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On Husimi Distribution for Systems with Continuous Spectrum

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Abstract *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. In the present article, we see the Husimi distribution as a representation of the density operator in terms of a basis of coherent states. There are other ways to obtain it, but we do not consider here. We specially discuss the problem of the continuous harmonic oscillator.*

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1 Introduction

Several distributions in phase space have been possible to define, but two of them, developed by Husimi[1] and Wigner[2] are particularly common. The Husimi function, introduced long ago, is well-known as the Husimi distribution (HD). Thus, we will focus our attention on it, because its particular properties suggest that the HD is preferable to the Wigner distribution, considering that this can take negative values, when it is evaluated in some regions of phase space. In general, the HD can be viewed as Gaussian smoothing of the Wigner distribution. In this line, useful properties of the HD and its implications are frequently discussed in the literature. We emphasize among these properties that, it is always positive definite and unique, conversely it cannot be considered as a true probability distribution over the quantum-mechanical phase space[3] (reason why the HD is often considered as a quasiprobability distribution). Although HD 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.[4]

The HD may be obtained in several ways; one strategy is to derive it as the expectation value of the density operator in a basis of coherent states.[5] Therefore, to investigate this matter it is essential to pay attention into the formulation of coherent states.[5] Thus, in Ref. [5] Gazeau–Klauder discuss, among other things, what an appropriate formulation of coherent states needs. For instance, they suggest a suitable set of requirements.

The HD has been useful to describe systems in different areas of physics such as quantum mechanics, quantum optics, information theory, etc. (see, for instance,[6−11] and references therein). Also, in nanotechnology, a clear description of localization (which, in the present perspective, corresponds to classicality) is crucial to correctly determining the size of systems when the particle dynamics takes into account mobility boundaries.[12] Hence, the relationship between classicality and thermodynamics is interesting, in order to obtain physical properties in the most realistic frame, i.e., temperatures other than zero, which are typically found in nature.

Coherent states are generally acknowledged to provide a close connection between classical and quantum formulations of a given system. This work is, in part, an extension of a work published by Gazeau–Klauder,[5] where they presented a formulation of coherent states with continuous spectrum. Specifically, the aim of the present paper, in relation to this kind of systems, is twofold: i) to show how the coherent states formulation is applied to a particular case and general spectra, and ii) to evaluate its corresponding HD obtaining some approximate expressions in limiting cases.

The paper is organized as follows. In Sec. 2 we summarize the most important aspects concerning on the HD, introduce the notion of coherent states and present requirements that they have to satisfy. Also, we concentrate particularly on coherent states for a particular case. In Sec. 3 we generalize the HD for systems with continuous spectrum. In Sec. 4 we discuss a particular weight, which allows one to consider the harmonic oscillator in the continuous limit. In addition, we emphasize two limiting cases, the $s \to 0$ and $s \to \infty$ behavior. In Sec. 5, we add two important remarks that one needs to take into account when this kind of systems are studied. Its usefulness may be seen when the motivation is to obtain its semiclassical values in nonvanishing temperatures. Finally, we summarize our paper in Sec. 6.

2 Considerations on Husimi Distribution and Coherent States

2.1 *Husimi Distribution*

The HD[1] can be represented by

$$Q(z) = \langle z|\hat{\rho}|z\rangle\,, \tag{1}$$

where $\{|z\rangle\}$ denotes a complete 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 $z \in \mathbb{C}$.[5]

The HD is normalized to unity according to

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

where the integration is carried out over the complex z plane and the differential $d^2z = dxdp/2\hbar$ is a real element of area in phase space.

Let $\hat{\rho} = Z^{-1}e^{-\beta\hat{H}}$ the density matrix be thermal, where $Z = \mathrm{Tr}(e^{-\beta\hat{H}})$ is the partition function of the system, and $\beta = 1/k_BT$, T the temperature and k_B the Boltzmann constant. Thus, the function for arbitrary Hamiltonian with discrete spectra takes the form

$$Q(z) = \frac{1}{Z}\sum_n e^{-\beta E_n}|\langle z|n\rangle|^2\,, \tag{3}$$

where $\{|n\rangle\}$ is the set of energy eigenstates with eigenvalues E_n.[7–8]

Next, relevant requirements needed to develop a formulation of continuous coherent states will be summarized in order to obtain the desired HD.

