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2000 J. Phys. A: Math. Gen. 33 921

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## Properties of nonclassical maximum-entropy states

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Received 4 October 1999, in final form 18 November 1999

**Abstract.** The density matrix in the position and momentum representation, the position–momentum uncertainty product, the Wigner and  $Q$  functions, and thermal properties of the family of the nonclassical maximum-entropy states of a single harmonic oscillator are determined. Any such state, having the mean number of quanta  $\bar{n}$ , has the uncertainty product  $\delta x \cdot \delta p = (2\bar{n} + 1)^{1/2}$ , and this product attains its minimum value for the temperature parameter  $\xi \rightarrow 0$ . Generically, the Wigner function has alternating sign so that the underlying maximum-entropy state is truly nonclassical. The von Neumann entropy and the heat capacity, expressed via the temperature parameter  $\xi$ , coincide with the corresponding quantities for the thermal state. The properties discussed here are of interest for the description and analysis of the vibrational motion of a trapped ion in a harmonic-oscillator potential since the equilibrium states which result under certain conditions are the maximum-entropy states.

### 1. Introduction

In this paper we examine certain properties of the family of the nonclassical maximum-entropy states of a simple harmonic oscillator, of frequency  $\omega$ , recently introduced in [1]. These *mixed* states arise when only number states,  $|n\rangle$ , differing by a multiple of a certain integer  $k$  ( $k \geq 1$ ) are allowed to be occupied, beginning with the lowest number state  $|q\rangle$  labelled by the integer parameter  $q$  ( $0 \leq q \leq k - 1$ ). A specific maximum-entropy state, distinguished by the ordered pair of integers  $(k, q)$ , has then the (steady-state) density operator

$$\hat{\rho}^{(k,q)} = \sum_{m=0}^{+\infty} p_{mk+q} |mk+q\rangle \langle mk+q|. \quad (1)$$

In equilibrium state the von Neumann entropy  $S^{(k,q)} = -\text{tr}[\hat{\rho}^{(k,q)} \ln \hat{\rho}^{(k,q)}]$  takes its maximum value. Under the constraints  $\text{tr}[\hat{\rho}^{(k,q)}] = 1$  and  $\text{tr}[\hat{n}\hat{\rho}^{(k,q)}] = \bar{n}$ , with  $\hat{n} \equiv \hat{a}^\dagger \hat{a}$  denoting the number operator and  $\bar{n}$  the mean number of quanta, one finds the number probability distribution of the maximum-entropy states [1]

$$p_{mk+q} = (1 - \xi)\xi^m. \quad (2)$$

Here  $\xi$  denotes the real parameter

$$\xi \equiv \frac{\bar{n} - q}{\bar{n} - q + k} \quad (3)$$

so that  $0 < \xi < 1$ . The special case  $(k, q) = (1, 0)$  corresponds to the familiar *thermal* state [2]. The relevance of the maximum-entropy states to the field of quantum optics, and also for the description of the vibrational centre-of-mass motion of a trapped ion in a harmonic-oscillator potential, was discussed in [1]. These states can be obtained as the stationary solutions of

a master equation which takes into account  $k$ -quantum absorption and  $k$ -quantum emission processes only. For the vibrational motion of a trapped ion, the states could be produced with the help of the recently proposed method of laser-assisted quantum reservoir engineering [3]. In section 2, we determine the closed-form expressions for the density matrix in the position and momentum representation,  $\langle x|\hat{\rho}^{(k,q)}|x'\rangle$  and  $\langle p|\hat{\rho}^{(k,q)}|p'\rangle$  respectively, generally for a  $(k, q)$  maximum-entropy state, and further establish with their help that the corresponding position–momentum uncertainty product has the value  $\delta x \cdot \delta p = (2\bar{n} + 1)\frac{\hbar}{2}$  for any  $(k, q)$ . In section 3 we obtain the Wigner function,  $W^{(k,q)}(x, p)$ , for the maximum-entropy states and find that in almost all cases it can be negative, so that the underlying maximum-entropy state is truly nonclassical. Additionally, we determine the  $Q$  function and with its help discuss briefly the phase properties of the maximum-entropy states. Finally, in order to clarify the physical significance of the parameter  $\xi$ , equation (3), we examine in some detail the thermal properties of these states. By using the appropriate expressions for the entropy and the mean energy,  $\overline{E^{(k,q)}}$ , we introduce the absolute temperature  $T$  and find that the parameter  $\xi$  is a monotonic increasing function of the temperature. We note that the  $(k, q)$  maximum-entropy state of the quantum oscillator may be regarded as being in thermal equilibrium with a reservoir, at absolute temperature  $T$ , with which it can exchange energy in lumps of  $k$ -quanta only, and establish that the entropy and heat capacity are certain universal functions of the temperature parameter  $\xi$ .

