DISTRIBUTION FUNCTIONS IN PHYSICS: FUNDAMENTALS

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Abstract:
This is the first part of what will be a two-part review of distribution functions in physics. Here we deal with fundamentals and the second part will deal with applications. We discuss in detail the properties of the distribution function defined earlier by one of us (EPW) and we derive some new results. Next, we treat various other distribution functions. Among the latter we emphasize the so-called P distribution, as well as the generalized P distribution, because of their importance in quantum optics.

1. Introduction

It is well known that the uncertainty principle makes the concept of phase space in quantum mechanics problematic. Because a particle cannot simultaneously have a well defined position and momentum, one cannot define a probability that a particle has a position q and a momentum p, i.e. one cannot define a true phase space probability distribution for a quantum mechanical particle. Nonetheless, functions which bear some resemblance to phase space distribution functions, "quasiprobability distribution functions", have proven to be of great use in the study of quantum mechanical systems. They are useful not only as calculational tools but can also provide insights into the connections between classical and quantum mechanics.

The reason for this latter point is that quasiprobability distributions allow one to express quantum mechanical averages in a form which is very similar to that for classical averages. As a specific example let us consider a particle in one dimension with its position denoted by q and its momentum by p. Classically, the particle is described by a phase space distribution $P_{\mathrm{Cl}}(q, p)$. The average of a function of the position and momentum $A(q, p)$ can then be expressed as

$$\langle A\rangle_{\mathrm{Cl}} = \int \mathrm{d}q \int \mathrm{d}p\, A(q, p)\, P_{\mathrm{Cl}}(q, p)\,. \tag{1.1}$$

The integrations in this equation are from $-\infty$ to $+\infty$. This will be the case with all integrations in this paper unless otherwise indicated. A quantum mechanical particle is described by a density matrix $\hat{\rho}$ (we will designate all operators by a ^) and the average of a function of the position and momentum operators, $\hat{A}(\hat{q}, \hat{p})$ is

$$\langle \hat{A}\rangle_{\mathrm{quant}} = \mathrm{Tr}(\hat{A}\hat{\rho}) \tag{1.2}$$

($\mathrm{Tr}\,\hat{Q}$ means the trace of the operator $\hat{Q}$). It must be admitted that, given a classical expression $A(q, p)$, the corresponding self-adjoint operator $\hat{A}$ is not uniquely defined – and it is not quite clear what the purpose of such a definition is. The use of a quasiprobability distribution, $P_{\mathrm{Q}}(q, p)$, however, does give such a definition by expressing the quantum mechanical average as

$$\langle \hat{A}\rangle_{\mathrm{quant}} = \int \mathrm{d}q \int \mathrm{d}p\, A(q, p)\, P_{\mathrm{Q}}(q, p) \tag{1.3}$$

where the function $A(q, p)$ can be derived from the operator $\hat{A}(\hat{q}, \hat{p})$ by a well defined correspondence rule. This allows one to cast quantum mechanical results into a form in which they resemble classical ones.

The first of these quasiprobability distributions was introduced by Wigner [1932a] to study quantum corrections to classical statistical mechanics. This particular distribution has come to be known as the

Wigner distribution,† and we will designate it as P_w. This is, and was meant to be, a reformulation of Schrödinger's quantum mechanics which describes states by functions in configuration space. It is non-relativistic in nature because it is not invariant under the Lorentz group; also, configuration space quantum mechanics for more than one particle would be difficult to formulate relativistically. However, it has found many applications primarily in statistical mechanics but also in areas such as quantum chemistry and quantum optics. In the case where P_O in eq. (1.3) is chosen to be P_w, then the correspondence between $A(q, p)$ and $\hat{A}$ is that proposed by Weyl [1927], as was first demonstrated by Moyal [1949]. Quantum optics has given rise to a number of quasiprobability distributions, the most well-known being the P representation of Glauber [1963a] and Sudarshan [1963], which have also found extensive use. As far as the description of the electromagnetic field is concerned, these do exhibit (special) relativistic invariance. Other distribution functions have also been proposed (Husimi [1940]; Margenau and Hill [1961]; Cohen [1966]) but have found more limited use, although, more recently, extensive use has been made of the generalized P representations by Drummond, Gardiner and Walls [1980, 1981]. In this paper we will discuss the basic formalism of these quasiprobability distributions and illustrate them with a few simple examples. We will defer any detailed consideration of applications to a later paper.

We now proceed to the basic problem: how do we go about constructing a quantum mechanical analogue of a phase space density? Let us again consider, for simplicity, a one particle system in one dimension which is described by a density matrix $\hat{\rho}$. In this paper we will work, for simplicity, in one dimension; the generalization to higher dimensions will be given in a few cases but is in most circumstances obvious. It is possible to express the position and momentum distributions of the particle as

$$P_{\text{pos}}(q) = \text{Tr}(\hat{\rho}\delta(q - \hat{q})) \tag{1.4a}$$

$$P_{\text{mom}}(p) = \text{Tr}(\hat{\rho}\,\delta(p - \hat{p})) \tag{1.4b}$$

where $\delta(q - \hat{q})$ is the operator which transforms $|q'\rangle$ as follows:

$$\delta(q - \hat{q})\,|q'\rangle \equiv |q\rangle\,\langle q|q'\rangle = \delta(q - q')\,|q'\rangle \tag{1.5}$$

and similarly for $\delta(p - \hat{p})$. We introduce the function $\rho(q', q'')$ defined by

$$\rho(q', q'') = \langle q'|\hat{\rho}|q''\rangle = \sum_{\lambda} w_\lambda\,\psi_\lambda(q')\,\psi_\lambda(q'')^* \tag{1.6}$$

where w_λ is the probability of the system being in the state ψ_λ, and the $\{\psi_\lambda\}$ form a complete set. Then

$$P_{\text{pos}}(q) = \rho(q, q) \tag{1.7a}$$

and

$$P_{\text{mom}}(p) = (2\pi\hbar)^{-1} \int \mathrm{d}x \int \mathrm{d}x'\,\rho(x, x')\exp\{\mathrm{i}p(x' - x)/\hbar\}\,. \tag{1.7b}$$

† We use this designation here and throughout the paper despite the strenuous objections of one of us since the majority of us feel we should adhere to what is now common nomenclature.

To show that this corresponds to the usual definition we will examine $P_{\text{pos}}(q)$. We have that, in the Dirac bracket notation,

$$P_{\text{pos}}(q) = \text{Tr}(\hat{\rho}\,\delta(q-\hat{q})) = \int \mathrm{d}q'\,\langle q'|\hat{\rho}\,\delta(q-\hat{q})|q'\rangle$$

$$= \int \mathrm{d}q'\,\delta(q-q')\,\langle q'|\hat{\rho}|q'\rangle = \langle q|\hat{\rho}|q\rangle \tag{1.8}$$

which is a more conventional expression for the position density. A first guess for some kind of a phase space density might then be

$$P_1(q,p) = \text{Tr}(\hat{\rho}\,\delta(q-\hat{q})\,\delta(p-\hat{p}))\,. \tag{1.9}$$

On the other hand, we might choose instead

$$P_2(q,p) = \text{Tr}(\hat{\rho}\,\delta(p-\hat{p})\,\delta(q-\hat{q}))\,. \tag{1.10}$$

But these expressions are not equal and although either of them, or a combination of both, could be used to evaluate expectation values of functions of $\hat{q}$ and $\hat{p}$ (provided the operators are ordered properly, the ordering for P_1 being different than that for P_2), they do not possess what we regard as desirable properties (see section 2). In fact, they are, in general, not real.

The association of distribution functions with operator ordering rules (or, equivalently, the association of operators with classical expressions) is one which will recur throughout this paper. Each of the distribution functions which we will discuss can be used to evaluate expectation values of products of operators ordered according to a certain rule. We will consider distribution functions which can be used to compute expectation values of products of the position and momentum operators $\hat{q}$ and $\hat{p}$, and also distribution functions which can be used to compute expectation values of products of the creation and annihilation operators, $\hat{a}^+$ and $\hat{a}$. The latter are useful in problems involving electromagnetic fields. Because the creation and annihilation operators are simply related to $\hat{q}$ and $\hat{p}$ there is a relation between these two types of distribution functions. The Wigner distribution, for example, has proved useful in both the $\hat{a}$, $\hat{a}^+$ and $\hat{p}$, $\hat{q}$ contexts. The basic criterion for the choice of a distribution function for a particular problem is convenience.

In the next two sections we will continue to examine distribution functions expressed in terms of both the position and momentum variables. The Wigner function, P_{w}, will be discussed first in section 2 for not only was it the first quantum mechanical phase space distribution to be considered, but also it satisfies a number of properties which make it quite useful in applications. First of all, we will discuss its properties and then show that Wigner's distribution function gives the same expectation value for every function of p and q as does the corresponding operator, as proposed by Weyl [1927], for the density matrix which describes the same state to which the distribution function corresponds. As was mentioned before, this was first observed by Moyal [1949]. Next we derive an equation, in many different forms, for the time dependence of P_{w}. Finally, we apply the formalism we have developed to the calculation of P_{w} for the eigenstates of the harmonic oscillator and also for the case of a canonical ensemble of harmonic oscillators at temperature T.

In section 3 we discuss distribution functions other than P_{w} which correspond to operator ordering

schemes different from that of Weyl–Wigner. Then in section 4 we treat distribution functions in terms of creation and annihilation operators, with emphasis on normal, symmetric and anti-normal ordering. In particular, we emphasize the normal ordering from which arises the well-known P distribution of quantum optics. We also discuss the generalized P representations. Finally, in section 5 we present our conclusions.

Applications will be treated in a future paper but we would be remiss not to mention the recent extensive review of quantum collision theory using phase space distributions (Carruthers and Zachariasan [1983]) and the work on relativistic kinetic theory – in addition to extensive discussions on the Wigner–Weyl correspondence – by the Amsterdam group (Suttorp and de Groot [1970]; Suttorp [1972]; de Groot [1974]; de Groot, van Leeuwen and van Weert [1980]). Also, a *brief* overview of some applications is presented in O'Connell [1983a,b].

2. Wigner distribution

2.1. Properties

In a 1932 paper (Wigner [1932a]) the distribution

$$P_{\mathrm{w}}(q,p)=\frac{1}{\pi\hbar}\int_{-\infty}^{\infty}\mathrm{d}y\,\langle q-y|\hat{\rho}|q+y\rangle\,\mathrm{e}^{2\mathrm{i}py/\hbar} \tag{2.1}$$

was proposed to represent a system in a mixed state represented by a density matrix $\hat{\rho}$. In the case of a pure state, ψ, it follows from eq. (1.6) that $\rho(q',q'')=\psi(q')\,\psi^*(q'')$ and hence

$$P_{\mathrm{w}}(q,p)=\frac{1}{\pi\hbar}\int_{-\infty}^{\infty}\mathrm{d}y\,\psi^*(q+y)\,\psi(q-y)\,\mathrm{e}^{2\mathrm{i}py/\hbar}\,. \tag{2.2a}$$

The latter result refers to one dimension. In the case of more than one dimension, the $\pi\hbar$ must be replaced by $(\pi\hbar)^{-n}$, where n is the number of the variables of ψ (or the number of variables of the rows or columns of $\hat{\rho}$) and q, y and p are n-dimensional vectors, with py the scalar product of the two. The integration is then over all components of y. Explicitly, eq. (2.2a) generalizes to

$$\begin{aligned}P_{\mathrm{w}}(q_1,\ldots q_n;p_1,\ldots p_n)=(\pi\hbar)^{-n}\int_{-\infty}^{\infty}\cdots\int_{-\infty}^{\infty}\mathrm{d}y_1\cdots\mathrm{d}y_n\,\psi^*(q_1+y_1,\ldots q_n+y_n)\\ \times\psi(q_1-y_1,\ldots q_n-y_n)\exp[2\mathrm{i}(p_1y_1+\cdots+p_ny_n)/\hbar]\,.\end{aligned} \tag{2.2b}$$

It was mentioned that this choice for a distribution function was by no means unique and that this particular choice was made because it seemed to be the simplest of those for which each Galilei transformation corresponds to the same Galilei transformation of the quantum mechanical wave functions. In later work Wigner [1979] returned to this issue by considering properties which one would want such a distribution to satisfy. He then showed that the distribution given by eq. (2.1) was the only

one which satisfied these properties. A subsequent paper by O'Connell and Wigner [1981a] considered a somewhat different list of properties and showed that these, too, led to the expression in eq. (2.1).