2.2 *Gazeau–Klauder Coherent States*

2.2.1 *Some requirements*

Let us consider the harmonic oscillator coherent states, which are given by[5]

$$|z\rangle = e^{-|z|^2/2}\sum_{n=0}^{\infty}\frac{z^n}{\sqrt{n!}}\,|n\rangle\,, \tag{4}$$

where $\{|n\rangle\}$ is a set of eigenvectors of the Hamiltonian $\hat{H} = \hbar\omega[\hat{a}^\dagger\hat{a} + 1/2]$, which satisfies the relation $\hat{H}|n\rangle = E_n|n\rangle$, with the set of eigenvalues $\{E_n\}$ and $n = 0, 1, 2, \ldots$

Eigenvectors $\{|n\rangle\}$ can always be chosen orthonormal, this is

$$\langle n|n'\rangle = \delta_{n,n'}\,, \tag{5}$$

where $\delta_{n,n'}$ is the Kronecker delta function. By definition, Hermitian operator $\hat{H}$ is observable if this orthonormal system of vectors forms a basis in the state space. This can be expressed by the closure relation

$$\sum_{n=0}^{\infty}|n\rangle\langle n| = \hat{1}\,, \tag{6}$$

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

It is well 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–Klauder have suggested that a suitable formalism for coherent states should satisfy at least the following requirements:[5]

(i) *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 $z' \to z$.

(ii) *Resolution of Unity*: A positive measure $\tau(z)$ on $\mathcal{L}$ exists such that the unity operator admits the representation

$$\int_{\mathcal{L}} |z\rangle\langle z| d\tau(z) = 1\,, \tag{7}$$

where $|z\rangle\langle z|$ denotes a projector, which takes a state vector into a multiple of the vector $|z\rangle$.

(iii) *Temporal Stability*: The evolution of any coherent state $|z\rangle$ always remains a coherent state, which leads to a relation of the form

$$|z(t)\rangle = e^{-i\hat{H}t/\hbar}|z\rangle\,, \tag{8}$$

where $z(0) = z$, for all $z \in \mathcal{L}$ and t.

(iv) *Action Identity*: This property requires that

$$\langle z|\hat{H}|z\rangle = |z|^2\hbar\omega\,. \tag{9}$$

At this point, we remark that requirements (iii) and (iv) 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.[5] In addition, there are some shortcomings about these requirements; for instance, Gazeau–Klauder states cannot be used for degenerate systems.[13] Furthermore, it is questionable that action identity leads to the classical action-angle variable interpretation.[13]

2.2.2 *Continuous spectrum*

Gazeau–Klauder[5] proposed a formulation of coherent states for systems with continuous spectrum. They introduced a Hamiltonian $\hat{H} > 0$, with a non-degenerate continuous spectrum, thus

$$\hat{H}|\epsilon\rangle = \omega\epsilon|\epsilon\rangle, \quad 0 < \epsilon < \epsilon_M\,, \tag{10}$$

where $\{|\epsilon\rangle\}$ 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.[14] In such a case, we can always choose a normalized basis of eigenvectors to rephrase Eqs. (5) and (6) in the following manner[14]

$$\langle\epsilon|\epsilon'\rangle = \delta(\epsilon - \epsilon')\,, \tag{11}$$

$$\int_0^{\epsilon_M} |\epsilon'\rangle\langle\epsilon| = \hat{1}\,, \tag{12}$$

where $\epsilon_M \le \infty$.[5] Hereafter we use units in which $\hbar = 1$.

