Semiclassical statistical mechanics’ tools for deformed algebras

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In order to enlarge the present arsenal of semiclassical tools we explicitly obtain here the Husimi distributions and Wehrl entropy within the context of deformed algebras built up on the basis of a new family of \( q \)-deformed coherent states, those of Quesne [J. Phys. A 35, 9213 (2002)]. We introduce also a generalization of the Wehrl entropy constructed with escort distributions. The two generalizations are investigated with emphasis on i) their behavior as a function of temperature and ii) the results obtained when the deformation-parameter tends to unity.

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I. INTRODUCTION

The semiclassical approach has had a long and distinguished history and is a very important weapon in the physicist’s armory. Indeed, semiclassical approximations to quantum mechanics remain an indispensable tool in many areas of physics and chemistry. Despite the extraordinary evolution of computer technology in the last years, exact numerical solution of the Schrödinger equation is still quite difficult for problems with more than a few degrees of freedom. Another great advantage of the semiclassical approximation lies in that it facilitates an intuitive understanding of the underlying physics, which is usually hidden in blind numerical solutions of the Schrödinger equation. Although semiclassical mechanics is as old as the quantum theory itself, the field is continuously evolving. There still exist many open problems in the mathematical aspects of the approximation as well as in the quest for new effective ways to apply the approximation to various physical systems (see, for instance, [1, 2] and references therein).

In a different vein, applications of the so-called \( q \)-calculus to statistical mechanics have accrued increasing interest lately [3]. This \( q \)-calculus [4] has its origin in the \( q \)-deformed harmonic oscillator theory, which, in turn, is based on the construction of a \( SU_q(2) \) algebra of \( q \)-deformed commutation or anti-commutation relations between creation and annihilation operators [5, 6, 7]. The above mentioned applications also employ “deformed information measures” (DIM) that have been applied to different scientific disciplines (see, for example, [8, 9] and references therein). DIMs were introduced long ago in the cybernetic-information communities by Harvda-Charvat [10] and Vadja [11] in 1967-68, being rediscovered by Daroczy in 1970 [12] with several echoes mostly in the field of image processing. For a historic summary and the pertinent references see Ref. [13]. In astronomy, physics, economics, biology, etc., these deformed information measures are often called \( q \)-entropies since 1988 [8].

In this work we are concerned with semiclassical statistical physics’ problems and wish to add tools to the semiclassical armory by, in particular, investigating putative \( q \)-deformed extensions of two of its most important quantities, namely, Husimi distributions (HD) and Wehrl entropies (WE). We will work within the context of deformed algebras built up with the new family of \( q \)-deformed coherent states introduced recently by Quesne [14], analyzing the main HD and WE properties.

Our attention will be focused on the thermal description of the harmonic oscillator (HO) (together with its phase-space delocalization as temperature grows), in the understanding that the HO is, of course, much more than a mere example, since in addition to the extensive use Glauber states in molecular physics and chemistry [15, 16], nowadays the HO is of particular interest for the dynamics of bosonic or fermionic atoms contained in magnetic traps [17, 18], as well as for any system that exhibits an equidistant level spacing in the vicinity of the ground state, like nuclei or Luttinger liquids.

The paper is organized as follows: in Section II we introduce the behavior of the HD and the WE for the HO, studying the fluctuations in thermal equilibrium while, in Section III the new \( q \)-deformed coherent states are introduced. We study the behavior of our generalizations of both the HD and the WE in Sections IV and VI respectively. Generalized WE’s bounds are analyzed in Section VII, while, in Section VIII we deal with escort distributions, which allow us to build up an alternative generalization of the WE. Finally, some conclusions are drawn in Section VIII.
II. SEMICLASSICAL DISTRIBUTION IN PHASE-SPACE

Wehrl’s entropy $W$ is a very useful measure of localization in phase-space \[19\]. It is built up using coherent states \[19, 20, 21\] and constitutes a powerful tool in statistical physics. The pertinent definition reads

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

where $\mu(x, p) = \langle z | \rho | z \rangle$ is a “semi-classical” phase-space distribution function associated to the density matrix $\rho$ of the system \[15, 20\]. Coherent states are eigenstates of the annihilation operator $a$, i.e., satisfies $a | z \rangle = z | z \rangle$.

