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ABOUT COLLECTIVITY AND ENTROPY MEASURES FOR COHERENT AND CLOSELY RELATED STATES

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A simple scheme is proposed for computing phase space entropy measures for quantum systems treated within the Wigner function formalism. The approach is applied to eigenstates and coherent states of harmonic oscillator, and to the quantum optical "Schroedinger cat" states. Along with the phase space representation, the Fock space (energetic) representation is invoked for the same problems. The essentially different behaviour of quantum entropies in the two mentioned representations is analysed.

Introduction

Coherent states were in fact introduced for quantum oscillator by Schroedinger who could build up the most localized states without spatial spreading over time [1]. The coherent states (CSs) now play a prominent role in quantum theory, in particular in field theory, optics, quantum information processing etc. [2-9]. There are some applications of CSs in molecular electronic structure theory and chemical dynamics [10-12].

From a formal viewpoint, the CSs are collective states of the quantum oscillator and related systems. This invokes the idea to treat collective properties of CSs by the same technique (collectivity numbers and the corresponding logarithmic indices) that we used previously in Refs. [13-18] for molecular excited and correlated states. Many works appeared recently in this field, and we mention some papers [19-26] that are most related to our study here. Along with this, certain ambiguous issues and difficulties (e.g., compare Refs. [21] and [22]) are additionally compelling about studying the problem more carefully.

Thus, the purpose of this paper is to examine CSs states (exhibiting classical-like behaviour) and nonclassical ones (being coherent superposition of CSs) by applying to them the above mentioned collectivity and entropy measures. In calculations we make use of discrete (countable) probability distributions (in the Fock space representation) as well as continuous distribution functions (in the Wigner picture of quantum mechanics). In so doing, we present a modified approach to evaluating quantum entropies in the phase space representation. The approach is illustrated by analytical and numerical studies of the measures in question.

1. Main Definitions

The previous experience with the electronic states [15-18] tell us that it is convenient to frame a wave function analysis in the "entropy language". Thus we must describe appropriate notions in a more wide context.

1 a. Case of discrete distributions

We first recall the definition of the collectivity index from Ref [13,14]. Let $\{\mu_j\}_{1\le j\le \dim}$ be a normalized set of probabilities or occupation numbers arising in physical and quantum-chemical applications. The collectivity number κ is introduced as

$$\kappa = (\sum_{j=1}^{\dim} \mu_j^2)^{-1} \tag{1}$$

We treat this quantity as an average rank of a wave function for which a set $\{\sqrt{\mu_j}\}_{1\le j\le \dim}$ serves as amplitude probabilities (phases are ignored). Notice that in the contemporary statistics such quantity is frequently termed as the so-called participation ratio. It is also used as a localization measure in solid state physics [27]. For the molecular electronic structure theory the corresponding logarithmic measures are considered in Refs. [15,28].

We write down the appropriate entropy measure as follows:

$$R = \log\kappa = -\log[\sum_{j=1}^{\dim} \mu_j^2], \tag{2}$$

here and elsewhere $\log$ is taken base 2, that is $\log \equiv (1/\ln 2)\ln$. The above expression (2) actually corresponds to another known quantity called the Renyi entropy (e.g., see detailed studies in Refs. [23-25]). More applied is to use the conventional Shannon entropy as the basic information measure:

$$S = -\sum_{j=1}^{\dim} \mu_j \log \mu_j \tag{3}$$

For current applications to molecular problems see papers [17,18] and references therein. In the case of countable probability distributions, the above expressions are supposed to be convergent series.

1 b. Case of continuous distributions

First of all, specify the type of continuous distribution we use in this work. For the purposes of our study the Wigner function (WF) is most relevant as it provides an opportunity to investigate quantum-mechanical problems in phase space [4, 29-34]. In the case of one-degree-of-freedom systems, the WF, $W(p,q)$, is identified with a special Fourier transformation of the corresponding density matrix $\rho(q,q')$ where variables p and q are interpreted as classical momentum and coordinates. For a pure state determined by a normalized wave function $|\psi\rangle$, we have

$$W(p,q) = \frac{1}{2\pi}\int_{-\infty}^{\infty} e^{ipx}\psi(q-x/2)\psi^*(q+x/2)dx \tag{4}$$

where atomic unities are implied. The $W(p,q)$, such defined, is automatically normalised to 1. In the Wigner formalism, the usual operator normalization of the density matrix ($\|\rho\|^2 = 1$ for pure states) is equivalent to the identity

$$2\pi\int_{-\infty}^{\infty}\int_{-\infty}^{\infty} W(p,q)^2 dpdq = 1\,. \tag{5}$$

