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When does a given function in phase space belong to the class of Husimi distributions?

D M Davidović and D Lalović

Institute for Nuclear Sciences Vinča, Laboratory for Theoretical Physics, PO Box 522, 11001 Beograd, Serbia, Yugoslavia

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Abstract. The problem of finding a density matrix corresponding to a Husimi distribution is solved in a simple, new way. It is shown how the proposed procedure may be effectively used to answer the question raised in the title.

1. Introduction

The oldest and the most elaborated phase space formulation of quantum mechanics was originated by Wigner in his 1932 seminal paper [1], in which every quantum mechanical state was represented by a corresponding function in phase space—its Wigner function. This formulation is now an indispensable language of many branches of physics. Although in calculations of quantum mechanical averages the Wigner function plays a role analogous to that of the classical distribution function [2], it cannot be interpreted as a probability distribution because in the general case it necessarily assumes negative values. To overcome this difficulty in interpretation and due to other more concrete reasons, several non-negative distribution functions were introduced.

The first to be introduced and the most widely used non-negative distribution function is the well known Husimi function [3]. Being non-negative by definition, the Husimi function can always be interpreted as some probability distribution on phase space. But this is not only a formal possibility. It has been shown that the Husimi function may be interpreted as the probability distribution for the statistics in a particular physical model for simultaneous measurement of coordinate and momentum [4, 5]. In a mathematically general and systematic way, Holevo [6] has shown that the Husimi function of any quantum mechanical state arises naturally whenever the simultaneous measurement of coordinate and momentum is performed on this state with maximal accuracy allowed by the uncertainty relations.

Quantum mechanics can be completely formulated in terms of the Husimi distribution [7–11]. However, unlike with the case of quantum mechanics in standard formulation, when one solves, for example, an eigenvalue equation in Husimi representation, one can obtain solutions which are mathematically acceptable but which do not have physical meaning [12]. Only those solutions have a physical meaning for which the corresponding quantum mechanical states, described by wavefunctions or more generally by density matrices, exist. For this reason it is necessary to have an efficient method enabling one to single out those functions in phase space which may correspond to some quantum mechanical states.

A similar necessity arises in the investigations of the correspondence between distribution functions in classical statistical mechanics and distributions in phase space representations of quantum mechanics. So, examining the general properties of entropy, Wehrl [13] noticed the striking paradox that the entropy defined quantum mechanically is always positive and cannot be greater than the entropy obtained in classical approximation defined in an appropriate way, while the latter for some distributions may well be negative. The reason for this paradox is that not every classical probability distribution has its quantum mechanical counterpart, and thus cannot be observed in nature.

In the present paper we first establish a new method for obtaining the corresponding density matrix from a given Husimi function and compare it with existing methods. Then we show how the proposed method may be effectively used in answering the question whether a given function in phase space may be a Husimi distribution. We also treat one concrete example. For simplicity we restrict our considerations to the one-dimensional case.

2. Obtaining the density matrix from the Husimi function

Up to a numerical factor, the Husimi distribution function $D_{\mathrm{H}}(q,p)$ may be defined as the diagonal matrix element of the density matrix $\hat{\rho}$ in the harmonic oscillator coherent states basis $|\alpha\rangle$. We can write

$$D_{\mathrm{H}}(q,p)=1/(2\pi h)\langle\alpha|\hat{\rho}|\alpha\rangle. \tag{1}$$

For $|\alpha\rangle$ in the coordinate representation we have

$$\langle x|\alpha\rangle=(b/\pi)^{1/4}\exp[-b/2(x-q)^2+\mathrm{i}px/\hbar] \tag{2}$$

where $b=mw/\hbar$, $\alpha=(b/2)^{1/2}q+\mathrm{i}/\hbar(2b)^{-1/2}p$.

