Chapter 25

The Husimi Distribution: Development and Applications

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1. Introduction

The Husimi distribution, introduced by Kôdi Husimi in 1940 [1], is a quasi-probability distribution commonly used to study the correspondence between quantum and classical dynamics [2]. Also, it is employed to describe systems in different areas of physics such as Quantum Mechanics, Quantum Optics, Information Theory [3–8]. Additionally, in nanotechnology it is possible to obtain a clear description of localization –which corresponds to classicality– and is crucial to determine correctly the size of systems when the particle dynamics takes into account mobility boundaries [9]. Among its properties, it is always positive definite and unique, conversely it cannot be considered as a true probability distribution over the quantum-mechanical phase space, reason why it is often considered as a quasi probability distribution. Although it possesses no correct marginal properties, its usefulness is to allow the assessment of the expectation values in quantum mechanics in a way similar to the classical case [10]. The semiclassical Husimi probability distribution refers to a special type of probability, this is for simultaneous but approximate location of position and momentum in phase space.

The Husimi distribution may be obtained in several ways; the strategy that we choose here is to derive it as the expectation value of the density operator in a basis of coherent states [11]. Therefore, the line of working in this chapter is illustrated in the following sequence:

$$\underbrace{\text{Coherent states}}_{}\\ \Downarrow \\ \overbrace{\underbrace{\text{Husimi Distribution}}_{}}^{} \\ \Downarrow \\ \overbrace{\text{Information measures,}}^{}$$

where the transcendence of defining correctly a set of coherent states and the Husimi distribution is evident, being the calculation of measures as Wehrl entropy and/or Fisher information a consequence of this procedure.

Coherent states provide a close connection between classical and quantum formulations of a given system. They were introduced early by Erwin Schrödinger in 1926 [12], but the name *coherent state* appeared for first time in Glauber's papers [13, 14]– see a detailed study about this in Ref. [15]. It is known that is difficult to construct coherent states for arbitrary quantum mechanical systems. Klauder shows an elegant method for construct it in Ref. [16]. Furthermore, in Ref. [11] Gazeau and Klauder consider essential, among other things, to discuss what an appropriate formulation of coherent states needs [11]. For instance, they suggest a suitable set of requirements. Then, the main interest in this chapter is to discuss, starting from a well defined set of coherent states, some interesting problems related to the Husimi distribution applied to important systems in physics, such as, the harmonics oscillator [5], the Landau diamagnetism model [17, 18] and, the rigid rotator [6, 18]. Also, we will discuss some properties related to systems with continuous spectrum [19]. In each case, the Wehrl entropy is calculated as a possible application.

This chapter is organized as follows. In section 2 we start presenting the background material and methodology that will be employed in the following chapters. In section 3 we revise the Husimi distribution and the Wehrl entropy for the problem of a particle in a magnetic field. In section 4 we discuss phase space delocalization for the rigid rotator within a semiclassical context by recourse to the Husimi distributions of both the linear and the $3D-$anisotropic instances. In section 5 we propose a procedure to generalize the Husimi distribution to systems with continuous spectrum. We start examining a pioneering work, by Gazeau and Klauder, where the concept of coherent states for systems with discrete spectrum was extended to systems with continuous one. Finally, some concluding remarks and open problems are commented in section 6 .

2. Background material and methodology

In this section we center our attention in 3 topics that we consider relevant to understand the problems that will be discussed in the following sections. These are *i)* the Husimi distribution and the most direct application, i.e., Wehrl entropy, *ii)* a special basis to formulate a suitable set of coherent states and *iii)* a generalization of this concepts to systems with continuous spectrum.

2.1. Husimi distribution and Wehrl entropy

The standard statistical mechanics starts conventionally using the Gibbs's canonical distribution, whose thermal density matrix is represented by

$$\hat{\rho} = Z^{-1} e^{-\beta \hat{H}}, \tag{1}$$

where $Z = \mathrm{Tr}(e^{-\beta \hat{H}})$ is the partition function, $\hat{H}$ is the Hamiltonian of the system, $\beta = 1/k_B T$ the inverse temperature T, and k_B the Boltzmann constant [20].

The Husimi distribution is obtained as the expectation value of the density operator in a basis of coherent states as follows [1]

$$\mu(z) = \langle z | \hat{\rho} | z \rangle, \tag{2}$$

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where $\{|z\rangle\}$ denotes the set of coherent states, which are the eigenstates of the annihilation operator $\hat{a}$, i.e., $\hat{a}|z\rangle = z|z\rangle$ defined for all $z \in \mathbb{C}$ [11]. This distribution is normalized to unity according to

$$\frac{1}{\pi}\int \mathrm{d}^2 z \mu(z) = 1, \tag{3}$$

where the integration is carried out over the complex z plane and the differential is a real element of area proportional to phase space element given by $\mathrm{d}^2 z = \mathrm{d}x\mathrm{d}p/2\hbar$.

For an arbitrary Hamiltonian $\hat{H}$, with the discrete spectra $\{E_n\}$, being n a positive integer, the Husimi distribution takes the form

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

where $\{|n\rangle|\}$ is the set of energy eigenstates with eigenvalues E_n [4, 5].

The Wehrl entropy is a direct application that we introduce here, which is a useful measure of localization in phase-space [21, 22], whose pertinent definition reads

$$W = -\frac{1}{\pi}\int \mathrm{d}^2 z \mu(z)\, \ln\mu(z), \tag{5}$$

The uncertainty principle manifests itself through the inequality $W \geq 1$ which was first conjectured by Wehrl [21] and later proved by Lieb (see, for instance Ref. [4]).

In the special case of the Harmonic Oscillator –whose Hamiltonian is $\hat{H} = \hbar\omega[\hat{a}^\dagger\hat{a} + 1/2]$– its set of Glauber's coherent states is defined in the form [14]

$$|z\rangle = e^{-|z|^2/2}\sum_{n=0}^{\infty}\frac{z^n}{\sqrt{n!}}|n\rangle, \tag{6}$$

where $\{|n\rangle\}$ are a complete orthonormal set of phonon-eigenstates, that is,

$$\langle n|n'\rangle = \delta_{n,n'} \tag{7}$$

where $\delta_{n,n'}$ is the Kronecker delta function, and the energy-spectrum is given by $E_n = \hbar\omega(n + 1/2)$, with $n = 0, 1, \ldots$ By definition, Hermitian operator $\hat{H}$ is an observable if this orthonormal system of vectors forms a basis in the state space. This can be expressed by the closure relation

$$\sum_{n=0}^{\infty}|n'\rangle\langle n| = \hat{1}, \tag{8}$$

where $\hat{1}$ stands for the identity operator in the space formed by eigenvectors.

In this situation one conveniently resorts to

$$\mu_{HO}(z) = (\hat{1} - e^{-\beta\hbar\omega})\, e^{-(1-e^{-\beta\hbar\omega})|z|^2}, \tag{9}$$

$$W_{HO} = 1 - \ln(1 - e^{-\beta\hbar\omega}). \tag{10}$$

which respectively are the useful analytical expressions for Husimi distribution and Wehrl entropy [4].

