A NEW PARAMETRIZED QUANTUM DISTRIBUTION FUNCTION AND ITS TIME DEVELOPMENT

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Received 15 August 1984
Revised manuscript received 3 October 1984

We discuss a new general class of quantum distribution functions characterized by an arbitrary parameter b. The values $b = -1, 0, 1$ correspond to the anti-standard (Kirkwood), the Wigner, and the standard distribution functions, respectively. An analytic form of the equation of motion is derived. We conclude that, for time-dependent problems involving a potential which is a function of coordinates only, the Wigner distribution function is the optimum one to use, from a simplicity standpoint.

1. Introduction. A phase formulation of quantum mechanics has been extensively used in many sub-fields of quantum physics, particularly in statistical mechanics and quantum optics [1–3]. In addition to the original distribution of Wigner [4], other common choices are the normal [5] and the anti-normal [6] distribution functions, also the standard and the anti-standard distribution functions [7]. A general class of distribution functions, P_G say, was introduced by Cahill and Glauber [8], and include the Wigner, normal and anti-normal functions as special cases.

One of us has recently discussed the relations between these various distribution functions and, in addition, introduced a new class of generalized distribution functions [9], $P_G(q, p; b)$ say, which includes the anti-standard, the Wigner, and the standard distribution functions as special cases when the parameter b assumes the values $-1, 0, +1$, respectively. As demonstrated in our recent work [9], the standard distribution is equivalent to the Kirkwood distribution [10], and with the exception of the Wigner distribution, the latter has been the most commonly used function in traditional statistical mechanics [‡1].

We would like to address the question of whether these are valid reasons for choosing one distribution function as distinct from another. As we have emphasized already [12–14] [‡2] one criterion for deciding on an optimum distribution is the simplicity of the associated time dependence, which of course is of paramount interest when one is dealing with non-equilibrium situations.

The purpose of the present paper is to derive an analytic expression for the time dependence of $P_G(q, p; b)$. We restrict ourselves to one dimension since a generalization to a multi-dimensional state is straightforward.

In section 2 we discuss the parametrized distribution function $P_G(q, p; b)$ with emphasis on how it may be written in terms of characteristic functions. The analytic form of its time development is derived in section 3. Finally, in section 4 we discuss our results.

2. A new parametrized distribution function. A new general class of quantum distribution functions has recently been introduced [9]. It is defined as follows:

$$P_G(q, p; b) = (2\pi\hbar)^{-2} \times \iint \mathrm{d}\sigma\, \mathrm{d}\tau\, \exp[-\mathrm{i}(\sigma q + \tau p)/\hbar]\, C_G(\sigma, \tau; b), \quad (1)$$

where the characteristic function C_G, which is the

‡1 For a more recent application employing the Kirkwood function, see ref. [11].

‡2 In the third line from the bottom of p. 244 and in the first line of section 4 on p. 245 of ref. [14], the subscript "a" should be replaced by "n".

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(North-Holland Physics Publishing Division)

Fourier transform of P_G, is given by

$$C_G(\sigma,\tau;b) = \langle\psi|\exp[-ib\sigma\tau/2\hbar + i(\sigma\hat{q}+\tau\hat{p})/\hbar]|\psi\rangle, \tag{2}$$

where $|\psi\rangle$ represents the state of the system of interest.

We recall that the characteristic function of the Wigner distribution function is [1,12]

$$C_w(\sigma,\tau) = \langle\psi|\exp[i(\sigma\hat{q}+\tau\hat{p})/\hbar]|\psi\rangle, \tag{3}$$

and those of the standard and the anti-standard distribution functions are [7]

$$C_{ST}(\sigma,\tau) = \langle\psi|\exp(i\sigma\hat{q}/\hbar)\exp(i\tau\hat{p}/\hbar)|\psi\rangle, \tag{4}$$

and

$$C_{AS}(\sigma,\tau) = \langle\psi|\exp(i\tau\hat{p}/\hbar)\exp(i\sigma\hat{q}/\hbar)|\psi\rangle. \tag{5}$$