The properties for a distribution function, $P(q, p)$, which were considered of special interest, for the case of a pure state (generalization to the case of a mixed state is straightforward), are as follows (O'Connell and Wigner [1981a]):

(i) $P(q, p)$ should be a Hermitean form of the state vector $\psi(q)$, i.e. P is given by

$$P(q, p) = \langle\psi|\hat{M}(q, p)|\psi\rangle \tag{2.3}$$

where $\hat{M}(q, p)$ is a self-adjoint operator depending on p and q. Therefore, $P(q, p)$ is real.

(ii)

$$\int \mathrm{d}p\, P(q, p) = |\psi(q)|^2 = \langle q|\hat{\rho}|q\rangle \tag{2.4}$$

$$\int \mathrm{d}q\, P(q, p) = \langle p|\hat{\rho}|p\rangle \tag{2.5}$$

$$\int \mathrm{d}q \int \mathrm{d}p\, P(q, p) = \mathrm{Tr}(\hat{\rho}) = 1\,. \tag{2.6}$$

(iii) $P(q, p)$ should be Galilei invariant, i.e. if $\psi(q) \to \psi(q + a)$ then $P(q, p) \to P(q + a, p)$ and if $\psi(q) \to \exp(\mathrm{i}p'q/\hbar)\,\psi(q)$ then $P(q, p) \to P(q, p - p')$.

(iv) $P(q, p)$ should be invariant with respect to space and time reflections, i.e. if $\psi(q) \to \psi(-q)$ then $P(q, p) \to P(-q, -p)$ and if $\psi(q) \to \psi^*(q)$ then $P(q, p) \to P(q, -p)$.

It should be admitted, however, that neither of these transformations is relativistic and also that they do not yet involve the spin variable.

(v) In the force-free case the equation of motion is the classical one

$$\frac{\partial P}{\partial t} = -\frac{p}{m}\frac{\partial P}{\partial q}\,. \tag{2.7}$$

(vi) If $P_\psi(q, p)$ and $P_\phi(q, p)$ are the distributions corresponding to the states $\psi(q)$ and $\phi(q)$ respectively then

$$\left|\int \mathrm{d}q\, \psi^*(q)\, \phi(q)\right|^2 = (2\pi\hbar) \int \mathrm{d}q \int \mathrm{d}p\, P_\psi(q, p)\, P_\phi(q, p)\,. \tag{2.8}$$

Property (vi) has two interesting consequences. If we set $\phi(q) = \psi(q)$ we get

$$\int \mathrm{d}q \int \mathrm{d}p\, [P_\psi(q, p)]^2 = \frac{1}{2\pi\hbar} \tag{2.9}$$

and, in the case of a mixed state, the right-hand side of eq. (2.9) is multiplied by $\Sigma_\beta\, w_k^2$ where the w_k are the probabilities for the different states (the characteristic values of $\hat{\rho}$). This implies that $P_\psi(q, p)$ is not too highly peaked and rules out such distributions as $P_\psi(q, p) = \delta(q - \hat{q})\,\delta(p - \hat{p})$ which would be

possible classically. We can also choose ϕ and ψ so that they are orthogonal. We then have that

$$\int \mathrm{d}q \int \mathrm{d}p\, P_\psi(q,p)\, P_\phi(q,p) = 0 \tag{2.10}$$

which implies that $P(q,p)$ cannot be everywhere positive. This conclusion is actually rather general. Wigner [1979] has shown that any distribution function as long as it satisfies properties (i) and (ii) assumes also negative values for some p and q.

(vii)

$$\int \mathrm{d}q \int \mathrm{d}p\, A(q,p)\, B(q,p) = (2\pi\hbar)\,\mathrm{Tr}(\hat{A}\hat{B}) \tag{2.11}$$

where $A(q,p)$ is the classical function corresponding to the quantum operator $\hat{A}$, and is given, according to Wigner's prescription, by

$$A(q,p) = \int \mathrm{d}z\, \mathrm{e}^{\mathrm{i}pz/\hbar}\, \langle q - \tfrac{1}{2}z|\hat{A}|q + \tfrac{1}{2}z\rangle \tag{2.12}$$

so that $\int\int \mathrm{d}q\, \mathrm{d}p\, A(q,p) = 2\pi\hbar\, \mathrm{Tr}(\hat{A})$. A similar relation exists between $B(q,p)$ and $\hat{B}$.

The proof of eq. (2.11) will be shown below to follow as a particular case of a more general relation (eq. (2.23)) for $F(q,p)$, in terms of $A(q,p)$ and $B(q,p)$, where $\hat{F} = \hat{A}\hat{B}$. From eq. (2.12), it is at once evident that the phase space description $A(q,p)$ of the operator $\hat{A}$ is real if $\hat{A}$ is self-adjoint (Hermitean) and is imaginary if $\hat{A}$ is skew Hermitean. Since in neither case does $A(q,p)$ vanish, it is evident that if it is real, its operator $\hat{A}$ is self-adjoint, if it is imaginary $\hat{A}$ is skew symmetric. It is also evident that the phase space description of the Hermitean adjoint $\hat{A}^+$ of $\hat{A}$ is the complex conjugate of the similar description of $\hat{A}$. Similarly, if the phase space descriptions of two operators are complex conjugates of each other, then the operators are Hermitean adjoints of each other.

By comparison of eqs. (2.1) and (2.12), it is clear that $P(q,p)$, derived from the density matrix, is $(2\pi\hbar)^{-1}$ times the phase space operator which corresponds to the same matrix. Also, for $\hat{A} = \hat{\rho}$ and $\hat{B}$ equal to the unit matrix, eq. (2.6) immediately follows from eq. (2.11). Furthermore, for $\hat{B} = \hat{\rho}$, eq. (2.11) reduces to

$$\int \mathrm{d}q \int \mathrm{d}p\, A(q,p)\, P_{\mathrm{w}}(q,p) = \mathrm{Tr}(\hat{\rho}\, \hat{A}(\hat{q},\hat{p}))\,, \tag{2.13}$$

which is equivalent to eqs. (1.2) and (1.3). This result was originally obtained (Wigner [1932]) for the special case of $\hat{A}$ being the sum of a function of $\hat{p}$ only and a function of $\hat{q}$ only but Moyal [1949] showed it was actually true in the case where $\hat{A}$ is any function of $\hat{q}$ and $\hat{p}$, if $\hat{A}(\hat{q},\hat{p})$ is the Weyl operator (discussed below in section 2.2) for $A(q,p)$. In addition, if we take $\hat{A} = \hat{B} = \hat{\rho}$ in eq. (2.11) and use the fact that, if $\hat{\rho}$ represents a pure state, $\mathrm{Tr}(\hat{\rho})^2 = \mathrm{Tr}\,\hat{\rho} = 1$, we obtain eq. (2.9) again.

(viii) If we define the Fourier transform of the wave function

$$\phi(p) = (2\pi\hbar)^{-1} \int \mathrm{d}q\, \psi(q)\, \mathrm{e}^{-\mathrm{i}qp/\hbar}\,, \tag{2.14}$$

then eq. (2.2a) can be re-written in the form

$$P(q,p)=(\pi\hbar)^{-1}\int \mathrm{d}p'\,\phi^*(p+p')\,\phi(p-p')\,\mathrm{e}^{-2\mathrm{i}qp'/\hbar}\,, \tag{2.15}$$

exhibiting the basic symmetry under the interchange $q \leftrightarrow p$.

It may be worth observing also that the contraction of the distribution function from n to $n-1$ variables

$$\begin{aligned}
&\int\int P(q_1,\ldots q_{n-1},q_n;p_1,\ldots p_{n-1},p_n)\,\mathrm{d}q_n\,\mathrm{d}p_n\\
&\quad=(\pi\hbar)^n\int\cdots\int \rho(q_1-y_1,\ldots q_{n-1}-y_{n-1},q_n-y_n;q_1+y_1,\ldots q_{n-1}+y_{n-1},q_n+y_n)\\
&\qquad\times\exp[2\mathrm{i}(p_1y_1+\cdots+p_{n-1}y_{n-1}+p_ny_n)/\hbar]\,\mathrm{d}y_1\cdots\mathrm{d}y_{n-1}\,\mathrm{d}y_n\,\mathrm{d}q_n\,\mathrm{d}p_n\\
&\quad=(\pi\hbar)^{n-1}\int\cdots\int \rho(q_1-y_1,\ldots q_{n-1}-y_{n-1},q_n-y_n;q_1+y_1,\ldots q_{n-1}+y_{n-1},q_n+y_n)\\
&\qquad\times\exp[2\mathrm{i}(p_1y_1+\cdots+p_{n-1}y_{n-1})/\hbar]\,\delta(y_n)\,\mathrm{d}y_1\cdots\mathrm{d}y_{n-1}\,\mathrm{d}y_n\,\mathrm{d}q_n\\
&\quad=(\pi\hbar)^{n-1}\int\cdots\int [\rho(q_1-y_1,\ldots q_{n-1}-y_{n-1},q_n;q_1+y_1,\ldots q_{n-1}+y_{n-1},q_n)\,\mathrm{d}q_n]\\
&\qquad\times\exp[2\mathrm{i}(p_1y_1+\cdots+p_{n-1}y_{n-1})/\hbar]\,\mathrm{d}y_1\cdots\mathrm{d}y_{n-1}
\end{aligned} \tag{2.16}$$

gives the distribution function which corresponds to the properly contracted ρ (in square brackets). Actually, this is true also for the other distribution functions which will be considered in section 3.

Wigner in his 1971 paper also showed that properties (i)–(v) determined the distribution function uniquely. O'Connell and Wigner [1981a] showed that properties (i)–(iv) and (vi) also accomplish this. In both cases the distribution function was that given by eq. (2.1).

Finally, we draw attention to two restrictions on the distribution function discussed above. First of all, as already mentioned, it is non-relativistic. Secondly, not all functions $P(q,p)$ are allowed, as we will now demonstrate by turning to the question of the admissability of P and asking what condition is necessary so that P implies the existence of the density function $\hat{\rho}$, the expectation values of which are, naturally, positive or zero. Our starting-point is eq. (2.2a) from which it follows that

$$\int \mathrm{d}p\,\mathrm{e}^{-2\mathrm{i}py/\hbar}\,P(q,p)=\rho(q-y,q+y)\,. \tag{2.17}$$

Hence, changing variables to $u=q+y$ and $v=q-y$, we obtain

$$\rho(v,u)=\int \mathrm{d}p\,\mathrm{e}^{-\mathrm{i}p(u-v)/\hbar}\,P(\tfrac{1}{2}(u+v),p)\,. \tag{2.18}$$

We remark that since p on the right-side of eq. (2.18) is a dummy variable it is clear that it could be replaced by q.

Now the condition for $P(q,p)$ to be a permissible distribution function is that the corresponding

density matrix be positive definite, i.e.

$$\int \mathrm{d}x \int \mathrm{d}x' \, \psi^*(x) \, \rho(x, x') \, \psi(x') \geq 0 \tag{2.19a}$$

for all ψ. Using eq. (2.18) and eq. (2.19a), it follows that the condition that $P(q, p)$ be permissible is that

$$\int \mathrm{d}q \int \mathrm{d}p \, P(q, p) \, P'(q, p) \geq 0 \tag{2.19b}$$

for *any* $P'(q, p)$ which corresponds to a pure state. This is evident already from eq. (2.8). It also follows from eq. (2.11) and the fact that $\mathrm{Tr}(\hat{\rho}\hat{\rho}') \geq 0$. Eq. (2.19b) holds, of course, for any P' which is itself permissible but the permissibility of P follows already if it is valid for *all* P' which correspond to a pure state.