The last relation plays a key role in our analysis of the quantum phase space entropies. Really, the WF itself can not directly treated as the usual probability distribution in lieu of the negative values allowing for WFs (it is proved that the WF of Gaussian wave functions is positive definite only). Owing to this cause, $W(p,q)$ is usually named as a quasi-probability thereby emphasizing a nonclassicality of quantum states in any correct description. However, this peculiarity precludes the use of the WFs as probabilities for evaluating statistical averages such as Shannon's entropy where a positive semi-definiteness of the distribution functions is mandatory. It is compelled to use some smoothed distributions ensuring a positiveness (the Husimi functions [30], first of all).

In this paper we propose a more simple and more direct approach to remove the WF negativeness. By using the integrand in Eq. (5) it is possible to define an admissible distribution which is straightforwardly produced by WF. Namely, we introduce the function

$$W_{sq}(p,q) = 2\pi\, W(p,q)^2 \tag{6}$$

which is naturally normalized to 1 due to Eq. (5). There are additional reasons motivating to involve in this analysis the squared WF (6). They are connected with the relation between the squared density matrix $\rho(q,q')$ and exchange density. This relation was given by Ruedenberg in Ref. [35] for many-electron systems, but here we do not discuss this issue further (for more details about $[\rho(q,q')]^2$ see Ref. [36] and references therein).

Now we can readily compute the phase space entropy measures by using the squared WF (3). The corresponding Renyi and Shannon entropies are respectively given by

$$R_W = -\log\left(\iint [W_{sq}(p,q)]^2 dpdq\right) \tag{7}$$

and

$$S_W = -\iint W_{sq}(p,q)\log[W_{sq}(p,q)]dpdq \tag{8}$$

It is not difficult to prove the inequality [24]

$$0 \le R_W \le S_W\,. \tag{9}$$

In practice it means that these two quantities are rather similar by properties but the Renyi index is evidently more simple for an analytical study. It is rather obvious how to generalize Eqs. (4)-(8) to the case of multidimensional systems.

2. Entropy Measures for Coherent and "Schroedinger cat" States

2 a. Using Fock space representation

We restrict ourselves by studying the harmonic oscillator as a typical system in the coherent state (CS) theory (recall also a mathematical equivalence of radiation field to the common quantum oscillator). When applying atomic units we shall now also take the oscillator frequency $\omega = 1$. Then by definition the oscillator coherent state $|\alpha\rangle$ is an eigenstate of annihilation operator $\hat{a} = (q + ip)/\sqrt{2}$ with eigenvalue α, the latter being any number (generally complex). For obtaining Fock's representation the infinite set of the oscillator eigenstates $\{|n\rangle\}$ is used. For CS $|\alpha\rangle$ it leads to the expansion

$$|\alpha\rangle = e^{-|\alpha|^2/2} \sum_{n=0}^{\infty} \frac{\alpha^n}{\sqrt{n!}} |n\rangle . \quad (10)$$

We shall further call the eigenstates "pure states" (this is a somewhat different usage of the term "pure" than in density matrix theory)

The coherent states satisfy the minimal uncertainty condition thus providing a set of the most classical-like states, and it is one of the main reasons why they are so popular in the current theory when examining a hard problem of quantum-classical correspondence. In this context the so-called "Schroedinder cat" states, which are essentially non-classical, are especially attractive [7]. In terms of CSs the simplest (even) optical "Schroedinder cat" state is usually taken as follows

$$|\alpha_{CAT}\rangle = \frac{1}{\sqrt{2(1+e^{-2|\alpha|^2})}} (|\alpha\rangle + |-\alpha\rangle) , \quad (11)$$

for another choice see Refs [4,5,26,31,37-39].

