4]{\frac{a_2}{a_1}} \left(\frac{1}{2} \coth \frac{\beta}{2} \sqrt{a_1 a_2} + \frac{\lambda^2}{2} |q|^2 \coth^2 \frac{\beta}{2} \sqrt{a_1 a_2} \right) \tag{38}$$

and, respectively, in the variable ξ:

$$\langle \xi \rangle = \sqrt[4]{\frac{a_1}{a_2}} \frac{\lambda}{\sqrt{2}} |q| \left(\coth \frac{\beta}{2} \sqrt{a_1 a_2} - 1 \right), \tag{39}$$

$$\langle \xi^2 \rangle = \left(\sqrt{\frac{a_1}{a_2}} \right) \left[\frac{1}{2} \coth \frac{\beta}{2} \sqrt{a_1 a_2} + \left(\frac{\lambda}{\sqrt{2}} |q| \right)^2 \left(\coth \frac{\beta}{2} \sqrt{a_1 a_2} - 1 \right)^2 \right]. \tag{40}$$

Because the position and momentum operators are canonical operators, characterized by nonzero commutation relation (8), it is interesting to calculate, besides the nth order moments of variable ξ, the average of the nth order derivatives with respect to this variable also:

$$\begin{aligned}\left\langle \frac{\partial^n}{\partial \xi^n} \right\rangle &= \frac{1}{Z_\lambda(\beta)} \int_{-\infty}^{+\infty} \frac{\partial^n}{\partial \xi'^n} \rho_\lambda(\xi, \xi'; \beta)|_{\xi'=\xi}\, d\xi \\ &= \left(\sqrt[4]{\frac{a_2}{a_1}} \right)^{n-1} \frac{1}{Z_\lambda(\beta)} \int_{-\infty}^{+\infty} \frac{\partial^n}{\partial \eta'^n} \rho_\lambda(\eta, \eta'; \beta)|_{\eta'=\eta}\, d\eta, \end{aligned} \tag{41}$$

where we must respect the succesive operations as previously indicated for Eq. (32).

The averages of the first two derivatives are

$$\left\langle \frac{\partial}{\partial \xi} \right\rangle = 0, \tag{42}$$

$$\left\langle \frac{\partial^2}{\partial \xi^2} \right\rangle = -\frac{1}{2}\sqrt{\frac{a_2}{a_1}}\ \coth\frac{\beta}{2}\sqrt{a_1 a_2}. \tag{43}$$

At this point, it is useful to observe that in the previous averages we dealt with the double average: the quantum-mechanical and the quantum-statistical, which cannot be separated. Consequently, it is easy to extend a series of considerations that refer to the quantum averages to thermal averages (Popov, 1998).

For a pair of noncommuting quantum observables (Hermitian operators in the Hilbert space) A and B, the uncertainty principle is given in the form of Robertson's relation (Robertson, 1930):

$$(\Delta A)^2(\Delta B)^2 \geq \frac{1}{4}\left(\langle C\rangle^2 + 4\sigma_{AB}^2\right), \quad C = -i[A,\ B], \tag{44}$$

where the variance of the observable A is

$$(\Delta A)^2 = \langle A^2\rangle - \langle A\rangle^2 \tag{45}$$

and similarly for the observable B.

The covariance of the observables A and B is defined as

$$\sigma_{AB} = \frac{1}{2}\langle AB + BA\rangle - \langle A\rangle\langle B\rangle. \tag{46}$$

When this covariance vanishes, $\sigma_{AB} = 0$, the Robertson uncertainty relation reduces to the Heisenberg uncertainty relation, that is, to the following uncertainty product:

$$(\Delta A)^2(\Delta B)^2 \geq \frac{1}{4}\langle C\rangle^2. \tag{47}$$

An interesting historical examination of the uncertainty relations problem was made by Majernik and Richterek (1997) (see also the references therein). Even if in the uncertainty relations the averages can be performed for a pure or a mixed state, Majernik and Richterek (1997) in their works preferred the pure states for the averages.

Formerly, we have extended the uncertainty relations to the mixed states, particularly for the thermal states, for the few exactly solvable potentials (Popov, 1999). Let us now apply these results also to the case of the BDS-Hamiltonian.