Since every density matrix by definition may be represented in the form

$$\hat{\rho}(x,y)=\sum_k \lambda_k\Psi_k(x)\Psi_k^*(y) \qquad \lambda_k\geqslant 0 \tag{3}$$

it is necessarily a positive definite function. Using the above relations, after simple rearrangements of terms we obtain

$$KD_{\mathrm{H}}(q,p)=\mathrm{e}^{-bq^2}\left\{\sum_k \lambda_k\int\Psi_k(x)\exp[-b/2x^2+x(bq+\mathrm{i}p/\hbar)]\,\mathrm{d}x\right.$$
$$\left.\times\int\Psi_k^*(y)\exp[-b/2y^2+y(bq-\mathrm{i}p/\hbar)]\,\mathrm{d}y\right\} \tag{4}$$

where $K=2\pi\hbar\ (\pi/b)^{1/2}$. From the last equality it is obvious that $D_{\mathrm{H}}(q,p)$ has all derivatives over q and p so that it is an entire function of q and p and may be analytically continuated to complex values of q and p [7]. This feature of the Husimi function may be used to find the relation between non-diagonal matrix elements in the coherent state basis and the values of the Husimi function in the complex domain. This relation is useful for obtaining the corresponding density matrix from a given Husimi function. To show this we shall choose complex values for the arguments of the Husimi function which will be denoted by $\tilde{q}$ and $\tilde{p}$, such that the following relations hold:

$$b\tilde{q}+i\tilde{p}/\hbar=bq_1+ip_1/\hbar$$

$$b\tilde{q}-i\tilde{p}/\hbar=bq_2-ip_2/\hbar$$

or equivalently

$$\begin{aligned}\tilde{q}&=\tfrac{1}{2}(q_1+q_2)+i(p_1-p_2)/(2b\hbar)\\ \tilde{p}&=\tfrac{1}{2}(p_1+p_2)+i\hbar b(q_2-q_1)/2.\end{aligned} \tag{5}$$

With (5), from the relation (4) we obtain

$$KD_{\mathrm{H}}(\tilde{q},\tilde{p})\ e^{b\tilde{q}^2}=\sum_k \lambda_k \int \Psi_k(x) \times\exp[-b/2x^2+x(bq_1+ip_1/\hbar)]\ dx \int \Psi_k^*(y) \times\exp[-b/2y^2+y(bq_2-ip_2/\hbar)]\ dy. \tag{6}$$

The right-hand side of the last equation is equal to the non-diagonal matrix element of the density matrix we were looking for, up to a multiplication factor. Putting $q_1=q_2=0$ in (6) and keeping in mind (5) we obtain

$$KD_{\mathrm{H}}(i(p_1-p_2)/(2b\hbar)\qquad (p_1+p_2)/2)\ \exp(-(p_1-p_2)^2/(4b\hbar^2))=\sum \lambda_k \int \Psi_k(x) \times\exp\left(-\frac{b}{2}x^2+ip_1x/\hbar\right)dx \int \Psi_k^*(y)\ \exp\left(-\frac{b}{2}y^2-ip_2y/\hbar\right)dy. \tag{7}$$

Inverting the Fourier transforms appearing in this relation we obtain the density matrix in the form

$$\begin{aligned}\hat{\rho}(x,y)&=\sum_k \lambda_k\Psi_k(x)\Psi_k(y)^*\\ &=K\exp[b(x^2+y^2)/2]/(2\pi\hbar)^2\int D_{\mathrm{H}}(i(p_1-p_2)/(2b\hbar),\\ &\quad (p_1+p_2)/2)\ \exp[-(p_1-p_2)^2/(4b\hbar^2)-ip_1x/h+ip_2y/\hbar]\ dp_1\ dp_2.\end{aligned} \tag{8}$$

When the Husimi distribution is available in the analytic form, the last relation can be effectively used to invert the Husimi function and so obtain the corresponding density matrix.

We shall now briefly describe the formulae for inversion of the Husimi function available in the literature, in order to compare them with our result.

