# Properties of nonclassical maximum-entropy states

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# Properties of nonclassical maximum-entropy states

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**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 $\delta x \cdot \delta p = (2\bar{n}+1)\frac{\hbar}{2}$, and this product attains its minimum value for the temperature parameter $\xi \to 0$. 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 $k$ ($k \geqslant 1$) are allowed to be occupied, beginning with the lowest number state $|q\rangle$ labelled by the integer parameter $q$ ($0 \leqslant q \leqslant k-1$). A specific maximum-entropy state, distinguished by the ordered pair of integers $(k, q)$, has then the (steady-state) density operator

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

In equilibrium state the von Neumann entropy $S^{(k,q)} = -\operatorname{tr}[\hat{\rho}^{(k,q)} \ln \hat{\rho}^{(k,q)}]$ takes its maximum value. Under the constraints $\operatorname{tr}[\hat{\rho}^{(k,q)}] = 1$ and $\operatorname{tr}[\hat{n}\hat{\rho}^{(k,q)}] = \bar{n}$, 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]

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

Here $\xi$ denotes the real parameter

$$\xi \equiv \frac{\bar{n} - q}{\bar{n} - q + k} \tag{3}$$

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

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

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)

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

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

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

$$\times \exp\left(-\frac{x^2+x'^2-2\xi^{1/k}\theta_j x x'}{2\sigma^2\tau_{jk}}\right) \tag{6}$$

where

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

and

$$\sigma^2 \equiv \hbar/(2\omega M) \tag{8}$$

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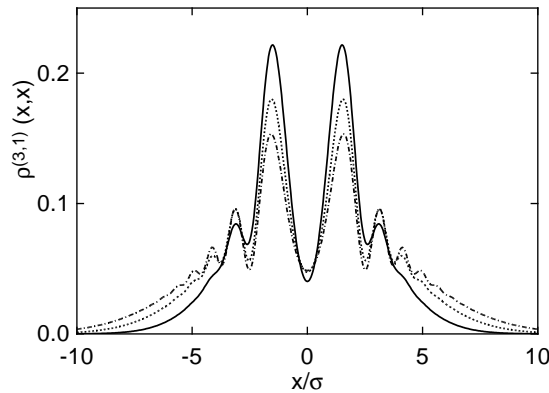
**Figure 1.** Position probability density, $\langle x|\hat{\rho}^{(3,1)}|x\rangle$, for the $(k, q) = (3, 1)$ maximum-entropy state with the mean number of quanta $\bar{n} = 3$ (full curve), $\bar{n} = 5$ (broken curve) and $\bar{n} = 7$ (chain curve).

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 $x \to p$, $x' \to p'$ and $\sigma \to \sigma' \equiv (\hbar\omega M/2)^{1/2}$.

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 $\widehat{x^n} = \text{tr}[\hat{x}^n \hat{\rho}^{(k,q)}]$ vanishes for any odd $n$. Therefore the dispersion of position for the $(k, q)$ maximum-entropy state is $(\delta x)^2 = \widehat{x^2} = (2\bar{n} + 1)\sigma^2$, 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 $\xi \to 0$. 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 $m = 1, 2, 3, \ldots$. Hence, the mixed state $\hat{\rho}^{(k,q)}$, equation (1), degenerates into the pure state $|q\rangle$ with the density operator $\hat{\rho}^{(k,q)} \to |q\rangle\langle q|$. Later we shall see that the limit $\xi \to 0$ corresponds to the zero absolute temperature, $T \to 0$.

## 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],

$$W^{(k,q)}(x, p) \equiv \frac{1}{2\pi\hbar} \int_{-\infty}^{+\infty} \mathrm{d}y \exp\left(\frac{\mathrm{i}}{\hbar} py\right) \left\langle x - \frac{y}{2}\right| \hat{\rho}^{(k,q)} \left|x + \frac{y}{2}\right\rangle.$$
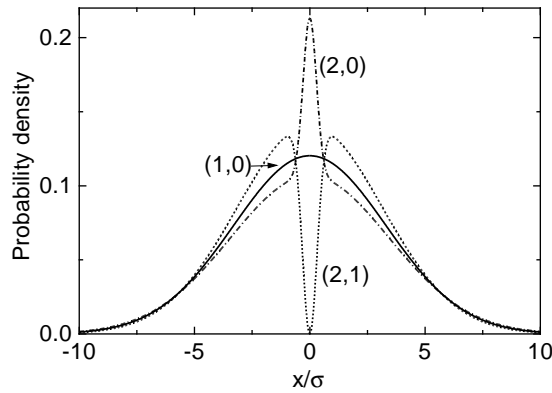
**Figure 2.** Position probability densities, $\langle x|\hat{\rho}^{(k,q)}|x\rangle$, for the $(k, q) = (1, 0)$, $(2, 0)$ and $(2, 1)$ maximum-entropy states, all with the same mean number of quanta $\bar{n} = 5$, and the same dispersion $(\delta x/\sigma)^2 = 11$. The two peaks in the $(2, 1)$ probability 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

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

where

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

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

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

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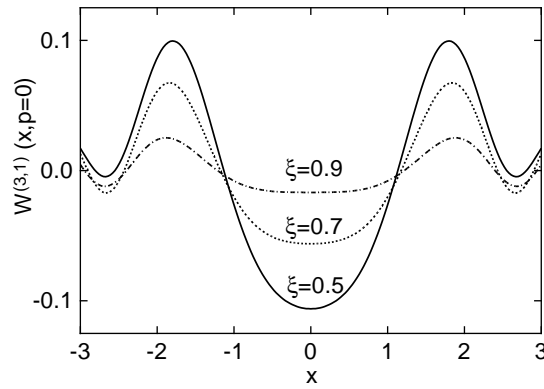
**Figure 3.** The Wigner function, $W^{(k,q)}(x, p)$, for the $(k, q) = (3, 1)$ maximum-entropy state, with momentum $p = 0$, for three different values of the temperature parameter $\xi$.
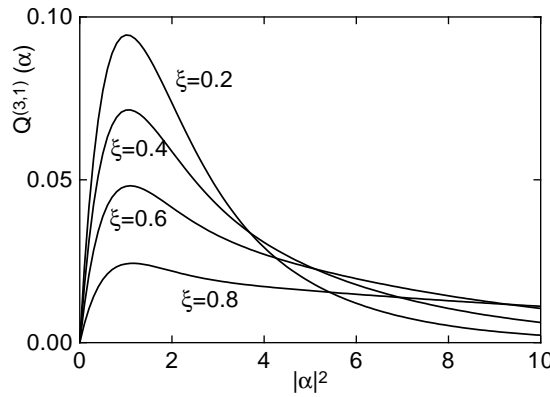


**Figure 4.** The $Q$ function for the $(k, q) = (3, 1)$ maximum-entropy state versus $|\alpha|^2 \in [0, 10]$, for four different values of the temperature parameter $\xi$.

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

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

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

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

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, $\xi \to 0$ corresponds to $T \to 0$, and $\xi \to +1$ to $T \to +\infty$. 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:

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

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

and

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

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

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

at the temperature

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

## 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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