SOME PROPERTIES OF A NON-NEGATIVE QUANTUM-MECHANICAL DISTRIBUTION FUNCTION

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We consider the distribution function obtained by smoothing the original distribution function, defined in an earlier publication, with a ground-state harmonic oscillator wave function. We derive its time dependence and show that, in particular, the field-free result does not correspond to the classical result. We point out that the non-negative property of the smoothed function follows immediately from the fact that the integral of the product of two of the original distribution functions is equal, except for a factor $2\pi\hbar$, to the transition probability between the two states they represent.

1. Definition of a non-negative ("smoothed") quantum mechanical distribution function. In a recent publication [1], we examined the conditions which are necessary for providing a unique definition for a quantum-mechanical distribution function $P(q,p)$, where q and p are positional and momentum coordinates. The conditions we listed lead uniquely to the result that, for every normalized state vector ψ,

$$P(q,p) = (\pi\hbar)^{-1} \int \psi(q+y)^* \psi(q-y) e^{2ipy/\hbar}\, dy\ , \tag{1}$$

which is the original distribution function given in ref. [2]. Some of the properties of P are [1–3]:

(a) It is a hermitian, that is bilinear, form of the wave-function ψ. Hence it is real for all q and p. The hermitian operator is, of course a function of q and p.

(b) If integrated over p, it gives the proper probabilities for the different values of q, and similarly with $p \leftrightarrow q$.

(c) The transition probability between two states ψ and ϕ is given, in terms of the corresponding distribution functions, P_ψ and P_ϕ say, as follows:

$$\left| \int \psi(x)^* \phi(x)\, dx \right|^2 = 2\pi\hbar \iint P_\psi(q,p) P_\phi(q,p)\, dq\, dp\ . \tag{2}$$

As pointed out in ref. [2] and proven in ref. [3], conditions (a) and (b) are incompatible with the requirement that the distribution function be everywhere nonnegative. In fact it is clear from condition (c) that the distribution function given by eq. (1) has to be able to assume negative values.

Starting with Husimi [4], many authors obtained non-negative distribution functions by dropping condition (a). In most cases this is essentially achieved, for all points (q,p), by smoothing $P(q',p')$ with a density function $D(q', p')$ and integrating over all p' and q'.

A natural and popular choice of the density function D is a gaussian distribution [4–8], recently considered anew by Cartwright [9].

Our considerations here will be restricted to one dimension but it will be clear that they can be generalized to higher dimensions. Consider a linear harmonic oscillator, centered at the point q and moving with an average momentum p. Then, as is well known, the ground-state wave-function, at the position q and average momentum p

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becomes, as function of q',

$$\psi_{q,p}(q',\alpha) = (\pi\alpha)^{-1/4}\, e^{-(q'-q)^2/2\alpha} e^{ipq'/\hbar} , \tag{3}$$

where $(\Delta q')^2 = \alpha/2$. Using this expression for $\psi_{q,p}$ in eq. (1), it may easily be verified that the corresponding distribution function, $P_{q,p}(q', p', \alpha)$ say, is

$$P_{q,p}(q', p', \alpha) = (\pi\hbar)^{-1}\, e^{-(q'-q)^2/\alpha} e^{-\alpha(p'-p)^2/\hbar^2} . \tag{4}$$

This function has the property that

$$(\Delta q')^2 = \alpha/2 \quad \text{and} \quad (\Delta q')(\Delta p') = \hbar/2 . \tag{4a}$$

This is the density function which, following Husimi [4], we will use to smooth $P(q', p')$. Thus, the resultant smoothed distribution function, $P_s(q, p, \alpha)$ say, is simply

$$P_s(q, p, \alpha) = \iint P(q', p') P_{q,p}(q', p', \alpha)\, dp'\, dq' . \tag{5}$$

Carrying out an explicit calculation, Cartwright [9] showed that $P_s(q, p, \alpha)$ is everywhere non-negative. However, it is clear that since the rhs of eq. (5) is a particular case of the rhs of eq. (2), and since the lhs of eq. (2) is non-negative it follows immediately that

$$P_s(q, p, \alpha) \geqslant 0 , \tag{6}$$

for all q and p.