In this section we discuss the entropic measures for CSs and nonclassical states determined by their Fock representations (10) and (11) respectively. For simplicity α is implied to be real. The Renyi entropies, denoted for Eqs. (10) and (11) by $R[\alpha]$ and $R[\alpha_{CAT}]$ respectively, is easy to compute explicitly:

$$R[\alpha] = 2\alpha^2 / \ln[2] - \log[I_0(2\alpha^2)] , \quad (12)$$

$$R[\alpha_{CAT}] = \log[\frac{2[\cosh(\alpha^2)]^2}{J_0(2\alpha^2) + I_0(2\alpha^2)}] , \quad (13)$$

where the Bessel $J_0(z)$, and modified Bessel $I_0(z)$ functions naturally appear. Due to known asymptotics of these functions, we have for large α the estimations

$$R[|\alpha\rangle] \to 1 + \log[2\alpha\sqrt{\pi}] , \quad (14)$$

$$R[\alpha_{CAT}] \to \log[\alpha\sqrt{\pi}] \; . \quad (15)$$

We see that asymptotically the Renyi entropy of these two types of states is different by 1 logarithmic unit ("bit"):

$$R[\alpha_{CAT}] - R[\alpha] \to -1 . \quad (16)$$

The same is true for the Shannon entropy (3)

$$S[\alpha_{CAT}] - S[\alpha] \to -1 \quad (17)$$

although in this case we cannot find a full set of analytical expressions. These results are in agreement with the numerical calculations displayed on the plots in Fig. 1. As a result, the coherent states tend to be more delocalized over "configurational" space of the oscillator excited states.

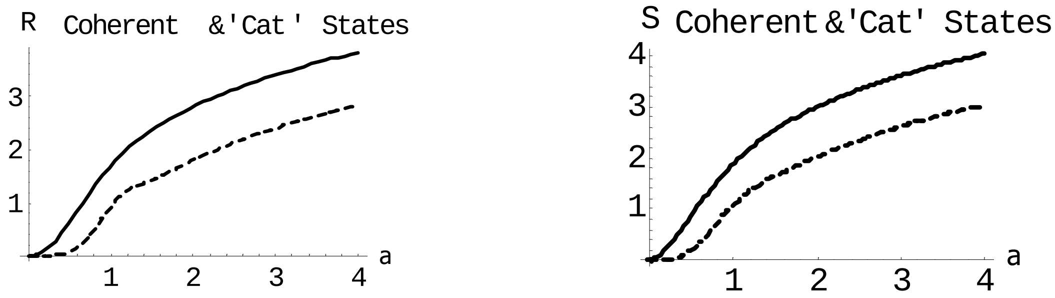

Figure 1. Renyi's [Eq. (2)] and Shannon's [Eq. (3)] entropies of CSs (10) (solid line) and "Schroedinder cat" states (11) (dashed line) in the Fock space representation.

2 b. Phase space representation

Now we examine the entropy measures in the phase space representation using Eqs. (7) and (8). The needed Wigner functions can be found in many works [5,29-31,40]. Here we reproduce them for the real α values referred to the associated CSs (10):

$$W[\alpha] = \frac{e^{-(p^2+(q-\sqrt{2}\alpha)^2)}}{\pi}, \tag{18}$$

and, respectively, to the "Schroedinder cat" states (11):

$$W[\alpha_{CAT}] = \frac{e^{-(p^2+q^2)}}{\pi(1+e^{-2\alpha^2})}\{e^{-2\alpha^2}\cosh(2\sqrt{2}\alpha\, q) + \cos(2\sqrt{2}\alpha\, p)\}. \tag{19}$$

For the pure eigenstates $\{|n\rangle\}$ the corresponding expression is

$$W[n] = \frac{(-1)^n}{\pi} e^{-(p^2+q^2)} L_n[2(p^2+q^2)] \tag{20}$$

where $L_n(z)$ is the Laguerre polynomial of order *n*. In this case, Renyi's entropies (7) for the lowest states are of the form

$$R_W[0] = \log\pi\,,\ \ R_W[1] = \log\pi + 1,\ \ R_W[2] = \log\frac{\pi}{11} + 5,$$

$$R_W[3] = \log\frac{\pi}{17} + 6,\ \ R_W[4] = \log\frac{\pi}{1787} + 13, \qquad etc. \tag{21}$$

