

## Thermal uncertainty relations and LMC structural quantifiers

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In this paper we establish information theoretical bridges between 1) Thermal Heisenberg uncertainties  $\Delta x \Delta p$  (at temperature  $T$ ), and 2) LMC structural quantifiers. After having achieved such purpose, we determine to what an extent our bridges can be extended to both the semi classical and classical realms. Also, we find a strict bound relating a special LMC structural quantifier to quantum uncertainties.

Keywords: Thermal uncertainties, Disequilibrium, Husimi distributions.

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### I. INTRODUCTION

#### A. Thermal uncertainty relations

Thermodynamics uncertainty-relations (TUR) were the subject of great effort and exceedingly interesting work (one can look, for instance, at [1–8]). A recommendable review was provided by Uffink and van Lith [9]. These thermal uncertainties [10] will be the focus of the present work, particularly in connection with the disequilibrium notion to be explained below. Our motivation arises from consideration of the TUR. We wish to encompass within this framework the behavior of the LMC structural quantifiers [11–25].

#### B. LMC structural quantifiers

Based on a recent discussion by Nagata [1], who analyzes finite-temperature uncertainties and their relation with the LMC structural quantifiers  $C$  (statistical complexity) and  $D$  (disequilibrium) [11–25]. We will connect them with TUR tenets.

In most systems a certain level of randomness (usually quantified by an entropy  $S$ ) coexists with some amount of correlation-structures. This fact can be viewed as an intermediate stage between two opposite extreme situations: (A) perfect order or (B) maximal randomness (no correlations exist). This intermediate stage has been successfully quantified in the last 20 years by a quantity that came to be called the statistical complexity  $C$ , advanced in Ref. [11], that can be properly regarded as a structure-content quantifier [11–25]. In [11], its authors established a kind of “distance” in probability space (PS) that they baptized the disequilibrium  $D$ . What does it measure? If  $f$  is the probability density that describes the system at hand, and  $f_u$  is the uniform probability density, then  $D$  tells us how far the two distributions,  $f$  and  $f_u$ , differ from each other [12]. In density matrix parlance,  $D$  measures the distance between the extant density matrix and the maximally mixed one and is associated with order, that grows with the  $D$ -value.

In addition,  $D$  provides a notion of hierarchy that makes it non-null if there are privileged states among the accessible

ones.  $D$  would then be maximal for (A) and vanish for (B) above. In the entropy-case, things are exactly reversed.  $S$  is minimal for (A), while it reaches a maximum for (B). Reasoning in this way L. Ruiz, Mancini, and Calvet (LMC) [11–13] formulated what constitutes today the standard way of casting a statistical complexity measure or structure-content quantifier  $C$ , written as

$$C = DS, \quad (1)$$

a functional of the density distributions (DD) [11]. Such proposal received great attention (see Refs. [11–25] as a quite small sample). It was used in different scenarios for both the canonical, microcanonical, and grand canonical ensembles. As already mentioned, in the present context we refer to  $C$  as a structure-content quantifier because we will apply it to the harmonic oscillator, which by no means regarded as “complex”. In fact,  $C$  has been of utility in the realm of non complex systems (see Ref. [24, 25] and references therein).

## II. THE THERMAL QUANTUM CASE

With regards to quantum mixed one-dimensional states, after consulting and relating references [1, 12, 26, 27], to see that one can cast the pertinent density matrix  $\hat{\rho}$  and the associated disequilibrium  $D$  in simple fashion. One starts with

$$\hat{\rho} = (1 - e^{-\beta\hbar\omega})e^{-\beta\hat{n}}, \quad (2)$$

being  $\beta = 1/k_B T$ , with  $k_B$  the Boltzmann constant and  $\hat{n}$  the number operator [26]. In this paper, we set the Boltzmann constant equal unity hereafter ( $k_B = 1$ ). Then, one can express the quantum disequilibrium in the fashion [12, 26, 27],

$$D = \text{Tr}\hat{\rho}^2. \quad (3)$$

Note that here  $D$  is exactly equal to the purity (or degree of mixedness)  $\mathcal{P}(\rho)$  of  $\hat{\rho}$ , so that  $0 \leq D \leq 1$ , since the dimension of the Hilbert space is infinity. With some simple manipulations one can as well ascertain that [1, 12, 26, 27]

$$D = \tanh(\beta\hbar\omega/2). \quad (4)$$

Further, the *quantal* HO-expression for the entropy  $S$  is [26]