If we set $M(s) = e^{|z|^2/2}$ and $z = se^{-i\gamma\epsilon}$ into coherent states (4), we find

$$|s,\gamma\rangle = M(s)^{-1}\int_0^{\epsilon_M} d\epsilon\,\frac{s^\epsilon e^{-i\gamma\epsilon}}{\sqrt{\rho(\epsilon)}}\,|\epsilon\rangle\,, \tag{13}$$

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

$$M(s)^2 = \int_0^{\epsilon_M} d\epsilon\,\frac{s^{2\epsilon}}{\rho(\epsilon)}\,, \tag{14}$$

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

Coherent states (13) must satisfy resolution of identity. In such a case, it is possible to introduce[5] the following relation

$$\rho(\epsilon) = \int_0^s ds'\, s'^{2\epsilon}\sigma(s')\,, \tag{15}$$

where s' is a variable of integration with $0 \leq s' < s \leq \infty$. In addition, a non-negative weight function $\sigma(s') \geq 0$ is introduced to satisfy the second requirement. Then, the measure of integration takes the form[5]

$$d\tau(s,\gamma) = \sigma(s) M(s)^2 \, ds \, \frac{d\gamma}{2\pi} \,. \tag{16}$$

Gazeau–Klauder showed that resolution of unity is satisfied for systems with continuous spectrum in the present formulation of coherent states.[5]

3 Husimi Distribution for Systems with Continuous Spectrum

Starting from Eq. (3), as we have aforementioned, we propose a continuous appearance of HD replacing the discrete form by the continuous version of variables, functions and operators. Hence, we define the continuous HD in the following manner:

$$Q(s,\gamma) = \frac{1}{Z} \int_0^{\epsilon_M} d\epsilon \; e^{-\beta\omega\epsilon} \, |\langle s,\gamma|\epsilon\rangle|^2 \,, \tag{17}$$

where ϵ stands for a continuous parameter. The HD satisfies the normalization condition according to

$$\int_0^S \int_{-\infty}^{\infty} d\tau(s,\gamma) Q(s,\gamma) = 1 \,, \tag{18}$$

where the measure $d\tau(s,\gamma)$ is given by Eq. (16).

We see easily from Eq. (13) that, the projection of eigenstates of the Hamiltonian over coherent states, is given by

$$\langle s,\gamma|\epsilon\rangle = M(s)^{-1} \, \frac{s^{\epsilon} e^{-i\gamma\epsilon}}{\sqrt{\rho(\epsilon)}} \,, \tag{19}$$

where the orthogonality condition of continuous states $\{|\epsilon\rangle\}$ has been imposed through Eq. (11). Introducing the above expression into Eq. (17) we arrive to

$$Q(s) = \frac{M(s)^{-2}}{Z} \int_0^{\epsilon_M} d\epsilon \; \frac{e^{-\beta\omega\epsilon} s^{2\epsilon}}{\rho(\epsilon)} \,, \tag{20}$$

where we have dropped out the dependence on γ. The continuous partition function obviously is[15]

$$Z = \int_0^{\epsilon_M} \mathrm{d}\epsilon \, e^{-\beta\omega\epsilon} \,. \tag{21}$$

It is important to remark that Eq. (20) is consistently normalized in accordance with Eq. (18), whose final form can be re-expressed by the following single integral

$$\int_0^S \mathrm{d}\tau(s) \, Q(s) = 1 \,, \tag{22}$$

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

4 Exponential Weight Function: Harmonic Oscillator

After developing a line of working and modifying certain mathematical tools to evaluate the continuous HD, we start choosing a non-negative weight function like $\sigma(s') = \exp(-s')$ trying to connecting to a particular physical system. The assessment of the function $\rho(\epsilon)$ is through Eq. (15). This choice, is not fully arbitrary, relies on at least two reasons: (i) it is related to the harmonic oscillator and, (ii) it is a useful function that permits exactly to solve the integral (15). The latter reason allows to express such integral in the following way

$$\begin{aligned} \rho(\epsilon) &= \int_0^s ds' s'^{2\epsilon} \exp(-s') \,, \\ &= e^{-s/2} \frac{s^{\epsilon}}{2\epsilon+1} \mathcal{M}(\epsilon, \epsilon+1/2, s) \,, \end{aligned} \tag{23}$$

where $\mathcal{M}(a,b,x)$ is the Whittaker function.[16] Besides, in relation to the first reason, when we consider $\epsilon = n$, where n is integer, in the limit $s \to \infty$; the equation (23) drops into the known quantum result for the harmonic oscillator, $\rho(n) = n!$.[5]

Moreover, the measure in phase space can be explicitly expressed from equation (16) as follows

$$d\tau(s) = ds \, e^{-s/2} \int_0^{\epsilon_F} d\epsilon \frac{(2\epsilon+1)s^{\epsilon}}{\mathcal{M}(\epsilon,\epsilon+1/2,s)} \,. \tag{24}$$

Although obtaining this explicit form of the measure, a most general expression for the integral of Eq. (24) strongly depends on the particular spectrum of the system. In the present case, a spectrum like $\epsilon \propto \omega$, the harmonic oscillator in the continuous limit, is considered.

