

Quantum statistical information contained in a semi-classical Fisher–Husimi measure

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We study here the difference between quantum statistical treatments and semi-classical ones, using as the main research tool a semi-classical, shift-invariant Fisher information measure built up with Husimi distributions. Its semi-classical character notwithstanding, this measure also contains information of a purely quantal nature. Such a tool allows us to refine the celebrated Lieb bound for Wehrl entropies and to discover thermodynamic-like relations that involve the degree of delocalization. Fisher-related thermal uncertainty relations are developed and the degree of purity of canonical distributions, regarded as mixed states, is connected to this Fisher measure as well.

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I. INTRODUCTION

A quarter of century before Shannon, R.A. Fisher advanced a method to measure the information content of continuous, rather than digital inputs, using not the binary computer codes but rather the statistical distribution of classical probability theory [1, 2]. Already in 1980 Wootters pointed out that Fisher’s information measure (FIM) and quantum mechanics share a common formalism and both relate probabilities to the squares of continuous functions [3]. Since then, much interesting work has been devoted to the manifold physical FIM–applications. For examples (not an exhaustive list, of course), see, for instance, Refs. [1, 4, 5, 6, 7]).

Our emphasis in this communication will be placed on the study of the differences between (i) statistical treatments of a purely quantal nature, on the one hand, and (ii) semi-classical ones, on the other one. We will show that these differences can be neatly expressed entirely in terms of a semi-classical, shift-invariant Fisher measure. Additionally, this measure helps to refine the so-called Lieb–bound [8] and connects this refinement with a Fisher-description of delocalization in phase-space, that, of course, can be visualized as information loss. Relations will also be established with an interesting measure that was early introduced to characterize delocalization: that of Wehrl’s [8], for which Lieb established the above cited lower bound [9].

In the wake of a discussion advanced in Ref. [10], *we will be mainly concerned with building “Husimi–Fisher” bridges*. It is well-known that the oldest and most elaborate phase-space (PS) formulation of quantum mechanics is that of Wigner [11, 12]. To every quantum state a PS function (the Wigner one) can be assigned. This PS func-

tion can, regrettably enough, assume negative values so that a probabilistic interpretation becomes questionable. Such limitation was overcome by Husimi [13] (among others). In terms of the concomitant Husimi probability distributions, quantum mechanics can be completely reformulated [14, 15].

The focus of our attention will be, following Ref. [16], the thermal description of the harmonic oscillator (HO) and its phase-space delocalization as temperature grows, in the understanding that the HO is, of course, much more than a mere example, since nowadays it is of particular interest for the dynamics of bosonic or fermionic atoms contained in magnetic traps [17, 18, 19], as well as for any system that exhibits an equidistant level spacing in the vicinity of the ground state, like nuclei or Luttinger liquids. However, a *generalization scheme that allows for going beyond the HO* will be discussed as well (Cf. Sect. VII).

The paper is organized as follows. In Section II we briefly review basic notions about i) Fisher’s information measure and ii) coherent states and Husimi distributions for a system’s thermal state. The nucleus of this communication is developed in Section III: appropriately employing the semi-classical, shift-invariant Fisher measure so as to uncover the rather surprising amount of purely quantum information that it carries. Thermodynamic-like relations are derived in Section IV. A survey on thermal uncertainty relations is introduced in Section V in order to show that, via Fisher, quantum and semi-classical uncertainties can be linked. We are able to establish some special connections between degrees of purity in Section VI, and to go beyond the harmonic oscillator in Section VII. Finally, some conclusions are drawn in Section VIII.

II. BACKGROUND MATERIAL

A. Fisher's information measure

One important information measure is that advanced by R. A. Fisher in the twenties (for a detailed study see Ref. [1, 4]). Consider a $[\theta - \mathbf{x}]$ “scenario” in which we deal with a system specified by a physical parameter θ , while \mathbf{x} is a stochastic variable ($\mathbf{x} \in \mathbb{R}^N$), and $f_\theta(\mathbf{x})$ the probability density for \mathbf{x} (that depends also on θ). One makes a measurement of \mathbf{x} and has to best infer θ from this measurement, calling the resulting estimate $\tilde{\theta} = \tilde{\theta}(\mathbf{x})$. How well θ can be determined? Estimation theory [20] states that the best possible estimator $\tilde{\theta}(\mathbf{x})$, after a very large number of \mathbf{x} -samples is examined, suffers a mean-square error e^2 from θ that obeys a relationship involving Fisher's I , namely, $Ie^2 = 1$, where the Fisher information measure I is of the form

$$I(\theta) = \int d\mathbf{x} f_\theta(\mathbf{x}) \left\{ \frac{\partial \ln f_\theta(\mathbf{x})}{\partial \theta} \right\}^2, \text{ i.e.,} \\ I(\theta) \equiv \left\langle \left\{ \frac{\partial \ln f_\theta(\mathbf{x})}{\partial \theta} \right\}^2 \right\rangle_f. \quad (1)$$