Eight properties of the distribution function were discussed above, eqs. (2.3) to (2.16), with the emphasis on the use of this function to form another description of a quantum mechanical state, i.e. be a substitute for the density matrix. Just as eq. (2.1) permits one to give a phase space formulation to the density matrix $\hat{\rho}$, we emphasize that eq. (2.12) permits one also to give a phase space formulation to any matrix – or operator – and it may be useful to consider the properties of eq. (2.12).

In particular, we wish to derive an expression for the function $F(q, p)$ which corresponds to the product $\hat{F} = \hat{A}\hat{B}$ of two operators $\hat{A}$ and $\hat{B}$ to which the q, p functions $A(q, p)$ and $B(q, p)$ correspond. We assume that the operators $\hat{A}$ and $\hat{B}$ are matrices, the rows and columns of which can be characterized by a single variable, but the generalization to a many-dimensional configuration space is obvious. We can write, therefore

$$\hat{F}(x, x'') = \int \hat{A}(x, x') \, \hat{B}(x', x'') \, \mathrm{d}x' \, . \tag{2.20}$$

Analogous to eqs. (2.17) and (2.18), eq. (2.20) can be written as (taking $\hbar = 1$ for this derivation)

$$\begin{aligned} \int \mathrm{d}p_1 \, F(\tfrac{1}{2}(x + x''), p_1) \, \mathrm{e}^{-\mathrm{i}p_1(x''-x)} &= (2\pi)^{-1} \int\int\int \mathrm{d}x' \, \mathrm{d}p' \, \mathrm{d}p'' \, A(\tfrac{1}{2}(x + x'), p') \, \mathrm{e}^{-\mathrm{i}p'(x'-x)} \\ &\quad \times B(\tfrac{1}{2}(x' + x''), p'') \, \mathrm{e}^{-\mathrm{i}p''(x''-x')} \, . \end{aligned} \tag{2.21}$$

Substituting $x = q + q'$, $x'' = q - q'$, multiplying with $\mathrm{e}^{-2\mathrm{i}q'p}$ and integrating over q' one obtains

$$\begin{aligned} F(q, p) = 2\,(2\pi)^{-2} &\int\int\int\int \mathrm{d}q' \, \mathrm{d}x' \, \mathrm{d}p' \, \mathrm{d}p'' \, A(\tfrac{1}{2}(q + q' + x'), p') \, B(\tfrac{1}{2}(q - q' + x'), p'') \\ &\times \exp\{-\mathrm{i}q'(2p - p' - p'') - \mathrm{i}(p'' - p')(q - x')\} \, . \end{aligned} \tag{2.22}$$

Introducing finally new variables $y = \frac{1}{2}(q + x')$, $y' = \frac{1}{2}q'$, $p' = \rho - \rho'$, $p'' = \rho + \rho'$, one obtains

$$\begin{aligned} F(q, p) &= 16\,(2\pi)^{-2} \int\int\int\int \mathrm{d}y \, \mathrm{d}y' \, \mathrm{d}\rho \, \mathrm{d}\rho' \, A(y + y', \rho - \rho') \, B(y - y', \rho + \rho') \\ &\quad \times \exp\{-4\mathrm{i}\, y'(p - \rho) - 4\mathrm{i}\, \rho'(q - y)\} \\ &= 16\,(2\pi)^{-2} \int\int\int\int \mathrm{d}y \, \mathrm{d}y' \, \mathrm{d}\rho \, \mathrm{d}\rho' \, A(q + y + y', p + \rho - \rho') \, B(q + y - y', p + \rho + \rho') \, \mathrm{e}^{4\mathrm{i}(\rho y' + y\rho')} \, . \end{aligned} \tag{2.23}$$

This expression for $F(q,p)$, which is a new result, also shows the similarity of the roles of p and q in Hamiltonian mechanics. In the next subsection, another expression (eq. (2.59)) for $F(q,p)$ will be presented.

If we integrate $F(q,p)$ in eq. (2.23) over q and p, we obtain

$$\int\int F(q,p)\,\mathrm{d}q\,\mathrm{d}p = 16\,(2\pi)^{-2}\int\int\int\int \mathrm{d}y\,\mathrm{d}y'\,\mathrm{d}\rho\,\mathrm{d}\rho'\,A(y+y',\rho-\rho')\,B(y-y',\rho+\rho')$$
$$\times\exp\{4\mathrm{i}y'\rho+4\mathrm{i}\rho'y\}\,(4\pi^2/16)\,\delta(y')\,\delta(\rho')\,. \tag{2.24}$$

Hence

$$\int\int F(q,p)\,\mathrm{d}q\,\mathrm{d}p = \int\int A(q,p)\,B(q,p)\,\mathrm{d}q\,\mathrm{d}p\,. \tag{2.25}$$

Since the left-hand side of this equation is the same as $(2\pi\hbar)\,\mathrm{Tr}(\hat{F})$, it is clear that eq. (2.25) is the same as eq. (2.11). In the case of n dimensions, the nth power of $(4/\pi^2)$ appears in the expression corresponding to eq. (2.23).

Eq. (2.23) provides also a means to ascertain, in terms of the phase space descriptions of $\hat{A}$ and $\hat{B}$, whether these two operators commute. Naturally, the condition for the commutative nature is

$$\int\int\int\int \mathrm{d}y\,\mathrm{d}y'\,\mathrm{d}\rho\,\mathrm{d}\rho'\,A(y+y',\rho-\rho')\,B(y-y',\rho+\rho')\exp\{-4\mathrm{i}\,y'(p-\rho)-4\mathrm{i}\,\rho'(q-y)\}$$
$$=\int\int\int\int \mathrm{d}y\,\mathrm{d}y'\,\mathrm{d}\rho\,\mathrm{d}\rho'\,B(y+y',\rho-\rho')\,A(y-y',\rho+\rho')\exp\{-4\mathrm{i}\,y'(p-\rho)-4\mathrm{i}\,\rho'(q-y)\}\,. \tag{2.26}$$

Since this is valid for all p and q, the integration over the variables which are their factors in the exponent (i.e. y' and ρ') can be omitted. This gives as condition for the commutability of $\hat{A}$ and $\hat{B}$ (we replace y, y' by q, q' and ρ, ρ' by p, p'):

$$\int\int \mathrm{d}p\,\mathrm{d}q\,[A(q+q',p-p')\,B(q-q',p+p')-A(q-q',p+p')\,B(q+q',p-p')]$$
$$\times\exp\{4\mathrm{i}(q'p+p'q)\}=0\,, \tag{2.27}$$

a somewhat unexpected expression.

The last quantum mechanical relation that will be translated into phase space language is the equation $\hat{A}\hat{\rho}=\lambda\hat{\rho}$ specifying that the wave functions of which $\hat{\rho}$ consists are characteristic functions (eigenfunctions) of $\hat{A}$ with the characteristic value λ. Whether $\hat{\rho}$ contains only one or more such characteristic functions depends whether or not its phase space representation, P_{w}, satisfies eq. (2.9), i.e. whether its square integral is equal to or smaller than $(2\pi\hbar)^{-1}$.

The $\hat{A}\hat{\rho}=\lambda\hat{\rho}$ relation, with $\hat{\rho}$ represented by P_{w}, reads, according to eq. (2.23), in phase space language:

$$(4/\pi^2)\int\int\int\int \mathrm{d}y\,\mathrm{d}y'\,\mathrm{d}\rho\,\mathrm{d}\rho'\,A(y+y',\rho-\rho')\,P_{\mathrm{w}}(y-y',\rho+\rho')\exp\{4\mathrm{i}\,y'(\rho-p)+4\mathrm{i}\,\rho'(y-q)\}$$
$$=\lambda\,P_{\mathrm{w}}(q,p)\,. \tag{2.28}$$

In order to simplify this, one can multiply with $\exp\{4\mathrm{i}(q'p+p'q)\}$ and integrate over p and q to obtain, substituting also q and p for the integration variables y and ρ,

$$\int\int \mathrm{d}q\,\mathrm{d}p\,A(q+q',p-p')\,P_{\mathrm{w}}(q-q',p+p')\exp\{4\mathrm{i}(q'p+p'q)\}$$
$$=\lambda\int\int \mathrm{d}q\,\mathrm{d}p\,P_{\mathrm{w}}(q,p)\exp\{4\mathrm{i}(q'p+p'q)\}\,. \tag{2.29}$$

Both eqs. (2.27) and (2.29) are a good deal more complicated than the quantum mechanical equations for which they substitute. It is questionable whether they are really useful. We thought that they should be derived in spite of this because the final form is considerably simpler than the original one and because they clearly demonstrate the essential phase space equivalence of q and p. It may be worth remarking finally that in the case of several dimensions all variables should be considered as vectors, and products like $q'p$ or $p'q$ should be replaced by scalar products of these vectors.

2.2. Associated operator ordering

We will now discuss the connection between a classical function of q and p and a quantum mechanical operator which is supposed to correspond to it. The result of the measurement of a quantum mechanical operator is well defined: it is supposed to transfer the state of the system on which the measurement is carried out into one of the characteristic vectors of the operator in question, and the probabilities with which the different characteristic vectors would result from the measurement are also well defined. They are the squares of the scalar products of the normalized initial state of the system on which the measurement is carried out and of the operator's normalized characteristic vector into which the state of the system is transformed. It must be admitted, even in this case, that, given an arbitrary operator, it is in many cases difficult, in others impossible, to construct an apparatus which can carry out the measurement, i.e. the desired change of the state of the system on which the measurement is to be carried out.

But as far as the measurement of a classical function of p and q is concerned, no similar postulate exists which can be formulated in classical terms. But Weyl did propose the association of a quantum mechanical operator to every function of q and p and defined the measurement of the classical quantity as being identical with the above described quantum mechanical measurement of the operator which he associated to the classical function of q and p. This association will be described below. What is remarkable, however, and what has been first pointed out by Moyal [1949], is the close connection between Weyl's proposal and the distribution function as defined above. In particular, the expectation value of the result of the measurement of the operator $\hat{A}$, which Weyl associates with the classical function $A(q,p)$ if carried out on a system in the state ψ,

$$\langle\psi|\hat{A}|\psi\rangle=\int \mathrm{d}q\int \mathrm{d}p\,P_{\mathrm{w}}(q,p)\,A(q,p) \tag{2.30}$$

is equal to the expectation value of the classical function $A(q, p)$ to which $\hat{A}$ corresponds assuming that the system is described by the distribution function $P_w(q, p)$ which corresponds to $\hat{\rho}$. This is the content of eq. (2.30) and it is valid, as will be demonstrated below, for every state vector ψ and also for any density matrix $\hat{\rho}$

$$\mathrm{Tr}(\hat{\rho}\hat{A}) = \int \mathrm{d}q \int \mathrm{d}p\, P_w(q, p)\, A(q, p)\,. \tag{2.31}$$

Actually eq. (2.31) is an easy consequence of eq. (2.30) and only the latter will be proved below.