$$S = \frac{\beta\hbar\omega}{e^{\beta\hbar\omega} - 1} - \ln(1 - e^{-\beta\hbar\omega}), \quad (5)$$

so that, with  $S$  and  $D$  at hand, the quantum structural quantifier  $C = DS$  becomes

$$C = \tanh(\beta\hbar\omega/2) \left( \frac{\beta\hbar\omega}{e^{\beta\hbar\omega} - 1} - \ln(1 - e^{-\beta\hbar\omega}) \right), \quad (6)$$

which vanishes both at  $T = 0$  and at  $T = \infty$  as one should expect. In addition, we believe convenient to add here the useful well-known HO-expressions for both the Helmholtz free energy  $F$ , the mean value of energy  $U$  and the specific heat  $C_V$ , respectively [26]

$$F = \frac{\hbar\omega}{2} + T \ln(1 - e^{-\beta\hbar\omega}), \quad (7)$$

$$U = \langle \hat{H} \rangle = \hbar\omega \left( \langle \hat{n} \rangle + \frac{1}{2} \right) \equiv \frac{\hbar\omega}{2 \tanh(\beta\hbar\omega/2)}. \quad (8)$$

and

$$C_V = \left( \frac{\hbar\omega\beta}{e^{\beta\hbar\omega} - 1} \right)^2 e^{\beta\hbar\omega} \quad (9)$$

Finally, the the mean particle number  $\langle \hat{n} \rangle$  is easily seen to be

$$\langle \hat{n} \rangle = \frac{1}{e^{\beta \hbar \omega} - 1}. \quad (10)$$

We have now enough materials to derive our desired equality below.

### III. A STRICT BOUND RELATING $D$ TO QUANTUM UNCERTAINTIES

Our present results arise at this stage. Remind that  $D$ , being equal to the ratio  $C/S$ , can also be regarded as the ratio between a structural and a random quantifiers. The thermal Heisenberg' uncertainty relation is of the form [10, 27]

$$\Delta x \Delta p = \frac{\hbar}{2} \coth(\beta \hbar \omega / 2), \quad (11)$$

so that it can be cast in the fashion

$$D = \frac{\hbar/2}{\Delta x \Delta p} = U_r \quad (12)$$

where  $\Delta x$  and  $\Delta p$  are the quantum variances for the canonically conjugated observables  $x$  and  $p$  [27] and thus  $D$  equals the ratio  $U_r = (\hbar\omega/2)/U$  between the minimum possible uncertainty value (attributable to coherent states) and the actual uncertainty value of the mixed state under consideration. This ratio, in turn, is also the purity  $\mathcal{P}(\hat{\rho})$ . We are then immediately led to our first significant result (we repeat that  $D$ , being equal to the ratio  $C/S$ , can also be regarded as the ratio between a structural and a random quantifiers)

$$D \Delta x \Delta p = \frac{\hbar}{2}. \quad (13)$$

Surprisingly enough, there exist semi classical and even classical counterparts of the above equality, as we will show below.

Eq. (13) can be cast also in purity terms, in the fashion

$$\mathcal{P}(\rho) \Delta x \Delta p = \frac{\hbar}{2}, \quad (14)$$

which constitutes, let us insist, an strict quantum equality (for the HO), that we believe to have newly established here. This relation tells us also that the ratio “structure/randomness” times thermal uncertainty equals  $\hbar/2$ .

#### 1. Graphs

We depict now some statistical quantifiers versus either Heisenberg's uncertainty  $q_1 = \Delta x \Delta p / \hbar$  or  $q_2 = \hbar \omega / k_B T$ . We begin with von Neumann's entropy in Fig. 1, that exhibits maxima at  $q_1 = 1 = q_2$ . Fig. 2 displays several thermal quantifiers versus uncertainty. These curves will be compared below with their semi classical Husimi counterparts.

We highlight here this fact regarding the right panel: the quantum structural quantifier does not attain its maximum at minimal uncertainty  $\hbar/2$  but at twice such value. This value is the minimum one that can be reached for semi classical uncertainties, as we will see below. Thus, the quantum structural quantifier seems to “sense” that the correlation-structure that it depicts is maximal as we enter the semi classical domain. The left panel tells us that structural quantifier becomes maximal when the vibrational energy equals the thermal-kinetic one.

Let us abound on this last result. Both the cases of  $T \rightarrow \infty$  and  $T = 0$  (one has the vibrational energy  $\hbar/2$ ) have zero structural quantifier  $C$ . The maximum  $C$  should be attained in an scenario “intermediate” between these two extreme instances. This happens precisely when the vibrational energy equals the thermal-kinetic one.