The distribution $\mu(x, p)$ is normalized in the fashion

$$ \int (dx dp/2\pi \hbar) \mu(x, p) = 1, \quad (2) $$

and it is often referred to as the Husimi distribution \[22\].

The last two equations clearly indicate that the Wehrl entropy is simply the “classical entropy” \[1\] of a Wigner-distribution. Indeed, $\mu(x, p)$ is a Wigner-distribution $D_W$ smeared over an $\hbar$ sized region of phase space \[21\]. 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 and momentum in phase space \[21\]. The uncertainty principle manifests itself through the inequality $1 \leq W$, which was first conjectured by Wehrl \[19\] and later proved by Lieb \[23\].

The usual treatment of equilibrium in statistical mechanics makes use of the Gibbs’s canonical distribution, whose associated, “thermal” density matrix is given by

$$ \rho = Z^{-1} e^{-\beta H}, \quad (3) $$

with $Z = \text{Tr}(e^{-\beta H})$ the partition function, $\beta = 1/k_B T$ the inverse temperature $T$, and $k_B$ the Boltzmann constant. In order to conveniently write down an expression for $W$ consider an arbitrary Hamiltonian $H$ of eigen-energies $E_n$ and eigenstates $|n\rangle$ ($n$ stands for a collection of all the pertinent quantum numbers required to label the states). One can always write \[21\]

$$ \mu(x, p) = \frac{1}{Z} \sum_n e^{-\beta E_n} |\langle z | n \rangle|^2. \quad (4) $$

A useful route to $W$ starts then with Eq. \[4\] and continues with Eq. \[1\]. In the special case of the harmonic oscillator the coherent states are of the form \[20\]

$$ |z\rangle = e^{-|z|^2/2} \sum_{n=0}^{\infty} \frac{z^n}{\sqrt{n!}} |n\rangle, \quad (5) $$

where $|n\rangle$ are a complete orthonormal set of eigenstates and whose spectrum of energy is $E_n = (n+1/2) \hbar \omega$, $n = 0, 1, \ldots$ In this situation the analytic expression for the HD and the WE were obtained in Ref. \[21\]

$$ \mu(z) = (1 - e^{-\beta \hbar \omega}) e^{-\left(1-e^{-\beta \hbar \omega}\right)|z|^2}, \quad (6) $$

$$ W = 1 - \ln(1 - e^{-\beta \hbar \omega}). \quad (7) $$

When $T \to 0$, the entropy takes its minimum value $W = 1$, expressing purely quantum fluctuations. On the other hand when $T \to \infty$, the entropy tends to the value $-\ln(\beta \hbar \omega)$ which expresses purely thermal fluctuations.

III. QUESNE’S NEW $q$-DEFORMED COHERENT STATES

Quesne advanced in Ref. \[14\] a new family of harmonic oscillator physical states, labelled by $0 < q < 1$ and $z \in \mathbb{C}$,

$$ |z\rangle_q = N_q^{-1/2} \sum_{n=0}^{\infty} \frac{z^n}{\sqrt{n!}} |n\rangle, \quad (8) $$

where $|n\rangle = (n!)^{-1/2} |n\rangle |0\rangle$ is the $n$-boson state and one introduces quasi-factorials \[14\]

$$ [n]_q! \equiv \begin{cases} [n]_q[n-1]_q \ldots [1]_q & \text{if } n = 1, 2, 3 \ldots \\ 1 & \text{if } n = 0 \end{cases} \quad (9) $$

with

$$ [n]_q! \equiv \frac{1 - q^{-n}}{q - 1} = q^{-n} [n]_q! \quad (10) $$

where $[n]_q$ is called the “$q$-basic number” and generates its own factorial (the $q$-factorial) \[14\]. The $q$-factorial can also be written in terms of the $q$-gamma function $\Gamma_q(x)$ \[14\]

$$ [n]_q! = q^\frac{[n+q]_q}{2} \Gamma_q(n+1) = q^{-\frac{[n+q]_q}{2}} [n]_q! \quad (11) $$