This “best” estimator is the so-called *efficient* estimator. Any other estimator exhibits a larger mean-square error. The only caveat to the above result is that all estimators be unbiased, i.e., satisfy $\langle \tilde{\theta}(\mathbf{x}) \rangle = \theta$. Fisher's information measure has a lower bound: no matter what parameter of the system one chooses to measure, I has to be larger or equal than the inverse of the mean-square error associated with the concomitant experiment. This result,

$$Ie^2 \geq 1, \quad (2)$$

is referred to as the Cramer–Rao bound [1].

1. Shift invariant I -measure

A particular I -case is of great importance: that of translation families [1, 5], i.e., distribution functions (DF) whose *form* does not change under θ -displacements. These DF are shift-invariant (à la Mach, no absolute origin for θ), and for them Fisher's information measure adopts the somewhat simpler appearance [1]

$$I_\tau = \int d\mathbf{x} [1/f(\mathbf{x})] \{ \nabla f(\mathbf{x}) \}^2. \quad (3)$$

The shift-invariant measure I_τ as a function of phase-space coordinates $\tau \equiv (x, p)$ will be the protagonist of this communication. Notice that I_τ is an *additive* measure [1]. Thus, since x and p are independent variables, we will have $I_\tau(x + p) = I_\tau(x) + I_\tau(p)$. We postpone writing down the pertinent Fisher expression until after having briefly reviewed coherent states [see Eq. (24) below].

B. Coherent states and Husimi distribution

The semi-classical Wehrl entropy W is a useful measure of localization in phase-space [8, 21]. It is built up using coherent states $|z\rangle$ [8, 16, 22] and constitutes a powerful tool in statistical physics. Of course, coherent states are eigenstates of a general annihilation operator a , appropriate for the problem at hand, i.e., $a|z\rangle = z|z\rangle$ [22, 23, 24]. The pertinent W -definition reads

$$W = - \int \frac{dx dp}{2\pi\hbar} \mu(x, p) \ln \mu(x, p), \quad (4)$$

clearly a Shannon-like measure [25] to which MxEnt considerations can be applied (see Sect. III B below).

The functions μ , commonly referred to as Husimi distributions [13], are the diagonal elements of the density matrix in the coherent-state basis $|z\rangle$, i.e.,

$$\mu(x, p) = \langle z|\rho|z\rangle. \quad (5)$$

They are “semi-classical” phase-space distribution functions associated to the density matrix ρ of the system [22, 23, 24]. The distribution $\mu(x, p)$ is normalized in the fashion

$$\int \frac{dx dp}{2\pi\hbar} \mu(x, p) = 1. \quad (6)$$

Indeed, $\mu(x, p)$ is a Wigner–distribution D_W , smeared over an \hbar sized region of phase-space [16]. The smearing renders $\mu(x, p)$ a positive function, even if D_W does not have such a character. The semi-classical Husimi probability distribution refers to a *special type* of probability: that for simultaneous but approximate location of position and momentum in phase space [16]. The uncertainty principle manifests itself through the inequality

$$W \geq 1, \quad (7)$$

which was first conjectured by Wehrl [8] and later proved by Lieb [9]. Equality holds if ρ is a coherent state [8, 9].

For dealing with equilibrium states at a temperature T in statistical mechanics one usually represents the system's state as an incoherent superposition (*mixed state*) of eigenenergies E_n weighted by the exponential Boltzmann factor $\exp(-\beta E_n)$, with $\beta = 1/kT$ the inverse temperature and, and k the Boltzmann constant (we take $k = 1$ hereafter). In other words, use is made of Gibbs's canonical distribution, whose associated, “thermal” density matrix is given by

$$\rho = Z^{-1} e^{-\beta \mathcal{H}}, \quad (8)$$

with $Z = Tr(e^{-\beta \mathcal{H}})$ the partition function. In order to conveniently write down an expression for W one considers, for the Hamiltonian \mathcal{H} , its eigenstates $|n\rangle$ and eigenenergies E_n , because one can always write [16]

$$\mu(x, p) = \langle z | \rho | z \rangle = \frac{1}{Z} \sum_n e^{-\beta E_n} |\langle z | n \rangle|^2, \quad (9)$$

with

$$\text{Tr } \rho \equiv \int \frac{dx dp}{2\pi\hbar} \mu(x, p) = 1. \quad (10)$$

A useful route to W starts then with Eq. (9) and continues with Eq. (4). Quantum-mechanical phase-space distributions expressed in terms of the coherent states $|z\rangle$ of the harmonic oscillator have proved to be useful in different contexts [22, 23, 24]. Particular reference is to be made to the illuminating work of Andersen and Halliwell [16], who discuss, among other things, the concepts of Husimi distributions and Wehrl entropy.