4.1 $s \to 0$ *Approximation for Husimi Distribution*

In order to know the shape of the HD in $s = 0$, we need to calculate some important quantities. First, we evaluate $\rho(\epsilon)$ given by equation (23) expanding the exponential which appears inside the integral, as follows

$$\rho(\epsilon) \approx \lim_{s\to 0} \int_0^s ds' s'^{2\epsilon} (1 - s' + \cdots) \tag{25}$$

$$\approx \frac{s^{2\epsilon+1}}{2\epsilon+1} \Big(1 - \frac{2\epsilon+1}{2\epsilon+2} s + \cdots \Big) \,. \tag{26}$$

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

$$\frac{1}{\rho(\epsilon)} \approx \frac{2\epsilon+1}{s^{2\epsilon+1}} \Big(1 + \frac{2\epsilon+1}{2\epsilon+2} s + \cdots \Big) \,. \tag{27}$$

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

$$Q(0) = \frac{1}{Z} \, \frac{\int_0^{\epsilon_M} d\epsilon \, (2\epsilon+1) e^{-\beta\omega\epsilon}}{\int_0^{\epsilon_M} d\epsilon \, (2\epsilon+1)} \,. \tag{28}$$

Now, after integrating equation (21) the partition function is expressed as follows

$$Z = \frac{1 - \exp(-\beta\omega\epsilon_M)}{\beta\omega} \,. \tag{29}$$

Then, the substitution of the equation (29) into (28) leads us to the appearance

$$Q(0) = \frac{(2e^{-\beta\omega\epsilon_M} \beta\omega\epsilon_M + 2e^{-\beta\omega\epsilon_M} + e^{-\beta\omega\epsilon_M} \beta\omega - 2 - \beta\omega)}{\beta\omega\epsilon_M (e^{-\beta\omega\epsilon_M} - 1)(\epsilon_M + 1)} \,. \tag{30}$$

In the high temperature limit, this becomes

$$Q(0) \approx \frac{1}{\epsilon_M} - \frac{\beta\omega\epsilon_M}{6(\epsilon_M+1)}\,. \tag{31}$$

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

4.2 *Asymptotic Behavior of Husimi Function*

In this part of the work, we are considering a particular range for ϵ; i.e., $0 \le \epsilon \le \epsilon_M = 1$ and we study the asymptotic behavior of the HD. This trend might be obtained from the Eq. (23) in the limiting case of the Whittaker function[16] defined for $s \to \infty$, as follows:

$$\lim_{s\to\infty} \frac{e^{-s/2} s^{\epsilon} \mathcal{M}(\epsilon, \epsilon+1/2, s)}{2\epsilon+1} = \Gamma(2\epsilon+1)\,. \tag{32}$$

If we replace this result into Eq. (14) we obtain

$$M(s)^2 = e^{s/2} \int_0^{\epsilon_M} d\epsilon \frac{s^{2\epsilon}}{\Gamma(2\epsilon+1)}\,, \tag{33}$$

and, from Eq. (20) we write

$$Q(s) = \frac{M(s)^{-2}}{Z} e^{s/2} \int_0^{\epsilon_M} d\epsilon \frac{e^{-\omega\beta\epsilon} s^{2\epsilon}}{\Gamma(2\epsilon+1)}\,. \tag{34}$$

Now, we follow expanding to third order the inverse of the gamma function, $1/\Gamma(2\epsilon+1)$, around its maximum[16]

$$\frac{1}{\Gamma(2\epsilon+1)} \approx \sum_{n=0}^{3} A_n \epsilon^n\,, \tag{35}$$

where $A_0 = 0.996\ 353\ 019\ 5$, $A_1 = 1.221\ 909\ 147$, $A_2 = -3.108\ 524\ 622$, and $A_3 = 1.333\ 217\ 620$.