2.2. Gazeau and Klauder's coherent states

Now, we go back to the set of coherent states defined in Eq. (6). Certainly, it is known that coherent states can be constructed in several ways by recourse to different techniques being its formulation of a not unique character. Nevertheless, contrary to this idea and in order to get a unifying perspective, Gazeau and Klauder have suggested that a suitable formalism for coherent states should satisfy at least the following requirements [11]:

1. *Continuity of labeling* refers to the map from the label space $\mathcal{L}$ into Hilbert space. This condition means that the expression $\| |z'\rangle - |z\rangle \| \to 0$ whenever $z' \to z$.
2. *Resolution of Unity*: a positive measure $\tau(z)$ on $\mathcal{L}$ exists such that the unity operator admits the representation

$$\int_{\mathcal{L}} |z\rangle\langle z| d\tau(z) = 1, \tag{11}$$

   where $|z\rangle\langle z|$ denotes a projector, which takes a state vector into a multiple of the vector $|z\rangle$.
3. *Temporal Stability*: the evolution of any coherent state $|z\rangle$ always remains a coherent state, which leads to a relation of the form

$$|z(t)\rangle = e^{-i\hat{H}t/\hbar}|z\rangle, \tag{12}$$

   where $z(0) = z$, for all $z \in \mathcal{L}$ and t.
4. *Action Identity*: this property requires that

$$\langle z|\hat{H}|z\rangle = \hbar\omega|z|^2. \tag{13}$$

At this point, we remark that requirements (3) and (4) are directly satisfied when the spectrum of the Hamiltonian $\hat{H}$ of the system, has the form $E_n \sim n\hbar\omega$, where n is the quantum number and ω is the frequency of the oscillator [11]. In addition, there are some shortcomings about these requirements; for instance, Gazeau and Klauder states cannot be used for degenerate systems. Furthermore, it is questionable that action identity leads to the classical action-angle variable interpretation [23].

2.3. Continuous spectrum

Gazeau and Klauder proposed in Ref. [11] a formulation of coherent states for systems with continuous spectrum. They introduced a Hamiltonian $\hat{H} > 0$, with a non-degenerate continuous spectrum, thus

$$\hat{H}|\varepsilon\rangle = \omega\varepsilon|\varepsilon\rangle, \quad 0 < \varepsilon < \varepsilon_M \tag{14}$$

where $\{|\varepsilon\rangle\}$ stands for a basis of eigenstates, which we can generalize replacing suitably discrete parameters by continuous ones, sums by integrals and Kronecker by Dirac delta function [46]. In such a case, we can always chose a normalized basis of eigenvectors to rephrase Eqs. (7) and (8) in the following manner [46]

$$\langle\varepsilon|\varepsilon'\rangle = \delta(\varepsilon-\varepsilon'), \tag{15}$$

and

$$\int_0^{\varepsilon_M} |\varepsilon'\rangle\langle\varepsilon| = \hat{1}, \tag{16}$$

where $\varepsilon_M \leq \infty$ [11]. In the section 5 and here we use units in which $\hbar = 1$.

If we set $M(s) = e^{|z|^2/2}$ and $z = se^{-i\gamma\varepsilon}$ into coherent states (6), we find

$$|s,\gamma\rangle = M(s)^{-1} \int_0^{\varepsilon_M} \mathrm{d}\varepsilon \, \frac{s^{\varepsilon} e^{-i\gamma\varepsilon}}{\sqrt{\rho(\varepsilon)}} |\varepsilon\rangle, \tag{17}$$

where $s > 0$. Since $\{|s,\gamma\rangle\}$ are orthonormals, the normalization factor $M(s)$ is given by

$$M(s)^2 = \int_0^{\varepsilon_M} \mathrm{d}\varepsilon \, \frac{s^{2\varepsilon}}{\rho(\varepsilon)}, \tag{18}$$

for $M(s)^2 < \infty$.

Coherent states (17) must satisfy resolution of identity. In this case, it was introduced in Ref. [11] the following relation

$$\rho(\varepsilon) = \int_0^{s} \mathrm{d}s' \, s'^{2\varepsilon} \sigma(s'), \tag{19}$$

where s' is a variable of integration with $0 \leq s' < s \leq \infty$. In addition, a non-negative weight function $\sigma(s') \geq 0$ was introduced in order to satisfy the second requirement. Then, the measure of integration takes the form [11]

$$\mathrm{d}\tau(s,\gamma) = \sigma(s) M(s)^2 \, \mathrm{d}s \, \frac{\mathrm{d}\gamma}{2\pi}. \tag{20}$$

Gazeau and Klauder shown that resolution of unity is satisfied for systems with continuous spectrum in the present formulation of coherent states [11]. In Ref. [19] the authors have proposed a continuous appearance of Eq. (4), replacing the discrete form by the continuous version of variables, functions and operators involved in the formalism. Hence, we are ready to define the Husimi distribution for systems with continuous spectrum in the following manner:

$$\mu_Q(s,\gamma) = \frac{1}{Z} \int_0^{\varepsilon_M} \mathrm{d}\varepsilon \, e^{-\beta\omega\varepsilon} |\langle s,\gamma|\varepsilon\rangle|^2, \tag{21}$$

where ε stands for a continuous parameter. The Husimi distribution is normalized according to

$$\int_0^\infty \int_{-\infty}^\infty d\tau(s,\gamma)\mu_Q(s,\gamma) = 1, \tag{22}$$

where the measure $d\tau(s,\gamma)$ is given by Eq. (20).

We see easily from Eq. (17) that, the projection of eingensatates of the Hamiltonian over coherent states, is given by

$$\langle s,\gamma|\varepsilon\rangle = M(s)^{-1}\frac{s^\varepsilon e^{-i\gamma\varepsilon}}{\sqrt{\rho(\varepsilon)}}, \tag{23}$$

where we have considered from Eq. (15) the orthogonality of the continuous states $\{|\varepsilon\rangle\}$. Introducing the above expression into Eq. (21) we finally arrive to [19]

$$\mu_Q(s) = \frac{M(s)^{-2}}{Z}\int_0^{\varepsilon_M} d\varepsilon\, \frac{e^{-\beta\omega\varepsilon}s^{2\varepsilon}}{\rho(\varepsilon)}, \tag{24}$$

where we have dropped out the dependence on γ. The continuous partition function obviously is [20]

$$Z = \int_0^{\varepsilon_M} d\varepsilon\, e^{-\beta\omega\varepsilon}. \tag{25}$$

It is important to note that Eq. (24) is consistently normalized in accordance with

$$\int_0^\infty d\tau(s)\,\mu_Q(s) = 1, \tag{26}$$

and in this case, the measure is $d\tau(s) = \sigma(s)M(s)^2\,ds$.

3. Landau diamagnetism: Charged particle in a uniform magnetic field

Diamagnetism was a problem firstly appointed by Landau who showed the discreteness of energy levels for a charged particle in a magnetic field [24]. By the observation of the diverse scenarios in the framework provided by the Landau diamagnetism we can study some relevant physical properties [25–27] as thermodynamic limit, role of boundaries, decoherence induced by the environment. The main motivation for several specialists work even today it is to make an accurate description of its theoretical and practical consequences.

In the past the appropriate partition function for this problem was calculated by Feldman and Kahn appealing to the concept of Glauber's coherent states as a set of basis states [28]. This formulation allows the use of classical concepts to describe electron orbits, even containing all quantum effects [28]. In a previous effort, this approach was used to obtain the Wehrl entropy [21, 22] and Fisher information [29] with the purpose of studying the thermodynamics of the Landau diamagnetism problem, namely, a free spinless charged particle in a uniform magnetic field [7]. In such contribution the authors focussed only in the transverse motion of a particle. For this reason, it was necessary to normalize the Husimi distribution in order to arrive to a consistent expression for semiclassical measures [7, 8, 32].

Certainly, because the relevant effects seem to come only from the transverse motion, several efforts are made to describe this problem in two dimensions [7, 8, 27, 28, 32-34]. Furthermore, since the discovery of interesting phenomena, as the quantum Hall effect, there has been much interest in understanding the dynamics of electrons confined to move in two dimensions in the presence of a magnetic field perpendicular to the motion plane [31]. The confinement is possible at the *interface* between two materials, typically a semiconductor and an insulator, where a quantum well that traps the particles is formed, forbidding their motion in the direction perpendicular to the interface plane at low energies.