It seems that there exist a general formula for arbitrary integer *n*, but we could not find it. In the case of Shannon's entropy, only the first 3 terms can be handled analytically:

$$S_W[0] = (\ln\pi + 1)/\ln 2 - 1,\ S_W[1] = \{\frac{4}{e}\,\mathrm{Ei}(1) - \ln\frac{\pi}{2} - 1]\}/\ln 2,$$

$$S_W[1] = \{4[\tau_+ e^{-\sigma_+}\,\mathrm{Ei}(\sigma_+) + \tau_- 4e^{-\sigma_-}\,\mathrm{Ei}(\sigma_-)\ \ln\pi - 15]\}/\ln 2 - 1 \tag{22}$$

where $\sigma_\pm = 2 \pm \sqrt{2}$, $\tau_\pm = 3\sqrt{2} \pm 5$, and $\mathrm{Ei}(z)$ is the exponential integral function.

Now we turn to states (10) and (11). By manipulating with Eq. (18), it is a simple matter to realize that the resulting expressions are independent of α values, that is

$$R_W[\alpha] \equiv R_W[0] = \log\pi\,, \tag{23}$$

$$S_W[\alpha] \equiv S_W[0] = \log\frac{\pi}{2} + 1. \tag{24}$$

This fact is not so unusual for the coherent states. For instance, many physical quantities of CSs, such as fluctuations of coordinate and momentum, are of the same behaviour. Another behaviour is observed for the "cat" states (11). It can be examined by the explicit expression derived from Eqs. (7) and (19):

$$R_W[\alpha_{CAT}] = \log\pi + 1 - \log[1 + \frac{\cosh(2\alpha^2)}{[\cosh(\alpha^2)]^4}] \tag{25}$$

Evidently, when α increases this entropy measure goes to $\log\pi + 1$. The same is in fact true for Shannon's entropy for the same 'cat' state (11), but again an analytical consideration cannot be done for this type of problem. As results, we have

$$R[\alpha_{CAT}] - R[\alpha] \to 1, \tag{26}$$

$$S[\alpha_{CAT}] - S[\alpha] \to \cong 1.73\,. \tag{27}$$

These relations are opposite to those for the Fock space representation of the same quantities [Eqs. (16), (17)]. We see that Eqs. (16), (17) reflect rather formal algebraic properties of the states in study whereas Eqs. (26), (27) provide the phase space description leading to a proper physical understanding. The plots in Fig. 2 confirm the above given consideration.

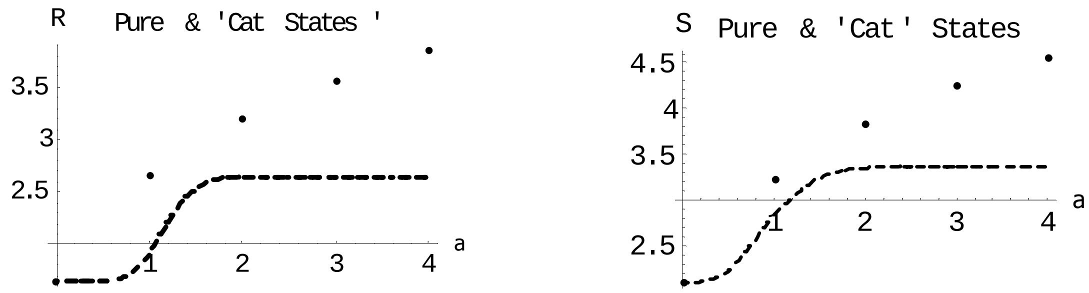

Figure 2. Renyi's [Eq. (7)] and Shannon's [Eq. (8)] entropies of pure eigenstates (points) and "Schroedinder cat" states (11) (dashed line) in the Wigner representation.

We can also suggest a rather plausible conjecture that for more complex cat-like states with ν essentially different coherent components we may expect the following generalization of Eq. (26):

$$R[\alpha_{CAT}] - R[\alpha] \to \log\nu\,. \tag{26}$$

However, a study of this problem is beyond the scope of the present paper.