C. Harmonic oscillator Husimi results

The above considerations are of a general character. In the special case of the harmonic oscillator, whose Hamiltonian has the form

$$\mathcal{H}_{HO} = \hbar\omega [a^\dagger a + 1/2] = (\hbar\omega/2) [a^\dagger a + a a^\dagger], \quad (11)$$

the (complex) *eigenvalues* z of the annihilation operator a are given by

$$z = \frac{1}{2} \left(\frac{x}{\sigma_x} + i \frac{p}{\sigma_p} \right), \quad (12)$$

where the variables x and p , are scaled by their respective variances (σ) for the HO ground state

$$\sigma_x = (\hbar/2m\omega)^{1/2}; \quad \sigma_p = (\hbar m\omega/2)^{1/2}; \quad \sigma_x \sigma_p = \hbar/2.$$

The Husimi distribution $\mu(x, p)$ adopts the appearance [10, 16]

$$\mu(x, p) \equiv \mu(z) = (1 - e^{-\beta\hbar\omega}) e^{-(1 - e^{-\beta\hbar\omega})|z|^2}, \quad (13)$$

which is normalized in the fashion

$$\int \frac{d^2 z}{\pi} \mu(z) = 1, \quad (14)$$

where $d^2 z / \pi = d(\text{Re } z) d(\text{Im } z) = dx dp / (2\pi\hbar)$ is the differential element of area in the z plane [22] and z is given by Eq. (12). The HO-Wehrl's measure becomes then [10]

$$W = 1 - \ln [1 - e^{-\beta\hbar\omega}]. \quad (15)$$

1. Semi-classical purity

The degree of purity of a density matrix ρ is given by $\text{Tr } \rho^2$ [26]. Its inverse, the so-called *participation ratio*

$$R(\rho) = \frac{1}{\text{Tr } \rho^2}, \quad (16)$$

is particularly convenient for calculations [27]. It varies from unity for pure states to N for totally mixed states [27]. It may be interpreted as the effective number of pure states that enter a quantum mixture. Here we will consider the ‘‘degree of purity’’ d_μ of a semi-classical distribution, given by

$$d_\mu = \int \frac{d^2 z}{\pi} \mu^2(z) \leq 1, \quad (17)$$

to be evaluated below [Cf. (50)].

2. Quantal purity

For the quantum mixed HO-state

$$\rho_{HO} = e^{-\beta\mathcal{H}_{HO}} / Z, \quad (18)$$

with $Z = e^{\beta\hbar\omega/2} / (e^{\beta\hbar\omega} - 1)$ the partition function [28], we have a degree of purity d_ρ given by (see the detailed study by Dodonov [29])

$$d_\rho = \frac{e^{-\beta\hbar\omega}}{Z^2} \sum_{n=0}^{\infty} e^{-2\beta\hbar\omega n}, \quad (19)$$

leading to

$$d_\rho = \tanh(\beta\hbar\omega/2), \quad (20)$$

where $0 \leq d_\rho \leq 1$. Thus, Heisenberg's uncertainty relation can be cast in the fashion

$$\Delta_x \Delta_p = \frac{\hbar}{2} \coth(\beta\hbar\omega/2), \quad (21)$$

where Δx and Δp are the quantum variances for the canonically conjugated observables x and p [29]

$$\Delta x \Delta p = \frac{\hbar}{2} \frac{1}{d_\rho}, \quad (22)$$

which is to be compared to the semi-classical result that we will derive below [Cf. (62)], on the basis of Eq. (17).