By making use of the Baker–Hausdorff theorem it follows that

$$C_{ST}(\sigma,\tau) = C_G(\sigma,\tau;+1) \tag{6}$$

and

$$C_{AS}(\sigma,\tau) = C_G(\sigma,\tau;-1). \tag{7}$$

It is also clear that

$$C_w(\sigma,\tau) = C_G(\sigma,\tau;0) \tag{8}$$

and

$$C_G(\sigma,\tau;b) = \exp(-ib\sigma\tau/2\hbar)C_w(\sigma,\tau). \tag{9}$$

Combining eqs. (1) and (9) we obtain the differential relation between the parametrized distribution function P_G and the Wigner distribution function P_w:

$$P_G(q,p;b) = \exp[\tfrac{1}{2}i\hbar b(\partial/\partial q)(\partial/\partial p)]P_w(q,p)$$
$$\equiv AP_w(q,p), \tag{10}$$

where

$$P_w(q,p) = (2\pi\hbar)^{-2}$$
$$\times \iint d\sigma\, d\tau \exp[-i(\sigma q+\tau p)/\hbar]\, C_w(\sigma,\tau). \tag{11}$$

With the help of eq. (10) it is easy to see that

$$P_G^*(q,p;b) = P_G(q,p;-b). \tag{12}$$

Explicitly we obtain

$$P_{ST}^*(q,p) = P_{AS}(q,p) \tag{13}$$

and

$$P_w^*(q,p) = P_w(q,p), \tag{14}$$

as pointed out in refs. [7] and [9].

In ref. [9] it was also shown that

$$P_{AS}(q,p) = P_k(q,p)$$
$$= (2\pi\hbar)^{-1}\int \psi^*(q')\psi(q)\exp[ip(q'-q)/\hbar]\, dq', \tag{15}$$

i.e. the Kirkwood [10] and anti-standard distibution functions are equivalent.

Finally, we emphasize that eq. (10) is a key result, giving the relation between the new generalized distribution function P_G and the Wigner distribution P_w. It will be used in the next section to obtain the time dependence of P_G from the time dependence of P_w. However, we will now show how it can be used to obtain the phase-space function, $F_G(q,p;b)$ say, corresponding to an arbitrary operator $\hat{F}(\hat{q},\hat{p})$. This is well known [1] in the case $b=0$, corresponding to the Wigner distribution, and is chosen to ensure that (see eqs. (2.12) and (2.13) of ref. [1]) that

$$\iint dq\, dp\, F_w(q,p)P_w(q,p) = \mathrm{Tr}\{\hat{\rho}\hat{F}(\hat{q},\hat{p})\}, \tag{16}$$

where $\hat{\rho}$ is the density matrix. If we now demand that the same relation hold in the more general case where the subscript w is replaced by G, then it follows from integration by parts that

$$F_G(q,p;b) = A^{-1}F_w(q,p), \tag{17}$$

where A is defined in eq. (10). Relations similar to those given by eqs. (10) and (17) hold for P_G and F_G except, of course, that A and A^{-1} are replaced by the approximate phase-space operators, displayed explicitly in eq. (20) of ref. [12].

3. Time dependence of the general class of distribution functions. The time dependence of the Wigner distribution function can be written in the following form [4]:

$$\partial P_w/\partial t = \partial_k P_w/\partial t + \partial_V P_w/\partial t, \tag{18}$$

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

Also, it has been shown that [4]

$$\partial_k P_W/\partial t = -(p/m)\,\partial p_W/\partial q\,, \qquad (19)$$

i.e., the field-free case corresponds to the classical result. In addition,

$$\frac{\partial_V P_W}{\partial t} = \sum_\lambda \frac{(\hbar/2i)^{\lambda-1}}{\lambda!}\,\frac{\partial^\lambda V(q)}{\partial q^\lambda}\,\frac{\partial^\lambda p_W}{\partial p^\lambda}\,, \qquad (20)$$

where the summation over λ is to be extended over all odd positive integers. Eqs. (18)–(20) constitute Wigner's form for the time dependence. Other forms have been displayed by Groenewold [15] and Moyal [16] but, as we have noted recently, their results are basically an abbreviated form of Wigner's result. From the point of view of applications, Wigner's form is the easiest to work with and thus we confine our attention to it.