However, we propose here to discuss this problem in the most complete form (three dimensions), some results related to the behavior of the Wehrl entropy. From the present line of reasoning, it is concluded that the two-dimensional formulation is sufficient unto itself to explain the problem whenever the length of the cylindrical geometry of the system is large enough. Nevertheless, as suggested before, electronic devices are based in interfaces. Thus, this fact theoretically imposes a natural lower temperature bound that emerges from the analysis when three dimensions are considered [18].

3.1. The model of one charged particle in a magnetic field

We enter the present application by revisiting the complete set of coherent states of a spinless charged particle in a uniform magnetic field. Consider the classical kinetic momentum

$$\vec{\pi} = \vec{p} + \frac{q}{c}\vec{A}, \tag{27}$$

of a particle of charge q, mass m_q, and linear momentum $\vec{p}$, subject to the action of a vector potential $\vec{A}$. These are the essential ingredients of the well-known Landau model for diamagnetism: a spinless charged particle in a magnetic field B (we follow the presentation of Feldman et al. [28]). The Hamiltonian reads [28]

$$H = \frac{\vec{\pi}\cdot\vec{\pi}}{2m_q}, \tag{28}$$

and the magnetic field is $\vec{B} = \vec{\nabla} \times \vec{A}$. The vector potential is chosen in the symmetric gauge as $\vec{A} = (-By/2, Bx/2, 0)$, which corresponds to a uniform magnetic field along the $z-$direction.

By using the quantum formulation of the step-ladder operators [28], one needs to define the step operators as follows [28]

$$\hat{\pi}_{\pm} = \hat{p}_x \pm i\hat{p}_y \pm \frac{i\hbar}{2\ell_{\mathrm{B}}^2}(\hat{x} \pm i\hat{y}), \tag{29}$$

where the length

$$\ell_{\mathrm{B}} = (\hbar c/qB)^{1/2} \tag{30}$$

is the classical radius of the ground-state Landau orbit [28]. Motion along the $z-$axis is free [28]. For the transverse motion, the Hamiltonian specializes to [28]

$$\hat{H}_t = \frac{\hat{\pi}_+ \hat{\pi}_-}{2m_q} + \frac{1}{2}\hbar\Omega\hat{1}, \tag{31}$$

where an important quantity characterizes the problem, namely,

$$\Omega = qB/m_q c, \tag{32}$$

the cyclotron frequency [33]. The eigenstates $|N,m\rangle$ are determined by two quantum numbers: N (associated to the energy) and m (to the $z-$ projection of the angular momentum). As a consequence, they are simultaneously eigenstates of both $\hat{H}_t$ and the angular momentum operator $\hat{L}_z$ [28], so that

$$\hat{H}_t|N,m\rangle = \left(N + \frac{1}{2}\right)\hbar\Omega\,|N,m\rangle = E_N|N,m\rangle \tag{33}$$

and

$$\hat{L}_z|N,m\rangle = m\hbar|N,m\rangle. \tag{34}$$

We note that the eigenvalues of $\hat{L}_z$ are not bounded by below (m takes the values $-\infty,\ldots,-1,0,1,\ldots,N$) [28]. This agrees with the fact that the energies $(N+1/2)\hbar\Omega$ are infinitely degenerate [33]. Such a fact diminishes the physical relevance of phase-space localization for estimation purposes, as we shall see below. Moreover, L_z is not an independent constant of the motion [33].

There exists a analogous formulation of an charged particle in a magnetic field by Kowalski that takes into account the geometry of a circle [30] (and for a comparison with the Feldman formulation see Ref.[8]), but at this point, we choose the Feldman formulation to work because the measure is easily defined and the normalization condition and other semiclassical measures are well described.

3.2. Husimi distribution and Wehrl entropy

We will start our present endeavor defining the Hamiltonian $\hat{H} = \hat{H}_t + \hat{H}_l$ for a particle of mass m_q and charge q in a magnetic field B, where $\hat{H}_t = \hbar\Omega(\hat{N}+1/2)$ describes the transverse motion, being Ω the cyclotron frequency as defined by the Eq. (32) and $\hat{N}$ the number operator. In addition, the Hamiltonian $\hat{H}_l = \hat{p}_z^2/2m_q$ represents a longitudinal one-dimensional free motion. After constructing a coherent state basis, a possible way to define the Husimi function η, for the complete motion, is given by

$$\eta(x,p_x;y,p_y;p_z) = \langle\alpha,\xi,k_z|\hat{\rho}|\alpha,\xi,k_z\rangle, \tag{35}$$

where $\hat{\rho}$ is the thermal density operator and the set $\{|\alpha,\xi,k_z\rangle\}$ represents the coherent states for the motion in three dimensions. Taking the direct product $|\alpha,\xi,k_z\rangle \equiv |\alpha,\xi\rangle \bigotimes |k_z\rangle$, the set $\{|\alpha,\xi\rangle\}$ corresponds to the coherent states of the transverse motion and $\{|k_z\rangle\}$ to the longitudinal motion. Therefore, the thermal density operator is given by

$$\hat{\rho} = \frac{1}{Z}\mathrm{e}^{-\beta(\hat{H}_l+\hat{H}_t)}, \tag{36}$$

where $\beta = 1/k_B T$, k_B the Boltzmann constant and T the temperature. Besides, Z is the partition function for the particle total motion. If Z is separated in a similar way as other physical properties are separated, it is possible to assure that $Z = Z_l Z_t$, where Z_t is the contribution for the transverse motion and Z_l the contribution for the one-dimensional free motion. Thus, the Husimi function [1] is written as

$$\eta = \frac{e^{-\beta p_z^2/2m_q}}{Z_l Z_t} \sum_{n,m} e^{-\beta\hbar\Omega(n+1/2)} |\langle n,m|\alpha,\xi\rangle|^2. \tag{37}$$

where

$$Z_l = (\mathcal{L}/h)(2\pi m_q k_B T)^{1/2} \quad \text{and} \tag{38}$$

$$Z_t = \mathcal{A} m_q \Omega / (4\pi\hbar \sinh(\beta\hbar\Omega/2)), \tag{39}$$

being $\mathcal{L}$ the length of the cylinder, $\mathcal{A} = \pi R^2$ the area for cylindrical geometry [28]. In addition, the matrix element $|\langle n,m|\alpha,\xi\rangle|^2$ represents the probability of finding the charged particle in the coherent state $|\alpha,\xi\rangle$ and we can find its expression as defined previously [34].

It should be noticed that the distribution η can be written as follows

$$\eta = \eta_l(p_z)\,\eta_t(x, p_x; y, p_y), \tag{40}$$

where η has been separated as a function of two distributions, namely, $\eta_l = \eta_l(p_z)$ and $\eta_t = \eta_t(x, p_x; y, p_y)$. The dependence on the variable z has been missed due to the explicit form of the hamiltonian $\hat{H}_l$. Accordingly, after summing in Eq. (37) we find

$$\eta_l = \frac{e^{-\beta p_z^2/2m_q}}{Z_l}, \tag{41}$$

$$\eta_t = \frac{2\pi\hbar}{\mathcal{A} m_q \Omega}(1 - e^{-\beta\hbar\Omega})\, e^{-(1-e^{-\beta\hbar\Omega})|\alpha|^2/2\ell_B^2}, \tag{42}$$

where the length ℓ_B is defined by the Eq. (30). From expressions (41) and (42), we emphasize again that $\eta_l(p_z)$ describes the free motion of the particle in the magnetic field direction and $\eta_t(x, p_x; y, p_y)$ the Landau levels due to the circular motion in a transverse plane to the magnetic field, similar to the harmonic oscillator of Eq. (9) since $|z|^2 \to |\alpha|^2/2\ell_B^2$. Consequently Eqs. (40), (41) and (42) together contain the complete description of the system. We noticed both distributions are naturally normalized in a standard form, i.e.,

$$\int \frac{dz\,dp_z}{h} \eta_l(p_z) = 1, \tag{43}$$

and

$$\int \frac{d^2\alpha\, d^2\xi}{4\pi^2 \ell_B^4} \eta_t(x, p_x; y, p_y) = 1. \tag{44}$$

In consequence, both Eqs. (41) and (42), under conditions (43) and (44), bring a promising way to get the exact form of the Wehrl entropy. Furthermore, using the additivity as the most basic property of the entropy, we can state $W_{\text{total}} = W_l + W_t$. Hence,

$$W_l = -\int \frac{\mathrm{d}z\mathrm{d}p_z}{h} \eta_l(p_z) \ln \eta_l(p_z), \tag{45}$$

$$W_t = -\int \frac{\mathrm{d}^2\alpha \mathrm{d}^2\xi}{4\pi^2 \ell_{\mathrm{B}}^4} \eta_t(x,p_x;y,p_y) \ln \eta_t(x,p_x;y,p_y), \tag{46}$$

where, as before, the subindex l stands for the longitudinal motion and t the transverse.