3. Basic quantal HO relations

We write down now, for future reference, well-known *quantal* HO-expressions for, respectively, the entropy S , the mean energy U , the mean excitation energy E , and the specific heat C [28]

$$\begin{aligned} S &= \beta \frac{\hbar\omega}{e^{\beta\hbar\omega} - 1} - \ln \{1 - e^{-\beta\hbar\omega}\}, \\ U &= \frac{\hbar\omega}{2} + E = \left[\frac{\hbar\omega}{2} + \frac{\hbar\omega}{e^{\beta\hbar\omega} - 1} \right], \\ C &= -\beta^2 (\partial U / \partial \beta) = \left[\frac{\hbar\omega\beta}{e^{\beta\hbar\omega} - 1} \right]^2 e^{\beta\hbar\omega}. \end{aligned} \quad (23)$$

III. SEMI-CLASSICAL FISHER'S MEASURE

According to the preceding considerations, the Fisher measure (3) associated to the probability distribution $\mu(x, p) \equiv \mu(\tau)$ will be of the form [5]

$$I_\tau = \int \frac{d^2z}{\pi} \mu(z) \left\{ \sigma_x^2 \left[\frac{\partial \ln \mu(z)}{\partial x} \right]^2 + \sigma_p^2 \left[\frac{\partial \ln \mu(z)}{\partial p} \right]^2 \right\}. \quad (24)$$

In the HO instance I_τ becomes, given the μ -expression (13) [10],

$$I_\tau = 1 - e^{-\beta\hbar\omega}. \quad (25)$$

Since the temperature lies between zero and infinity, the range of values of I_τ is

$$0 \leq I_\tau \leq 1. \quad (26)$$

The above entails, via Eq. (23), that the *quantal* HO expressions for E and S can be expressed in terms of the *semi-classical* measure I_τ

$$\begin{aligned} \frac{E}{\hbar\omega} &= \frac{1 - I_\tau}{I_\tau} \\ S &= \beta\hbar\omega \frac{1 - I_\tau}{I_\tau} - \ln I_\tau, \end{aligned} \quad (27)$$

which shows that the semi-classical, Husimi based I_τ -information measure does contain purely quantum-statistical information. The fact that the quantal HO-thermodynamic quantities (q.t.q.) $U = \hbar\omega/2 + E$ and S can be entirely expressed in terms of I_τ , implies that, a posteriori, all q.t.q.'s can be written in these terms. We emphasize thus, as a new result (the first of this communication), the fact that the semi-classical quantity I_τ contains all the relevant HO-statistical quantum information.

In the wake of Eq. (15), for the equilibrium thermal state ρ , the entropy W and the shift invariant Fisher measure I_τ are related according to [10]

$$W + \ln I_\tau = 1, \quad (28)$$

i.e.,

$$e^W I_\tau = e, \quad (29)$$

so that the two measures become complementary informational quantities, which entails that the quantal expressions for E and S can also be cast in terms of W . How stable are the results (27)? To answer this question we resort to a numerical procedure. We build a two-dimensional lattice large enough to accommodate numerical integration in phase-space with precision 1 in 10^{-16} and vary, at each lattice-point, $\mu(z)$ by a random, small amount $\delta\mu(z) = \xi R_{nd}\mu(z)$, with R_{nd} random and ξ a small quantity. We then evaluate the concomitant δW and find $\delta W \propto \xi^2$. Thus, first-order changes in $\mu(z)$ lead to second-order changes in δW , and, consequently, in $\ln I_\tau$. The results (27) are stable against small changes in the Husimi PD.

A. MaxEnt approach

Note also that, from Eq. (13), we can conveniently recast the HO-expression for μ into the Gaussian fashion

$$\mu(z) = I_\tau e^{-I_\tau |z|^2}, \quad (30)$$

peaked at the origin. The Fisher measure I_τ of Eq. (30) is clearly of the maximum entropy (MaxEnt) [25] form (compare, for instance, with Eq. (4.2) of Ref. [30]). As a consequence, it can be viewed in the following light. Assume we know a priori the value $\mathcal{E}_\nu = \langle \hbar\omega |z|^2 \rangle_\nu$. We wish to determine the distribution $\nu(z)$ that maximizes the Wehrl entropy W under this \mathcal{E}_ν -value constraint. Accordingly, the MaxEnt distribution will be [25]

$$\nu(z) = e^{-\lambda_o} e^{-\eta E(z)}, \quad (31)$$

with λ_o the normalization Lagrange multiplier and η the one associated to \mathcal{E}_ν . According to MaxEnt tenets we have [25]

$$\lambda_o = \lambda_o(\eta) = \ln \int \frac{d^2z}{\pi} e^{-\eta \hbar\omega |z|^2} = -\ln(\eta \hbar\omega). \quad (32)$$

Now, the η -multiplier is determined by the relation [25]

$$-\mathcal{E}_\nu = \frac{\partial \lambda_o}{\partial \eta} = -\frac{1}{\eta}. \quad (33)$$

If we choose the Fisher-Husimi constraint given by Eq. (44) $\mathcal{E}_\mu = \hbar\omega/I_\tau$, this results in

$$\begin{aligned}
\eta &= I_\tau/(\hbar\omega), \text{ and, from (32)} \\
\lambda_o &= -\ln I_\tau \text{ i.e.,} \\
e^{-\lambda_o} &= I_\tau \text{ and} \\
\nu(z) &= I_\tau e^{-I_\tau |z|^2} \equiv \mu(z). \tag{34}
\end{aligned}$$