So, with the help of the above moments, the variance of the variable ξ for the thermal states of the $HO(\lambda)$ is

$$\Delta\xi = \sqrt{\langle \xi^2\rangle - \langle \xi\rangle^2}. \tag{48}$$

Finally, we obtain

$$(\Delta\xi)^2 = \sqrt{\frac{a_1}{a_2}}\frac{1}{2}\ \coth\frac{\beta}{2}\sqrt{a_1a_2}; \quad \Delta\xi = \sqrt{\langle\xi^2\rangle^{(0)}}. \tag{49}$$

It is easy to observe that this thermal variance does not depend on the parameter λ, as the eigenvalues of the $HO(\lambda)$. So, the variance of the $HO(\lambda)$ is just the square root of the 2-order moment of the usual HO.

By particularizing the expression of the thermal variance for the variable ξ, according to Table I, we obtain the corresponding variances for the position x and momentum p-variables:

$$(\Delta x)^2 = \frac{1}{2}\frac{\hbar}{m\omega}\ \coth\frac{\beta}{2}\hbar\omega; \qquad (\Delta p)^2 = \frac{1}{2}m\hbar\omega\ \coth\frac{\beta}{2}\hbar\omega, \tag{50}$$

so that the uncertainty product for the thermal averages is

$$\Delta x\ \Delta p = \frac{\hbar}{2}\ \coth\frac{\beta}{2}\hbar\omega \geq \frac{\hbar}{2}. \tag{51}$$

It is evident that the uncertainty product for the thermal states is greater than the constant $\hbar/2$ and, of course, is dependent on the temperature T (throught the variable β).

Moreover, the variance of the momentum p can be obtained by using the averages (42) and (43):

$$(\Delta p)^2 = \langle p^2\rangle - \langle p\rangle^2 = -\hbar^2\left\langle\frac{\partial^2}{\partial x^2}\right\rangle + i\hbar\left\langle\frac{\partial}{\partial x}\right\rangle = \frac{1}{2}m\hbar\omega\ \coth\frac{\beta}{2}\hbar\omega. \tag{52}$$

This is same as the result obtained for the usual HO by extending the usual uncertainty product to the mixed states (Popov, 1999).

4. ENTROPIC UNCERTAINTY RELATIONS

In the past, there was a considerable interest in evaluating, in a nontraditional manner, the various measures for uncertainty of two noncommuting observables A and B. Because the most natural measure of uncertainty in the result of a measurement is the entropy, the entropic uncertainty relations were formulated, which are an inequality of the form (Majernik and Opatrný, 1996; Yáñez *et al.*, 1994):

$$S^{(A)} + S^{(B)} \geq S_{AB}, \tag{53}$$

where S_{AB} is a positive constant, which represent the lower bound of the left-hand side.

For a certain physical pure state $|v\rangle$ of the system, in the $\{\xi\}$-representation, the physical entropy is defined as (Yáñez *et al.*, 1994)

$$S_v^{(\xi)} = -k_{\mathrm{B}}\int \rho_v(\xi)\ \ln\rho_v(\xi)\, d\xi = -k_{\mathrm{B}}\int |\Psi_v(\xi)|^2\ \ln|\Psi_v(\xi)|^2\, d\xi, \tag{54}$$

which depend, of course, on the quantum number v.

We extend this definition to the mixed states, particularly, to the thermal states of $HO(\lambda)$. For these kind of states, which are described by the density matrix (24), the averages must be calculated by using Eq. (32) and so, the entropy is

$$S_\lambda^{(\xi)}(\beta) = -k_\mathrm{B}\left\langle \ln\rho_\lambda^{(N)}\right\rangle = -k_\mathrm{B}\int_{-\infty}^{+\infty}\left[\ln\rho_\lambda^{(N)}\right]\rho_\lambda^{(N)}(\xi,\xi';\,\beta)|_{\xi'=\xi}\,d\xi. \tag{55}$$

As we see, the entropy is defined as the thermal average of the logarithm of the normalized canonical operator:

$$\rho_\lambda^{(N)} = \frac{1}{Z_\lambda(\beta)}\rho_\lambda = \frac{1}{Z_\lambda(\beta)}\ \exp[-\beta H_\lambda(\xi)], \tag{56}$$

which leads to the expression

$$S_\lambda^{(\xi)}(\beta) = k_\mathrm{B}\ \ln Z_\lambda(\beta) + k_\mathrm{B}\beta\frac{1}{Z_\lambda(\beta)}\int_{-\infty}^{+\infty} H_\lambda(\xi)\rho_\lambda^{(N)}(\xi,\xi';\,\beta)|_{\xi'=\xi}\,d\xi. \tag{57}$$