After evaluating the respective integrals in Eqs. (45) and (46), it is feasible to identify the two particular entropies

$$W_l = \frac{1}{2} + \ln\left(\frac{\mathcal{L}}{\lambda}\right), \tag{47}$$

$$W_t = 1 - \ln\left(1 - \mathrm{e}^{-\beta\hbar\Omega}\right) + \ln(g), \tag{48}$$

where $\lambda = h/(2\pi m_q k_{\mathrm{B}} T)^{1/2}$ is the mean thermal wavelength of the particle and $g = \mathcal{A}/2\pi\ell_{\mathrm{B}}^2$ stands for the degeneracy of a Landau level [35]. Indeed, Eq. (47) coincides with the classical entropy for a free particle in one dimension. Eq. (48) is the Wehrl entropy for the transverse motion and possesses a form for the one close to the harmonic oscillator entropy given by the Eq. (10), with the exception of a term associated with the degeneracy.

3.3. Semiclassical behavior and consequences

Although the total Wehrl entropy is expressed simply as follows

$$W_{\text{total}} = \frac{3}{2} - \ln(1 - \mathrm{e}^{-\beta\hbar\Omega}) + \ln(g) + \ln\left(\frac{\mathcal{L}}{\lambda}\right), \tag{49}$$

we notice that some of its properties are directly derived from Eqs. (47) and (48). First, as we commented before, W_l coincides with the classical entropy for the free motion in one dimension. From this glance, we can add that W_l has to be nonnegative, $W_l \geq 0$ at all temperatures. This last condition imposes a minimum temperature, given by

$$T_0 = \frac{h^2}{2\pi m_q e k_B \mathcal{L}^2}, \tag{50}$$

where $e = 2.718281828$. The standard behavior of W_l obligates the system to take high values of temperature, wherever the temperature T ought to be greater than T_0, in such case the conduct of the system is classical. This is equivalent to assert that, if $T/T_0 \geq 1$, the length of a thermal wave λ lower than the average of the spacing among particles and quantum considerations are not relevant [36]. In addition, T_0 only depends on the size of the system and does not depend on other external or

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internal physical parameters such as transverse area, external magnetic field, charge of the particle, etc. If the system is large then the minimum temperature is low. However, modern electronic systems has junctions where $\mathcal{L}$ is practically zero. In such case the required minimum temperature to make applicable our description is numerically high enough [39].

Nevertheless, the entropy associated with transverse motion satisfies $W_t \geq 1 + \ln(g)$ for all temperatures in the system of a particle in a magnetic field where the symmetry is polar, which is almost the Lieb condition for systems in one dimension [37] with an additional term associated with the degeneracy g. Roughly speaking, the transverse motion is bi-dimensional, but in the Landau approach the quantum motion of the particle in a magnetic field is reduced to a degenerate spectrum in one dimension. This degeneracy essentially recovers the physics of the missing dimension. Resuming the discussion of the behavior of the Wehrl entropy, it is not plausible to adventure any conclusion about the applicability of the present treatment because the Lieb condition is always satisfied. This is the main problem stems from the restricted vision presented in other contributions over this topic which only put its emphasis on the transverse motion [8, 28, 30] and represent the main difference from the vision obtained in that other contributions that discuss this topic. From the combined reasoning of both motions we conclude that the present description, this is the calculation of W_t, has sense when the imposition over the temperature is satisfied. Under T_0 the behavior is intrinsically anomalous and the present proposal is not applicable.

If we consider $k_B T \gg \hbar\Omega$, we can apply the first order of approximation as $\ln(g/(1-e^{-\beta\hbar\Omega})) \approx \ln(\mathcal{A}T/T_0\mathcal{L}^2)$. Indeed, taking into account that the thermal wave length can be rewritten in terms of the temperature T_0 this way $\lambda = \mathcal{L}(eT_0/T)^{1/2}$, the expression (49) after a bit of algebra reduces to

$$W_{\text{total}}^{(1)} \approx \frac{3}{2}\ln\left(\frac{T}{T_0}\right) + \ln\left(\frac{\mathcal{A}}{\mathcal{L}^2}\right). \tag{51}$$

Considering that $\mathcal{V} = \mathcal{A}\mathcal{L}$ in Eq. (51), the total Wehrl entropy can be expressed as follows

$$W_{\text{total}}^{(1)} = \frac{3}{2} + \ln\left(\frac{\mathcal{V}}{\lambda^3}\right). \tag{52}$$

This is a particular expression for the entropy of a free particle in three dimensions related to the motion of a charged particle into a region of the magnetic field making mention of some geometrical properties of the system.

In second order of approximation for high temperatures, considering the special condition $\mathcal{A} \sim \mathcal{L}^2$, Wehrl entropy is expressed as follows

$$W_{\text{total}}^{(2)} \approx \frac{T_0}{T}g + \frac{3}{2} + \frac{3}{2}\ln\left(\frac{T}{T_0}\right) = \frac{T_0}{T}g + W_{\text{total}}^{(1)}. \tag{53}$$

As explained before, the Wehrl entropy takes values that are permitted by the Lieb condition, namely, $W \geq 1$. According to Eq. (53) the slope decreases as temperature increases. This fact illustrates why the disorder slowly increases as the magnetic field increases too. Consequently, at extremely high temperatures as expected, the slope of the present linear dependence tends to zero apparently taking a constant value close to the corresponding classical entropy of the free particle in three dimensions.

The lower bound of temperature is related to $T/T_0 \to 1^+$, because this approach does not consider temperature values under T_0. The total Wehrl entropy is reduced to logarithm behavior of the magnetic field.

To study what occurs close to zero temperature, in accordance with Eq. (50), we need to take systems with $L \to \infty$ and after this consideration the transverse entropy of Eq. (48) can be seen as follows

$$W_t^{T \to 0^+} = 1 + \ln(g). \tag{54}$$

As we discussed before, this Wehrl entropy is also a kind of harmonic oscillator entropy and the lower bound complies with being greater than a bound limiting value of the temperature, which has been suggested by Wehrl and shown by Lieb, $W \geq 1$ [37]. Starting from this condition it must arrive to the following inequality for the magnetic field

$$g \geq 1, \tag{55}$$

where $g = q\mathcal{A}B/hc$ also accounts for the ratio between the flux of the magnetic field $\mathcal{A}B$ and the quantum of the magnetic flux given by $hc/q = 4.14 \times 10^{-7}[gauss/cm^2]$ [17]. Then the inequality (55) adopts the form

$$B \geq \frac{1}{\mathcal{A}}\frac{hc}{q} = B_0. \tag{56}$$

Therefore, the quantity $B_0 = hc/\mathcal{A}q$ becomes a bound limiting field that represents the minimum value for the external magnetic field. To study what occurs close to zero magnetic field we need to take systems with $\mathcal{A} \to \infty$.