Departing from coherent states expressed through the eigen-energy states of the harmonic oscillator [14], one easily obtains

$$\langle\alpha|\hat{\rho}|\alpha\rangle=\sum_{n,m}\langle n|\hat{\rho}|m\rangle\ e^{-|\alpha|^2}\alpha^{*n}\alpha^m/(n!m!)^{1/2}$$

and from there

$$\langle n|\hat{\rho}|m\rangle=(n!m!)^{1/2}[\partial^n/\partial\alpha^{*n}\,\partial^m/\partial\alpha^m\,e^{\alpha\alpha^*}\langle\alpha|\hat{\rho}|\alpha\rangle]_{0,0}.$$

A formula for inversion of the Husimi function was derived for the first time by Kano [15] and is very similar to the one just presented.

Another formula for inversion may be obtained from the differential relation between the Husimi function and the Wigner function. One can write [16]

$$D_{\rm H}(q,p)=\exp(a\,\partial^2/\partial q^2+1/a\,\partial^2/\partial p^2)W(q,p)$$

and from there

$$E(q,p)=\exp(-a\,\partial^2/\partial q^2-1/a\,\partial^2/\partial p^2)D_{\rm H}(q,p).$$

From the Wigner function, which in our case is expressed through the Husimi function, one can obtain the density matrix using the Weyl transformation [17].

Both formulae are used mainly in theoretical considerations and although formally simple, are of little practical use due to the appearance of an infinite series of operators.

From the integral relation between the Husimi function and Wigner function

$$D_{\rm H}(q,p)=\int e^{-a(q-q')^2-1/a(p-p')^2}W(q',p')\,dq'\,dp'$$

using the Fourier transform twice in an obvious way, the Wigner function may be obtained and then, from it, the density matrix.

Mizrahi, who in a series of papers [8–10] gave the first systematic formulation of quantum mechanics in terms of Husimi function, proposed the following formula for inversion of the Husimi function

$$\rho(x',x)=\exp[a^2/2(x'-x)^2]\sum_{n=0}^{\infty}(-)^n/(n!2^n)$$
$$\times\int dq\,dp\,H_{2n}[a(q-(x+x')^2/2)]K(q,p;x,x')D_{\rm H}(q,p)$$

where $K(q,p;x,x')=(a^2/\pi)^{1/2}\exp[-a^2(q-(x+x')/2)^2-a^2(x-x')^2+ip(x-x')]$.

To obtain the density matrix in our formalism it is sufficient to make a simple change of variables and then the Fourier transform. Compared with the complicated procedures one has to perform in all the described approaches, it is evident that our method is essentially simpler. In the next section we will demonstrate the use of our method on one concrete example.

3. Applications

We have just shown how a density matrix may be obtained for a given Husimi function. Now we shall show how the same method may be used to find the conditions under which a given function in phase space $F(q,p)$ belongs to the class of Husimi distributions. First, this function must be non-negative and an entire function of its variables. Further, from the structure of the right-hand side of (7), it is evident that the expression appearing on its left side is a positive definite function for every Husimi distribution. So, the necessary condition for $F(q,p)$ to be a Husimi distribution is that the same expression for it is positive definite. In detail, when we take

$$\tilde{q} = i(p_1 - p_2)/(2b\hbar)$$
$$\tilde{p} = (p_1 + p_2)/2 \tag{9}$$

the expression

$$F(\tilde{q}, \tilde{p})\, e^{b\tilde{q}^2} = F[i(p_1 - p_2)/(2b\hbar), (p_1 + p_2)/2] \exp\left(-\frac{(p_1 - p_2)^2}{4b\hbar^2}\right)$$
$$= \exp\left(-\frac{p_1^2 + p_2^2}{4b\hbar^2}\right) f(p_1, p_2) \tag{10}$$

must for some positive values of a parameter b be positive definite. This condition is at the same time sufficient. Namely, the expression (10) has such analytic structure and asymptotic behaviour at infinity, that the function which one obtains from it after the transformation appearing in (8) does not diverge and has all the necessary features of a density matrix. In this way, in order to find whether a given non-negative normalized entire function is a Husimi distribution, we have only to see whether the expression (10) for this function is positive definite.