This integral can be calculated in much simpler way if we use the Bloch equation (14). After straighforward calculations, the left-hand side of this equation leads to:

$$\begin{aligned}
-\frac{\partial}{\partial\beta}\rho_\lambda(\xi,\xi';\,\beta)|_{\xi'=\xi} &= -\sqrt{a_1a_2}\frac{\partial}{\partial f}\rho_\lambda(\eta,\eta';\,f)|_{\eta'=\eta}\\
&= \frac{1}{2}\sqrt{a_1a_2}\left(\coth f + \frac{1}{\cosh^2\frac{f}{2}}\eta^2\right)\rho_\lambda(\eta,\eta;\ f).
\end{aligned} \tag{58}$$

By replacing the integrand of Eq. (57) by the above expression, we obtain

$$S_\lambda^{(\xi)}(\beta) = k_\mathrm{B}\ \ln Z_\lambda(\beta) + k_\mathrm{B}\frac{\beta}{2}\sqrt{a_1a_2}\left(\coth f + \frac{1}{\cosh^2\frac{\beta}{2}\sqrt{a_1a_2}}\sqrt[4]{\frac{a_1}{a_2}}\langle\eta^2\rangle\right). \tag{59}$$

Using the expression (38) of the second moment of variable η and performing some simple trigonometrical transformations, we obtain the final expression for the entropy of the thermal states:

$$\begin{aligned}
S_\lambda^{(\xi)}(\beta) &= k_\mathrm{B}\left(\frac{\beta}{2}\sqrt{a_1a_2}\ \coth\frac{\beta}{2}\sqrt{a_1a_2} - \ln 2\ \sinh\frac{\beta}{2}\sqrt{a_1a_2}\right)\\
&\quad + k_\mathrm{B}\frac{\lambda^2}{2}|q|^2\left(\coth\frac{\beta}{2}\sqrt{a_1a_2} + \frac{\beta}{2}\sqrt{a_1a_2}\frac{1}{\sinh^2\frac{\beta}{2}\sqrt{a_1a_2}}\right).
\end{aligned} \tag{60}$$

At the harmonic limit ($\lambda \to 0$), this entropy leads to the corresponding expression of the harmonic oscillator (Feynman, 1972):

$$\lim_{\lambda\to 0} S_\lambda^{(\xi)}(\beta) = k_\mathrm{B}\left(\frac{\beta}{2}\sqrt{a_1a_2}\ \coth\frac{\beta}{2}\sqrt{a_1a_2} - \ln 2\ \sinh\frac{\beta}{2}\sqrt{a_1a_2}\right) \equiv S^{(0)}(\beta). \tag{61}$$

According to Table I, the parameter q has the same value, that is, $|q|^2 = 1$, for both the representations $\{x\}$ and $\{p\}$. We thus obtain that the entropies of the thermal states are equal for both variables x and p, that is, are independent on the representation

$$S_\lambda^{(x)}(\beta) = S_\lambda^{(p)}(\beta) = k_B\left(\beta\frac{\hbar\omega}{2}\ \coth\beta\frac{\hbar\omega}{2} - \ln 2\ \sinh\beta\frac{\hbar\omega}{2}\right)$$
$$+ k_B\frac{\lambda^2}{2}\left(\coth\beta\frac{\hbar\omega}{2} + \beta\frac{\hbar\omega}{2}\frac{1}{\sinh\beta\frac{\hbar\omega}{2}}\right). \tag{62}$$

So, the searched sum of the entropies of two noncommuting observables, position x and momentum p, for the $HO(\lambda)$ is

$$S_\lambda^{(x)}(\beta) + S_\lambda^{(p)}(\beta) = 2S^{(0)}(\beta) + k_B\lambda^2\left(\coth\beta\frac{\hbar\omega}{2} + \beta\frac{\hbar\omega}{2}\frac{1}{\sinh\beta\frac{\hbar\omega}{2}}\right). \tag{63}$$

Because the parameter λ is positive for a certain temperature T, that is, for a certain β, the lower bound of this sum for the $HO(\lambda)$ is just the double of the entropy of the usual *HO*, so that

$$S_\lambda^{(x)}(\beta) + S_\lambda^{(p)}(\beta) \geq 2S^{(0)}(\beta). \tag{64}$$

As expected, the right-hand side of this expression depends on the temperature T through the variable β.

Moreover, we recall that the absolute lower bound of this expression must be searched for $T \to 0$ (or for $\beta \to \infty$):

$$\lim_{\beta\to\infty} S^{(0)}(\beta) = 0, \tag{65}$$

that is, this result is in accordance with the Nernst theorem (the third law of thermodynamics).