For finite values of $\mathcal{A}$ and B lower than B_0 is manifested the Haas-van Alphen effect, which describes oscillations in the magnetization because at temperatures low enough the particles will tend to occupy the lowest energy states. Whereas if the value of the magnetic field decreases a less number of particles can be in the lowest state due to degeneracy is directly proportional to B [35]. Then, the transverse Wehrl entropy W_t is well defined for values of the magnetic field over B_0, this is $B/B_0 \geq 1$ and/or $g \to 1^+$.

We can assert that this description of the system is not quantum, we say that it is semiclassical; for instance, it does not contain the Haas-van Alphen effect, the same condition marks the beginning of one description and the ending of the other.

Other relevant effect that emerges from the Landau quantization [38] is the quantum Hall effect [39] which is a quantum-mechanical version of the Hall effect [31], observed in two-dimensional electron systems subjected to low temperatures and strong magnetic fields. The degeneracy is given by [17]

$$\phi = \nu\phi_0, \tag{57}$$

where $\phi_0 = hc/q$ is the quantum of the magnetic flux. The factor ν is related to the “filling factor" that takes integer values (ν = 1, 2, 3, ...). The discovery of the fractional quantum Hall effect [32] extend these values to rational fractions (ν = 1/3, 1/5, 5/2, 12/5, ...). The integer quantum Hall effect is simply explained in terms of the conductivity quantization $\sigma = \nu q^2/h$. However, the fractional quantum Hall effect relies on other phenomena related to interactions. Consistently, we see that the degeneracy is equal to ν, which must be greater than 1 due to the inequality (55) obtaining an infinite family of Wehrl entropies

$$W_t = 1 - \ln(1 - e^{-\beta\hbar\Omega}) + \ln\nu. \tag{58}$$

Again, Eq. (55) provides the limiting value of ν and, as before, the transverse entropy always satisfies the Lieb bound for all temperatures and large enough systems when the quantum Hall effect is manifested at least for the integer quantum Hall effect. Conversely, fractional values of ν less than 1 are left out the present approach.

4. Description of the molecular rotation: Rigid rotator

The rigid rotator is a system of a single particle whose quantum spectrum of energy is exactly known. Therefore, the study of typical thermodynamic properties can be analytically derived [40]. Applications lead to the treatment of important aspects of molecular systems [41] and several applications to materials [42].

4.1. Linear rigid rotator

We start the present study by exploring a simple model, the linear rigid rotator, based on the excellent discussion concerning the coherent states for angular momenta given in Ref. [43]. The Hamiltonian of the linear rigid rotator is [20]

$$\hat{H} = \frac{\hat{L}^2}{2I_{xy}}, \tag{59}$$

where $\hat{L}^2 = \hat{L}_x^2 + \hat{L}_y^2$ is the angular momentum operator and I_x and I_y are the associated moments of inertia. We have assumed that $I_{xy} \equiv I_x = I_y$. Calling $|IK\rangle$ the set of H-eigenstates, we recall that they verify the relations

$$\begin{aligned} \hat{L}^2|IK\rangle &= I(I+1)\hbar^2|IK\rangle \\ \hat{L}_z|IK\rangle &= K\hbar|IK\rangle, \end{aligned} \tag{60}$$

with $I = 0, 1, 2\ldots$, for $-I \leq K \leq I$, the eigenstates' energy spectrum being given by

$$\varepsilon_I = \frac{I(I+1)\hbar^2}{2I_{xy}}. \tag{61}$$

Coherent states are constructed in Ref. [44, 45] for the lineal rigid rotator, using Schwinger's oscillator model of angular momentum, in the fashion

$$|IK\rangle = \frac{(\hat{a}_+^\dagger)^{I+K}(\hat{a}_-^\dagger)^{I-K}}{\sqrt{(I+K)!(I-K)!}}|0\rangle, \tag{62}$$

with $\hat{a}_+$, $\hat{a}_-$ the pertinent creation and annihilation operators, respectively, and $|0\rangle \equiv |0,0\rangle$ the vacuum state. The states $|IK\rangle$ are orthogonal and satisfy the closure relation, i.e.,

$$\langle I^{'}K^{'}|IK\rangle = \delta_{I',I}\delta_{K',K}, \tag{63}$$

$$\sum_{I=0}^{\infty}\sum_{K=-I}^{I}|IK\rangle\langle IK| = \hat{1}. \tag{64}$$

Since we deal with two degrees of freedom the ensuing coherent states are of the tensor product form (involving $|z_1\rangle$ and $|z_2\rangle$) [43, 46]

$$|z_1z_2\rangle = |z_1\rangle \otimes |z_2\rangle, \tag{65}$$

where

$$\hat{a}_+|z_1z_2\rangle = z_1|z_1z_2\rangle, \tag{66}$$

$$\hat{a}_-|z_1z_2\rangle = z_2|z_1z_2\rangle. \tag{67}$$

Therefore, the coherent state $|z_1z_2\rangle$ writes [43]

$$|z_1z_2\rangle = e^{-\frac{|z|^2}{2}}e^{z_1\hat{a}_+^{\dagger}}e^{z_2\hat{a}_-^{\dagger}}|0\rangle, \tag{68}$$

with

$$|z_1\rangle = e^{-\frac{|z_1|^2}{2}}e^{z_1\hat{a}_+^{\dagger}}|0\rangle, \tag{69}$$

$$|z_2\rangle = e^{-\frac{|z_2|^2}{2}}e^{z_2\hat{a}_-^{\dagger}}|0\rangle. \tag{70}$$

We have introduced the convenient notation

$$|z|^2 = |z_1|^2 + |z_2|^2. \tag{71}$$

Using Eqs. (62) and (68) we easily calculate $|z_1z_2\rangle$ and, after a bit of algebra, find

$$|z_1z_2\rangle = e^{-\frac{|z|^2}{2}}\sum_{n_+,n_-}\frac{z_1^{n_+}}{\sqrt{n_+!}}\frac{z_2^{n_-}}{\sqrt{n_-!}}|IK\rangle \tag{72}$$

where $n_+ = I + K$ and $n_- = I - K$. Therefore, the probability of observing the state $|IK\rangle$ in the coherent state $|z_1 z_2\rangle$ is of the form

$$|\langle IK|z_1 z_2\rangle|^2 = e^{-|z|^2} \frac{|z_1|^{2n_+}}{n_+!} \frac{|z_2|^{2n_-}}{n_-!}. \tag{73}$$

The present coherent states satisfy resolution of unity

$$\int \frac{d^2 z_1}{\pi} \frac{d^2 z_2}{\pi} |z_1 z_2\rangle\langle z_1 z_2| = 1. \tag{74}$$

Furthermore, z_1 and z_2 are continuous variables.