From Eq. (33), we derive an approximate result for $M(s)^2$, which is given by

$$M(s)^2 = e^{s/2} \frac{s}{2} \sum_{n=0}^{3} A_n \times \frac{\mathcal{M}(n/2, n/2+1/2, -2\ln(s))}{(n+1)(-2\ln(s))^{1+n/2}}\,, \tag{36}$$

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

$$Q(s) = \frac{M(s)^{-2}}{Z} e^{s/2-\beta\omega/2} \frac{s}{2} \sum_{n=0}^{3} A_n \times \frac{\mathcal{M}(n/2, n/2+1/2, \beta\omega-2\ln(s))}{(n+1)(\beta\omega-2\ln(s))^{1+n/2}}\,, \tag{37}$$

where $\mathcal{M}(a,b,c)$ is again the Whittaker function.[16]

In the high temperature approximation, Eq. (37) is given by

$$Q(s) \approx \beta\omega \frac{\exp(-\beta\omega/2)}{1-\exp(-\beta\omega)} \approx \exp(-\beta\omega/2)\,. \tag{38}$$

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

5 Remarks

5.1 *On the Mean Energy*

In Ref. [5], 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 arrived 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 $Q(s)$ as a weigh function. Hence, we have

$$\langle\mathcal{H}\rangle = \int d\tau(s)\, Q(s)\, \mathcal{H}(s)\,, \tag{39}$$

where $\mathcal{H}$, expressed in terms of the variable s, denotes the classical Hamiltonian of the system. Inserting the HD (20) into Eq. (39) and making use the relation (15) we finally get

$$\langle\mathcal{H}\rangle = \frac{1}{Z} \int_0^{\epsilon_M} d\epsilon\, e^{-\beta\omega\epsilon}\, \mathcal{H}(\epsilon)\,, \tag{40}$$

that is the classical mean energy.[15] We emphasize that the HD, 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.

5.2 *On the Density of States*

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

$$E = A\epsilon^{\nu}\,, \tag{41}$$

where A and ν are constants. 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 continuous limit of a particle in a Coulomb potential. Therefore, it is necessary to introduce a density of states $g(E)$ to rephrase Eq. (40) and we immediately propose the following modification for the mean value of the HD

$$\langle\mathcal{H}\rangle = \frac{1}{Z} \int_0^{E_M} dE\, g(E) e^{-\beta E}\, \mathcal{H}(E)\,, \tag{42}$$

where we have considered

$$g(E) = \frac{E^{1/\nu-1}}{\nu A^{1/\nu}}\,, \tag{43}$$

which is trivially derived from the spectrum of Eq. (41).

6 Summary

In this paper we have considered some concepts needed to evaluate the HD. Several ways are possible to follow when the HD is evaluated. In particular, we have obtained it as the expectation value of the density operator in a basis of coherent states. Next, we have reviewed requirements that a suitable formalism of coherent states ought to satisfy. In addition, we have payed special attention to a possible extension of such a formalism to systems with continuous spectrum proposed before by Gazeau–Klauder.

After reviewing the above concepts, we briefly summarize our contributions. We present a general expression for the HD making use of the representation of coherent states for systems with continuous spectrum. As already said, we make an effort to connect our results to a well known system, the harmonic oscillator. This fact is based in the exponential weight of Eq. (23), whose use gives us to the continuous limit of factorial numbers, which typically appears in the formulation of coherent states of quantum systems. The measure in phase space is explicitly obtained in Eq. (24). In addition, two limiting cases of the HD are obtained; these are: the $s \to \infty$ (asymptotic) and the $s \to 0$ approximations.

Also, we have commented about the density of states, whose usefulness is worthy to consider, when systems different to harmonic oscillator are studied. Furthermore, we have remarked that the mean value of the Hamiltonian using the HD as a weight function leads us directly to the classical mean value of energy. Certainly, it is possible to extend the validity of this remark to all quantum observables of physical systems.

Finally, we think it is possible to study other systems with continuous spectrum (14) making use of the representation of coherent states proposed before by Gazeau–Klauder.

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