Before turning to a consideration of other properties of P_s, not heretofore considered in the literature, it is convenient to use eqs. (4) and (5) to write explicitly

$$P_s(q, p, \alpha) = (\pi\hbar)^{-1} \iint P(q', p') e^{-(q'-q)^2/\alpha}\, e^{-\alpha(p'-p)^2/\hbar^2}\, dq'\, dp' , \tag{7}$$

where the P without the index is the old distribution function (1). It may be of some interest to remark here already that P_s is an "entire function" of q and p, i.e. that the range of these variables may be extended to the whole complex plane without encountering any irregularities. First of all, by simple differentiation, it is easy to verify that

$$\alpha \partial P_s/\partial\alpha = (\alpha/4)\partial^2 P_s/\partial q^2 - (\hbar^2/4\alpha)\partial^2 P_s/\partial p^2 . \tag{8}$$

2. *Time dependence of the smoothed distribution function.* We next consider the equation of motion of P_s. The time dependence of P_s may be decomposed into two parts,

$$\partial P_s/\partial t = \partial_k P_s/\partial t + \partial_v P_s/\partial t , \tag{9}$$

the first part resulting from the $(i\hbar/2m)\partial^2/\partial q^2$, the second from the potential energy $V/i\hbar$ part of the expression for $\partial\psi/\partial t$.

It has already been shown [2] that the time dependence of $P(q', p')$ corresponds to the classical result in the field-free case, i.e.

$$\partial_k P(q', P')/\partial t = -(p'/m)\partial P(q', p')/\partial q' , \tag{10}$$

and in the presence of a potential we have the extra contribution

$$\partial_v P(q', P')/\partial t = \int dj\, P(q'; p' + j) J(q', j) , \tag{11}$$

where

$$J(q',j) = (\mathrm{i}/\pi\hbar^2) \int [V(q'+y) - V(q'-y)]\, \mathrm{e}^{-2\mathrm{i}yj/\hbar}\, \mathrm{d}y \tag{12}$$

is the probability of a jump of the momentum by an amount j if the positional coordinate is q'.

Applying the results to eq. (7), we have, first of all, that

$$\frac{\partial_k P_s(q,p,\alpha)}{\partial t} = -(\pi\hbar)^{-1} \iint \frac{p'}{m} \frac{\partial P(q',p')}{\partial q'} \{\mathrm{e}^{-(q'-q)^2/\alpha}\, \mathrm{e}^{-\alpha(p'-p)^2/\hbar^2}\}\, \mathrm{d}q'\, \mathrm{d}p'$$
$$= (\pi\hbar)^{-1} \iint \frac{p'}{m} P(q',p') \frac{\partial}{\partial q'} \{\mathrm{e}^{-(q'-q)^2/\alpha}\, \mathrm{e}^{-\alpha(p'-p)^2/\hbar^2}\}\, \mathrm{d}q'\, \mathrm{d}p', \tag{13}$$

the right side having been obtained by partial integration. But since the $\partial/\partial q'$, as applied to the expression in the curly bracket can be replaced by $-\partial/\partial q$, we also have

$$\frac{\partial_k P_s(q,p,\alpha)}{\partial t} = -(\pi\hbar)^{-1} \frac{\partial}{\partial q} \iint \frac{p'}{m} P(q',p') \{\mathrm{e}^{-(q'-q)^2/\alpha}\, \mathrm{e}^{-\alpha(p'-p)^2/\hbar^2}\}\, \mathrm{d}q'\, \mathrm{d}p'. \tag{14}$$

The classical expression for $\partial_k P_s(q,p,\alpha)/\partial t$ would be

$$-\frac{p}{m} \frac{\partial P_s(q,p,\alpha)}{\partial q} = -(\pi\hbar)^{-1} \frac{\partial}{\partial q} \iint \frac{p}{m} P(q',p') \{\mathrm{e}^{-(q'-q)^2/\alpha}\, \mathrm{e}^{-\alpha(p'-p)^2/\hbar^2}\}\, \mathrm{d}q'\, \mathrm{d}p'. \tag{14a}$$

The difference between the two expressions (14) and (14a) is

$$(\pi\hbar)^{-1} \frac{\partial}{\partial q} \iint \frac{p-p'}{m} P(q',p',\alpha) \{\mathrm{e}^{-(q'-q)^2/\alpha}\, \mathrm{e}^{-\alpha(p'-p)^2/\hbar^2}\}\, \mathrm{d}q'\, \mathrm{d}p'$$
$$= -(\pi\hbar)^{-1} \frac{\hbar^2}{2\alpha m} \frac{\partial^2}{\partial q \partial p} \iint P(q',p',\alpha) \{\mathrm{e}^{-(q'-q)^2/\alpha}\, \mathrm{e}^{-\alpha(p'-p)^2/\hbar^2}\}\, \mathrm{d}q'\, \mathrm{d}p' = -\frac{\hbar^2}{2\alpha m} \frac{\partial^2}{\partial q\, \partial p} P(q,p,\alpha). \tag{15}$$