We would like to obtain the time dependence of P_G by making use of eqs. (10), (18), (19) and (20). For convenience we define

$$\mu = i\hbar b/2\,. \qquad (21)$$

Thus eq. (10) can be written as follows

$$P_W = A^{-1}P_G\,, \qquad (22)$$

with the inverse operator

$$A^{-1} = \exp[-\mu(\partial/\partial q)(\partial/\partial p)]\,. \qquad (23)$$

In analogy to eq. (18) the time dependence of P_G can also be decomposed into two parts

$$\partial P_G/\partial t = \partial_V P_G/\partial t + \partial_k P_G/\partial t\,. \qquad (24)$$

Noting that A is independent of time, we substitute eqs. (10) and (22) into eq. (19) to obtain the kinetic part of the time dependence of P_G:

$$\partial_k P_G/\partial t = A(\partial_k P_W/\partial t) = A(-p/m)\,\partial P_W/\partial q$$
$$= (-1/m)(ApA^{-1}\,\partial P_G/\partial q)\,. \qquad (25)$$

Similarly the potential part is

$$\frac{\partial_V P_G}{\partial t} = \sum_\lambda \frac{(\hbar/2i)^{\lambda-1}}{\lambda!}\,A\,\frac{\partial^\lambda V(q)}{\partial q^\lambda}\,A^{-1}\,\frac{\partial^\lambda P_G}{\partial p^\lambda}\,. \qquad (26)$$

To simplify eqs. (25) and (26) further we use the following identity, which is proved in the appendix,

$$Af(p)A^{-1} = \sum_{n=0}^{\infty} [f^{(n)}(p')/n!]\,(p - p' + \mu\partial/\partial q)^n\,, \qquad (27)$$

where $f(p)$ is an arbitrary function of p containing derivatives of arbitrary order at $p = p'$.

In the case of $f(p) = p$, p' can be chosen to be zero. Only the $n = 1$ term contributes, hence

$$ApA^{-1} = p + \mu\partial/\partial q\,. \qquad (28)$$

Substituting eqs. (28) and (21) into eq. (25) we get the equation of motion in the field-free case:

$$\partial_k P_G/\partial t = (-1/m)(p + \tfrac{1}{2}i\hbar b\,\partial/\partial q)\,\partial P_G/\partial q\,. \qquad (29)$$

Again we make use of eq. (26) but now with the variable p replaced by q, and choose $f(q) = V^{(\lambda)}(q)$ so that

$$\partial_V P_G/\partial t = \sum_\lambda \sum_{n=0}^{\infty} \frac{(\hbar/2i)^{\lambda-1}}{\lambda!\,n!}\,V^{(\lambda+n)}(q')$$
$$\times\,(q - q' + \tfrac{1}{2}i\hbar b\,\partial/\partial p)^n\,\partial^\lambda P_G/\partial q^\lambda\,, \qquad (30)$$

where q' is chosen such that the potential $V(q)$ is infinitely differentiable at q', but otherwise arbitrary.

4. Discussion and conclusion. We discussed a new general class of quantum distribution function $P_G(q, p; b)$ with a parameter $b = -1, 0, 1$ corresponding to the anti-standard, the Wigner and the standard distribution functions. The differential relation between $P_G(q, p; b)$ and $P_W(q, p)$ was given and used to obtain an explicit form of the time dependence of P_G.

In eq. (29) if and only if $b = 0$ does the equation of motion coincide with the classical one. It is a unique property of the Wigner distribution function. By contrast, the corresponding results for the anti-standard and standard distribution functions contain additional $\hbar$ terms which are not of quantum origin. We emphasize that a similar remark applies to eq. (30). Only for $b = 0$ (the Wigner case) can the double summation be replaced by the single summation appearing in eq. (20), giving the simplest form of the time dependence. The same thing happens in the time dependence of P_G, as recently pointed out [12–14].