We have thus shown that the HO-Husimi distributions are MaxEnt-ones with the semi-classical excitation energy (44) as a constraint, our 2th new result. It is clear from Eq. (34) that I_τ plays there the role of an “inverse temperature”. This means that we can think of a quantity T_W associated to the Wehrl measure on account of

$$\mu(z) = I_\tau e^{-(I_\tau/\hbar\omega) \hbar\omega|z|^2} = I_\tau e^{-\mathcal{E}_\mu/T_W}, \tag{35}$$

which entails

$$T_W = \hbar\omega/I_\tau; \quad (\hbar\omega \leq T_W \leq \infty). \tag{36}$$

Due to the semi-classical nature of both W and μ , T_W has a lower bound greater than zero. At this stage we introduce a “delocalization factor” D

$$\begin{aligned}
D &= T_W/\hbar\omega \Rightarrow \\
W &= 1 + \ln T_W - \ln \hbar\omega = 1 + \ln D, \tag{37}
\end{aligned}$$

to be discussed next.

B. Delocalization revisited

As stressed above, W has been conceived as a delocalization measure. The preceding considerations clearly motivate one to regard, as well, the Fisher measure built up with Husimi distributions $|z\rangle$ (Cf. Eq. (12)) as a “localization estimator” in phase space. It has been shown already in Ref. [10] that efficient estimation (meaning that the Cramer–Rao lowest bound is reached) is possible for all temperatures T . The HO-Gaussian expression for μ (30) illuminates the fact that the Fisher measure controls height, on the one hand, and spread, on the other one (that is $\sim [2I_\tau]^{-1}$). Obviously, spread is here a “phase-space delocalization indicator”. This fact is reflected by the quantity D introduced above.

Thus, an original physical interpretation of Fisher’s measure emerges: localization control. The inverse of the Fisher measure, D , turns out then to be a delocalization-indicator. Notice also that

$$\frac{dI_\tau}{dT} = -\frac{\hbar\omega}{T^2} e^{-\beta\hbar\omega}, \tag{38}$$

so that Fisher’s information decreases exponentially as the temperature grows. Our Gaussian distribution loses phase-space “localization” as energy and/or temperature are injected into our system, as reflected via T_W or D . Remark that (37) complements the Lieb bound $W \geq 1$. W exceeds unity by virtue of delocalization effects, and this can be expressed using the shift-invariant Fisher measure (our 3rd. new result). We will now show that D is proportional to the system’s energy fluctuations.

C. Second moment of the Husimi distribution

The second moment of the Husimi distribution $\mu(z)$ given by Eq. (30) is defined as [31]

$$M_2 = \int \frac{d^2z}{\pi} \mu^2(z), \tag{39}$$

that, after explicit evaluation of M_2 reads

$$M_2 = \frac{I_\tau}{2}. \tag{40}$$

Using now (37) we conclude that

$$M_2(D) = \frac{1}{2D}. \tag{41}$$

In order to give physical meaning to this result consider the energy-fluctuations evaluated via the distribution function $\mu(z)$. The semi-classical energy \mathcal{E}_μ is

$$\mathcal{E}_\mu = \int \frac{d^2z}{\pi} \mu(z) E(z), \tag{42}$$

with [32]

$$E(z) = \langle z|H|z\rangle - \frac{\hbar\omega}{2} = \hbar\omega|z|^2 = \langle z|\hbar\omega a^\dagger a|z\rangle. \tag{43}$$

Thus,

$$\mathcal{E}_\mu = \frac{\hbar\omega}{I_\tau}. \tag{44}$$

Comparing now with Eq. (23) we see that

$$\mathcal{E}_\mu - E = \hbar\omega, \tag{45}$$

i.e., the difference between the semi-classical energy \mathcal{E}_μ and the mean quantum energy U equals $\hbar\omega/2$, the vacuum-energy, independently of T . For our purposes we need also the semi-classical mean value of $(\mathcal{E}^2)_\mu$

$$(\mathcal{E}^2)_\mu = \int \frac{d^2z}{\pi} \mu(z) E(z)^2, \tag{46}$$

i.e.,

$$(\mathcal{E}^2)_\mu = 2 \left(\frac{\hbar\omega}{I_\tau} \right)^2, \tag{47}$$

so that, finally, our energy-fluctuations turn out to be

$$\Delta_\mu E = \frac{\hbar\omega}{I_\tau} = \hbar\omega D, \tag{48}$$

with $(\Delta_\mu E)^2 = (\mathcal{E}^2)_\mu - \mathcal{E}_\mu^2$. As a consequence, we get

$$D = \frac{\Delta_\mu E}{\hbar\omega}. \tag{49}$$

An important new result (our 4th. one) is thus obtained: the delocalization factor D represents energy-fluctuations expressed in $\hbar\omega$ -terms. Delocalization is clearly seen to be the counterpart of energy fluctuations!