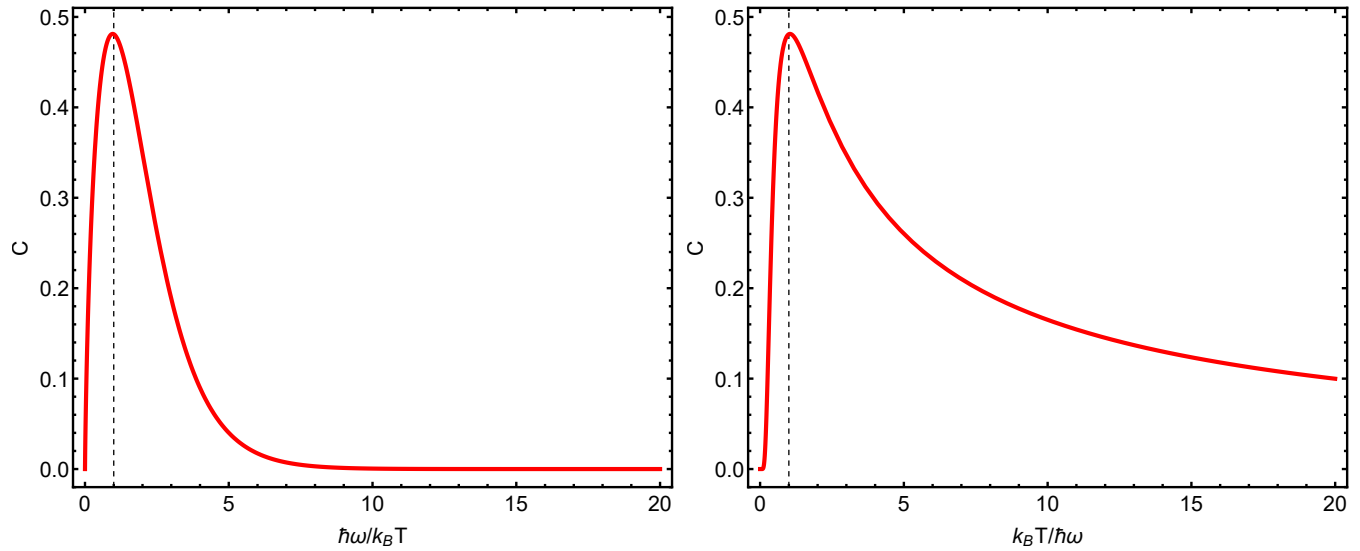


FIG. 1: Left panel: Quantum structural quantifier  $C$  versus  $\hbar\omega/k_B T$ . The maximum equal to 0.477 is detected when the thermal energy equals the vibrational one, at  $\hbar\omega/k_B T = 1$ , as indicated by the vertical line. Right panel: Quantum structural quantifier  $C$  versus  $k_B T/\hbar\omega$ . Also, the maximum is located in  $\hbar\omega/k_B T = 1$ .