We should emphasize that our considerations have been restricted to the case of a potential which is a function of coordinates only, whereas in the areas of quantum optics and synergetics one often encounters momentum-dependent forces. On the other hand, in the area of more traditional non-equilibrium statistical mechanics, this is often the more common situation. Thus, for time-dependent problems involving a potential $V(q)$, we conclude that it is simpler to use the Wigner distribution function than any other, such as the Kirkwood, or any of the new generalized class of functions introduced here or the generalized class of Cahill–Glauber.

This research was partially supported by the Department of Energy under Grant No. DE-FG05-84ER45135.

Appendix. Proof of Identity (27). Let

$$F(\mu) = Af(p)A^{-1}\,, \tag{A1}$$

where

$$A = \exp[\mu(\partial/\partial q)(\partial/\partial p)]\,. \tag{A2}$$

Hence

$$\frac{\mathrm{d}F(\mu)}{\mathrm{d}\mu} = \exp\left(\mu\frac{\partial}{\partial q}\frac{\partial}{\partial p}\right)\frac{\partial}{\partial q}\frac{\partial}{\partial p}f(p)\exp\left(-\mu\frac{\partial}{\partial q}\frac{\partial}{\partial p}\right)$$
$$-\exp\left(\mu\frac{\partial}{\partial q}\frac{\partial}{\partial p}\right)f(p)\frac{\partial}{\partial q}\frac{\partial}{\partial p}\exp\left(-\mu\frac{\partial}{\partial q}\frac{\partial}{\partial p}\right)$$
$$=\exp\left(\mu\frac{\partial}{\partial q}\frac{\partial}{\partial p}\right)\frac{\partial f(p)}{\partial p}\frac{\partial}{\partial q}\exp\left(-\mu\frac{\partial}{\partial q}\frac{\partial}{\partial p}\right). \tag{A3}$$

Similarly we verify

$$\frac{\mathrm{d}^nF(\mu)}{\mathrm{d}\mu^n} = \exp\left(\mu\frac{\partial}{\partial q}\frac{\partial}{\partial p}\right)f^{(n)}(p)\frac{\partial^n}{\partial q^n}\exp\left(-\mu\frac{\partial}{\partial q}\frac{\partial}{\partial p}\right). \tag{A4}$$

If we choose $f(p) = p^n/n!$ we get

$$\mathrm{d}^nF(\mu)/\mathrm{d}\mu^n = \partial^n/\partial q^n\,. \tag{A5}$$

Solving (A5) for $F(\mu)$ we obtain

$$F(\mu) = C_n\mu^n + C_{n-1}\mu^{n-1} + \ldots + C_1\mu + C_0\,, \tag{A6}$$

where

$$C_m = (1/m!)[\mathrm{d}^mF(\mu)/\mathrm{d}\mu^m]\,|_{\mu=0}$$
$$= [n(n-1)\ldots(n-m+1)/m!n!]p^{n-m}(\partial^m/\partial q^m)\,, \tag{A7}$$

and $m = 0, 1, \ldots, n$.

Finally we have

$$F(\mu) = \sum_{m=0}^{n} C_m\mu^m$$
$$= \frac{1}{n!}\sum_{m=0}^{\infty}\frac{n!}{m!(n-m)!}\,p^{n-m}\frac{\partial^m}{\partial q^m}\mu^m$$
$$= (p + \mu\partial/\partial q)^n/n!\,. \tag{A8}$$

In general we expand an arbitrary $f(p)$ in power series around $p = 0$:

$$f(p) = \sum_{n=0}^{\infty} f^{(n)}(0)p^n/n!\,. \tag{A9}$$

Thus combining eqs. (A8) and (A9) we obtain

$$Af(p)A^{-1} = \sum_{n=0}^{\infty}[f^{(n)}(0)/n!]\,(p + \mu\partial/\partial q)^n\,. \tag{A10}$$

More generally, if we expand around $p = p'$ instead of $p = 0$ we obtain a result which corresponds to eq. (27) of the text. Choosing $\mu = 0$, $Af(p)A^{-1} = f(p)$, as it should, which provides a simple check of the result.

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