that, in the limit $q \to 1$, yields $[n]_q!, [n]_q!$, and $\Gamma_q(n)$ tending to $n, n!$, and $\Gamma(n)$, respectively. The states $|z\rangle_q$ allow one to build up $q$-deformed coherent states. They will be acceptable generalized coherent states if three basic mathematical properties are verified \[15\]. The states $|z\rangle_q$ should be: i) normalizable, ii) continuous in the $z$-label. Additionally, iii) one must ascertain the existence of a resolution of unity with a positive weight function. The normalization condition, $\langle z | z \rangle_q = 1$ leads to

$$ N_q(|z|^2) = \sum_{n=0}^{\infty} \frac{(|z|^2)^n}{[n]_q!} = E_q((1-q)q|z|^2), \quad (11) $$

where $E_q(x) = \prod_{k=0}^{\infty} (1+q^k x)$ is one of the so-called Jackson’s $q$-exponentials introduced in 1909 \[20\] such that
\[ \lim_{q \to 1} E_q[(1 - q)x] = e^x. \] Since \( N_q(\vert z \vert^2) \) is equal to \( E_q[(1 - q)q \vert z \vert^2] \) (a well defined function in \( 0 < q < 1 \)), the new states are normalizable on the whole complex plane. On the other hand, the states \( \vert z \rangle_q \) are always continuous in \( z \). Finally, for the resolution of unity one needs

\[ \int \int d^2z |z\rangle_q K_q(|z|^2) \langle z| = \sum_{n=0}^{\infty} |n\rangle \langle n| = I, \] (12)

with a weight function \( K_q(|z|^2) \) that can be obtained using the expressions for \( |z\rangle_q \) and its conjugate and then performing the integral by recourse to the \( q \)-analogue of the Euler gamma integral. Quesne finds

\[ K_q(|z|^2) = \frac{1 - q}{\pi \ln q^{-1}} \frac{E_q[(1 - q)q |z|^2]}{E_q[(1 - q)q |z|^2]}. \] (13)

It is seen that, in the limit \( q \to 1^- \), we have \( K_q(|z|^2) \to K(|z|^2) = 1/\pi \), corresponding to the weights for the conventional coherent states of the harmonic oscillator. This entails that we indeed have at hand new \( q \)-deformed coherent states that fulfill the standard properties. In the next section we start presenting the results of this communication, using these Quesne-coherent states to generalize our \( q \)-Husimi distribution.

### IV. The \( q \)-Husimi Distribution to \( 0 < q < 1 \)

We define the \( q \)-Husimi distribution (\( q \)-HD) in the rather "natural" fashion

\[ \mu_q(z) = q(z)\rho(z)_q, \] (14)

using Quesne’s HO-\( q \)-coherent states \( \langle q \rangle \). From these it is easy to find an analytic expression for our new \( q \)-Husimi distributions

\[ \mu_q(z) = (1 - e^{-\beta \hbar \omega}) \frac{E_q[(1 - q)q |z|^2 e^{-\beta \hbar \omega}]}{E_q[(1 - q)q |z|^2]}. \] (15)

It is important to remark that

\[ \lim_{q \to 1^-} \mu_q(z) = \mu(z), \] (16)

where \( \mu(z) \) is given by (6). We have numerically ascertained that our \( q \)-Husimi distribution is normalizing using the same weight function \( K_q(|z|^2) \) that Quesne employed for the resolution of unity of her \( q \)-coherent states.

\[ \int \int d^2z K_q(|z|^2) \mu_q(z) = 1. \] (17)

We see in Fig. 1 that a \( q \)-HD’s height depends only upon the temperature (not on \( q! \)). \( q \)-Deformation affects only shapes. Thus,

\[ 0 < \mu_q(z) \leq 1, \] (18)

and \( \mu_q(z) \) remains a legitimate semi-classical probability distribution (unlike Wigner’s one).