Hence we obtain

$$\frac{\partial_k P_s(q,p,\alpha)}{\partial t} = -\frac{1}{m}\left(p + \frac{\hbar^2}{2\alpha} \frac{\partial}{\partial p}\right) \frac{\partial}{\partial q} P_s(q,p,\alpha). \tag{16}$$

It is thus clear that, in the field-free case, the time dependence of $P_s(q,p,\alpha)$, in contrast to that of $P(q,p)$, is not given by the classical expression but contains a correction term of order $\hbar^2$. But this is not a quantum effect: the same expression would appear in the time derivative of the classical distribution function if this were "smoothed" as in (7).

We turn now to a consideration of

$$\frac{\partial_v P_s(q,p,\alpha)}{\partial t} = (\pi\hbar)^{-1} \iint \frac{\partial_v P(q',p')}{\partial t} \{\mathrm{e}^{-(q'-q)^2/\alpha}\, \mathrm{e}^{-\alpha(p'-p)^2/\hbar^2}\}\, \mathrm{d}q'\, \mathrm{d}p'. \tag{17}$$

Thus, utilizing eqs. (11) and (12) in eq. (17), we obtain

$$\frac{\partial_v P_s(q,p,\alpha)}{\partial t} = \frac{\mathrm{i}}{(\pi\hbar)(\pi\hbar^2)} \iiiint \mathrm{d}p'\, \mathrm{d}q'\, \mathrm{d}j\, \mathrm{d}y\, P(q',p'+j)[V(q'+y) - V(q'-y)]$$
$$\times \{\mathrm{e}^{-(q'-q)^2/\alpha}\, \mathrm{e}^{-\alpha(p'-p)^2/\hbar^2}\, \mathrm{e}^{-2\mathrm{i}jy/\hbar}\} \equiv -\frac{2}{\pi^2\hbar^3} \operatorname{Im} I, \tag{18}$$

where

$$I = \iiiint \mathrm{d}p'\,\mathrm{d}q'\,\mathrm{d}j\,\mathrm{d}y\,P(q';p'+j)\,V(q'+y)\{\mathrm{e}^{-(q'-q)^2/\alpha}\,\mathrm{e}^{-\alpha(p'-p)^2/\hbar^2}\,\mathrm{e}^{-2\mathrm{i}jy/\hbar}\}\,. \tag{19}$$

Replacing y by a new variable $z = y + q'$ and p' by $p'' = p' + j$ this becomes

$$I = \iiiint P(q', p'')\,\mathrm{e}^{-(q+\mathrm{i}\alpha j/\hbar - q')^2/\alpha}\,\mathrm{e}^{-\alpha(p+j-p'')^2/\hbar^2}\,V(z)\,\mathrm{e}^{-\alpha j^2/\hbar^2 + 2\mathrm{i}j(q-z)/\hbar}\,\mathrm{d}p''\,\mathrm{d}q'\,\mathrm{d}j\,\mathrm{d}z\,. \tag{20}$$

Because of eq. (7) and the possibility of extending P_s also to complex values of q and p, this can be written also as

$$I = \pi\hbar \iint \mathrm{d}j\,\mathrm{d}z\,P_s(q + \mathrm{i}\alpha j/\hbar\,, p + j, \alpha)\,V(z)\,\mathrm{e}^{-\alpha j^2/\hbar^2 + 2\mathrm{i}j(q-z)/\hbar}\,. \tag{21}$$

As was observed already before, P_s is an entire function so that it remains uniquely defined in spite of the complex nature of one of its arguments. It now follows from eqs. (9), (16), (18) and (21) that

$$\frac{\partial P_s(q,p,\alpha)}{\partial t} = \frac{\partial_k P_s(q,p,\alpha)}{\partial t} + \frac{\partial_v P_s(q,p,\alpha)}{\partial t} = -\frac{1}{m}\left(p + \frac{\hbar^2}{2\alpha}\frac{\partial}{\partial p}\right)\frac{\partial P_s(q,p,\alpha)}{\partial q}$$
$$-\mathrm{i}(\pi\hbar)^{-1}\iint [P_s(q - \mathrm{i}\alpha j, p + \hbar j, \alpha)\mathrm{e}^{-2\mathrm{i}j(q-z)} - P_s(q + \mathrm{i}\alpha j, p + \hbar j, \alpha)\mathrm{e}^{2\mathrm{i}j(q-z)}]\,V(z)\,\mathrm{e}^{-\alpha j^2}\,\mathrm{d}j\,\mathrm{d}z\,, \tag{22}$$

the integration variable j of (21) having been replaced by $\hbar j$.