In order to prove eq. (2.30), we start with Weyl's expansion of $A(q, p)$ into a Fourier integral (taking $\hbar = 1$ for the purpose of this proof):

$$A(q, p) = \int \mathrm{d}\sigma \int \mathrm{d}\tau\, \alpha(\sigma, \tau)\, \mathrm{e}^{\mathrm{i}(\sigma q + \tau p)}\,. \tag{2.32}$$

Weyl then defines the operator which corresponds to the exponential in the integrand on the right-hand side of eq. (2.32) as $\exp\{\mathrm{i}(\sigma\hat{q} + \tau\hat{p})\}$. The operator which corresponds to $A(q, p)$ is then given by

$$\hat{A}(\hat{q}, \hat{p}) = \int \mathrm{d}\sigma \int \mathrm{d}\tau\, \alpha(\sigma, \tau) \exp\{\mathrm{i}(\sigma\hat{q} + \tau\hat{p})\}\,. \tag{2.33}$$

If we substitute this result for $\hat{A}$ into the left-hand side of eq. (2.30) and replace $A(q, p)$ on the right-hand side by the right-hand side of eq. (2.32), it becomes evident that all we have to prove is that

$$\begin{aligned}\langle\psi|\exp\{\mathrm{i}(\sigma\hat{q} + \tau\hat{p})\}|\psi\rangle &= \int \mathrm{d}q \int \mathrm{d}p\, P_w(q, p) \exp\{\mathrm{i}(\sigma q + \tau p)\} \\ &= \frac{1}{2\pi} \int \mathrm{d}y \int \mathrm{d}q \int \mathrm{d}p\, \psi^*(q + \tfrac{1}{2}y)\, \psi(q - \tfrac{1}{2}y) \exp\{\mathrm{i}py + \mathrm{i}(\sigma q + \tau p)\}\,.\end{aligned} \tag{2.34}$$

The integration over p gives $2\pi\,\delta(y + \tau)$ and hence the right-hand side of eq. (2.34) becomes

$$\int \mathrm{d}q\, \psi^*(q - \tfrac{1}{2}\tau)\, \psi(q + \tfrac{1}{2}\tau)\, \mathrm{e}^{\mathrm{i}\sigma q}\,.$$

In order to evaluate the left-hand side of (2.34) we note that according to the Baker–Hausdorff theorem (Messiah [1961]), if the commutator $\hat{D} = [\hat{A}, \hat{B}]$ commutes with $\hat{A}$ and $\hat{B}$ then

$$\mathrm{e}^{\hat{A}+\hat{B}} = \mathrm{e}^{\hat{A}}\, \mathrm{e}^{\hat{B}}\, \mathrm{e}^{-\hat{D}/2}\,. \tag{2.35a}$$

It then follows that

$$\mathrm{e}^{\mathrm{i}(\sigma\hat{q} + \tau\hat{p})} = \mathrm{e}^{\mathrm{i}\sigma\hat{q}}\, \mathrm{e}^{\mathrm{i}\tau\hat{p}}\, \mathrm{e}^{\mathrm{i}\sigma\tau/2}\,. \tag{2.35b}$$

Hence, the left-hand side of eq. (2.34) becomes

$$e^{i\sigma\tau/2}\langle\psi|e^{i\sigma\hat{q}}\, e^{i\tau\hat{p}}|\psi\rangle\,.$$

Next, using the fact that

$$e^{i\tau\hat{p}}\,|\psi(x)\rangle = |\psi(x+\tau)\rangle \tag{2.36}$$

and transferring the $e^{i\sigma\hat{q}}$ to the left-hand side, this becomes

$$e^{i\sigma\tau/2}\langle e^{-i\sigma x}\,\psi(x)|\psi(x+\tau)\rangle = \int dx\, e^{i(\sigma x+\sigma\tau/2)}\,\psi^*(x)\,\psi(x+\tau)\,, \tag{2.37}$$

which is equal to the expression obtained above for the right-hand side of eq. (2.34). Thus, we have proved eq. (2.34) and hence also eq. (2.30).

In summary, if a classical function

$$A(q,p) = \int d\sigma \int d\tau\, e^{(i/\hbar)(\sigma q+\tau p)}\,\alpha(\sigma,\tau) \tag{2.38}$$

goes over to the quantum operator

$$\hat{A}(\hat{q},\hat{p}) = \int d\sigma \int d\tau\, e^{(i/\hbar)(\sigma\hat{q}+\tau\hat{p})}\,\alpha(\sigma,\tau) \tag{2.39}$$

then the relation between $A(q,p)$ and $\hat{A}$ is that given by Wigner in eq. (2.12). Furthermore, it is clear that if, for all $A(p,q)$

$$\int dq \int dp\, P(q,p)\, A(q,p) = \int dq \int dp\, P'(q,p)\, A(q,p) \tag{2.40}$$

then P' is identical with P.

In addition, we mention that under the Weyl correspondence the classical quantity $q^n p^m$ becomes

$$q^n p^m \to \frac{1}{2^n}\sum_{r=0}^{n}\binom{n}{r}\,\hat{q}^{n-r}\,\hat{p}^m\,\hat{q}^r \tag{2.41}$$

as can be seen by considering the $\sigma^n\tau^m$ coefficient in $(\sigma\hat{q}+\tau\hat{p})^{n+m}$.

Finally, we would like to mention the role played by the characteristic function. This is a description of the state $\hat{\rho}$ by means of a function of two new variables, σ and τ,

$$C(\sigma,\tau) = \mathrm{Tr}(\hat{\rho}\,\hat{C}(\sigma,\tau))\,, \tag{2.42}$$

where

$$\hat{C}(\sigma,\tau) = e^{(i/\hbar)(\sigma\hat{q}+\tau\hat{p})}\,. \tag{2.43}$$

Here we are following the nomenclature of Moyal which has now become standard in describing this quantity as a "characteristic function". This description stems from statistical terminology, and, in particular, should not be confused with the sometime usage of "characteristic function" in quantum mechanics to denote an eigenfunction.

$C(\sigma, \tau)$ is just the Fourier transform of $P(q, p)$. To see this we note that the function corresponding to $\hat{C}(\sigma, \tau)$ is just $\exp\{(\mathrm{i}/\hbar)(\sigma q + \tau p)\}$. Making use of eq. (2.11) gives

$$C(\sigma, \tau) = \mathrm{Tr}(\hat{\rho}\, \hat{C}(\sigma, \tau)) = \int \mathrm{d}q \int \mathrm{d}p\, \mathrm{e}^{(\mathrm{i}/\hbar)(\sigma q + \tau p)}\, P_{\mathrm{w}}(q, p) \tag{2.44}$$

so that

$$P_{\mathrm{w}}(q, p) = \left(\frac{1}{2\pi\hbar}\right)^2 \int \mathrm{d}\sigma \int \mathrm{d}\tau\, \mathrm{e}^{(-\mathrm{i}/\hbar)(\sigma q + \tau p)}\, C(\sigma, \tau)\,. \tag{2.45}$$

We can use the characteristic function to compute expectation values of Weyl-ordered products of p and q. We have that

$$\left(\frac{\hbar}{\mathrm{i}}\right)^{m+n} \frac{\partial^m}{\partial\sigma^m} \frac{\partial^n}{\partial\tau^n} C(\sigma, \tau)\bigg|_{\sigma=\tau=0} = \int \mathrm{d}q \int \mathrm{d}p\, q^m p^n\, P_{\mathrm{w}}(q, p)\,, \tag{2.46}$$

the right-hand side of which is just the average of the Weyl-ordered product $q^m p^n$.

2.3. Dynamics

We would now like to derive equations for the time-dependence of P_{w}. As before, our detailed considerations will be confined to one dimension but some results will also be quoted for the multi-dimensional case. The time-dependence of P_{w} may be decomposed into two parts (Wigner [1932a])

$$\frac{\partial P_{\mathrm{w}}}{\partial t} = \frac{\partial_k P_{\mathrm{w}}}{\partial t} + \frac{\partial_v P_{\mathrm{w}}}{\partial t} \tag{2.47}$$

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

From the definition of P_{w}, given by eq. (2.2a), it follows that

$$\frac{\partial_k P_{\mathrm{w}}}{\partial t} = -\frac{\mathrm{i}}{2\pi m} \int \mathrm{d}y \left[\underline{\frac{\partial^2\psi^*(q+y)}{\partial y^2}}\, \psi(q-y) - \psi^*(q+y) \frac{\partial^2\psi(q-y)}{\partial y^2}\right] \mathrm{e}^{2\mathrm{i}py/\hbar}\,, \tag{2.48}$$

where we have taken advantage of the functional dependence of ψ to replace $\partial^2/\partial q^2$ by $\partial^2/\partial y^2$. Next we perform one partial integration with respect to y to obtain

$$\frac{\partial_k P_{\mathrm{w}}}{\partial t} = -\frac{p}{\pi\hbar m} \int \mathrm{d}y \left[\frac{\partial\psi^*(q+y)}{\partial y}\, \psi(q-y) - \psi^*(q+y) \frac{\partial\psi(q-y)}{\partial y}\right] \mathrm{e}^{2\mathrm{i}py/\hbar}\,, \tag{2.49}$$

since the boundary term does not contribute. Switching back from $\partial/\partial y$ to $\partial/\partial q$, we finally obtain

$$\frac{\partial_k P_w}{\partial t} = -\frac{p}{m}\frac{\partial P_w(q,p)}{\partial q}. \tag{2.50}$$

This is identical with the classical (Liouville) equation for the corresponding part of $\partial P/\partial t$, as was mentioned at eq. (2.7). We next calculate

$$\begin{aligned}\frac{\partial_v P_w}{\partial t} &= \frac{i}{\pi\hbar^2}\int dy\,\{[V\psi^*(q+y)]\,\psi(q-y) - \psi^*(q+y)\,[V\psi(q-y)]\}\,e^{2ipy/\hbar}\\ &= \frac{i}{\pi\hbar^2}\int dy\,[V(q+y) - V(q-y)]\,\psi^*(q+y)\,\psi(q-y)\,e^{2ipy/\hbar}.\end{aligned} \tag{2.51}$$

Assuming that V can be expanded in a Taylor series, we write

$$V(q+y) = \sum_{\lambda=0}^{\infty}\frac{y^\lambda}{\lambda!}V^{(\lambda)}(q) \tag{2.52}$$

where $V^{(\lambda)}(q) = \partial^\lambda V/\partial q^\lambda$. It follows that

$$\frac{\partial_v P_w}{\partial t} = \frac{2i}{\pi\hbar^2}\int dy\,\sum_\lambda \frac{y^\lambda}{\lambda!}V^{(\lambda)}(q)\,\psi^*(q+y)\,\psi(q-y)\,e^{2ipy/\hbar}, \tag{2.53}$$

where now the summation over λ is restricted to all odd positive integers. It is clear that in the powers y^λ in the integrand we can replace y by $(\hbar/2i)(\partial/\partial p)$. It then follows that

$$\frac{\partial_v P_w}{\partial t} = \sum_\lambda \frac{1}{\lambda!}\left(\frac{\hbar}{2i}\right)^{\lambda-1}\frac{\partial^\lambda V(q)}{\partial q^\lambda}\frac{\partial^\lambda P_w(q,p)}{\partial p^\lambda}, \tag{2.54}$$

λ again being restricted to odd integers. An alternative form for $\partial_v P_w/\partial t$ is given by

$$\frac{\partial_v P_w}{\partial t} = \int dj\,P_w(q,p+j)\,J(q,j), \tag{2.55}$$

where

$$\begin{aligned}J(q,j) &= \frac{i}{\pi\hbar^2}\int dy\,[V(q+y) - V(q-y)]\,e^{-2ipy/\hbar}\\ &= \frac{i}{\pi\hbar^2}\int dy\,[V(q+y) - V(q-y)]\,\sin(2jy/\hbar)\end{aligned} \tag{2.55a}$$

is the probability of a jump in the momentum by an amount j if the positional coordinate is q. The first part of eq. (2.55a) may be verified by inserting the Fourier expansion, with respect to y, of $V(q+y)-$

$V(q-y)$ into eq. (2.51). The second part is obtained by replacing the exponential by cos + i sin and noting that the expansion in the square bracket is odd so that the integral of the cos part vanishes.

In the multi-dimensional case where $P_w = P_w(q_1, \ldots q_n; p_1, \ldots p_n)$, the corresponding results are

$$\frac{\partial P_w}{\partial t} = -\sum_{k=1}^{n} \frac{p_k}{m_k} \frac{\partial P_w}{\partial q_k} + \sum \frac{\partial^{\lambda_1+\cdots+\lambda_n} V}{\partial q_1^{\lambda_1} \cdots \partial q_n^{\lambda_n}} \frac{(\hbar/2i)^{\lambda_1+\cdots+\lambda_n-1}}{\lambda_1! \cdots \lambda_n!} \frac{\partial^{\lambda_1+\cdots+\lambda_n} P_w}{\partial p_1^{\lambda_1} \cdots \partial p_n^{\lambda_n}}, \tag{2.56}$$

where the last summation has to be extended over all positive integer values of $\lambda_1, \ldots \lambda_n$ for which the sum $\lambda_1 + \lambda_2 + \cdots + \lambda_n$ is odd.