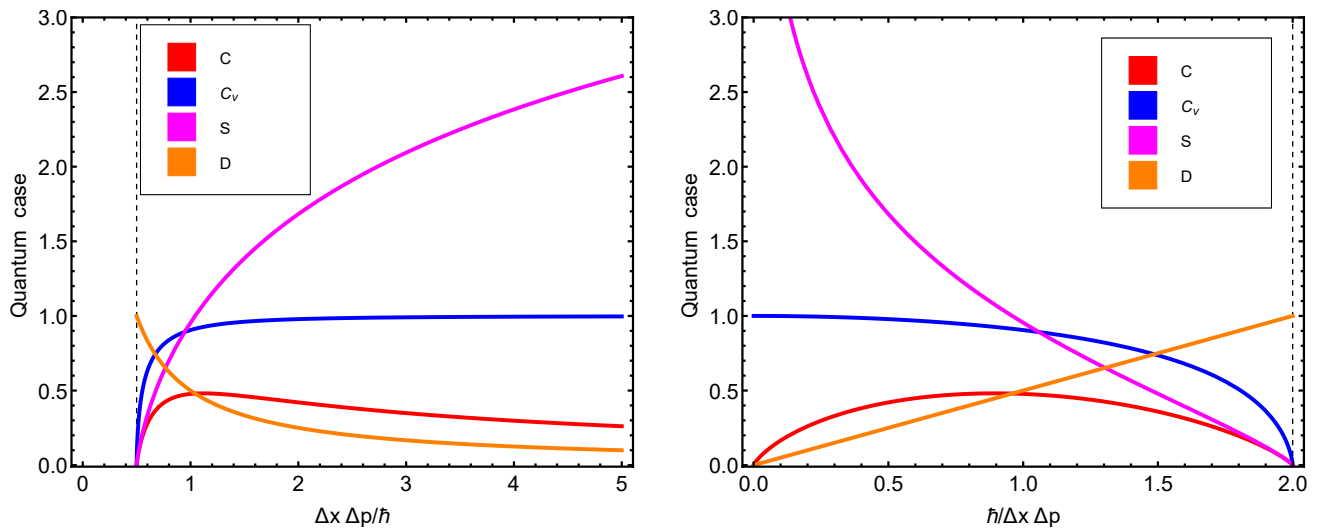


FIG. 2: Left panel: Thermal quantum quantifiers (TQF) versus  $\Delta x \Delta p/\hbar$ . Right panel: TQF versus  $\hbar/\Delta x \Delta p$  expressed in  $k_B$ -units. These plots should be compared to associated ones displayed in Ref. [1].

Fig. 2 displays several thermal quantifiers versus uncertainty in two distinct fashions for didactic purposes. Notice that at the minimum minimorum (MM) uncertainty value the entropy, specific heat, and structural quantifier all vanish. Interestingly enough, at four times the MM uncertainty value, we already enter the classical regime, as indicated by the  $C_V$  attainment of its constant classical value.

subsection Quantum HO- $D$  (or  $\mathcal{P}$ )-based thermodynamics

It may be of some interest to see that all relevant thermal quantifiers can be casted in terms of  $D = U_r = \mathcal{P}(\hat{\rho})$ . Indeed, we have

$$e^{-\beta\hbar\omega} = \frac{1-D}{1+D}, \quad (15)$$

which implies that

$$1 - e^{-\beta\hbar\omega} = \frac{2D}{1+D}. \quad (16)$$

Therefore, and this is, we believe, a new way of casting HO-thermal quantities, solely in terms of  $D = U_r$ , we have the panoply of expressions:

$$S = \left(\frac{1-D}{2D}\right) \ln\left(\frac{1+D}{1-D}\right) + \ln\left(\frac{1+D}{2D}\right), \quad (17)$$

while the structural quantifier reads

$$C = \left(\frac{1-D}{2}\right) \ln\left(\frac{1+D}{1-D}\right) + D \ln\left(\frac{1+D}{2D}\right), \quad (18)$$

the free energy turns out to be

$$F = \hbar\omega \frac{\ln\left(\frac{\sqrt{1-D^2}}{2D}\right)}{\ln\left(\frac{1-D}{1+D}\right)}, \quad (19)$$

the energy is

$$U = \frac{\hbar\omega}{2D}, \quad (20)$$

and the specific heat becomes

$$C_V = \frac{1}{4} \left(\frac{1-D^2}{D^2}\right) \left[\ln\left(\frac{1+D}{1-D}\right)\right]^2. \quad (21)$$

Finally, the number of particles becomes

$$\langle \hat{n} \rangle = \frac{1-D}{2D}. \quad (22)$$

The whole HO-thermodynamics can be expressed in terms of either  $D$  or the purity. These may be trivial, but novel results.

#### IV. EXTENDING BRIDGES TO A SEMI CLASSICAL ENVIRONMENT

##### A. Introduction: Coherent states and Husimi distributions

The well known semi-classical Wehrl entropic quantifier  $W$  constitutes a phase-space measure of localization [28, 29]. It is constructed via coherent states  $|z\rangle$  [28, 30, 32] and is regarded as a powerful tool in statistical physics. Remind that coherent states are eigenstates of an appropriate annihilation operator  $\hat{a}$  that satisfy the relation  $\hat{a}|z\rangle = z|z\rangle$  [31–33]. The  $W$ -definition is

$$W = - \int \frac{dx dp}{2\pi\hbar} \mu(x, p) \ln \mu(x, p), \quad (23)$$

being thus a Shannon-like information measure [34] to which Jaynes' MaxEnt elaborations can be applied.