## 2. Density matrix and position–momentum uncertainty product

First, we determine the density matrix in the position representation for the  $(k, q)$  maximum-entropy state. From equations (1) and (2) one has

$$\langle x|\hat{\rho}^{(k,q)}|x'\rangle = (1 - \xi) \sum_{m=0}^{+\infty} \xi^m u_{mk+q}(x) u_{mk+q}^*(x') \quad (4)$$

with  $u_n(x) \equiv \langle x|n\rangle$  denoting the familiar harmonic oscillator eigenfunctions [4]. With the help of (i) the integral representation of Hermite polynomial [5], (ii) the sum ( $q < k, y$  real)

$$\sum_{m=0}^{+\infty} \frac{y^{mk+q}}{(mk+q)!} = \frac{1}{k} \sum_{j=0}^{k-1} \frac{e^{y\theta_j}}{\theta_j^q} \quad (5)$$

where  $\theta_j \equiv \exp(2ij\pi/k)$ , and (iii) the integral quoted in [5], we obtain

$$\begin{aligned} \langle x|\hat{\rho}^{(k,q)}|x'\rangle &= \frac{1 - \xi}{\sqrt{2\pi\sigma k\xi^{q/k}}} \exp\left(\frac{x^2 + x'^2}{4\sigma^2}\right) \sum_{j=0}^{k-1} \theta_j^{-q} \tau_{jk}^{-1/2} \\ &\times \exp\left(-\frac{x^2 + x'^2 - 2\xi^{1/k}\theta_j x x'}{2\sigma^2 \tau_{jk}}\right) \end{aligned} \quad (6)$$

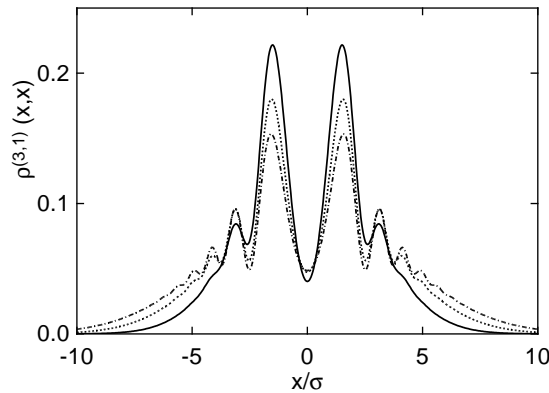
where

$$\tau_{jk} \equiv 1 - \xi^{2/k} \theta_j^2 \quad (7)$$

and

$$\sigma^2 \equiv \hbar/(2\omega M) \quad (8)$$

with  $M$  denoting the oscillator mass. Since the harmonic oscillator functions  $u_n(x)$  are real, it is clear from (4) that the density matrix in the position representation is real not only for  $x = x'$  but also for any  $x \neq x'$ . Nonzero off-diagonal matrix elements of  $\hat{\rho}^{(k,q)}$  are related to the quantum coherences [6], while the diagonal matrix elements are the probabilities of finding



**Figure 1.** Position probability density,  $\langle x | \hat{\rho}^{(3,1)} | x \rangle$ , for the  $(k, q) = (3, 1)$  maximum-entropy state with the mean number of quanta  $\bar{n} = 3$  (full curve),  $\bar{n} = 5$  (broken curve) and  $\bar{n} = 7$  (chain curve).

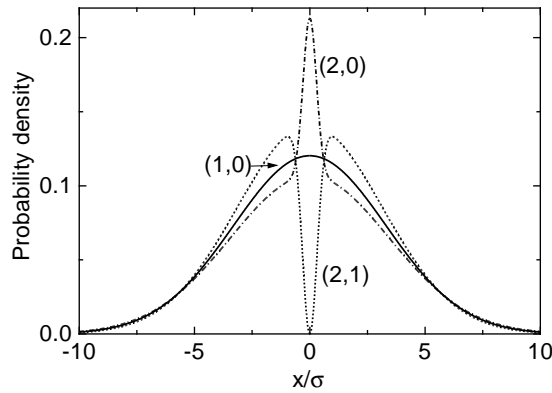
the oscillator at the coordinate  $x = x'$ ; see figure 1. Recalling the form of the momentum space eigenfunctions,  $v_n(p) \equiv \langle p | n \rangle$ , of the harmonic oscillator [4], one obtains the density matrix in the momentum representation,  $\langle p | \hat{\rho}^{(k,q)} | p' \rangle$ , from  $\langle x | \hat{\rho}^{(k,q)} | x' \rangle$  simply by replacing  $x \rightarrow p$ ,  $x' \rightarrow p'$  and  $\sigma \rightarrow \sigma' \equiv (\hbar\omega M/2)^{1/2}$ .