D. Purity and delocalization

Uncertainty arguments can also be used for “purity” purposes [26] (Cf. (17)). The semi-classical degree of purity is given by

$$d_\mu = \int \frac{d^2z}{\pi} \mu^2(z) = \frac{I_\tau}{2} = \frac{1}{2D}, \quad (50)$$

so that $0 \leq d_\mu \leq 1/2$. Notice that I_τ is [Cf. Eq. (3)] is a mean value evaluated with a semi-classical distribution, which helps to achieve a first understanding of the low value (1/2) of the degree of purity’s upper bound. A more complete discussion is given below.

IV. THERMODYNAMICS-LIKE RELATIONS

We now go back to Eq. (23) and take a hard look at the entropic expression and see that we can recast the entropy S in terms of the quantal mean excitation energy E and the delocalization factor D (the information I_τ) as

$$\frac{E}{T} = S - \ln D, \quad (51)$$

i.e., if one injects into the system some excitation energy E , expressed in “natural” T units (remember that we have set $k = 1$), it is apportioned partly as heat dissipation via S and partly via delocalization. More precisely, the part of this energy not dissipated is that employed to delocalize the system in phase space. Now, since $W = 1 - \ln I_\tau = 1 + \ln D$, the above equation can be recast in alternative forms, as

$$S = \frac{E}{T} + \ln D = \frac{E}{T} - \ln I_\tau; \quad \text{or :} \quad (52)$$

$$W = 1 + S - \frac{E}{T}, \quad (53)$$

implying

$$W - S \mapsto 0 \quad \text{for } T \mapsto \infty, \quad (54)$$

which is a physically sensible one and

$$W - S \mapsto 1 \quad \text{for } T \mapsto 0, \quad (55)$$

as it should, since $S = 0$ at $T = 0$ (third law of thermodynamics), while W attains there its Lieb’s lower bound of unity.

One finds in Eq. (52) some degree of resemblance to thermodynamics’s fist law. To reassure ourselves on this point, we slightly changed our underlying canonical probabilities (8), multiplying them by a factor $\mathcal{F} =$

random number/100, i.e., we generated random numbers according to the normal distribution divided by 100 to obtain the above factors. This entails new “perturbed” probabilities P_i , conveniently normalized ($\sum P_i = 1$). With them we evaluate the concomitant changes dS , dE (we did this 50 times, with different random numbers in each instance) and verified that, numerically, the difference $dS - \beta dE \sim 0$. The concomitant results are plotted in Fig. 1. Since, as stated, numerically $dS = (1/T) dE$, this entails, from Eq. (52), $dI_\tau/I_\tau \simeq 0$. The physical connotations are as follows: if the *only* modification effected is that of a “population” change δp_i in the p_i , this implies that the system undergoes a heat transfer process [28] for which thermodynamics’ first law implies $dU = TdS$ and this is numerically confirmed in the plots of Fig. 1. The null contribution of $\ln I_\tau$ to this process suggests that delocalization (not a thermodynamic effect, but a dynamic one) can be looked at as behaving (thermodynamically) like a kind of “work”.

Now, since (a) [Cf. (25)] $I_\tau = 1 - e^{-\beta\hbar\omega}$, and (b) the mean energy of excitation is $E = \hbar\omega/[\exp(\beta\hbar\omega) - 1]$ one also finds, for the quantum-semi-classical difference (QsCD) $S - W$ the original (as far as we know) result

$$W - S = 1 - [(I_\tau - 1)/I_\tau] \ln(1 - I_\tau) = F_1(I_\tau) \quad (56)$$

Moreover, since $0 \leq F_1(I_\tau) \leq 1$, we see that, always, $W \geq S$, as expected, since the semi-classical treatment contains less information than the quantal one. Note that the QsCD can be expressed exclusively on Fisher’s information measure. This is, the quantum-semi-classical entropic difference $S - W$ may be given in I_τ -terms only, which is a new Fisher-property (our 5th. new result). Fig. 2 depicts S , βE , and $\ln D$ vs. the dimensionless quantity $t = T/\hbar\omega$. According to Eq. (51), entropy is apportioned in such a way that

- part of it originates from excitation energy and
- the remaining is accounted for by phase-space delocalization.