To prove the above statement in detail let us note that when the expression (10) is positive definite it may, due to its analyticity, be represented as follows

$$\exp\left(-\frac{p_1^2 + p_2^2}{4b\hbar^2}\right) f(p_1, p_2)$$
$$= \frac{1}{2\pi\hbar} \exp\left(-\frac{p_1^2 + p_2^2}{4b\hbar^2}\right) \sum_k \lambda_k \left(\sum_n \frac{C_{k,n}}{\sqrt{n!}} \left(\frac{i}{\hbar} \frac{p_1}{\sqrt{2b}}\right)^n\right)$$
$$\times \left(\sum_m \frac{C^*_{k,m}}{\sqrt{m!}} \left(\frac{-i}{\hbar} \frac{p_2}{\sqrt{2b}}\right)^m\right) \qquad \lambda_k > 0 \tag{11}$$

where the coefficients are written in a form convenient for further use. Performing here the transformation inverse to that in (9) we obtain

$$F(q, p) = \frac{1}{2\pi\hbar} \exp\left(-\frac{b}{2} q^2 - \frac{1}{2b} \frac{b^2}{\hbar^2}\right) \sum_k \lambda_k \left(\sum_n \frac{C_{k,n}}{\sqrt{n!}} \left(\sqrt{\frac{b}{2}}\, q + \frac{i}{\hbar} \frac{p}{\sqrt{2b}}\right)^n\right.$$
$$\times \left.\left(\sum_m \frac{C^*_{k,m}}{\sqrt{m!}} \left(\sqrt{\frac{b}{2}}\, q - \frac{i}{\hbar} \frac{p}{\sqrt{2b}}\right)^m\right)\right). \tag{12}$$

Any putative Husimi function must be normalized to unity. Thus, after integration of (12) in the q–p plane using polar coordinates, we obtain the following relation for coefficients:

$$\sum_k \lambda_k \left(\sum_n |C_{k,n}|^2\right) = 1. \tag{13}$$

Performing now in (11) the operation appearing in (8) and taking into account that

$$\int_{-\infty}^{+\infty} \left(\frac{\mathrm{i}}{\hbar}\frac{p}{\sqrt{b}}\right)^n \exp\left(-\frac{p^2}{4b\hbar^2} - \mathrm{i}\,\frac{px}{\hbar}\right) \mathrm{d}p = 2\hbar\sqrt{\pi b}\, H_n(\sqrt{b}x)\, \mathrm{e}^{-bx^2}$$

we obtain for a putative density matrix

$$\rho_b(x,y) = \sqrt{\frac{b}{\pi}} \exp\left(-\frac{b}{2}(x^2+y^2)\right) \sum_k \lambda_k \left(\sum_n \frac{C_{k,n}}{\sqrt{n!}} \frac{1}{(\sqrt{2})^n} H_n(\sqrt{b}x)\right) \times \left(\sum_m \frac{C^*_{k,m}}{\sqrt{m!}} \frac{1}{(\sqrt{2})^m} H_m(\sqrt{b}y)\right).$$

Since the Hermitean polynomials are orthogonal, the trace $\int \rho_p(x, y)\,\mathrm{d}x$ of this matrix is equal to unity because of the relation (13). As we saw, this relation follows from the normalization of $F(q, p)$ to unity. The structure of $\rho_p(x, y)$ is such that it is manifestly positive definite. So, it is a true density matrix. The Husimi function of this density matrix is obviously $F(q, p)$. In this way we have shown that whenever a positive parameter b may be chosen in such a way that the expression (10) becomes positive definite, there exists a density matrix for which $F(q, p)$ is its Husimi function.

Now we shall apply the developed formalism to a Gaussian distribution in phase space. Krüger [18] recently found the conditions which the parameters of a Gaussian distribution must satisfy in order that it is possible to interpret such a distribution as a Wigner function. Here, we shall find the conditions under which a Gaussian distribution may be interpreted as a Husimi function.