The Husimi distributions (HD)  $\mu(x, p)$  [35] are the diagonal elements of the density operator in the coherent-state basis  $|z\rangle$ . Accordingly,

$$\mu(x, p) = \langle z | \hat{\rho} | z \rangle. \quad (24)$$

The  $\mu$  are semi-classical distributions linked to a density matrix  $\hat{\rho}$  for the system [31–33], normalized in the fashion

$$\int \frac{dx dp}{2\pi\hbar} \mu(x, p) = 1. \quad (25)$$

It is well known that  $\mu(x, p)$  is a Wigner–distribution  $\rho_W$ , smeared over an  $\hbar$  sized region of phase-space [30]. Such bedaubing makes  $\mu(x, p) > 0$ , although  $\rho_W$  lacks such a positivity character. The HD is a special sort of distribution, concerning an approximate specification of location in phase space [30]. The uncertainty principle acquires the form

$$W \geq 1, \quad (26)$$

as conjectured by Wehrl [28] and proved by Lieb [36]. Equality is attained for  $\hat{\rho}$  a coherent state [28, 36].

In considering  $T$ –equilibrium states at a one usually regards the system’s state as an incoherent mixture of eigenenergies  $E_n$  weighted by the Boltzmann factor  $\exp(-\beta E_n)$ . The Gibbs’s canonical distribution is the thermal density matrix given by  $\hat{\rho} = \exp(-\beta E_n)/Z$  with  $Z = \sum_n \exp(-\beta E_n)$ .

If we want a  $W$ –expression for the Hamiltonian  $\hat{H}$ , of eigenstates  $|n\rangle$  and eigen-energies  $E_n$  one can always write [30]

$$\mu(x, p) = \langle z | \hat{\rho} | z \rangle = \frac{1}{Z} \sum_n e^{-\beta E_n} |\langle z | n \rangle|^2, \quad (27)$$

A useful path  $W$  begins then with Eq. (27) and follows with Eq. (23). Distributions cast in terms of the coherent states  $|z\rangle$  of the harmonic oscillator are useful in multiple contexts [30–33].

## B. HO-specialization

The above ruminations are of a general nature. Let us specialize things for the HO whose Hamiltonian reads

$$\hat{H} = \hbar\omega (\hat{a}^\dagger \hat{a} + 1/2) = (\hbar\omega/2)(\hat{a}^\dagger \hat{a} + \hat{a} \hat{a}^\dagger). \quad (28)$$

The complex *eigenvalues*  $z$  of the destruction operator  $\hat{a}$  are

$$z = \frac{1}{2} \left( \frac{x}{\sigma_x} + i \frac{p}{\sigma_p} \right), \quad (29)$$

where  $x$  and  $p$  are scaled by their respective variances ( $\sigma$ ) in the HO ground state  $\sigma_x = (\hbar/2m\omega)^{1/2}$ ,  $\sigma_p = (\hbar m\omega/2)^{1/2}$ ,  $\sigma_x \sigma_p = \hbar/2$ . Thus, the Husimi  $\mu(x, p)$  becomes [30, 37]

$$\mu(x, p) \equiv \mu(z) = (1 - e^{-\beta\hbar\omega}) e^{-(1 - e^{-\beta\hbar\omega})|z|^2}, \quad (30)$$

which is normalized according to Eq. (25). Also, the mean energy is [38],

$$\langle \hat{H} \rangle = \hbar\omega \left( \langle |z|^2 \rangle - \frac{1}{2} \right) = \hbar\omega \left( \frac{1}{1 - e^{-\beta\hbar\omega}} - \frac{1}{2} \right) \equiv \frac{\hbar\omega}{2 \tanh(\beta\hbar\omega/2)}, \quad (31)$$

that coincides with its quantum counterpart.

The HO-Wehrl’s measure acquires now the appearance [37]

$$W = 1 - \ln(1 - e^{-\beta\hbar\omega}). \quad (32)$$

## V. HO-SEMI CLASSICAL THERMAL TREATMENT AND UNCERTAINTY RELATIONS

We enter now our semi classical contributions at this stage. The semi classical disequilibrium is easily seen to be

$$D_{sc} = D_{semi-quant} = \int \frac{d^2z}{\pi} \mu^2(z), \quad (33)$$

where  $d^2z/\pi = d(Re z)d(Im z) = dx dp/(2\pi\hbar)$  is the differential  $z$  plane's area-element [32]. We will use the subscript  $sc$  for the semiclassical case.

After evaluation of that integral becomes

$$D_{semi-quant} = \frac{1}{2}(1 - e^{-\beta\hbar\omega}), \quad (34)$$

and comparing to (16) we see that

$$D_{semi-quant} = \frac{D}{1 + D}, \quad (35)$$

entailing that

$$D_{semi-quant} \leq D, \quad (36)$$

an unsuspected relationship that makes sense however, since as a classical density distribution (DD) one expects it to be closer to the uniform distribution than a quantal DD derived from a density operator.