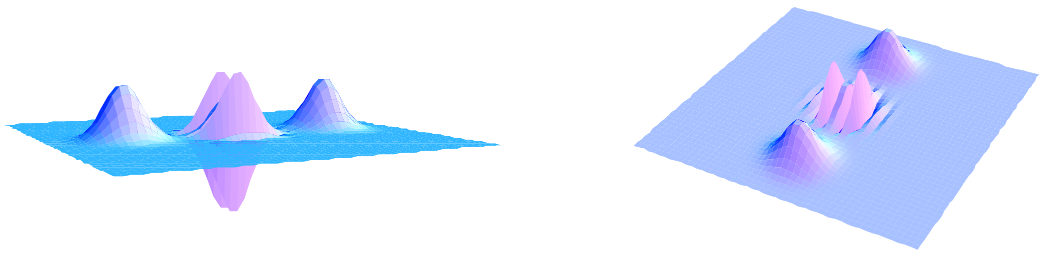

Figure 3. The Wigner function (19) for the "Schroedinder cat" state (11) with $\alpha = 3$.
In the first plot the region of negative values is under the plane (p, q).

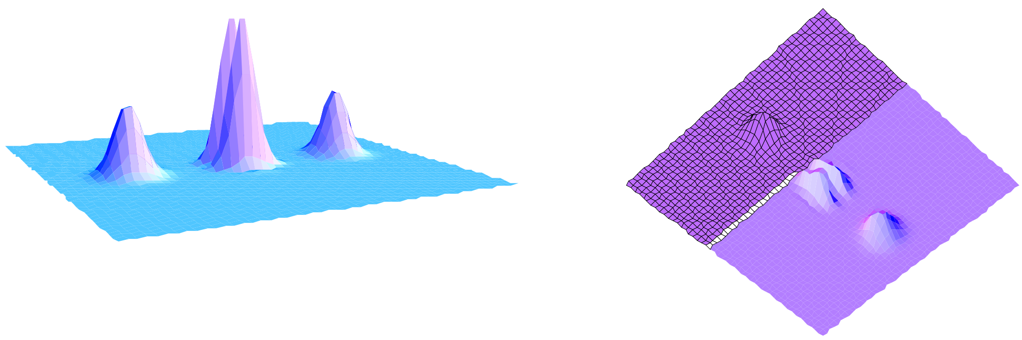

Figure 4. The squared Wigner function (6) for the "Schroedinder cat" state (11) with $\alpha = 3$.

To conclude this section, we show some 3D plots of the WF and squared WF functions for the Schroedinder cat state. We observe a sizeable region of negative values for the WF in Fig. 3. At the same time, the squared WF reproduces a rather complicated topography of the starting distribution (19).

3. Concluding remarks

With this paper we have presented a modified scheme for calculating some typical entropy measures for nonclassical (ground and excited eigenstates as well as the "Schroedinder cat" states) and for classical-like coherent states. We explored the 'configurational' entropy using the conventional Fock space representation, and concurrently the phase space entropy measure by using the Wigner function formalism. In the latter case we introduced the squared Wigner function $W_{sq}(p,q)$ (6) as a naturally normalized positive definite distribution. It allows us to directly evaluate entropy measures from the Wigner functions without any smearing procedures.

The results obtained are rather clear interpreted. In the entropy language, with increasing excitation level (quantum number n) the pure eigenstates become very smeared over phase space. On contrary, the CSs as the most classical states have a minimal and identical entropy measure. Even the nonclassical "Schroedinder cat" states turn out to be limitedly spreading over the phase space. It means that our scheme seems to be reliable for treating quantum entropies. We hope that using the proposed squared Wigner function method can be further extended to more complex quantum models such as molecular electronic structure problems.

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Kharkov University Bulletin 2007. № 770. Chemical Series. Issue 15(38). А.В. Лузанов. О коллективности и энтропийных мерах для когерентных и близких им квантовых состояний.

Предложен простой подход для мероопределения квантовой энтропии в фазовом пространстве на основе вигнеровского формализма. Метод применен к собственным и когерентным состояниям гармонического осциллятора и к квантовым состояниям так называемого оптического "шредингеровского кота". Для тех же задач наряду с представлением в фазовом пространстве используется Фоковское представление. Анализируется существенно различное поведение энтропийных мер для данных двух типов представлений.