Eq. (22) is, probably, the shortest expression for the time derivative of P_s. It may be observed that the time derivative of the smoothed distribution is not very simple even in classical theory – not even if we restrict ourselves, as was done in all the preceding discussion, to the non-relativistic limit.

The extension of P_s into the complex plane in (22) can be made unnecessary by expanding the P_s under the integral sign into a power series of $\mathrm{i}\alpha j$. The exponentials of $\mathrm{i}j(q-z)$ are then replaced, for the successive q derivatives of P_s, by $\sin 2j(q-z)$, $\cos 2j(q-z)$, $-\sin 2j(q-z)$, $-\cos 2j(q-z)$, again $\sin 2j(q-z)$, and so on. For the factor accompanying the nth derivative of P_s this can be written as $\sin[2j(q-z) + \frac{1}{2}n\pi]$. Hence one obtains

$$\frac{\partial P_s(q,p,\alpha)}{\partial t} = -\frac{1}{m}\left(p + \frac{\hbar^2}{2\alpha}\frac{\partial}{\partial p}\right)\frac{\partial P_s(q,p,\alpha)}{\partial q}$$
$$-\frac{1}{\pi\hbar}\sum_n \frac{1}{n!}\iint \frac{\partial^n P_s(q, p + \hbar j, \alpha)}{\partial q^n}\sin[2j(q-z) + \tfrac{1}{2}n\pi]\,V(z)\,\mathrm{e}^{-\alpha j^2}\,\mathrm{d}j\,\mathrm{d}z\,. \tag{22a}$$

There are two, apparently different but mathematically identical, expressions for the time derivative of the old distribution function P of (1): the one given by eq. (11) of ref. [2] (eqs. (10) and (11) of the present article), the other by eq. (8) of the same article. The latter expression is a power series in $\hbar^2$ and shows the analogy to the classical expression for $\partial P/\partial t$ more clearly. The next section will derive the analogue of this for $\partial P_s/\partial t$, using the old expression (8) of ref. [2] for $\partial P/\partial t$.

3. Other expression for the time derivative of P_s. The alternate expression for $\partial P_s/\partial t$ is also a sum of the two parts, as given by (9). Since the first part is again given by (16), only the second part, i.e. $\partial_v P_s/\partial t$ will be recalculated. According to eq. (8) of ref. [2]

$$\frac{\partial_v P(q,p)}{\partial t} = \sum_\lambda \frac{1}{\lambda!}\left(\frac{\hbar}{2\mathrm{i}}\right)^{\lambda-1}\frac{\partial^\lambda V(q)}{\partial q^\lambda}\frac{\partial^\lambda P(q,p)}{\partial p^\lambda}\,. \tag{23}$$

The summation over λ is to be extended over all odd positive integers. We have, therefore,

$$\frac{\partial_v P_s(q,p,\alpha)}{\partial t} = \frac{1}{\pi\hbar}\sum_\lambda \frac{1}{\lambda!}\left(\frac{\hbar}{2i}\right)^{\lambda-1} \times \iint \frac{\partial^\lambda V(q')}{\partial q'^\lambda}\frac{\partial^\lambda P(q',p')}{\partial p'^\lambda}\{e^{-(q'-q)^2/\alpha}\, e^{-\alpha(p'-p)^2/\hbar^2}\}\, dq'\, dp' . \tag{24}$$

By partial integrations with respect to p' and replacement of the p' derivatives of the last factor by its negative p derivatives one obtains

$$\frac{\partial_v P_s(q,p,\alpha)}{\partial t} = \frac{1}{\pi\hbar}\sum_\lambda \frac{1}{\lambda!}\left(\frac{\hbar}{2i}\right)^{\lambda-1} \frac{\partial^\lambda}{\partial p^\lambda}\iint \frac{\partial^\lambda V(q')}{\partial q'^\lambda} P(q',p')\{e^{-(q'-q)^2/\alpha}\, e^{-\alpha(p'-p)^2/\hbar^2}\}\, dq'\, dp' . \tag{25}$$