Second, having obtained the density matrix in the position and momentum representation for the maximum-entropy states, one is able to determine the corresponding position–momentum uncertainty product. Since the diagonal matrix element,  $\langle x | \hat{\rho}^{(k,q)} | x \rangle$ , is an *even* function of  $x$ , the expectation value  $\overline{\hat{x}^n} = \text{tr}[\hat{x}^n \hat{\rho}^{(k,q)}]$  vanishes for any odd  $n$ . Therefore the dispersion of position for the  $(k, q)$  maximum-entropy state is  $(\delta x)^2 = \overline{\hat{x}^2} = (2\bar{n} + 1)\sigma^2$ , where the last equality is obtained with the help of the special case  $x = x'$  of equation (6). It is seen that  $(\delta x)^2$  is, for a given  $\bar{n}$ , independent of  $(k, q)$ . This is illustrated in figure 2 where the position probability densities, for  $\bar{n} = 5$ , and for the first few  $(k, q)$  values are plotted; these probability densities all have the same dispersion  $(\delta x/\sigma)^2 = 11$ . The dispersion of momentum is  $(\delta p)^2 = (2\bar{n} + 1)\sigma'^2$ , so that the position–momentum uncertainty product for the  $(k, q)$  maximum-entropy state is  $\delta x \cdot \delta p = (2\bar{n} + 1)\frac{\hbar}{2}$ . Thus, the uncertainty product is independent of  $k$  and  $q$ , and increases linearly with the mean number of quanta  $\bar{n}$ . In particular, any  $(k, q)$  maximum-entropy state, with an *integer* mean number of quanta  $\bar{n} = n$ , has the same uncertainty product as the corresponding number state  $|n\rangle$ . Since  $\bar{n} = q + k\xi/(1 - \xi) > q$ , one obtains the *minimum* uncertainty product,  $(\delta x \cdot \delta p)_{\min} = (2q + 1)\frac{\hbar}{2}$ , for  $\xi \rightarrow 0$ . In this limiting case the probability of finding the oscillator in the ground state,  $|q\rangle$ , becomes  $p_q = 1$  while at the same time  $p_{mk+q} = 0$  for  $m = 1, 2, 3, \dots$ . Hence, the mixed state  $\hat{\rho}^{(k,q)}$ , equation (1), degenerates into the pure state  $|q\rangle$  with the density operator  $\hat{\rho}^{(k,q)} \rightarrow |q\rangle\langle q|$ . Later we shall see that the limit  $\xi \rightarrow 0$  corresponds to the zero absolute temperature,  $T \rightarrow 0$ .

### 3. Wigner function and Q function

With the help of the density matrix in the position representation one can obtain the Wigner function for the maximum-entropy states [7],

$$W^{(k,q)}(x, p) \equiv \frac{1}{2\pi\hbar} \int_{-\infty}^{+\infty} dy \exp\left(\frac{i}{\hbar}py\right) \left\langle x - \frac{y}{2} \left| \hat{\rho}^{(k,q)} \right| x + \frac{y}{2} \right\rangle.$$



**Figure 2.** Position probability densities,  $\langle x | \hat{\rho}^{(k,q)} | x \rangle$ , for the  $(k, q) = (1, 0)$ ,  $(2, 0)$  and  $(2, 1)$  maximum-entropy states, all with the same mean number of quanta  $\bar{n} = 5$ , and the same dispersion  $(\delta x/\sigma)^2 = 11$ . The two peaks in the  $(2, 1)$  probability distribution correspond to the two possible localizations of the trapped ion in that state.

