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Husimi distribution for the linear rigid rotator

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Abstract. We find the Husimi distribution for the linear rigid rotator. The Husimi function can be viewed in a variety of ways. In particular, we obtain it as the expectation value of the density operator in a suitable basis of coherent states. We employ the Schwinger's oscillator model for the construction of the angular momentum coherent states.

1. Introduction

We are interested in the semiclassical description of the rotational dynamics of molecular systems. A pioneer effort in this sense is that of Morales *et al.* in Ref. [1], who studied the connection between such dynamics and coherent states [2, 3].

In this communication, the main goal is to obtain analytically the Husimi distribution for the linear rigid rotator. Advantages about the Husimi distribution for the interpretation of the electronic structure in hydrogen and nitrogen atoms are discussed in Refs. [4, 5]. Authors suggest that their work may be extended to the molecular instance. Following this suggestion we address here the simplest applicable model, i.e., the rigid rotator. Its usefulness for describing diatomic molecules is well-known [6].

The paper is organized as follows: In Section 2 we introduce basic aspects and properties which must be satisfied by coherent states. In Section 3 we explore the linear rigid rotator. We write the probability of finding a quantum state in a coherent state that is used to obtain an explicit expression for the Husimi distribution, and finally in Section 4, we draw some concluding remarks.

2. Coherent States and Husimi distribution

Glauber's coherent states are eigenstates of an annihilation operator \hat{a} [2]

$$\hat{a}|z\rangle = z|z\rangle, \quad (1)$$

where the Hamiltonian of the harmonic oscillator reads $\hat{H} = \hbar\omega[\hat{a}^\dagger\hat{a} + 1/2]$ and the complex eigenvalues of the operator \hat{a} are $z = (m\omega/2\hbar)^{1/2}x + i(2\hbar\omega m)^{-1/2}p$.

It is well-known that coherent states can be constructed in several ways and by recourse to different techniques, its formulation being of a not-unique character. Gazeau and Klauder

suggest that a suitable formalism for coherent states should satisfy at least the following requirements [7]:

- (i) Continuity of labelling refers to the map from the label space \mathcal{L} into Hilbert space. This condition means that the expression $\| |z'\rangle - |z\rangle \| \rightarrow 0$ whenever $z' \rightarrow z$.
- (ii) Resolution of Unity: A positive measure $\mu(z)$ on \mathcal{L} exists such that the unity operator admits the representation

$$\int_{\mathcal{L}} |z\rangle\langle z| d\mu(z) = 1, \quad (2)$$

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

The “*semi-classical*” phase-space distribution function associated to the density matrix $\hat{\rho}$ of the system [2, 3], often referred to as the Husimi distribution [8] is

$$\mu(x, p) = \langle z | \hat{\rho} | z \rangle, \quad (3)$$

which is normalized in compliance with

$$\int (dx dp / 2\pi\hbar) \mu(x, p) = 1. \quad (4)$$

Indeed, $\mu(x, p)$ is a Wigner-distribution D_W smeared over an \hbar sized region of phase space [10]. The smearing renders $\mu(x, p)$ a positive function, even if D_W does not have such a character.

The usual treatment of equilibrium in statistical mechanics makes use of the Gibbs’s canonical distribution, whose associated, “*thermal*” density matrix is $\hat{\rho} = Z^{-1} e^{-\beta\hat{H}}$, with $Z = Tr(e^{-\beta\hat{H}})$ the partition function, $\beta = 1/k_B T$ the inverse temperature T , and k_B the Boltzmann constant. For an arbitrary Hamiltonian \hat{H} of eigen-energies E_n and eigenstates $|n\rangle$, being n a collection of all the pertinent quantum numbers required to label the states, one can always write [10, 9]

$$\mu(x, p) = \langle z | \hat{\rho} | z \rangle = \frac{1}{Z} \sum_n e^{-\beta E_n} |\langle z | n \rangle|^2. \quad (5)$$

3. Linear rigid rotator

For pedagogical purpose, we develop a simple model, the linear rigid rotator, based on the excellent discussion concerning the coherent states for angular momenta given in Ref. [11, 12]. The Hamiltonian is $\hat{H} = \hat{L}^2 / 2I_{xy}$ 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 [6]. We have assumed that $I_{xy} \equiv I_x = I_y$. Calling $|I, K\rangle$ the set of H -eigenstates, we recall that they verify the relations

$$\begin{aligned} \hat{L}^2 |IK\rangle &= I(I+1)\hbar^2 |IK\rangle \\ \hat{L}_z |IK\rangle &= K\hbar |IK\rangle, \end{aligned} \quad (6)$$

with $I = 0, 1, 2, \dots$, for $-I \leq K \leq I$, the eigenstates’ energy spectrum being given by $\varepsilon_I = I(I+1)\hbar^2 / 2I_{xy}$. Our coherent states are constructed in Ref. [11, 13] using Schwinger’s oscillator model of angular momentum, in the fashion

$$|IK\rangle = \frac{(\hat{a}_+^\dagger)^{I+K} (\hat{a}_-^\dagger)^{I-K}}{\sqrt{(I+K)!(I-K)!}} |0\rangle, \quad (7)$$

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.,

$$\langle I' K' | IK \rangle = \delta_{I', I} \delta_{K', K}, \quad (8)$$

$$\sum_{I=0}^{\infty} \sum_{K=-I}^I |IK\rangle \langle IK| = \hat{1}. \quad (9)$$