The lowest term of eq. (2.56) in which only one λ is 1 and the others vanish, and which has no $\hbar$ factors, is identical with the corresponding term of Liouville's equation. Hence eq. (2.56) reproduces the classical (but non-relativistic) equation if $\hbar$ is set equal to zero. The $\hbar^2$ terms give the quantum correction if this is very small. We will obtain a somewhat similar equation for the $1/T$ dependence of the distribution function of the canonical ensemble, which also is useful if the temperature T is not too low so that the quantum correction is small.

Eq. (2.56) is the generalization of eq. (2.50) and eq. (2.54) for an n-dimensional configuration space. The same generalization of eq. (2.50) with eq. (2.55) is

$$\frac{\partial P_w}{\partial t} = -\sum_{k} \frac{p_k}{m_k} \frac{\partial P_w}{\partial q_k} + \int \mathrm{d}j_1 \cdots \int \mathrm{d}j_n \, P_w(q_1, \ldots q_n; p_1 + j_1, \ldots p_n + j_n) \, J(q_1, \ldots q_n; p_1, \ldots p_n), \tag{2.57}$$

where $J(q_1, \ldots q_n; j_1, \ldots j_n)$ can be interpreted as the probability of a jump in the momenta with the amounts $j_1, \ldots j_n$ for the configuration $q_1, \ldots q_n$. The probability of this jump is given by

$$J(q_1, \ldots q_n; j_1, \ldots j_n) = \frac{\mathrm{i}}{\pi^n \hbar^{n+1}} \int \mathrm{d}y_1 \cdots \int \mathrm{d}y_n \, [V(q_1 + y_1, \ldots q_n + y_n) - V(q_1 - y_1, \ldots q_n - y_n)]$$
$$\times \exp\{-(2\mathrm{i}/\hbar)(y_1 j_1 + \cdots + y_n j_n)\} \tag{2.58}$$

that is, by the Fourier expansion coefficients of the potential $V(q_1, \ldots q_n)$.

From eq. (2.56) it is clear that the equation of motion is the same as the classical equation of motion when V has no third and higher derivatives as, for example, in the case of a uniform electric field or for a system of oscillators. However, there is still a subtle difference in that the possible initial conditions are restricted. This comes about because not all $P(q, p)$ are permissible (see eq. (2.19b)).

While we consider that the above form for the equations of motion (Wigner [1932]) are the simplest to use in practice, we will now discuss some other forms which occur frequently in the literature.

Before doing so it is useful to take note of another relation, in addition to that given by eq. (2.23), which expresses the Weyl function corresponding to an operator $\hat{F} = \hat{A}\hat{B}$ in terms of the Weyl functions corresponding to $\hat{A}$ and $\hat{B}$. This relation was first derived by Groenewold [1946] and was also discussed by Imre, Ozizmir, Rosenbaum and Zweifel [1967]. They find that the function corresponding to $\hat{F}$ is

$$\hat{A}\hat{B} = \hat{F} \to F(q, p) = A(q, p)\, \mathrm{e}^{(\hbar \Lambda/2\mathrm{i})}\, B(q, p)$$
$$= B(q, p)\, \mathrm{e}^{-(\hbar \Lambda/2\mathrm{i})}\, A(q, p), \tag{2.59}$$

where

$$\Lambda = \frac{\overleftarrow{\partial}}{\partial p}\frac{\overrightarrow{\partial}}{\partial q} - \frac{\overleftarrow{\partial}}{\partial q}\frac{\overrightarrow{\partial}}{\partial p} \tag{2.60}$$

and the arrows indicate in which direction the derivatives act. Also $(\partial/\partial p)(\partial/\partial q)$ is considered as the multi-dimensional scalar product of $\partial/\partial p$ and $\partial/\partial q$, or, in other words, it is equal to $(\partial/\partial p_i)(\partial/\partial q_i)$, where $i = (1, \ldots n)$ and n denotes the number of dimensions and, as usual, repeated indices denotes summation.

To derive this result we first note that

$$\langle q''|\hat{A}|q'\rangle = \int \mathrm{d}\sigma \exp\{(\mathrm{i}/\hbar)\,\sigma(q'+q'')/2\}\,\alpha(\sigma, q'-q''), \tag{2.61}$$

where α is defined by eq. (2.32). This result follows from eq. (2.33) by taking the matrix element of both sides. A similar result follows for $\langle q''|\hat{B}|q'\rangle$ except that α is replaced by β, the Fourier transform of $B(q, p)$:

$$\hat{B}(\hat{q}, \hat{p}) = \int \mathrm{d}\sigma \int \mathrm{d}\tau \exp\{(\mathrm{i}/\hbar)\,(\sigma\hat{q} + \tau\hat{p})\}\,\beta(\sigma, \tau). \tag{2.62}$$

We can now calculate $F(q, p)$. We have from eq. (2.12) that

$$\begin{aligned} F(q,p) &= \int \mathrm{d}z\, \mathrm{e}^{(\mathrm{i}/\hbar)pz} \left\langle q - \frac{z}{2}\middle| \hat{A}\hat{B} \middle| q + \frac{z}{2}\right\rangle \\ &= \int \mathrm{d}z \int \mathrm{d}q'\, \mathrm{e}^{(\mathrm{i}/\hbar)pz} \left\langle q - \frac{z}{2}\middle| \hat{A} \middle| q'\right\rangle \left\langle q'\middle| \hat{B} \middle| q + \frac{z}{2}\right\rangle \\ &= \int \mathrm{d}z \int \mathrm{d}q' \int \mathrm{d}\sigma \int \mathrm{d}\sigma'\, \mathrm{e}^{(\mathrm{i}/\hbar)\,\sigma(q'+q-z/2)/2}\, \mathrm{e}^{(\mathrm{i}/\hbar)\,\sigma'(q'+q+z/2)/2} \\ &\quad \times \alpha\left(\sigma, q'-q+\frac{z}{2}\right) \beta\left(\sigma', q-q'+\frac{z}{2}\right) \mathrm{e}^{(\mathrm{i}/\hbar)pz}. \end{aligned} \tag{2.63}$$

We now define two new variables of integration $\tau = q' - q + (z/2)$ and $\tau' = q - q' + (z/2)$ so that

$$F(q,p) = \int \mathrm{d}\tau \int \mathrm{d}\tau' \int \mathrm{d}\sigma \int \mathrm{d}\sigma'\, \mathrm{e}^{(\mathrm{i}/\hbar)\,(\sigma q + \tau p)}\, \alpha(\sigma, \tau)\, \mathrm{e}^{(\mathrm{i}/\hbar)\,(\sigma'\tau - \sigma\tau')/2}\, \mathrm{e}^{(\mathrm{i}/\hbar)\,(\sigma' q + \tau' p)}\, \beta(\sigma', \tau'). \tag{2.64}$$

It is possible to replace the exponential factor $\exp\{(\mathrm{i}/\hbar)\,(\sigma'\tau - \sigma\tau')/2\}$ by $\exp(\hbar\Lambda/2\mathrm{i})$ so that eq. (2.64) becomes

$$F(q,p) = A(q,p)\, \mathrm{e}^{\hbar\Lambda/2\mathrm{i}}\, B(q,p) \tag{2.65}$$

i.e. just the first expression appearing on the right-hand side of eq. (2.59). The second expression also follows readily from eq. (2.64).

We can also make use of eq. (2.64) to find an alternative expression for $F(q, p)$ involving the Bopp operators (Bopp [1961] and Kubo [1964])

$$Q = q - \frac{\hbar}{2\mathrm{i}}\frac{\partial}{\partial p}, \qquad P = p + \frac{\hbar}{2\mathrm{i}}\frac{\partial}{\partial q}. \tag{2.66}$$

We first note that

$$\exp\left\{\frac{\mathrm{i}}{\hbar}\left[\sigma\left(q - \frac{\hbar}{2\mathrm{i}}\frac{\partial}{\partial p}\right) + \tau\left(p + \frac{\hbar}{2\mathrm{i}}\frac{\partial}{\partial q}\right)\right]\right\} = \exp\left\{\frac{\mathrm{i}}{\hbar}(\sigma q + \tau p)\right\}\exp\left\{\tfrac{1}{2}\left(\tau\frac{\partial}{\partial q} - \sigma\frac{\partial}{\partial p}\right)\right\} \tag{2.67}$$

so that

$$\exp\left\{\frac{\mathrm{i}}{\hbar}\left[\sigma\left(q - \frac{\hbar}{2\mathrm{i}}\frac{\partial}{\partial p}\right) + \tau\left(p + \frac{\hbar}{2\mathrm{i}}\frac{\partial}{\partial q}\right)\right]\right\}\mathrm{e}^{(\mathrm{i}/\hbar)(\sigma' q + \tau' p)} = \mathrm{e}^{(\mathrm{i}/\hbar)(\sigma q + \tau p)}\,\mathrm{e}^{(\mathrm{i}/\hbar)(\sigma'\tau - \sigma\tau')/2}. \tag{2.68}$$

Using this result in eq. (2.64) we then have that

$$F(q, p) = \int \mathrm{d}\tau \int \mathrm{d}\tau' \int \mathrm{d}\sigma \int \mathrm{d}\sigma'\, \mathrm{e}^{(\mathrm{i}/\hbar)(\sigma Q + \tau P)}\,\alpha(\sigma, \tau)\,\mathrm{e}^{(\mathrm{i}/\hbar)(\sigma' q + \tau' p)}\,\beta(\sigma', \tau'). \tag{2.69}$$

From eq. (2.33) we see that the expression

$$\tilde{A}(Q, P) \equiv \int \mathrm{d}\tau \int \mathrm{d}\sigma\, \mathrm{e}^{(\mathrm{i}/\hbar)(\sigma Q + \tau P)}\,\alpha(\sigma, \tau) \tag{2.70}$$

is just the Weyl-ordered operator $\hat{A}(\hat{q}, \hat{p})$ with $\hat{q} \to Q$ and $\hat{p} \to P$. $\tilde{A}(Q, P)$ is also an operator but not on the Hilbert space on which $\hat{A}(\hat{q}, \hat{p})$ is an operator; it operates on functions in phase space. We can, therefore, express $F(q, p)$ as

$$F(q, p) = \tilde{A}(Q, P)\, B(q, p). \tag{2.71}$$

In a similar manner one can show that

$$F(q, p) = \tilde{B}(Q^*, P^*)\, A(q, p), \tag{2.72}$$

where

$$Q^* = q + \frac{\hbar}{2\mathrm{i}}\frac{\partial}{\partial p}, \qquad P^* = p - \frac{\hbar}{2\mathrm{i}}\frac{\partial}{\partial q}. \tag{2.73}$$

It is now possible to make use of the fact that the Wigner distribution is the function which is associated with $(1/2\pi\hbar)\hat{\rho}$. The equation of motion for $\hat{\rho}$ is just

$$\mathrm{i}\hbar\, \partial\hat{\rho}/\partial\tau = [\hat{H}, \hat{\rho}]. \tag{2.74}$$

This implies that we have for the Wigner function

$$\mathrm{i}\hbar\, \partial P_{\mathrm{w}}/\partial t = H(q,p)\, \mathrm{e}^{\hbar\Lambda/2\mathrm{i}}\, P_{\mathrm{w}}(q,p) - P_{\mathrm{w}}(q,p)\, \mathrm{e}^{\hbar\Lambda/2\mathrm{i}}\, H(q,p)$$

or

$$\hbar\, \partial P_{\mathrm{w}}/\partial t = -2\, H(q,p) \sin(\hbar\Lambda/2)\, P_{\mathrm{w}}(q,p)\,, \tag{2.75}$$

where $H(q,p)$ is the function corresponding to the Hamiltonian operator for the system, $\hat{H}$. Actually, this is an abbreviated form of eq. (2.56) as can be verified by expanding the sin into a power series. Note that if we take the $\hbar \to 0$ limit of this equation we obtain the classical Liouville equation

$$\partial P^{\mathrm{c}}_{\mathrm{w}}/\partial t + \{P^{\mathrm{c}}_{\mathrm{w}}, H\} = 0\,, \tag{2.76}$$

where $\{\,\}$ denote Poisson brackets and the superscript c on P_{w} indicates the classical limit. For an $H(q,p)$ which is at most quadratic in q and p, e.g. a free particle or an harmonic oscillator, eqs. (2.75) and (2.76) coincide. In these systems, then, the difference between a classical and a quantum ensemble is the restriction on the initial conditions in the case of latter (cf. eq. (2.19)).