The structural quantifier  $C_{sc} = D_{sc} W$ , derives from Eqs. (32) and (34) and reads

$$C_{sc} = \frac{1}{2}(1 - e^{-\beta\hbar\omega}) (1 - \ln(1 - e^{-\beta\hbar\omega})). \quad (37)$$

Thermal uncertainties express the effect of temperature on Heisenberg's celebrated relations (see, for instance [27, 39–41]). We use now a result obtained in Ref. [30] (equation (3.12)), where the authors cast Wehrl's information measure in terms of the "coordinates"'s variances  $\Delta_\mu x$  and  $\Delta_\mu p$ , obtaining

$$W = \ln \left( \frac{e}{\hbar} \Delta_\mu x \Delta_\mu p \right). \quad (38)$$

In the present context, the relation  $W = 1 - \ln(1 - e^{-\beta\hbar\omega})$  allows us to write [37]

$$\Delta_\mu x \Delta_\mu p = \frac{\hbar}{1 - e^{-\beta\hbar\omega}}, \quad (39)$$

that in view of Eq. (34) we can affirm that there is an exact semi classical replica of the quantum equality (13) above that reads

$$D_{sc} \Delta_\mu x \Delta_\mu p = \frac{\hbar}{2}. \quad (40)$$

Also, the structural quantifier has the form

$$C_{sc} = \frac{\ln \left( \frac{e \Delta_\mu x \Delta_\mu p}{\hbar} \right)}{\Delta_\mu x \Delta_\mu p / (\hbar/2)}. \quad (41)$$

We note that when  $\Delta_\mu x \Delta_\mu p = \hbar$ , then  $C_{sc} = 1/2$ , which is the maximum possible value attained by  $C_{sc}$ . Fig. 2 depicts the behavior of  $C_{sc}$  in terms of the uncertainty relation  $\Delta_\mu x \Delta_\mu p$ . Remark that  $W$  and its associated structural quantifier can be expressed exclusively in uncertainty terms.

In Fig. 3 we appreciate that (i) The Wehrl structural quantifier attains its maximum values at the same place at which the quantal structural quantifier does so. (ii) This place corresponds to maximum possible semi classical localization in phase space. (iii) Wehrl structural quantifier grows from zero vibrational energy) till it attains on-half the thermal-kinetic energy, and then remains constant.