Following the procedure developed by Anderson *et al.* [4], we can readily calculate the pertinent Husimi distribution [1]. For our system this is defined, from Eq. (4), as

$$\mu(z_1, z_2) = \langle z_1, z_2|\hat{\rho}|z_1, z_2\rangle, \tag{75}$$

where the density operator is

$$\hat{\rho} = Z_{2D}^{-1} \exp(-\beta \hat{H}). \tag{76}$$

The concomitant rotational partition function Z_{2D} is given in Ref. [20]

$$Z_{2D} = \sum_{I=0}^{\infty} (2I+1)\, e^{-I(I+1)\frac{\Theta}{T}}, \tag{77}$$

with $\Theta = \hbar^2/(2I_{xy}k_B)$. Remark that in the present context, speaking of the "trace operation" entails performing the sum $\mathrm{Tr} \equiv \sum_{I=0}^{\infty} \sum_{K=-I}^{I}$. Inserting now the closure relation into Eq. (75), and using Eq. (73), we finally get our Husimi distribution in the fashion

$$\mu(z_1, z_2) = e^{-|z|^2} \frac{\sum_{I=0}^{\infty} \frac{|z|^{4I}}{(2I)!} e^{-I(I+1)\frac{\Theta}{T}}}{\sum_{I=0}^{\infty} (2I+1)\, e^{-I(I+1)\frac{\Theta}{T}}}. \tag{78}$$

It is easy to show that this distribution is normalized to unity

$$\int \frac{d^2 z_1}{\pi} \frac{d^2 z_2}{\pi} \mu(z_1, z_2) = 1, \tag{79}$$

where z_1 and z_2 are given by Eqs. (66), (67), and (71). Note that we must deal with the binomial expression $(|z_1|^2 + |z_2|^2)^{4I}$ firstly and then integrate over the whole complex plane (in two dimensions) in order to verify the normalization condition (79). The differential element of area in the $z_1(z_2)$ plane is $d^2 z_1 = dx dp_x/2\hbar$ ($d^2 z_2 = dy dp_y/2\hbar$) [13]. Moreover, we have the phase-space relationships

$$|z_1|^2 = \frac{1}{4}\left(\frac{x^2}{\sigma_x^2} + \frac{p_x^2}{\sigma_{p_x}^2}\right), \tag{80}$$

$$|z_2|^2 = \frac{1}{4}\left(\frac{y^2}{\sigma_y^2} + \frac{p_y^2}{\sigma_{p_y}^2}\right), \tag{81}$$

where $\sigma_x \equiv \sigma_y = \sqrt{\hbar/2m\omega}$ and $\sigma_{p_x} \equiv \sigma_{p_y} = \sqrt{m\omega\hbar/2}$.

The profile of the Husimi function is similar to that of a Gaussian distribution.

The Wehrl entropy is a semiclassical measure of localization [21] (so is Fisher's one [5] as well). Indeed, Wehrl's measure is simply a logarithmic Shannon measure built up with Husimi distributions. For the present bi-dimensional model this entropy reads

$$\mathcal{W} = -\int \frac{\mathrm{d}^2 z_1}{\pi}\frac{\mathrm{d}^2 z_2}{\pi}\,\mu(z_1, z_2)\,\ln\mu(z_1, z_2), \tag{82}$$

where $\mu(z_1, z_2)$ is given by Eq. (78).

4.2. Rigid rotator in three dimensions

In the present section we consider a more general problem, the model of the rigid rotator in three dimensions, whose Hamiltonian writes [47]

$$\hat{H} = \frac{\hat{L}_x^2}{2I_x} + \frac{\hat{L}_y^2}{2I_y} + \frac{\hat{L}_z^2}{2I_z}, \tag{83}$$

where I_x, I_y, and I_z are the associated moments of inertia. A complete set of rotator eigenstates is $\{|IMK\rangle\}$. The following relations apply

$$\begin{aligned} \hat{L}^2|IMK\rangle &= I(I+1)\hbar^2|IMK\rangle \\ \hat{L}_z|IMK\rangle &= K\hbar|IMK\rangle \\ \hat{J}_z|IMK\rangle &= M\hbar|IMK\rangle, \end{aligned} \tag{84}$$

where $I = 0, \ldots, \infty, -I \le K \le I$, and $-I \le M \le I$. The states $|IMK\rangle$ satisfy orthogonality and closure relations [47]

$$\langle I^{'}M^{'}K^{'}|IMK\rangle = \delta_{I',I}\delta_{M',M}\delta_{K',K} \tag{85}$$

$$\sum_{I=0}^{\infty}\sum_{M=-I}^{I}\sum_{K=-I}^{I}|IMK\rangle\langle IMK| = \hat{1}. \tag{86}$$

If we take $\hat{L}^2 = \hat{L}_x^2 + \hat{L}_y^2 + \hat{L}_z^2$ and assume axial symmetry, i.e., $I_{xy} \equiv I_x = I_y$, we can recast the Hamiltonian as

$$\hat{H} = \frac{1}{2I_{xy}}\left[\hat{L}^2 + \left(\frac{I_{xy}}{I_z} - 1\right)\hat{L}_z^2\right], \tag{87}$$

where $\hat{L}^2$ is the angular momentum operator and $\hat{L}_z$ is its projection on the rotation axis z. The concomitant spectrum of energy becomes

$$\varepsilon_{I,K} = \frac{\hbar^2}{2I_{xy}}\left[I(I+1) + \left(\frac{I_{xy}}{I_z} - 1\right)K^2\right], \tag{88}$$

where $I = 0, 1, 2, \cdots$ and it represents the eigenvalue of the angular momentum operator $\hat{L}^2$, the numbers $m = -I, \cdots, -1, 0, 1, \cdots, I$ stand for the projections on the intrinsic rotation axis of the rotator. All states exhibit a $(2I+1)-$degeneracy. The parameters $I_x = I_y \equiv I_{xy}$ and I_z are the inertia momenta. Different “geometrical" instances are characterized through the I_{xy}/I_z-ratio. For example, the value $I_{xy}/I_z = 1$ corresponds to the spherical rotator. Limiting cases can also be considered. This is, $I_{xy}/I_z = 1/2$ and $I_{xy}/I_z \to \infty$, that correspond to the extremely oblate- and prolate cases, respectively.

4.2.1. Coherent states for the rigid rotator in three dimensions

In order to obtain the Husimi distribution for this problem we need first of all to have the associated coherent states. Morales *et al.* have constructed them in Ref. [47] and discussed their mathematical foundations. First, they introduced the auxiliary quantity

$$X_{I,M,K} = \sqrt{I!(I+M)!(I-M)!(I+K)!(I-K)!}, \tag{89}$$

and then write [47]

$$|z_1z_2z_3\rangle = e^{-\frac{|u|^2}{2}}\sum_{IMK}\frac{[(2I)!]^2 z_1^{(I+M)} z_2^I z_3^{(I+K)}}{X_{I,M,K}}|IMK\rangle, \tag{90}$$

where the following supplementary variable were introduced by Morales *et al.* in Ref. [47]

$$|u|^2 = |z_2|^2(1+|z_1|^2)^2(1+|z_3|^2)^2. \tag{91}$$

All coherent states share at least two requirements. Continuity of labeling and resolution of unity. In relation to the last property we add

$$\int d\Gamma |z_1z_2z_3\rangle\langle z_1z_2z_3| = 1 \tag{92}$$

where $\mathrm{d}\Gamma$ is the measure of integration given by [47]

$$\mathrm{d}\Gamma = \mathrm{d}\tau\left\{4[(1+|z_1|^2)(1+|z_3|^2)]^4|z_2|^4 - 8[(1+|z_1|^2)(1+|z_3|^2)]^2|z_2|^2+1\right\} \tag{93}$$

with

$$\mathrm{d}\tau = \frac{\mathrm{d}^2 z_1}{\pi}\frac{\mathrm{d}^2 z_2}{\pi}\frac{\mathrm{d}^2 z_3}{\pi}, \tag{94}$$

and, of course, in this case we have three degrees of freedom. The present formulation satisfy the weaker version of the second requirement, because the measure is defined non positive [47].