We also want to quote two alternate forms of eq. (2.75). The first follows immediately from our discussion of the Bopp operators. We have, using eqs. (2.65), (2.71), (2.72) and (2.75), that

$$\mathrm{i}\hbar\, \partial P_{\mathrm{w}}/\partial t = [\tilde{H}(Q,P) - \tilde{H}(Q^*,P^*)]\, P_{\mathrm{w}}(q,p)\,, \tag{2.77}$$

a result first obtained by Bopp [1961]. Analogous to the definition of $A(\tilde{Q},P)$, given by eq. (2.70), $\tilde{H}(Q,P)$ is the Weyl-ordered operator with $\hat{q} \to Q$ and $\hat{p} \to P$, where Q and P are defined in eq. (2.66). These equations do not exhaust the possible formulations of the dynamics of the Wigner function. One can also make use of propagation kernels. This approach is discussed by Moyal [1949] and Mori, Oppenheim and Ross [1962].

We turn now to a consideration of a canonical ensemble. If $\beta = 1/kT$ where k is Boltzmann's constant and T is the temperature, then the density matrix of the canonical ensemble is

$$\hat{\rho} = \frac{1}{Z(\beta)}\, \mathrm{e}^{-\beta\hat{H}} \equiv \frac{1}{Z(\beta)}\, \hat{\Omega} \tag{2.78}$$

and $Z(\beta) = \mathrm{Tr}(\mathrm{e}^{-\beta\hat{H}})$. The unnormalized density matrix, $\hat{\Omega}$, then satisfies the equation

$$\partial\hat{\Omega}/\partial\beta = -\hat{H}\hat{\Omega} = -\hat{\Omega}\hat{H}\,, \tag{2.79}$$

subject to the initial condition $\hat{\Omega}(\beta = 0) = \hat{I}$ where $\hat{I}$ is the identity operator. Eq. (2.79) is referred to as the Bloch [1932] equation for the density matrix of a canonical ensemble. Using the product rule given by eq. (2.59) we have that

$$\partial\Omega(q,p)/\partial\beta = -H(q,p)\, \mathrm{e}^{\hbar\Lambda/2\mathrm{i}}\, \Omega(q,p) = -H(q,p)\, \mathrm{e}^{-\hbar\Lambda/2\mathrm{i}}\, \Omega(q,p)\,, \tag{2.80}$$

Λ being given by eq. (2.60) so that

$$\partial\Omega(q,p)/\partial\beta = -H(q,p)\cos(\hbar\Lambda/2)\,\Omega(q,p)\,. \tag{2.81}$$

This is the Wigner translation of the Bloch equation, which was entensively studied by many authors and was first derived in this form by Oppenheim and Ross [1957]. It is useful in the calculation of quantum mechanical corrections to classical statistical mechanics. The initial condition for this equation is just the Wigner function corresponding to $\hat{\Omega}(\beta=0)=\hat{I}$. Inserting I in eq. (2.12) we find that the initial condition is just $\Omega(q,p)|_{\beta=0}=1$.

It is also worth noting that $P_{\mathrm{w}}(q,p)$ does not satisfy the Wigner translation of the Bloch equation simply because of the fact that it must be multiplied by the β-dependent factor $(2\pi\hbar)\,Z(\beta)$ in order to obtain $\Omega(q,p)$.

Finally, we emphasize that all equations from eq. (2.59) onwards hold in the multi-dimensional case, where we simply interpret (q,p) to be $(q_1,\ldots q_n;p_1,\ldots p_n)$ and the simple products in the exponents as scalar products. The solution of eq. (2.81) in the multi-dimensional case, is to order $\hbar^2$ (Wigner [1932a]),

$$\Omega_{\mathrm{w}}(q,p)=\mathrm{e}^{-\beta H(q,p)}\left\{1+(2\pi\hbar)^2\left[\sum_k\left(-\frac{\beta^2}{8m_k}\frac{\partial^2 V}{\partial q_k^2}+\frac{\beta^3}{24m_k}\left(\frac{\partial V}{\partial q_k}\right)^2\right)+\sum_{k,l}\frac{\beta^3 p_k p_l}{24m_k m_l}\frac{\partial^2 V}{\partial q_k\partial q_l}\right]\right\}. \tag{2.82}$$

Actually, the Wigner translation of the Bloch equation, eq. (2.18) above, can be simplified further into a form, analogous to that of eq. (2.56), which is more convenient for applications. This is achieved by writing the cos term as the real part of the operator

$$\hat{0}\equiv\exp\left[\frac{\mathrm{i}\hbar}{2}\left(\frac{\overleftarrow{\partial}}{\partial p}\frac{\overrightarrow{\partial}}{\partial q}-\frac{\overleftarrow{\partial}}{\partial q}\frac{\overrightarrow{\partial}}{\partial p}\right)\right], \tag{2.83}$$

where we have used the explicit form for Λ given in eq. (2.60), again noting that the arrows indicate in which direction the derivatives act and that the gradient operators are $3N$-dimensional. Next we decompose $\hat{0}$ by means of the Baker–Hausdorff theorem (eq. (2.35a)), and using the fact that

$$\frac{\partial}{\partial p}\frac{\partial}{\partial q}H(q,p)=0 \tag{2.84}$$

it follows that we may write

$$\hat{0}=\exp\left[\frac{\mathrm{i}\hbar}{2}\frac{\overleftarrow{\partial}}{\partial p}\frac{\overrightarrow{\partial}}{\partial q}\right]\exp\left[-\frac{\mathrm{i}\hbar}{2}\frac{\overleftarrow{\partial}}{\partial q}\frac{\overrightarrow{\partial}}{\partial p}\right], \tag{2.85}$$

where we have neglected terms which do not contribute in the present context. Again because of eq. (2.84), and also using the fact that we are only interested in the real part, it follows that the only terms in $\hat{0}$ which contribute are

$$\exp\left[-\frac{\mathrm{i}\hbar}{2}\frac{\overleftarrow{\partial}}{\partial q}\frac{\overrightarrow{\partial}}{\partial p}\right]-\frac{\hbar^2}{8}\frac{\overleftarrow{\partial}}{\partial p_i}\frac{\overleftarrow{\partial}}{\partial p_j}\frac{\overrightarrow{\partial}}{\partial q_i}\frac{\overrightarrow{\partial}}{\partial q_j} \tag{2.86}$$

where $i,j=1,\ldots n$ (and as usual, it is understood that $(\partial/\partial q)(\partial/\partial p)$ stands for $(\partial/\partial q_i)(\partial/\partial p_i)$). From henceforth, we will assume that we are dealing with a system of $(n/3)$ identical particles of mass m.

Hence, since $H = (p^2/2m) + V$, it follows that

$$H \hat{0} \Omega = \left\{ \exp\left[-\frac{i\hbar}{2} \frac{\vec{\partial}}{\partial q} \frac{\vec{\partial}}{\partial p} \right] V - \frac{\hbar^2}{2m} \frac{\vec{\partial}^2}{\partial q^2} + \frac{p^2}{2m} \right\} \Omega , \tag{2.87}$$

where it is to be understood that the $(\vec{\partial}/\partial q)$ term in the exponential operates only on V and not on Ω (whereas the $\vec{\partial}^2/\partial q^2$ term operates on Ω). Also, the $\vec{\partial}/\partial p$ term has no effect on V and thus operates only on Ω. Since all arrows now operate to the right, they will be omitted from henceforth so that we finally obtain

$$\frac{\partial \Omega(q,p)}{\partial \beta} = -\left\{ \frac{p^2}{2m} + \cos\left(\frac{\hbar}{2} \frac{\partial}{\partial q} \frac{\partial}{\partial p} \right) V - \frac{\hbar^2}{8m} \frac{\partial^2}{\partial q^2} \right\} \Omega \tag{2.88a}$$

$$= \left\{ -H + 2\sin^2\left(\frac{\hbar}{4} \frac{\partial}{\partial q} \frac{\partial}{\partial p} \right) V + \frac{\hbar^2}{8m} \frac{\partial^2}{\partial q^2} \right\} \Omega , \tag{2.88b}$$

where the $\partial/\partial q$ term in the cos and sin terms is to be understood as operating only on V. Such a form was given for the first time by Alastuey and Jancovici [1980] and, in fact, their result also takes account of the presence of a magnetic field. We recall that $(\partial/\partial p)(\partial/\partial q)$ is considered as the multi-dimensional scalar product of $\partial/\partial p$ and $\partial/\partial q$, or, in other words it is equal to $(\partial/\partial p_i)(\partial/\partial q_i)$ where i goes from 1 to n and n denotes the number of dimensions. Hence, the explicit form of eq. (2.88a) is

$$\frac{\partial \Omega(q,p)}{\partial \beta} = -\left\{ \frac{p_i p_i}{2m} - \frac{\hbar^2}{8m} \frac{\partial^2}{\partial q_i \partial q_i} + \sum \frac{(i\hbar/2)^{\lambda_1+\lambda_2+\cdots+\lambda_n}}{\lambda_1!\lambda_2!\cdots\lambda_n!} \frac{\partial^{\lambda_1+\cdots+\lambda_n} V}{\partial q_1^{\lambda_1}\cdots\partial q_n^{\lambda_n}} \frac{\partial^{\lambda_1+\cdots+\lambda_n}}{\partial p_1^{\lambda_1}\cdots p_n^{\lambda_n}} \right\} \Omega \tag{2.89}$$

where the last summation is to be extended over all positive integer values, as well as zero values, of $\lambda_1, \lambda_2, \ldots \lambda_n$, for which the sum $\lambda_1 + \lambda_2 + \cdots + \lambda_n$ is even. This form for the Wigner translation of the Bloch equation is the most convenient from the point of view of applications.

One of the earliest applications of these results was to the quantum corrections of the classical equations of state and to similar corrections to chemical reaction rates (Wigner [1932b, 1938]) and they have been extensively used in statistical mechanics (Oppenheim and Ross [1957]; Mori, Oppenheim and Ross [1962]; Nienhuis [1970], for example). However, we will defer a detailed discussion of applications to Part II of our review, to be published at a later date.

2.4. An example

We would now like to use some of the formalism which we have developed to actually calculate some distribution functions. The system which we will consider is the harmonic oscillator and we will consider both pure and mixed states. We will find the Wigner functions corresponding to the eigenstates of the harmonic oscillator and also the function corresponding to a canonical ensemble of harmonic oscillators at temperature T.