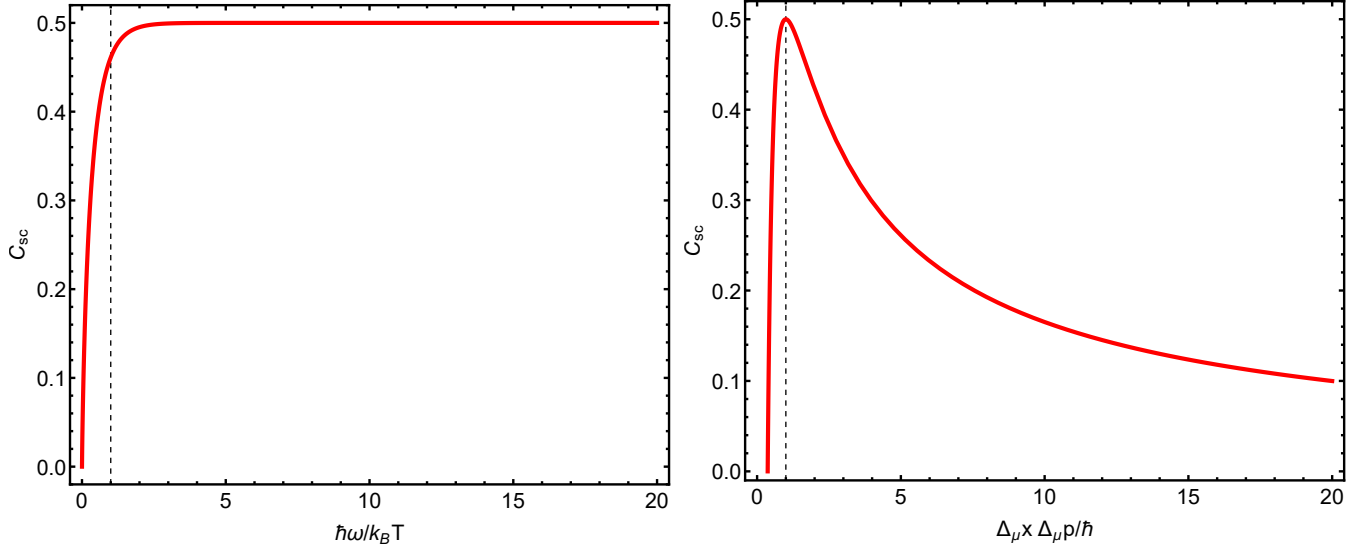


FIG. 3: Left panel: structural quantifier  $C_{sc}$  versus  $\hbar\omega/k_B T$ . The vertical line indicates equality between the thermal and the vibrational energies. Right panel: structural quantifier  $C_{sc}$  versus  $\Delta_\mu x \Delta_\mu p/\hbar$ . The vertical line indicates optimal semi classic localization.

## VI. POSSIBLE CLASSICAL EXTENSION

For completeness' sake, we add here a word regarding the classical scenario. We obtain from Refs. [12, 26, 27] the three relations ( note we will use here the subscript *class* for the classical case)

$$D_{class} = \beta\hbar\omega/2, \quad (42)$$

$$S_{class} = 1 - \ln(\beta\hbar\omega) = 1 - \ln(2D_{class}), \quad (43)$$

vanishing thus for (here  $e$  is the basis of natural logarithms)

$$D_{class} = e/2, \quad (44)$$

and becoming negative is  $D_{class} > e/2$ , a typical classical artifact.

Finally, the special equality obeyed by the uncertainty relation can be extended to the classical realm. In this case one has

$$\Delta_{class} x \Delta_{class} p = \frac{\hbar}{\beta\hbar\omega} = \frac{\hbar}{2D_{class}}, \quad (45)$$

or, significantly enough, we have a classical counterpart of the quantum equality (13) that reads



$$D_{class} \Delta_{class} x \Delta_{class} p = \frac{\hbar}{2}. \quad (46)$$

A word of caution may be pertinent here. In this instance,  $\hbar$  is just an arbitrary elementary action that one introduces in classical statistical mechanics in order to avoid Gibbs' paradox. It is gratifying though that (46) preserves the structure of Eq. (13).

Using relation (15) we see that

$$D_{class} = \ln(1 - D)^{1/2} - \ln(1 + D)^{1/2}, \quad (47)$$

so that  $D_{class}$  vanishes if its quantum counterpart does so. However, it diverges when  $D$  attains its maximum value of unity. Also, with some algebra the classical structural quantifier can be written in terms of the quantum uncertainties as

$$C_{class} = \frac{\ln(e \Delta_{class} x \Delta_{class} p / \hbar)}{2 \Delta_{class} x \Delta_{class} p / \hbar}. \quad (48)$$

We illustrate things in Fig. (5). Notice that, also classically, the structural quantifier becomes maximal when the two types of energies at play become equal. Remark on the extraordinary similitude between the quantum and the classical  $C$ -structural quantifiers.