Using equation (6), and the tabulated integral cited in [5], one finds

$$W^{(k,q)}(x, p) = \frac{1 - \xi}{\pi \hbar k \xi^{q/k}} \operatorname{Re} \left\{ \sum_{j=0}^{k-1} \frac{\theta_j^{-q}}{1 + \xi^{1/k} \theta_j} \exp \left[ -2|\alpha|^2 \frac{1 - \xi^{1/k} \theta_j}{1 + \xi^{1/k} \theta_j} \right] \right\} \quad (9)$$

where

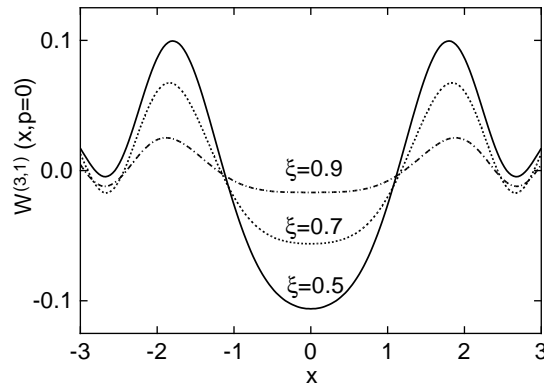
$$\alpha \equiv \frac{1}{2} \left( \frac{x}{\sigma} + i \frac{p}{\sigma'} \right) \quad (10)$$

denotes the complex displacement parameter. The Wigner function,  $W^{(k,q)}(x, p)$ , is real and exhibits in all but first two cases,  $(k, q) = (1, 0)$  and  $(2, 0)$ , alternating sign (see figure 3). Hence, the Wigner function cannot be regarded as a classical probability distribution in the phase space. As long as the negative values are present the underlying maximum-entropy state is truly nonclassical. Numerical calculations reveal that, for a given  $(k, q)$  and with increasing  $\xi$  (this then amounts to the increasing  $\bar{n}$ ; see equation (3)), the negative and positive ripples of the Wigner function reduce in amplitude, diffuse into each other and to a certain extent cancel out. Thus one observes gradual transition from quantum to classical behaviour of the  $(k, q)$  maximum-entropy state with increasing absolute temperature.

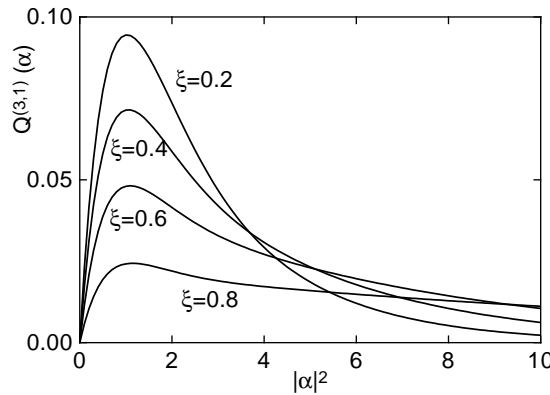
With the help of equation (5) one also obtains the general expression for the  $Q$  function,  $Q^{(k,q)}(\alpha) \equiv \langle \alpha | \hat{\rho}^{(k,q)} | \alpha \rangle / \pi$ , for the maximum-entropy states. Here  $|\alpha\rangle \equiv e^{-|\alpha|^2/2} \sum_{n=0}^{+\infty} (\alpha^n / \sqrt{n!}) |n\rangle$  denotes the familiar *coherent* state. One finds

$$Q^{(k,q)}(\alpha) = \frac{(1 - \xi) \exp(-|\alpha|^2)}{\pi k \xi^{q/k}} \operatorname{Re} \left\{ \sum_{j=0}^{k-1} \frac{\exp(\xi^{1/k} \theta_j |\alpha|^2)}{\theta_j^q} \right\}. \quad (11)$$

It is seen that the  $Q^{(k,q)}$  function depends, for any  $k$  and  $q$ , only on the square of the absolute value,  $|\alpha|^2$ , of the complex displacement parameter  $\alpha$ ; see figure 4. This is consistent with expression (9) since one can also make the usual transition from the  $Q$  function to the Wigner function via convolution. Since a measure of the phase uncertainty,  $\delta\phi$ , can be obtained from the half-width of the  $Q$  distribution in the azimuthal direction in the complex  $\alpha$  plane [8], it is apparent that the phase width for a maximum-entropy state has the largest possible value,  $\delta\phi = \pi$  (as is to be expected for a state that is an incoherent mixture of number states; the Pegg–Barnett Hermitian phase operator theory [9] leads to the same conclusion). Thus,



**Figure 3.** The Wigner function,  $W^{(k,q)}(x, p)$ , for the  $(k, q) = (3, 1)$  maximum-entropy state, with momentum  $p = 0$ , for three different values of the temperature parameter  $\xi$ .