4.2.2. Husimi function, Wehrl entropy

Using now Eq. (90) we find

$$|\langle IMK|z_1 z_2 z_3\rangle|^2 = \frac{e^{-|u|^2}}{X^2_{I,M,K}}[(2I)!]^2|z_1|^{2(I+M)}|z_2|^{2I}|z_3|^{2(I+K)} \tag{95}$$

and determine that, in this case, the rotational partition function reads

$$Z_{3D} = \sum_{I=0}^{\infty}\sum_{K=-I}^{I}\sum_{M=-I}^{I} e^{-\beta\varepsilon_{I,K}}, \tag{96}$$

i.e.,

$$Z_{3D} = \sum_{I=0}^{\infty}(2I+1)\,e^{-I(I+1)\frac{\Theta}{T}}\sum_{K=-I}^{I} e^{-\left(\frac{I_{xy}}{I_z}-1\right)K^2\frac{\Theta}{T}}. \tag{97}$$

Remark that if we take the "extremely prolate" limiting case $I_{xy}/I_z \to \infty$ just one term that survives in the right sum of the right side in Eq. (97), that for $K=0$, while all terms for $K \neq 0$ vanish. In this special instance case Z_{2D} is recovered from Z_{3D}. The pertinent Husimi distribution becomes

$$\mu(z_1,z_2,z_3) = \frac{e^{-|u|^2}}{Z_{3D}}\sum_{I=0}^{\infty}\frac{(2I)!}{I!}|v|^{2I}\,e^{-I(I+1)\frac{\Theta}{T}}\times g(I), \tag{98}$$

where

$$g(I) = \sum_{K=-I}^{I}\frac{|z_3|^{2(I+K)}}{(I+K)!(I-K)!}\,e^{-\left(\frac{I_{xy}}{I_z}-1\right)K^2\frac{\Theta}{T}}, \tag{99}$$

with

$$|v|^2 = (1+|z_1|^2)^2|z_2|^2, \tag{100}$$

$$|u|^2 = |v|^2(1+|z_3|^2)^2. \tag{101}$$

We can easily verify that $\mu(z_1,z_2,z_3)$ is normalized in the fashion

$$\int \mathrm{d}\Gamma\, \mu(z_1,z_2,z_3) = 1, \tag{102}$$

We compute now (i) the Wehrl entropy in the form

$$\mathcal{W} = \int \mathrm{d}\Gamma\, \mu(z_1,z_2,z_3)\, \ln\mu(z_1,z_2,z_3). \tag{103}$$

In the special instance $I_{xy}/I_z = 1$, that corresponds to the spherical rotator, we explicitly obtain

$$\mu(z_1,z_2,z_3) = e^{-|u|^2}\, \frac{\sum_{I=0}^{\infty} \frac{|u|^{2I}}{I!}\, e^{-I(I+1)\frac{\Theta}{T}}}{\sum_{I=0}^{\infty} (2I+1)^2\, e^{-I(I+1)\frac{\Theta}{T}}}. \tag{104}$$

Having the Husimi functions the Wehrl entropy is straightforwardly computed.

In order to emphasize some special cases associated to possible applications we consider several possibilities.

1. The spherical rotator $I_{xy} = I_x = I_y = I_z$, thus $I_{xy}/I_z = 1$ (*e.g.* CH_4).
2. The oblate rotator $I_{xy} = I_x = I_y < I_z$, specifically $1/2 \leq I_{xy}/I_z < 1$ (*e.g.* C_6H_6).
3. The prolate rotator $I_{xy} = I_x = I_y > I_z$, which corresponds to $I_{xy}/I_z > 1$ (*e.g.* PCl_5).
4. The extremely prolate rotator is equivalent to the linear case (all diatomic molecules, $I_z = 0$, this is $I_{xy}/I_z \to \infty$ (*e.g.* CO_2, C_2H_2).

5. Husimi distribution for systems with continuous spectrum

In this section we propose a procedure to generalize the Husimi distribution to systems with continuous spectrum. We start extending the concept of coherent states for systems with discrete spectrum to systems with continuous one. In the present section, we see the Husimi distribution as a representation of the density operator in terms of a basis of coherent states. We specially discuss the problem of the continuous harmonic oscillator [20].

5.1. The exponential weight function: Harmonic oscillator

From the $\rho(\varepsilon)$ definition expressed in Eq. (19), we can take a non-negative weight function like $\sigma(s') = \exp(-s')$. However, this choice is not fully arbitrary, because it relies on , at least, two reasons: 1) it is related to the harmonic oscillator and, 2) it is a useful function that permits exactly to solve the integral (19). The latter reason allows to express such integral in the following way

$$\rho(\varepsilon) = \int_0^s ds' s'^{2\varepsilon} \exp(-s'),$$
$$= e^{-s/2} \frac{s^\varepsilon}{2\varepsilon+1} \mathcal{M}(\varepsilon, \varepsilon+1/2, s) \tag{105}$$

where $\mathcal{M}(a,b,x)$ is the Whittaker function [48]. Besides, in relation to the first reason, when we consider $\varepsilon = n$, where n is integer, in the limit $s \to \infty$; the Eq. (105) drops into the known quantum result for the harmonic oscillator, $\rho(n) = n!$ [11].

Moreover, the measure in phase space can be explicitly expressed from Eq. (20) as follows

$$d\tau(s) = ds\, e^{-s/2} \int_0^{\varepsilon_F} d\varepsilon \frac{(2\varepsilon+1)s^\varepsilon}{\mathcal{M}(\varepsilon, \varepsilon+1/2, s)}. \tag{106}$$

Although obtaining this explicit form of the measure, a most general expression for the integral of Eq. (106) strongly depends on the particular spectrum of the system. In the present case, a spectrum like $\varepsilon \propto \omega$, the harmonic oscillator in the continuous limit, is considered.

5.2. $s \to 0$ approximation for the Husimi distribution

In order to know the shape of the Husimi distribution in $s = 0$, we need to calculate some important quantities. First, we evaluate $\rho(\varepsilon)$ given by Eq. (105) expanding the exponential which appears inside the integral, as follows

$$\rho(\varepsilon) \approx \lim_{s\to 0} \int_0^s ds' s'^{2\varepsilon}(1 - s' + \cdots), \tag{107}$$
$$\approx \frac{s^{2\varepsilon+1}}{2\varepsilon+1}\left(1 - \frac{2\varepsilon+1}{2\varepsilon+2}s + \cdots\right). \tag{108}$$

But, we are interested in evaluating the inverse of $\rho(\varepsilon)$, therefore

$$\frac{1}{\rho(\varepsilon)} \approx \frac{2\varepsilon+1}{s^{2\varepsilon+1}}\left(1 + \frac{2\varepsilon+1}{2\varepsilon+2}s + \cdots\right). \tag{109}$$

Second, we show easily that, in the limit $s \to 0$, the Husimi distribution is given by

$$\mu_Q(0) = \frac{1}{Z} \frac{\int_0^{\varepsilon_M} d\varepsilon\, (2\varepsilon+1)e^{-\beta\omega\varepsilon}}{\int_0^{\varepsilon_M} d\varepsilon\, (2\varepsilon+1)}. \tag{110}$$

Now, after integrating Eq. (25) the partition function is expressed as follows

$$Z = \frac{1 - \exp(-\beta\omega\varepsilon_M)}{\beta\omega}. \tag{111}$$

Then, the substitution of the Eq. (111) into (110) leads us to the appearance

$$\mu_Q(0) = \frac{(2e^{-\beta\omega\varepsilon_M}\beta\omega\varepsilon_M + 2e^{-\beta\omega\varepsilon_M} + e^{-\beta\omega\varepsilon_M}\beta\omega - 2 - \beta\omega)}{\beta\omega\varepsilon_M(e^{-\beta\omega\varepsilon_M} - 1)(\varepsilon_M + 1)}. \tag{112}$$

In the high temperature limit, this becomes

$$\mu_Q(0) \approx \frac{1}{\varepsilon_M} - \frac{\beta\omega\varepsilon_M}{6(\varepsilon_M + 1)}. \tag{113}$$

If we take into account a kind of particles filling a band in the lowest continuous levels of energy (for instance, $\varepsilon_M \to 1$), we find $\mu_Q(0) = 1 - \beta\omega/12$.