Let us consider the Gaussian distribution

$$F(q,p) = N \exp[-\beta p^2 - \gamma q^2 + \delta pq] \qquad N = (\beta\gamma - \delta^2/4)/\pi \tag{14}$$

where β, γ and δ are real parameters, $\beta > 0$, $\gamma > 0$, and $\beta\gamma > \delta^2/4$.

Performing the change of variables according to (9), the expression (10) becomes

$$F(\tilde{q}, \tilde{p})\, \mathrm{e}^{b\tilde{q}^2} = N \exp[-ap_1^2 - a^* p_2^2 + cp_1p_2] = f(p_1, p_2) \tag{15}$$

where

$$a = [\beta + 1/(bh^2) - \gamma/(b^2h^2) - \mathrm{i}\delta/(bh)]/4 \tag{16}$$

$$c = [-\beta + 1/(bh^2) - \gamma/(b^2h^2)]/4 \tag{17}$$

and where a^* denotes the complex conjugate of a. Now we have to find for which values of the parameters the function $f(p_1, p_2)$ is positive definite. If c is negative $f(p_1, p_2)$ cannot be positively definite. Namely, in this case we would have

$$f(p_1, p_2) = \sum_{k=0}^{\infty} (-1)^k p_1^k p_2^k |c|^k/(k!) \exp[-ap_1^2 - a^* p_2^2]. \tag{18}$$

For any real odd function because of the relation $\Psi(p) = -\Psi(-p)$, we would have

$$\int f(p_1, p_2)\Psi(p_1)\Psi(p_2)\,\mathrm{d}p_1\,\mathrm{d}p_2 = -\sum_k |c|^{2k+1} |z_{2k+1}|^2/(2k+1)! \tag{19}$$

where $z_k = \int p^k\, \mathrm{e}^{-ap^2}\Psi(p)\,\mathrm{d}p$ so that the expression (19) is negative. For $c \geqslant 0$ $f(p_1, p_2)$ is obviously positive definite. This condition reads, in detail

$$1/(bh^2) - \beta - \gamma/(b^2h^2) \geqslant 0$$

or

$$-\beta^2 b^2 h^2 + \beta b - \beta \gamma^2 \geqslant 0. \tag{20}$$

This inequality is satisfied when

$$1 - 4h^2 \beta \gamma \geqslant 0 \tag{21}$$

and

$$1 - (1 - 4h^2\beta\gamma)^{1/2} \leqslant 2h^2 b\beta \leqslant 1 + (1 - 4h^2\beta\gamma)^{1/2}. \tag{22}$$

We can thus conclude that the Gaussian distribution (14) may be interpreted as a Husimi function whenever $\beta\gamma \leqslant 1/(4h^2)$. When this condition is satisfied the existence of a density matrix is guaranteed and we can find it using the method developed in the preceding section. Using the well known integral $\int \exp(-at^2 - 2bt)\, dt = (\pi/4)^{1/2} \exp(-b^2/a)$ twice, we can easily transform the function from (15) according to (8) and obtain

$$\rho(x, y) = \pi N(aa^* - c^2)^{-1/2} \exp[-x^2(a^*/d - b/2) - y^2(a/d - b/2) + 2xyc/d] \tag{23}$$

where $d = 4h^2(aa^* - c^2)$.

Here, b must be chosen so that (22) is satisfied. We see that for fixed β and γ satisfying $4h^2\beta\gamma < 1$ (and of course $\beta\gamma > \delta^2/4$) we can choose two values of b for which (23) represents a pure state ($c = 0$) and the whole interval of values for b defined by (22) when (23) is a mixed state ($c > 0$). When $1 - 4h^2\beta\gamma = 0$ the inequality (22) has a unique solution for b and (23) becomes a pure state. Only in this case can we ascribe a unique quantum mechanical state to the Husimi function of the Gaussian type.

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