A bit of algebra allows one now to express the rate of entropic change per unit temperature increase as

$$\frac{dS}{dT} = \beta \frac{dE}{dT} = \beta C = \hbar\omega \frac{1}{T} \frac{dD}{dT}, \quad (57)$$

entailing

$$C = \hbar\omega \frac{dD}{dT}. \quad (58)$$

In the case of the one dimensional HO we see that the specific heat measures delocalization change per unit temperature increase. Also, $dE/dT \propto dD/dT$, providing us with a very simple relationship between (mean) excitation energy changes and delocalization ones (our 6th new result)

$$\frac{dE}{dD} = \hbar\omega. \quad (59)$$

V. “THERMAL” UNCERTAINTIES

Thermal uncertainties express the effect of temperature on Heisenberg’s celebrated relations (see, for instance [7, 29, 33, 34]). We use now a result obtained in Ref. [16] (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

$$W = \ln \left\{ \frac{e}{\hbar} \Delta_\mu x \Delta_\mu p \right\}. \quad (60)$$

In the present context, the relation $W = 1 - \ln I_\tau$ allows us to conclude that [10]

$$I_\tau \Delta_\mu x \Delta_\mu p = \hbar, \quad (61)$$

which can be regarded as a “Fisher uncertainty principle” and adds still another meaning to I_τ : since, necessarily, $\Delta_\mu x \Delta_\mu p \geq \hbar/2$, it is clear that $I_\tau/2$ is the “correcting factor” that permits one to reach the uncertainty’s lower bound $\hbar/2$.

As stated above, phase space “localization” is possible, with Husimi distributions, only up to \hbar . This is to be compared to the uncertainties evaluated in a purely quantal fashion, without using Husimi distributions. By recourse to the virial theorem [28] one easily ascertains that [10]

$$\begin{aligned} \Delta x \Delta p &= \frac{\hbar}{2d_\rho} = \frac{\hbar}{2} \frac{e^{\beta\hbar\omega} + 1}{e^{\beta\hbar\omega} - 1} \Rightarrow \\ \Delta_\mu x \Delta_\mu p &= \frac{2 \Delta x \Delta p}{1 + e^{-\beta\hbar\omega}}. \end{aligned} \quad (62)$$

As $\beta \rightarrow \infty$, $\Delta_\mu \equiv \Delta_\mu x \Delta_\mu p$ is twice the minimum quantum value for $\Delta x \Delta p$, and $\Delta_\mu \rightarrow \hbar$, the “minimal” phase-space cell. The quantum and semi-classical results do coincide at very high temperature, though. Indeed, one readily verifies [10] that Heisenberg’s uncertainty relation, as a function of both frequency and temperature, is governed by a thermal “uncertainty function” F that acquires the aspect

$$F(\beta, \omega) = \Delta x \Delta p = \frac{1}{2} \left[\Delta_\mu + \frac{E}{\omega} \right]. \quad (63)$$

Within the present context F can be recast as

$$F(\beta, \omega) = \frac{1}{2} \left[\hbar D + \frac{E}{\omega} \right], \quad (64)$$

so that, for T varying in $[0, \infty]$, the range of possible $\Delta x \Delta p$ -values is $[\hbar/2, \infty]$. Eq. (64) is a “Heisenberg–Fisher” thermal uncertainty (TU) relation (for a discussion of the TU concept see, for instance, [7, 33, 34]).

$F(\beta, \omega)$ grows with both E and D . The usual result $\hbar/2$ is attained for minimum D and zero excitation energy. As for dF/dT , one is able to set $F \equiv F(E, D)$, since $2dF = \hbar dD + \omega^{-1} dE$. Remarkably enough, the two contributions to dF/dT are easily seen to be equal and $dF/dT \rightarrow (1/\omega)$ for $T \rightarrow \infty$. One can also write

$$\left(\frac{\partial F}{\partial D} \right)_E = \frac{\hbar}{2}; \quad \left(\frac{\partial F}{\partial E} \right)_D = \frac{1}{2\omega}, \quad (65)$$

providing us with a thermodynamic “costume” for the uncertainty function F that sheds some new light onto the meaning of both \hbar and ω .