5.3. Asymptotic behavior of the Husimi function

In this part of the work, we are considering a particular range for ε; *i.e.,* $0 \le \varepsilon \le \varepsilon_M = 1$ and we study the asymptotic behavior of the Husimi distribution. This trend might be obtained from the limiting case of the Whittaker function [48] defined for $s \to \infty$, as follows:

$$\lim_{s\to\infty} \frac{e^{-s/2}s^{\varepsilon}\mathcal{M}(\varepsilon, \varepsilon + 1/2, s)}{2\varepsilon + 1} = \Gamma(2\varepsilon + 1). \tag{114}$$

If we replace this result into Eq. (124) we obtain

$$M(s)^2 = e^{s/2}\int_0^{\varepsilon_M} \mathrm{d}\varepsilon \frac{s^{2\varepsilon}}{\Gamma(2\varepsilon + 1)}, \tag{115}$$

and, from Eq. (24) we write

$$\mu_Q(s) = \frac{M(s)^{-2}}{Z}e^{s/2}\int_0^{\varepsilon_M} \mathrm{d}\varepsilon \frac{e^{-\omega\beta\varepsilon}s^{2\varepsilon}}{\Gamma(2\varepsilon + 1)}. \tag{116}$$

Now, we follow expanding to third order the inverse of the gamma function, $1/\Gamma(2\varepsilon + 1)$, around its maximum [48]

$$\frac{1}{\Gamma(2\varepsilon + 1)} \approx \sum_{n=0}^{3} A_n \varepsilon^n, \tag{117}$$

where $A_0 = .9963530195$, $A_1 = 1.221909147$, $A_2 = -3.108524622$, and $A_3 = 1.333217620$.

From Eq. (115), we derive a approximate result for $M(s)^2$, which is given by

$$M(s)^2 = e^{s/2}\frac{s}{2}\sum_{n=0}^{3} A_n \frac{\mathcal{M}\left(\frac{n}{2}, \frac{n}{2} + \frac{1}{2}, -2\ln(s)\right)}{(n+1)(-2\ln(s))^{1+n/2}}, \tag{118}$$

and combining all above expressions, we have finally found an expression to third order of approximation for Husimi distribution given by

$$\mu_Q(s) = \frac{M(s)^{-2}}{Z} e^{s/2-\beta\omega/2} \frac{s}{2} \sum_{n=0}^{3} A_n \frac{\mathcal{M}\left(\frac{n}{2}, \frac{n}{2}+\frac{1}{2}, \beta\omega - 2\ln(s)\right)}{(n+1)(\beta\omega - 2\ln(s))^{1+n/2}}, \tag{119}$$

where $\mathcal{M}(a,b,c)$ is again the Whittaker function [48].

In the high temperature approximation, Eq. (119) is given by

$$\mu_Q(s) \approx \beta\omega \frac{\exp(-\beta\omega/2)}{1-\exp(-\beta\omega)} \approx \exp(-\beta\omega/2). \tag{120}$$

The present result does not depend on the values of the parameter s. Furthermore, this approximation is valid whenever $0 \leq \varepsilon \leq 1$. We notice that the asymptotic trend of the Husimi distribution approaches to the Boltzmann weight in the ground state of the harmonic oscillator.

5.4. Some applications and consequences

In Ref. [11], the mean value of energy is obtained from the expectation value of the classical Hamiltonian $\mathcal{H}$ in a coherent state as follows $\mathcal{H}(s) = \langle s,\gamma|\mathcal{H}|s,\gamma\rangle$, therefore they arrive to the relation $\mathcal{H}(s) = s\partial \ln M(s)/\partial s$.

However, it is our interest here to calculate the mean value of energy in a different way, integrating in the variable s with $\mu_Q(s)$ as a weigh function. Hence, we have

$$\langle\mathcal{H}\rangle = \int d\tau(s)\, \mu_Q(s)\, \mathcal{H}(s), \tag{121}$$

where $\mathcal{H}$, expressed in terms of the variable s, denotes the classical Hamiltonian of the system. Inserting the Husimi distribution (24) into Eq. (121) and making use the relation (19) we finally get

$$\langle\mathcal{H}\rangle = \frac{1}{Z}\int_0^{\varepsilon_M} d\varepsilon\, e^{-\beta\varepsilon}\, \mathcal{H}(\varepsilon), \tag{122}$$

that is the classical mean energy [20]. We emphasize that the Husimi distribution, for a system with continuous spectrum, conduces in a natural way to the classical mean value of energy. Obviously, this is not true when the spectrum is discrete.

An extra motivation consists in extending the formulation of coherent states to systems with continuum spectrum considering its explicit form; for instance, we can take a spectrum whose appearance is $E = A\varepsilon^{\nu}$, where A and ν are constant. The values $\nu = \pm 1$ and $\nu = 2$ might define the continuous limit of three remarkable cases in physics. Certainly, in a general study other values of the parameter ν may be conveniently considered as an interesting analytical extension. Thus, for $\nu = 1$ and $A = \omega$ we have the continuous limit of a particle in a harmonic potential; this case is being in detail discussed in the present work. For $\nu = 2$ we have the continuous limit of a particle in a box. For $\nu = -1$ we have the

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continuous limit of a particle in a Coulomb potential. Therefore, it is necessary to introduce a density of states $g(E)$ in the formulation of continuous coherent states (17) and immediately get the following modification

$$|s,\gamma\rangle = M(s)^{-1} \int_0^{E_M} \mathrm{d}E\, g(E)\, \frac{s^{E/A} e^{-i\gamma E/A}}{\sqrt{\rho(E)}}\, |\varepsilon\rangle, \tag{123}$$

where the function $M(s)$

$$M(s)^2 = \int_0^{E_M} \mathrm{d}E\, g(E)^2\, \frac{s^{2E/A}}{\rho(E)} \tag{124}$$

represents the normalization factor.

6. Final remarks

We have included in the current work some motivational elements to develop possible future applications to information theory and condensed matter. We have focused attention primarily upon Husimi distribution and its analytical results, beyond the numerical, graphical, or approximate calculations. A semiclassical description undertaking can be tackled, (i) trying to estimate phase-space location via measures as Fisher information and (ii) evaluating the semiclassical Wehrl entropy. A crucial point, in such an estimation, is to define the Husimi distribution in a convenient set of coherent states. Hence, we introduce a formal view of general requirements for formulations of coherent states in the context of the Gazeau and Klauder formalism for the harmonic oscillator – we have included some mathematical details in order to make it easy to follow and instructive in courses of quantum mechanics for graduates– we show some practical elements to apply the present formalisms to specific calculations of semi-classical measures.

By using a suitable formulation of coherent states in every case, we show explicitly the form of the Husimi distribution for i) a spinless charged particle in a uniform magnetic field (Landau diamagnetism), (ii) the linear and the three dimensional rotator (molecular rotation) and (iii) a case of the limiting harmonic oscillator (continuous spectrum).

In addition, we can calculate the probability by projecting the states over the coherent states as a function of a variable related to the coherent states. We see that the localization of probability, in the phase space decreases as temperature increases. Also, as always, the localization of the Husimi distribution in the phase space decreases as temperature increases. The present derivation of Husimi distributions is based on the evaluation of the mean value of the density operator in the basis of a single-particle coherent state. While the Husimi function takes into account collective and environmental effects, the coherent states are independent-particle states. Thus, if the Husimi distribution is delocalized, we need many wave packets (independent-particle states) to represent the state. Furthermore, the thermodynamics of particles in systems, which come from environmentally induced effects, does not depend on the formulation of the coherent states. In this manner, we expect this behavior to become general.

In conclusion, quantal distributions in the phase space, such as the Husimi distribution, have long been recognized as powerful tools for studying the quantum-classical correspondence and semi-classical aspects of quantum mechanics, since they provide a phase-space picture of the density matrix. We aknowledge partial financial support by FONDECYT 1110827.

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