### V. Deformed Wehrl Entropies

In order to introduce deformed Wehrl entropies we start by reminding the reader of the concept of \( q \)-deformed measures, that read

\[ S_q = -k_B \int d\Omega f(x)^q \ln_q f(x), \] (19)

where \( k_B \) is the constant of Boltzmann’s, \( f(x) \) a normalized probability density, and one defines the \( q \)-logarithm function in the fashion \( \ln_q x = (1 - x^{1-q})/(q - 1) \) with \( x > 0; \ q \in \mathbb{R} \),

\[ \ln_q x = (1 - x^{1-q})/(q - 1) \] with \( x > 0; \ q \in \mathbb{R} \) (20)

where \( q \) is called the deformation index (the signature of the "deformed" nature of the measure). For \( q = 1 \) we reobtain the ordinary logarithm and the logarithmic Shannon measure. The measure (19) can also be generated using the \( q \)-calculus introduced by Jackson (20) in the following form (21)

\[ S_q = -k_B D_a^{(q)} g(\alpha)|_{\alpha = 1}, \] (21)

where \( g(\alpha) = \int dx f(x)^\alpha \) and \( D_a^{(q)} \) is Jackson’s \( q \)-derivative operator

\[ D_a^{(q)} = \frac{h(qx) - h(x)}{q x - x}, \] (22)

which reduces to the ordinary Leibnitz-one \( d/dx \) when the parameter \( q \) goes to unity (27).
Accordingly, the natural definition of a deformed Wehrl entropy reads as follows

\[ W_q \equiv - \int \tfrac{1}{2} d^2 z K_q (|z|^2) \mu_q (z) \ln \mu_q (z), \]  

(23)

and, inserting the explicit HO-form into the above expression, we find

\[ W_q = f(q) - \ln(1 - e^{-\beta \omega}) \equiv f(q) - 1 + W, \]  

(24)

where

\[ f(q) = - \int K_q d^2 z \mu_q \ln \left\{ \frac{\mu_q}{1 - e^{-\beta \omega}} \right\}. \]  

(25)

It easy to check that in the limit \( q \to 1 \) one has \( f(q) \to 1 \) and Eq. (24) leads to the usual Wehrl entropy. The \( q \)-Wehrl entropy can not be obtained in analytic fashion and needs numerical evaluation. In Fig. 2 we plot \( W_q \) vs. \( t (t = T/\hbar \omega) \) for several values of the parameter \( q \).

![Diagram](image)

**FIG. 2:** \( W_q (\mu_q) \) vs. \( t (t = T/\hbar \omega) \), for values ranging downwards from \( q = 0.95 \) to \( q = 0.50 \). The standard standard WE \( (q = 1) \) is also represented.

We see from and comparison with the conventional HO-Wehrl entropy \( W = 1 - \ln(1 - e^{-\beta \omega}) \) that deformation merely entails a constant-in-z additive function \( f(q) \), depending solely on \( q \), as depicted in Fig. 2 so that \( W_q \) behaves, as a function of deformation, exactly like the \( q \)-distributions of the previous Sections. At low enough temperatures our \( q \)-coherent states minimize the \( q \)-entropy, i.e., \( W_q \sim 1 \), yielding maximal localization. Delocalization grows with \( T \), of course.

At this stage we are in a position to draw an important consequence. In general, deformed (or Tsallis') entropies are quite different objects as compared with Shannon’s one, save for \( q \) close to unity. This is not the case for Wehrl entropies! \( q \)-deformation becomes in this case a smooth shape-deformation. At the semiclassical level the difference between Tsallis and Shannon entropies becomes weaker than either at the quantal or the classical levels.

**VI. WEHRL ENTROPY BOUNDS**

Using the definition of the \( q \)-WE given by Eq. (24) we can easily investigate possible bounds for the Wehrl entropy, i.e., for our localization power. We see that, when \( T \to 0 \), one has

\[ W_q \to A_q \equiv \frac{(q - 1)}{\ln(q)} g(q), \]  

(26)

where

\[ g(q) = \int_0^\infty d|z|^2 \ln \left( \frac{E_q (1 - q)|z|^2}{E_q (1 - q)|z|^2} \right). \]  

(27)

while, for \( T \to \infty \),

\[ W_q \to - \ln(\beta \hbar \omega) = \infty, \]  

(28)

having a lower bound only. Since, obviously, \( W_q \) is a monotonously growing function of \( T \) we can state that

\[ A_q \leq W_q, \]  

(29)

which constitutes the new deformed Lieb-relation. It is easy to check the limit \( q \to 1 \):

\[ \lim_{q \to 1} A_q = 1, \]  

(30)

and we reobtain the known Lieb bound of the standard Wehrl entropy \( 1 \leq W \). In Table 1 we illustrate the behavior of the function \( A_q \) vs. \( q \). We note that the function reproduces the values of the \( q \)-Wehrl entropy at \( T = 0 \), as expected.