5. CONCLUSIONS

It is well known that the usual or traditional uncertainty relations are available not only for pure states in which the system was prepared, but also for mixed states, that is, for the superposition of pure states. But in most of the papers relating to uncertainty relations the attention is directed to pure states.

On the other hand, in the past years, the most natural measure of the uncertainty in the result of a measurement (or preparation) of a single observable is considered to be the entropy, motivating the so-called entropic uncertainty relations (Beckers and Debergh, 1989; Majernik and Richterek, 1997; Popov, 1999; Yáñez *et al.*, 1994) also formulated only for the pure states.

In the present paper, we have extended both kind of uncertainty relations to the mixed states, particularly to the thermal states. As a quantum-mechanical model, we considered a quantum ideal gas of the harmonic oscillators with the BDS-Hamiltonian, depending on a real parameter λ, in thermodynamical equilibrium with the reservoir at the temperature T, that is, in the conditions of the quantum-canonical distributions. Due to the symmetry in the structure of this Hamiltonian, we have constructed the corresponding density matrix in a common way, in both representations, the position $\{x\}$ and momentum $\{p\}$.

For the mixed states, both the uncertainty product and the entropic uncertainty relation for these two canonical variables have a lower bound, which is dependent on the temperature T. This fact was expected, because, for the pure states, the lower bound was a constant. For the case of the $HO(\lambda)$, the lower bound for the mixed states (for $\lambda = 0$) is just the lower bound, which corresponds to the usual harmonic one-dimensional oscillator. The entropies calculated for two canonical observables x and p are equal, but the absolutely lower bound is, of course, equal to zero in accordance with the Nernst theorem. We can say that the HO(λ) is superior, from the entropy value, confronted by the usual *HO*.

From this point of view, that is, from the point of view of the right-hand side value of entropic uncertainty relations, these relations can be considered as a good criterion for the anharmonic oscillators classification.

6. APPENDIX

In order to solve Eq. (19), we impose that solution (21) must satisfy this equation and we check the expressions of the functions $A(f)$, $B(f)$, and $C(f)$. We obtain the following equation:

$$A'\eta^2 - B'\eta - C' = A - 2A^2\eta^2 + 2AB\eta - \frac{1}{2}B^2 + \frac{1}{2}\eta^2 + \frac{\lambda}{\sqrt{2}}|q|B - \frac{\lambda}{\sqrt{2}}2|q|A\eta - \frac{\lambda^2}{4}|q|^2, \tag{66}$$

where primes indicate derivatives of the corresponding functions with respect to the variable f.

By identifiyng the coefficients of the powers of the variable η, we obtain three new equations:

$$A' = \frac{1}{2} - 2A^2, \tag{67}$$

$$B' = \frac{\lambda}{\sqrt{2}}2|q|A - 2AB, \tag{68}$$

$$C' = \frac{1}{2}B^2 - \frac{\lambda}{\sqrt{2}}|q|B - A + \frac{\lambda^2}{4}|q|^2. \tag{69}$$

By integrating the first equation (67) and putting $f_0 = 0$, we obtain

$$A = \frac{1}{2}\coth f. \tag{70}$$

The second equation (68) can be written as follows:

$$\frac{dB}{df} + \coth f\, B = \frac{\lambda}{\sqrt{2}}|q| \coth f, \tag{71}$$

and its solution can be determined (see, e.g., Piskounov, 1972) by using the following notations:

$$P(f) = \coth f; \qquad \mu(f) = \exp\int P(f)\,df; \qquad Q(f) = \frac{\lambda}{\sqrt{2}}|q| \coth f, \tag{72}$$

$$B(f) = \frac{1}{\mu(f)}\left[\int Q(f)\mu(f)\,df + C_1\right]. \tag{73}$$

So, the function $B(f)$ becomes

$$B(f) = \frac{\lambda}{\sqrt{2}}|q| + C_1\frac{1}{\sinh f}. \tag{74}$$

By subsituting the expressions for $A(f)$ and $B(f)$ in the third equation (69), we obtain an ordinary differential equation for the function $C(f)$:

$$C(f) = C_0 - \frac{1}{2}C_1^2 \coth f - \frac{1}{2}\ln \sinh f. \tag{75}$$

Finally, the expression for the density matrix is

$$\rho = \frac{1}{\sqrt{\sinh f}} \exp\left[C_0 - \frac{1}{2}\coth f\left(\eta^2 + C_1^2\right) + \frac{1}{\sinh f}C_1\eta + \frac{\lambda}{\sqrt{2}}|q|\eta\right]. \tag{76}$$

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