The eigenstates of the harmonic oscillator are (Landau and Lifshitz [1965])

$$U_n(q) = \left(\frac{\alpha^2}{4}\right)^{1/4} \left(\frac{1}{2^n n!}\right)^{1/2} e^{-\alpha^2 q^2/2} H_n(\alpha q) , \tag{2.90}$$

where H_n is the nth Hermite polynomial and $\alpha = (m\omega/\hbar)^{1/2}$. Substituting this expression into the definition of the distribution function, eq. (2.2a), we find that

$$U_n^*(q+y)\,U_n(q-y) = \left(\frac{\alpha^2}{\pi}\right)^{1/2} \frac{1}{2^n n!} \exp\{-a^2[(q+y)^2+(q-y)^2]/2\}\, H_n(\alpha(q+y)) \cdot H_n(\alpha(q-y)) \tag{2.91}$$

so that

$$P_w(q,p) = \frac{1}{\pi\hbar}\frac{\alpha}{\sqrt{\pi}}\frac{1}{2^n n!}\,\mathrm{e}^{-\alpha^2 q^2} \int \mathrm{d}y\, \mathrm{e}^{2\mathrm{i}py/\hbar}\, \mathrm{e}^{-\alpha^2 y^2}\, H_n(\alpha(q+y))\, H_n(\alpha(q-y))\,. \tag{2.92}$$

We now note that

$$\alpha^2 y^2 - 2\mathrm{i}py/\hbar = \alpha^2(y - \mathrm{i}p/\alpha^2\hbar)^2 + p^2/\alpha^2\hbar^2 \tag{2.93}$$

and define a new variable

$$z = \alpha(y - \mathrm{i}p/\alpha^2\hbar)\,. \tag{2.94}$$

We then have that

$$P_w(q,p) = \frac{1}{\sqrt{\pi}}\frac{1}{\pi\hbar}\frac{1}{2^n n!}\,\mathrm{e}^{-\alpha q^2}\,\mathrm{e}^{\beta^2} \int \mathrm{d}z\, \mathrm{e}^{-z^2}\, H_n(\alpha q + z + \beta)\, H_n(\alpha q - z - \beta)\,, \tag{2.95}$$

where $\beta = \mathrm{i}p/\alpha\hbar$. Noting the $H_n(-x) = (-1)^n H_n(x)$ we find

$$P_w(q,p) = \frac{1}{\sqrt{\pi}}\frac{1}{\pi\hbar}\frac{(-1)^n}{2^n n!}\,\mathrm{e}^{-\alpha q^2}\,\mathrm{e}^{\beta^2} \int \mathrm{d}z\, \mathrm{e}^{-z^2}\, H_n(\alpha q + z + \beta)\, H_n(z + \beta - \alpha q)\,. \tag{2.96}$$

The above integral can be done (Gradshteyn and Ryzhik [1980]) and is

$$\int \mathrm{d}z\, \mathrm{e}^{-z^2}\, H_n(z+\beta+\alpha q)\, H_n(z+\beta-\alpha q) = 2^n \sqrt{\pi}\, n!\, L_n(2(\alpha^2 q^2 - \beta^2))\,, \tag{2.97}$$

where L_n is the nth Laguerre polynomial. Re-expressing α and β in terms of q and p we have

$$\alpha^2 q^2 - \beta^2 = \frac{2}{\hbar\omega}\left(\frac{p^2}{2m} + \frac{1}{2}m\omega^2 q^2\right) = \frac{2}{\hbar\omega} H(q,p) \tag{2.98}$$

so that (Groenewold [1946]; Takabayaski [1954]; Dahl [1982])

$$P_w(q,p) = (1/\pi\hbar)\,(-1)^n\, \mathrm{e}^{-2H/\hbar\omega}\, L_n(4H/\hbar\omega)\,. \tag{2.99}$$

Before discussing this result we will first calculate the distribution for an ensemble of oscillators at temperature T (Imre, Ozizmir, Rosenbaum and Zweifel [1967]). Here we proceed by way of the Wigner

translation of the Bloch equation (eq. (2.88b)) which for this system results in

$$\frac{\partial \Omega(q,p)}{\partial \beta} = \left\{ -\left(\frac{p^2}{2m} + \frac{1}{2} m\omega^2 q^2\right) + 2\sin^2\left(\frac{\hbar}{4}\frac{\partial}{\partial q}\frac{\partial}{\partial p}\right) V + \frac{\hbar^2}{8m}\frac{\partial^2}{\partial q^2}\right\} \Omega . \tag{2.100}$$

Because V is quadratic in q^2 it is clear that only the leading order term in the $\sin^2$ expansion will contribute, and since $\partial^2 V/\partial q^2 = m\omega^2$, it follows that the Wigner translation of the Bloch equation for the oscillator reduces to

$$\frac{\partial \Omega}{\partial \beta} = -\left(\frac{p^2}{2m} + \frac{1}{2} m\omega^2 q^2\right)\Omega + \frac{\hbar^2}{8}\left(\frac{1}{m}\frac{\partial^2 \Omega}{\partial q^2} + m\omega^2 \frac{\partial^2 \Omega}{\partial p^2}\right) . \tag{2.101}$$

To solve this equation we make the Ansatz

$$\Omega(q,p) = \exp\{-A(\beta)\, H + B(\beta)\} \tag{2.102}$$

where $A(0) = B(0) = 0$, and $H = (p^2/2m) + \frac{1}{2}m\omega^2 q^2$. Substituting this into eq. (2.101) gives us

$$\begin{aligned}\left(-\frac{\mathrm{d}A}{\mathrm{d}\beta} H + \frac{\mathrm{d}B}{\mathrm{d}\beta}\right)\Omega &= -H\Omega + \frac{\hbar^2}{8}\left[\frac{1}{m}\omega^2(-mA + m\omega^2 q^2 A^2) + m\omega^2\left(-\frac{A}{m} + \frac{p^2}{m}\right)A^2\right]\Omega \\ &= -H\Omega + \frac{(\hbar\omega)^2}{4}(-A + HA^2)\,\Omega . \end{aligned} \tag{2.103}$$

This equation can be re-expressed in the form

$$H(q,p)\left[-\frac{\mathrm{d}A}{\mathrm{d}\beta} + 1 - \frac{(\hbar\omega)^2}{4}A^2\right] + \left[\frac{\mathrm{d}B}{\mathrm{d}\beta} + \frac{(\hbar\omega)^2}{4}A\right] = 0 . \tag{2.104}$$

Because this equation must hold for all q and p, and the terms in the brackets are independent of q and p, they must vanish independently, i.e.

$$\frac{\mathrm{d}A}{\mathrm{d}\beta} + \frac{(\hbar\omega)^2}{4}A^2 - 1 = 0 \tag{2.105}$$

$$\frac{\mathrm{d}B}{\mathrm{d}\beta} + \frac{(\hbar\omega)^2}{4}A = 0 . \tag{2.106}$$

Eq. (2.105) can be integrated directly. One has that

$$\int \frac{\mathrm{d}A}{1 - (\hbar\omega/2)^2 A^2} = \int \mathrm{d}\beta \tag{2.107}$$

or

$$\beta = \frac{1}{\hbar\omega}\ln\left[\left(1 + \frac{\hbar\omega}{2}A\right)\Big/\left(1 - \frac{\hbar\omega}{2}A\right)\right] . \tag{2.108}$$

Inverting this equation gives us that

$$A(\beta) = (2/\hbar\omega)\tanh(\hbar\omega\beta/2)\,. \tag{2.109}$$

This can now be substituted into eq. (2.106) to give

$$B(\beta) = -\frac{\hbar\omega}{2}\int_0^\beta \mathrm{d}\beta'\tanh\left(\frac{\hbar\omega\beta'}{2}\right) = -\ln\cosh\left(\frac{\hbar\omega\beta}{2}\right). \tag{2.110}$$

Therefore, we have

$$\Omega(q,p) = \operatorname{sech}(\hbar\omega\beta/2)\exp[-(2/\hbar\omega)\tanh(\hbar\omega\beta/2)\,H(q,p)]\,. \tag{2.111}$$

To complete our derivation we need to normalize the above expression. As was noted before the Wigner function is the function which corresponds to the operator $(\hat{\rho}/2\pi\hbar)$. From eq. (2.78) we then have

$$P_{\mathrm{w}}(q,p) = \frac{1}{2\pi\hbar}\frac{1}{Z(\beta)}\Omega(q,p) \tag{2.112}$$

as $\Omega(q,p)$ is just the function corresponding to $\mathrm{e}^{-\beta\hat{H}}$. We also have from eq. (2.11) (setting $\hat{A} = \mathrm{e}^{-\beta\hat{H}}$ and $\hat{B} = \hat{I}$)

$$Z(\beta) = \mathrm{Tr}(\mathrm{e}^{-\beta\hat{H}}) = \frac{1}{2\pi\hbar}\int \mathrm{d}q\int \mathrm{d}p\,\Omega(q,p)\,. \tag{2.113}$$

Substituting eq. (2.111) into eq. (2.113) we find

$$Z(\beta) = \tfrac{1}{2}[\sinh(\hbar\omega\beta/2)]^{-1}\,. \tag{2.114}$$

Finally we obtain for $P_{\mathrm{w}}(q,p)$, from eqs. (2.111), (2.112) and (2.114),

$$P_{\mathrm{w}}(q,p) = (1/\pi\hbar)\tanh(\hbar\omega\beta/2)\exp[-(2/\hbar\omega)\tanh(\hbar\omega\beta/2)\,H(q,p)]\,. \tag{2.115}$$

We now want to compare the two expressions (eq. (2.99) and eq. (2.115)) for P_{w} for the pure and mixed states, respectively. Examining the first few Laguerre polynomials

$$\begin{aligned} L_0(x) &= 1 \\ L_1(x) &= 1 - x \\ L_2(x) &= 1 - 2x + x^2 \end{aligned} \tag{2.116}$$

we see that for the ground state of the oscillator $P_{\mathrm{w}}(q,p) > 0$ while for excited states $P_{\mathrm{w}}(q,p)$ can assume negative values. The result for the canonical ensemble, however, is always positive. It does not have the oscillatory structure which is present in the expressions given by eq. (2.99). The incoherence induced by a finite temperature leads to a much smoother distribution function.

2.5. *Statistics and second-quantized notation* (Klimintovich [1958]; Brittin and Chappell [1962]; Imre, Ozizmir, Rosenbaum and Zweifel [1967])

When one is dealing with more than one particle one has to include the effects of quantum statistics. To illustrate how these effects come in to the Wigner function we will first consider an example. We will then show how the Wigner function can be expressed in second-quantized notation. In this form it is easier to take the effects of statistics into account, but two of us have an article in preparation (O'Connell and Wigner [1983]) which not only will take the effect of statistics into account, but will also include spin effects.

Let us consider two identical particles in one dimension in a harmonic potential well. We will further assume that the particles are bosons. The Hamiltonian for the system is

$$\hat{H} = \frac{1}{2m}(\hat{p}_1^2 + \hat{p}_2^2) + \tfrac{1}{2}m\omega^2(\hat{q}_1^2 + \hat{q}_2^2)\,. \tag{2.117}$$

Suppose that we want to find the Wigner distribution for a canonical ensemble of these systems at a temperature T. We would again like to use the Wigner translation of the Bloch equation but now we must be more careful; the initial condition is no longer so simple.