| \( q \)  | \( A_q \)  |
|---|---|
| 0.50 | 1.5289 |
| 0.55 | 1.4337 |
| 0.60 | 1.3536 |
| 0.65 | 1.2852 |
| 0.70 | 1.2264 |
| 0.75 | 1.1753 |
| 0.80 | 1.1307 |
| 0.85 | 1.0916 |

**VII. ESCORT GENERALIZATIONS**

In this Section we consider a new possible deformation of the entropy, which we shall call \( q \)-escort Wehrl entropy.
(q-eWE). It is build up from a deformation of the HD advanced in Ref. [24], called the q-escort Husimi distribution (q-eHD). In general, given a normalized probability density (PD) \( f(x) \), its associated q-escort PD \( F(x) \) reads

\[
F(x) = \frac{f(x)^q}{\int dx f(x)^q}.
\]

(31)

If we replace here \( f(x) \) by the Husimi distribution one gets [24]

\[
\gamma_q(|z|) = q(1 - e^{-\beta \hbar \omega}) \exp[-q|z|^2(1 - e^{-\beta \hbar \omega})],
\]

(32)

where \( q \in (1, \sqrt{2}) \) [24].

Our goal is now to get the associated q-Wehrl’s entropy. Replacing Eq. (32) into Eq. (31), we immediately find

\[
W_q(\gamma_q) = q^2(1 - e^{-\beta \hbar \omega})^2 I_q - \ln[q(1 - e^{-\beta \hbar \omega})] N_q,
\]

(33)

where

\[
I_q = \int \frac{d^2z}{\pi} |z|^2 \exp[-q|z|^2(1 - e^{-\beta \hbar \omega})],
\]

(34)

and

\[
N_q = \int \frac{d^2z}{\pi} \gamma_q(|z|).
\]

(35)

Integrating over all phase space one finds \( N_q = 1 \), the normalization condition of the q-eHD. On the other hand we have \( I_q = 1/q^2(1 - e^{-\beta \hbar \omega})^2 \). Thus, our q-eWE, is given by

\[
W_q(\gamma_q) = 1 - \ln[q(1 - e^{-\beta \hbar \omega})] = W - \ln(q),
\]

(36)

a rather interesting result that entails, for our alternative escort q-deformation, that it simply adds a new term to the entropy, given by \( \ln(q) \) (vanishing, as it should, for \( q = 1 \)).

Analyzing the behavior of the q-eWE with temperature we can look for its bounds and easily ascertain that

\[
T \to 0 \Rightarrow W_q(\gamma_q) \to 1 - \ln(q)
\]

\[
T \to \infty \Rightarrow W_q(\gamma_q) \to - \ln(\beta \hbar \omega) = \infty,
\]

i.e., only a lower bound exists. In Table II we illustrate how the lower bound changes with \( q \). Fig. 3 depicts \( W_q(\gamma_q) \) vs. \( t \) for several values of \( q \). The q-escort entropies is able to “perforate” the Lieb lower bound for \( q \geq 1 \), without violating the uncertainty principle, since \( q \in (0, \sqrt{2}) \).

VIII. CONCLUSIONS

Semiclassical Husimi distributions and their associated Wehrl entropies have been here investigated within the frame of deformed algebras. As a summary of our results we can state that:

- we have advanced a q-generalization of the Husimi distribution \( \mu_q(z) \), which arises from the Quesne-family of q-coherent states and found that the q-deformation does not change the HD’s property of being legitimate probability distributions, i.e., \( 0 < \mu_q \leq 1 \).

- the above leads to a concomitant generalization of the WE \( W_q(\mu_q) \), whose lower bound coincides with the well-known Lieb one. These semiclassical q-entropies approach the standard one when \( q \) tends to unity.

- a different generalization of the Wehrl entropy, \( W_q(\gamma_q) \), called the escort-one has also been advanced in Section VIII starting from the q-eHD of Ref. [24]. We saw that this generalization closely resembles the standard WE, but its lower bound improves on the Lieb one, allowing (at least in principle) for a better localization in phase-space. This point should be further considered in future research.

IX. ACKNOWLEDGMENTS

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