**Figure 4.** The  $Q$  function for the  $(k, q) = (3, 1)$  maximum-entropy state versus  $|\alpha|^2 \in [0, 10]$ , for four different values of the temperature parameter  $\xi$ .

in spite of the fact that, for example, the  $(k, q) = (2, 0)$  state has the number probability distribution remarkably similar to that of the squeezed vacuum state with the same mean number of quanta [1], the corresponding phase distributions are completely dissimilar and they can be used to discriminate between the two states. We note that the phase uncertainty  $\delta\phi = \pi$ , together with the corresponding uncertainty of the number of quanta,  $\delta n$ , already determined in [1], leads to the number–phase uncertainty product for the  $(k, q)$ -maximum-entropy state,  $\delta n \cdot \delta\phi = \pi k \sqrt{\xi} / (1 - \xi)$ .

Finally, in order to clarify the physical significance of the parameter  $\xi$ , equation (3), we examine the thermal properties of the maximum-entropy states. From equations (1) and (2) one obtains

$$S^{(k,q)} = - \sum_{m=0}^{+\infty} p_{mk+q} \ln p_{mk+q} = - \ln(1 - \xi) - \frac{\xi \ln \xi}{1 - \xi}. \quad (12)$$

This, together with the mean energy,  $\overline{E^{(k,q)}} / \hbar\omega = \bar{n} + \frac{1}{2} = \frac{1}{2} + q + k\xi / (1 - \xi)$ , leads to the corresponding absolute temperature

$$\frac{1}{k_B T} = \frac{\partial S^{(k,q)}}{\partial \overline{E^{(k,q)}}} = - \frac{\ln \xi}{k \hbar \omega} \quad (13)$$

with  $k_B$  denoting the Boltzmann constant. It is seen that the parameter  $\xi$  is a monotonic increasing function of  $T$  so that, in particular,  $\xi \rightarrow 0$  corresponds to  $T \rightarrow 0$ , and  $\xi \rightarrow +1$  to  $T \rightarrow +\infty$ . Any  $(k, q)$  maximum-entropy state of the quantum oscillator, analogously to the  $(k, q) = (1, 0)$  special case of the thermal state, may be regarded as being in thermal equilibrium with a reservoir, at absolute temperature  $T$ , with which it can exchange energy in lumps of  $k$ -quanta only. Further, one determines the Helmholtz free energy, the heat capacity and the partition function:

$$\frac{F^{(k,q)}}{\hbar\omega} = \frac{\overline{E^{(k,q)}} - k_B T S^{(k,q)}}{\hbar\omega} = \frac{1}{2} + q - \frac{k \ln(1 - \xi)}{\ln \xi} \quad (14)$$

$$\frac{C^{(k,q)}}{k_B} = \frac{1}{k_B} \frac{\partial \overline{E^{(k,q)}}}{\partial T} = \xi \left( \frac{\ln \xi}{1 - \xi} \right)^2 \quad (15)$$

and

$$Z^{(k,q)} = e^{-F^{(k,q)}/k_B T} = \frac{\xi^{\frac{1}{k}(q+\frac{1}{2})}}{1 - \xi}. \quad (16)$$

It is apparent that the probabilities  $p_{mk+q}$ , the entropy  $S^{(k,q)}$ , and the heat capacity  $C^{(k,q)}$  are all universal functions of the temperature parameter  $\xi$ ; they are the same for any  $(k, q)$  and are in fact the same as for the familiar thermal state. By inverting equation (13) one can eliminate the temperature parameter,  $\xi = \exp(-k\hbar\omega/k_B T)$ , and use in all quantities the absolute temperature  $T$  instead. In particular, it is seen that the probability  $p_{mk+q}$ , of finding the oscillator in the number state  $|mk + q\rangle$ , attains its maximum value

$$(p_{mk+q})_{\max} = \frac{1}{m+1} \left( \frac{m}{m+1} \right)^m \quad (17)$$

at the temperature

$$T_{\max} = \frac{k\hbar\omega}{k_B \ln\left(\frac{m+1}{m}\right)}. \quad (18)$$

#### 4. Summary

In summary, we have examined certain properties of the nonclassical maximum-entropy states of a single harmonic oscillator. Specifically we have determined the corresponding density matrix in the position and momentum representation, the position–momentum uncertainty product, the Wigner and  $Q$  functions, and we have also investigated the thermal properties of these states. These results are of interest for the description and analysis of the vibrational centre-of-mass motion of a trapped ion in a harmonic oscillator potential, since the equilibrium states which result under certain conditions (discussed in [1]) are the maximum-entropy states described by the density operator, equation (1).

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