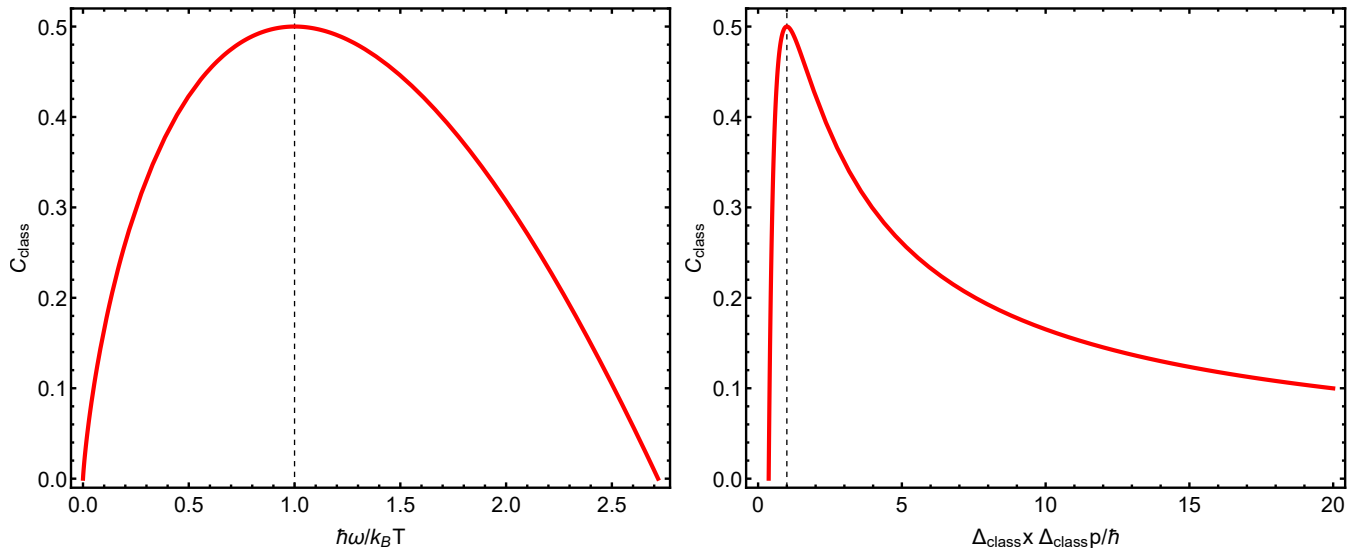


FIG. 4: Left panel: structural quantifier  $C_{class}$  versus  $\hbar\omega/k_B T$ . The maximum is attained at  $\hbar\omega/k_B T = 1$ , that is, equality between thermal and vibrational energies. Right panel: structural quantifier  $C_{class}$  versus  $\Delta_{class} x \Delta_{class} p = \hbar$ . Remarkably enough,  $C_{class}$  is maximal at the same uncertainties value which maximize its quantum counterpart.

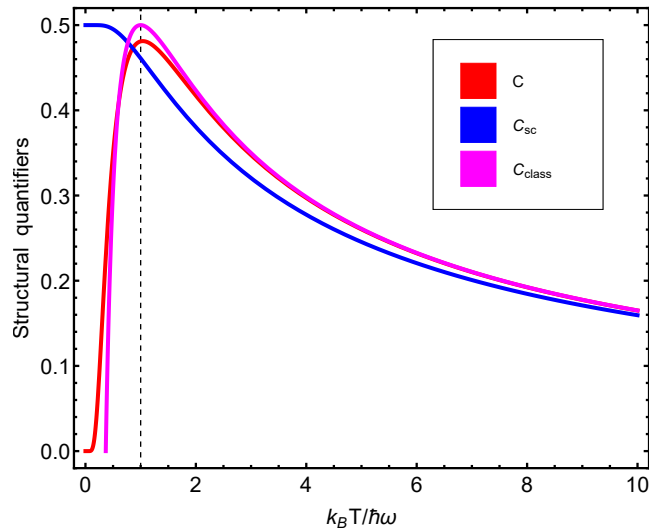


FIG. 5: Our three manners of calculating complexities (or structural quantifiers)  $C$  versus  $k_B T / \hbar \omega$ . The vertical line signals equality between thermal and vibrational energies.

## VII. CONCLUSIONS

This work had two parts. In the first one we have uncovered and/ or found some novel information-related Gibbs statistical description's facets. More specifically, we established for mixed states (at a temperature  $T$ ) the equality

$$\Delta x \Delta p \mathcal{P} = \Delta x \Delta p D = \hbar/2.$$

This equality was suitably extended, mutatis mutandis, both to the semi classical and to the classical realms, as we explained above. Further,

- At the minimum minimorum uncertainty value, the entropy, specific heat, and structural quantifier  $C$  all vanish.
- Obviously, the purer the state, the smaller the thermal uncertainty.
- The closer the extant density matrix to the maximally mixed one, the larger the thermal uncertainty.
- Note that all quantities involved in (14) are observable (in principle) so that we are dealing with a nature-equality.

The second part of this effort involves semi classical and classical scenarios. We highlight that

1. The Wehrl structural quantifier  $C_{sc}$  attains its maximum values at the same place at which the quantal structural quantifier  $C$  does so.
2. This place corresponds to maximum possible semi classical localization in phase space.
3. Wehrl's structural quantifier  $C_{sc}$  grows from zero at null vibrational energy (VE) till the VE attains one-half the thermal-kinetic energy, and then remains constant.
4.  $\Delta_\mu x \Delta_\mu p / \hbar$  can be regarded as the phase space localization error  $e$  (in its natural units) that accompanies the Husimi distribution.
5. The Wehrl structural quantifier  $C_{sc}$  becomes a maximum in these circumstances.
6. We emphasize that  $C_V$  attains its constant classical value as soon as the thermal energy equals the vibrational one.
7. The three different structural quantifiers  $C$  at play in this work behave in a remarkably similar fashion as the last graphs explicitated.

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