It is natural now to expand the derivatives of V into a power series of $q' - q$,

$$\frac{\partial^\lambda V(q')}{\partial q'^\lambda} = \sum_\mu \frac{1}{\mu!}\frac{\partial^{\lambda+\mu}V(q)}{\partial q^{\lambda+\mu}}(q'-q)^\mu . \tag{26}$$

We then use the identity [‡1]

$$x^\mu e^{-x^2/\alpha} = \frac{(-)^\mu \mu!}{2^\mu}\sum_\kappa \frac{\alpha^{\mu-\kappa}}{\kappa!(\mu-2\kappa)!}\frac{d^{\mu-2\kappa}e^{-x^2/\alpha}}{dx^{\mu-2\kappa}} , \tag{27}$$

in which the summation over κ is to be extended from 0 until $\mu - 2\kappa$ becomes negative. It may be observed that if μ is even, the last term of (27) contains the function $e^{-x^2/\alpha}$ itself, if μ is odd the last term contains the first derivative of this. Introducing now (27) into (25) with $x = q' - q$ and replacing the q' derivative of the last factor by the negative q derivative [which introduces a factor $(-)^\mu$], one obtains finally

$$\frac{\partial_v P_s(q,p,\alpha)}{\partial t} = \frac{1}{\pi\hbar}\sum_{\lambda\mu\kappa}\frac{(\hbar/2i)^{\lambda-1}\alpha^{\mu-\kappa}}{\lambda! 2^\mu \kappa!(\mu-2\kappa)!}\frac{\partial^{\lambda+\mu}V(q)}{\partial q^{\lambda+\mu}}\frac{\partial^\lambda}{\partial p^\lambda}\frac{\partial^{\mu-2\kappa}}{\partial q^{\mu-2\kappa}}\iint P(q',p')e^{-(q'-q)^2/\alpha}\, e^{-\alpha(p'-p)^2/\hbar^2}\, dp'\, dq' . \tag{28}$$

Hence

$$\frac{\partial P_s(q,p,\alpha)}{\partial t} = -\frac{1}{m}\left(p + \frac{\hbar^2}{2\alpha}\frac{\partial}{\partial p}\right)\frac{\partial}{\partial q}P_s + \sum_{\lambda\mu\kappa}\frac{(i\hbar)^{\lambda-1}\alpha^{\mu-\kappa}}{2^{\lambda+\mu-1}\lambda!\kappa!(\mu-2\kappa)!}\frac{\partial^{\lambda+\mu}V(q)}{\partial q^{\lambda+\mu}}\frac{\partial^\lambda}{\partial p^\lambda}\frac{\partial^{\mu-2\kappa}}{\partial q^{\mu-2\kappa}}P_s(q,p,\alpha) . \tag{29}$$

It may be good to recall that λ assumes all odd – but only odd – values from 1 to infinity, κ all integer values from 0 as long as $\mu - 2\kappa$ remains non-negative, μ all integer values from 0 to infinity.

The second part of (29) is surely not simple, neither is the corresponding expression in the classical limit ($\hbar = 0$). Eq. (29) was derived because it is easier to derive from the approximate expressions for $\partial P_s/\partial t$ than it is from (22). If the "smoothing" over the coordinate is very narrow, i.e. if α is assumed to be very small, the second part of $\partial P_s/\partial t$ naturally goes over into the expression for $\partial P/\partial t$ as given by eq. (23). If $\hbar$ is also assumed to be small, it goes over into the classical expression. But many other approximate expressions for $\partial P_s/\partial t$ can be derived from (29), as were also from (23).

The preceding calculations and the resulting equations are apparently restricted to the case of a single dimension. However, it is not difficult to generalise them for the general case of several dimensions. As to the more simple expression (22) for $\partial P_s/\partial t$, the variables q, p, j and z have to be treated as vectors of as many dimensions as there are dimensions in coordinate (or momentum) space. The exponents $j(q - z)$ are to be replaced by the scalar products of the vectors j and $q - z$, the j^2 by $j \cdot j$. In the case of (29) the situation is a bit more complex: the indices κ, λ, μ must be replaced by as many sets of indices $\kappa_n, \lambda_n, \mu_n$ as there are space (or momentum) dimensions and the summations extended over all these indices. The restrictions are then that the *sum* of all the λ must be odd and that all the $\mu_n - 2\kappa_n$ must be non-negative, as are also all $\kappa_n, \mu_n, \lambda_n$.

‡1 We could not find this equation in the literature, even though it must have been known. It is not difficult to verify it – for $\alpha = 1$ the factors of $\exp(-x^2)$ on the right side are Hermite polynomials.

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