In particular, we see that $\hbar/2$ is the derivative of the uncertainty function F with respect to the delocalization factor D . Increases dF of the thermal uncertainty function F are of two types (our 7th. new result)

- i) from the excitation energy, that supplies a C/ω contribution and
- ii) from the delocalization factor D

Additionally, on account of Eq. (61), on the one hand, and since the degree of purity reads [Cf. Eq. (50)] $d_\mu = I_\tau/2$, on the other one, we are led to *an uncertainty relation for mixed states in terms of d_μ* , namely,

$$\Delta_\mu x \Delta_\mu p = \frac{\hbar}{2} \frac{1}{d_\mu}, \quad (66)$$

that tells us just how uncertainty grows as participation ratio $R = 1/d_\mu$ augments (8th. new result). Eq. [(66)] is of semi-classical origin, which makes it a bit different from the one that results form a purely quantal treatment [see [29], Eq. (4)].

VI. DEGREES OF PURITY’S RELATIONS

We relate now the degree of purity of our thermal state with various physical quantities both in its quantal and semi-classical versions (our 9th. new result). This will explain the upper bound 1/2 of the semi-classical purity d_μ . Using Eqs. (62) and (66) we get

$$d_\mu = \frac{I_\tau}{2} = (1 - d_\mu) d_\rho, \quad (67)$$

which leads to

$$\begin{aligned} d_\rho &= \frac{d_\mu}{1 - d_\mu} = \frac{I_\tau}{2 - I_\tau}, \\ d_\mu &= \frac{d_\rho}{1 + d_\rho} \end{aligned} \quad (68)$$

such as clearly shows that (i) $d_\mu \leq d_\rho$, and (ii) for a pure state, its semi-classical counterpart has a degree of purity

equal 1/2. Moreover, notice how information concerning the purely quantal notion of purity d_ρ is already contained in the semi-classical measure I_τ .

We appreciate the fact that R increases as delocalization grows, a quite sensible result. Fig. 3 depicts $d_\mu(T)$, a monotonously decreasing function, which tells us that degree of purity acts here as a thermometer. Also, from Eq. (25) we see that $\beta\hbar\omega = -\ln(1 - I_\tau)$. Thus, we can rewrite Eq. (56) in the following form

$$W - S = 1 + \beta\hbar\omega \frac{2d_\mu - 1}{2d_\mu} = 1 + \beta\hbar\omega \frac{d_\rho - 1}{2d_\rho}, \quad (69)$$

which casts the difference between the quantal and semi-classical entropies in terms of the degrees of purity. From Eq. (69) we can also give the quantal mean energy in terms of d_μ using Eqs. (25) and (27)

$$E = \frac{\hbar\omega}{2} \frac{1 - 2d_\mu}{d_\mu} = \frac{\hbar\omega}{2} \frac{1 - d_\rho}{d_\rho}. \quad (70)$$

VII. GENERALIZATIONS

Eqs. (11) and (12) can be generalized. It is well known (see, for instance, [35] and references therein) that, for more general Hamiltonians \mathcal{H}_G with discrete spectra, one can always find a representation that writes

$$H_G = a_0 + a_1\eta^\dagger\eta + a_1^*\eta\eta^\dagger, \quad (a_0, a_1 \text{ given constants}), \quad (71)$$

where η , of eigenvalue z_η , is a generalized annihilation operator that can be obtained using a definite algorithm [35]. The equation $\eta|z_\eta\rangle = z_\eta|z_\eta\rangle$ generates generalized coherent states and, in turn, generalized Husimi distributions. Most of our results above follow by replacement of $\hbar\omega$ by a suitable combination of a_0 , a_1 , and a_1^* . Work in such direction is currently being performed.

VIII. CONCLUSIONS

Our statistical semi-classical study yielded, we believe, some new interesting physics that we proceed to summarize. We have, for the HO,

1. established that the semi-classical Fisher measure I_τ contains all relevant statistical quantum information,
2. shown that the Husimi distributions are MaxEnt ones, with the semi-classical excitation energy \mathcal{E} as the only constraint,
3. complemented the Lieb bound on the Wehrl entropy using I_τ ,
4. seen in detailed fashion how delocalization becomes the counterpart of energy fluctuations,
5. written down the difference $W - S$ between the semi-classical and quantal entropy also in I_τ -terms,
6. provided a relation between energy excitation and degree of delocalization,
7. shown that the derivative of twice the uncertainty function $F(\beta\omega) = \Delta x \Delta p$ with respect to I_τ^{-1} is the Planck constant \hbar ,
8. established a semi-classical uncertainty relation in terms of the semi-classical purity d_μ , and
9. expressed both d_μ and the quantal degree of purity in terms of I_τ .

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FIG. 1: Numerical computation results for the HO: changes dI_τ and dU vs. dS that ensue after randomly generating variations δp_i in the underlying microscopic canonical probabilities p_i .

FIG. 2: S , βE , and $\ln D$ as a function of $t = T/(\hbar\omega)$.

FIG. 3: Semi-classical purity d_μ vs. $T/h\nu$, a monotonous function.