Since we deal with two degrees of freedom the ensuing coherent states are of the tensorial product form $|z_1 z_2\rangle = |z_1\rangle \otimes |z_2\rangle$, where $\hat{a}_+ |z_1 z_2\rangle = z_1 |z_1 z_2\rangle$, $\hat{a}_- |z_1 z_2\rangle = z_2 |z_1 z_2\rangle$. Therefore, the coherent state is $|z_1 z_2\rangle = e^{-|z|^2/2} e^{z_1 \hat{a}_+^\dagger} e^{z_2 \hat{a}_-^\dagger} |0\rangle$, and $|z|^2 = |z_1|^2 + |z_2|^2$ [12]. Using Eqs. (7), after a bit of algebra, we immediately find

$$|z_1 z_2\rangle = e^{-\frac{|z|^2}{2}} \sum_{I=0}^{\infty} \sum_{K=-I}^I \frac{z_1^{n_+}}{\sqrt{n_+!}} \frac{z_2^{n_-}}{\sqrt{n_-!}} |IK\rangle \quad (10)$$

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

$$|\langle IK | z_1 z_2 \rangle|^2 = e^{-|z|^2} \frac{z_1^{2n_+}}{n_+!} \frac{z_2^{2n_-}}{n_-!}. \quad (11)$$

The Husimi distribution for this system is defined from Eq.(5), as $\mu(z_1, z_2) = \langle z_1, z_2 | \hat{\rho} | z_1, z_2 \rangle$, where $\hat{\rho} = Z_{2D}^{-1} \exp(-\beta \hat{H})$, and the rotational partition function is $Z_{2D} = \sum_{I=0}^{\infty} (2I + 1) e^{-I(I+1)\Theta/T}$, with $\Theta = \hbar^2/(2I_{xy} k_B)$ [6]. Using Eq. (11) and Eq. (5) we finally get our Husimi distribution

$$\mu(z_1, z_2) = e^{-|z|^2} \frac{\sum_{I=0}^{\infty} \frac{|z|^{4I}}{(2I)!} e^{-I(I+1)\frac{\Theta}{T}}}{\sum_{I=0}^{\infty} (2I + 1) e^{-I(I+1)\frac{\Theta}{T}}} \quad (12)$$

normalized according to $\int (d^2 z_1/\pi)(d^2 z_2/\pi) \mu(z_1, z_2) = 1$. The differential element of area in the $z_1(z_2)$ plane is $d^2 z_1 = dx dp_x/2\hbar$ ($d^2 z_2 = dy dp_y/2\hbar$) [2]. Moreover, we have the phase-space relationships

$$|z_1|^2 = \frac{1}{4} \left(\frac{x^2}{\sigma_x^2} + \frac{p_x^2}{\sigma_{p_x}^2} \right), \quad (13)$$

$$|z_2|^2 = \frac{1}{4} \left(\frac{y^2}{\sigma_y^2} + \frac{p_y^2}{\sigma_{p_y}^2} \right), \quad (14)$$

where $\sigma_x \equiv \sigma_y = \sqrt{\hbar/2m\omega}$ and $\sigma_{p_x} \equiv \sigma_{p_y} = \sqrt{\hbar m\omega/2}$. In Fig. 1, we depict the behavior of the Husimi distribution $\mu(z_1, z_2)$ as a function of $|z|$ at fixed temperature. The profile of the Husimi function looks like a Gaussian distribution. We see that the maximum value of the distribution increases as the temperature decreases.

4. Concluding remarks

A study has been performed on the basis of Schwinger's angular momenta construction [11] rotator-formulation.

We have obtained in analytical fashion the form of the appropriate semiclassical Husimi distribution.

Results from this kind of techniques can be relevant in the study of information on the localization of molecules in phase space. In addition, writing a suitable form of the Husimi distribution is crucial in future calculations, for instance the Wehrl entropy and the Fisher measure.

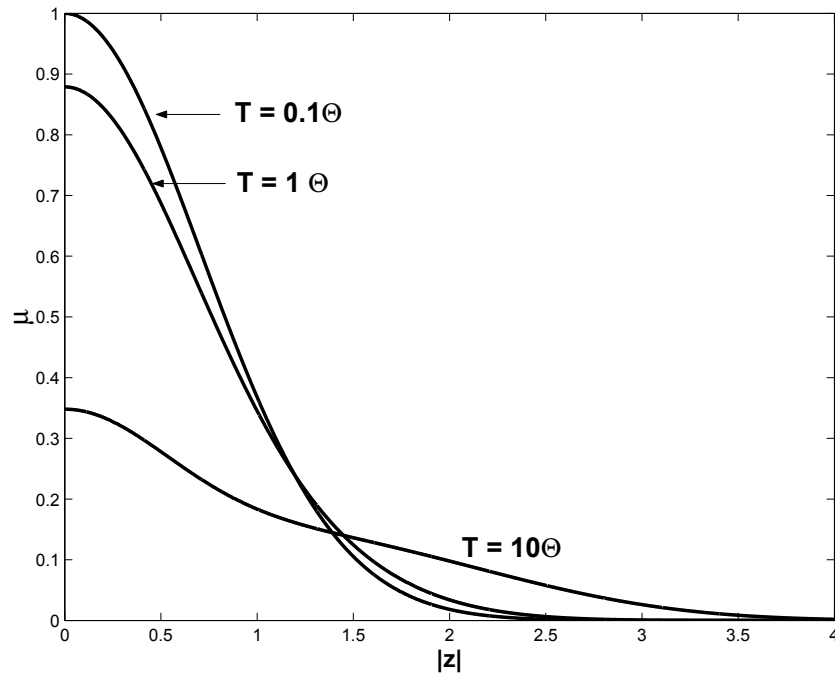


Figure 1. The Husimi distribution $\mu(z_1, z_2)$ is plotted as a function of $|z|$ for several values of the temperature: ($T = 0.1\Theta, \Theta, 10\Theta$). The behavior of the Husimi function resembles that of a Gaussian distribution. The peak of the distribution increases as the temperature decreases.

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