To see this we first find the density matrix for the system. The eigenstates of the Hamiltonian given by eq. (2.117) are

$$\phi_{n_1n_2}(q_1, q_2) = \begin{cases} \dfrac{1}{\sqrt{2}}(U_{n_1}(q_1)\,U_{n_2}(q_2) + U_{n_2}(q_1)\,U_{n_1}(q_2)) & \text{if } n_1 > n_2 \\[2ex] U_{n_1}(q_1)\,U_{n_1}(q_2) & \text{if } n_1 = n_2\,, \end{cases} \tag{2.118}$$

where $U_n(q)$ is given by eq. (2.90). This state has an energy $E_{n_1n_2}$ given by

$$E_{n_1n_2} = \hbar\omega\,(n_1 + n_2 + 1)\,. \tag{2.119}$$

The unnormalized density matrix for this system is just

$$\hat{\Omega} = \sum_{n_1 \geq n_2} \exp(-\beta E_{n_1n_2})\,|\phi_{n_1n_2}\rangle\,\langle\phi_{n_1n_2}|\,. \tag{2.120}$$

In the $\beta \to 0$ limit this becomes

$$\hat{\Omega}(\beta = 0) = \sum_{n_1 \geq n_2} |\phi_{n_1n_2}\rangle\,\langle\phi_{n_1n_2}|\,. \tag{2.121}$$

Taking matrix elements we find

$$\begin{aligned} \langle q_1', q_2'|\hat{\Omega}(\beta = 0)|q_1, q_2\rangle &= \sum_{n_1 > n_2} \tfrac{1}{2}(U_{n_1}(q_1')\,U_{n_2}(q_2') + U_{n_2}(q_1')\,U_{n_1}(q_2')) \\ &\quad \times (U_{n_1}^*(q_1)\,U_{n_2}^*(q_2) + U_{n_2}^*(q_1)\,U_{n_1}^*(q_2)) + \sum_n U_n(q_1')\,U_n(q_2')\,U_n^*(q_1)\,U_n^*(q_2) \\ &= \tfrac{1}{2}\sum_{n_1,n_2} (U_{n_1}(q_1')\,U_{n_2}(q_2')\,U_{n_1}^*(q_1)\,U_{n_2}^*(q_2) + U_{n_1}(q_1')\,U_{n_2}(q_2')\,U_{n_1}^*(q_2)\,U_{n_2}^*(q_1))\,. \end{aligned} \tag{2.122}$$

We can now make use of the identity

$$\sum_n U_n(q_1')\, U_n^*(q_1) = \delta(q_1 - q_1') \tag{2.123}$$

to give

$$\langle q_1', q_2'|\hat{\Omega}(\beta = 0)|q_1, q_2\rangle = \tfrac{1}{2}[\delta(q_1' - q_1)\,\delta(q_2' - q_2) + \delta(q_1' - q_2)\,\delta(q_2' - q_1)]\,, \tag{2.124}$$

as was to be expected. If we operate on an arbitrary two particle state, $|\psi\rangle$, with $\hat{\Omega}(\beta = 0)$ we have that

$$\begin{aligned}\langle q_1', q_2'|\hat{\Omega}(\beta = 0)|\psi\rangle &= \int \mathrm{d}q_1 \int \mathrm{d}q_2\, \langle q_1', q_2'|\hat{\Omega}(\beta = 0)|q_1, q_2\rangle\, \langle q_1, q_2|\psi\rangle \\ &= \tfrac{1}{2}[\psi(q_1', q_2') + \psi(q_2', q_1')]\,. \end{aligned} \tag{2.125}$$

If ψ is symmetric the result on the right-hand side of eq. (2.125) is ψ, if ψ is anti-symmetric the result is 0.

Therefore, $\hat{\Omega}(\beta = 0)$ is just the projection operator, $\hat{P}_S$ say, onto the state of symmetric two-particle wave functions. This result is also true for an arbitrary number of particles, N. Our result that $\hat{\Omega}(\beta = 0)$ is $\hat{P}_S$ was derived for bosons. Similarly, if the particles are fermions $\hat{\Omega}(\beta = 0)$ is $\hat{P}_A$, the projection onto the space of anti-symmetric N-particle wave functions, but in this case, the spin variable should also be included.

Returning now to our example we want to find the initial condition for the Wigner translation of Bloch equation, i.e. we must find the function corresponding to $\hat{P}_S$. Making use of the two-particle extension of eq. (2.12) we find

$$\begin{aligned}\Omega(q_1, q_2, p_1, p_2) &= \int \mathrm{d}y_1 \int \mathrm{d}y_2 \exp\{(\mathrm{i}/\hbar)\,(p_1 y_1 + p_2 y_2)\}\, \langle q_1 - \tfrac{1}{2}y_1, q_2 - \tfrac{1}{2}y_2|\hat{P}_S|q_1 + \tfrac{1}{2}y_1, q_2 + \tfrac{1}{2}y_2\rangle \\ &= \int \mathrm{d}y_1 \int \mathrm{d}y_2 \exp\{(\mathrm{i}/\hbar)\,(p_1 y_1 + p_2 y_2)\}\, \tfrac{1}{2}[\delta(y_1)\,\delta(y_2) \\ &\quad + \delta(q_2 - q_1 + \tfrac{1}{2}(y_2 + y_1))\,\delta(q_1 - q_2 + \tfrac{1}{2}(y_1 + y_2))] \\ &= \tfrac{1}{2} + \pi\hbar\,\delta(q_1 - q_2)\,\delta(p_1 - p_2)\,. \end{aligned} \tag{2.126}$$

The corresponding result for fermions has a minus sign in front of the second term. This initial condition is considerably more complicated than the initial condition, $\Omega(q, p) = 1$, which was obtained in the one-dimensional case. The situation rapidly becomes worse with larger numbers of particles.

Second-quantized notation provides, in principle, a convenient way to deal with the problems imposed by quantum statistics. We will consider a Fock space and designate the vacuum state of this space by $|0\rangle$, and the quantized field operators at the point $\boldsymbol{r}$ by $\hat{\psi}^+(\boldsymbol{r})$ and $\hat{\psi}(\boldsymbol{r})$. The interpretation of the field operators is that $\hat{\psi}^+(\boldsymbol{r})$ adds a particle at point $\boldsymbol{r}$ to the system whereas $\hat{\psi}(\boldsymbol{r})$ removes a particle at point $\boldsymbol{r}$. They are defined as

$$\hat{\psi}(\boldsymbol{r}) = \sum_{\boldsymbol{p}} \frac{1}{\sqrt{V}} \mathrm{e}^{\mathrm{i}\boldsymbol{p}\cdot\boldsymbol{r}}\, \hat{a}_{\boldsymbol{p}} \tag{2.127a}$$

$$\hat{\psi}^+(\boldsymbol{r}) = \sum_{\boldsymbol{p}} \frac{1}{\sqrt{V}} \mathrm{e}^{-\mathrm{i}\boldsymbol{p}\cdot\boldsymbol{r}}\, \hat{a}_{\boldsymbol{p}}^+ \tag{2.127b}$$

where the so-called annihilation and creation operators, $\hat{a}_p$ and $\hat{a}_p^+$, respectively (discussed in detail in section 4), act to remove or create a particle of momentum p in a box of volume V. For bosons these operators obey the commutation relation

$$[\hat{\psi}(\boldsymbol{r}), \hat{\psi}^\dagger(\boldsymbol{r}')] = \delta^{(3)}(\boldsymbol{r} - \boldsymbol{r}') \tag{2.128a}$$

$$[\hat{\psi}(\boldsymbol{r}), \hat{\psi}(\boldsymbol{r}')] = 0 \tag{2.128b}$$

and for fermions the anti-commutation relation

$$\{\hat{\psi}(\boldsymbol{r}), \hat{\psi}^\dagger(\boldsymbol{r}')\} = \delta^{(3)}(\boldsymbol{r} - \boldsymbol{r}') \tag{2.129a}$$

$$\{\hat{\psi}(\boldsymbol{r}), \hat{\psi}(\boldsymbol{r}')\} = 0\,. \tag{2.129b}$$

To every N-particle state $|\Psi_N\rangle$ in the Fock space corresponds an N-particle wave function given by (Schweber [1961])

$$\Psi_N(\boldsymbol{r}_1, \ldots \boldsymbol{r}_N) = \frac{1}{\sqrt{N!}} \langle 0|\hat{\psi}(\boldsymbol{r}_N) \cdots \hat{\psi}(\boldsymbol{r}_1)|\Psi_N\rangle\,. \tag{2.130}$$

The distribution function for the state $|\Psi_N\rangle$ then, is given by

$$\begin{aligned} P(\boldsymbol{r}_1, \ldots \boldsymbol{r}_N; \boldsymbol{p}_1, \ldots \boldsymbol{p}_N) &= \left(\frac{1}{2\pi\hbar}\right)^{3N} \int \mathrm{d}^3\boldsymbol{y}_1 \cdots \int \mathrm{d}^3\boldsymbol{y}_N \exp\{(\mathrm{i}/\hbar)(\boldsymbol{p}_1 \cdot \boldsymbol{y}_1 + \cdots + \boldsymbol{p}_N \cdot \boldsymbol{y}_N)\} \\ &\quad \times \Psi_N^*(\boldsymbol{r}_1 + \tfrac{1}{2}\boldsymbol{y}_1, \ldots \boldsymbol{r}_N + \tfrac{1}{2}\boldsymbol{y}_N)\, \Psi_N(\boldsymbol{r}_1 - \tfrac{1}{2}\boldsymbol{y}_1, \ldots \boldsymbol{r}_N - \tfrac{1}{2}\boldsymbol{y}_N) \\ &= = \left(\frac{1}{2\pi\hbar}\right)^{3N} \frac{1}{N!} \int \mathrm{d}^3\boldsymbol{y}_1 \cdots \int \mathrm{d}^3\boldsymbol{y}_N \exp\{(\mathrm{i}/\hbar)(\boldsymbol{p}_1 \cdot \boldsymbol{y}_1 + \cdots + \boldsymbol{p}_N \cdot \boldsymbol{y}_N)\} \\ &\quad \times \langle 0|\hat{\psi}(\boldsymbol{r}_N - \tfrac{1}{2}\boldsymbol{y}_N) \cdots \hat{\psi}(\boldsymbol{r}_1 - \tfrac{1}{2}\boldsymbol{y}_1)|\Psi_N\rangle \langle \Psi_N|\hat{\psi}^\dagger(\boldsymbol{r}_1 + \tfrac{1}{2}\boldsymbol{y}_1) \cdots \hat{\psi}^\dagger(\boldsymbol{r}_N + \tfrac{1}{2}\boldsymbol{y}_N)|0\rangle\,. \end{aligned} \tag{2.131}$$

This expression readily extends to N-particle density matrixes, $\hat{\rho}_N$, so that

$$\begin{aligned} P(\boldsymbol{r}_1, \ldots \boldsymbol{r}_N; \boldsymbol{p}_1, \ldots \boldsymbol{p}_N) &= \left(\frac{1}{2\pi\hbar}\right)^{3N} \frac{1}{N!} \int \mathrm{d}^3\boldsymbol{y}_1 \cdots \int \mathrm{d}^3\boldsymbol{y}_N \exp\{(\mathrm{i}/\hbar)(\boldsymbol{p}_1 \cdot \boldsymbol{y}_1 + \cdots + \boldsymbol{p}_N \cdot \boldsymbol{y}_N)\} \\ &\quad \times \langle 0|\hat{\psi}(\boldsymbol{r}_N - \tfrac{1}{2}\boldsymbol{y}_N) \cdots \hat{\psi}(\boldsymbol{r}_1 - \tfrac{1}{2}\boldsymbol{y}_1)\, \hat{\rho}_N\, \hat{\psi}^\dagger(\boldsymbol{r}_1 + \tfrac{1}{2}\boldsymbol{y}_1) \cdots \hat{\psi}^\dagger(\boldsymbol{r}_N + \tfrac{1}{2}\boldsymbol{y}_N)|0\rangle\,, \end{aligned} \tag{2.132}$$

where, in the case of a pure state,

$$\hat{\rho}_N = |\Phi_N\rangle \langle \Phi_N| \tag{2.133}$$

with $|\Phi_N\rangle$ denoting the N-particle ket basis vector. An N-particle density matrix has the property that if $\Phi_{N'}$ and $\Phi_{N''}$ are N'-particle and N''-particle states respectively, then $\langle \Phi_{N''}|\hat{\rho}_N|\Phi_{N'}\rangle = 0$ unless $N' = N'' = N$. Therefore, eq. (2.132) can be expressed as

$$P(\boldsymbol{r}_1,\ldots\boldsymbol{r}_N;\boldsymbol{p}_1,\ldots\boldsymbol{p}_N)=\left(\frac{1}{2\pi\hbar}\right)^{3N}\frac{1}{N!}\int \mathrm{d}^3\boldsymbol{y}_1\cdots\int \mathrm{d}^3\boldsymbol{y}_N\,\exp\{(\mathrm{i}/\hbar)(\boldsymbol{p}_1\cdot\boldsymbol{y}_1+\cdots+\boldsymbol{p}_N\cdot\boldsymbol{y}_N)\}$$
$$\times\,\mathrm{Tr}(\hat{\psi}(\boldsymbol{r}_N-\tfrac{1}{2}\boldsymbol{y}_N)\cdots\hat{\psi}(\boldsymbol{r}_1-\tfrac{1}{2}\boldsymbol{y}_1)\,\hat{\rho}_N\,\hat{\psi}^\dagger(\boldsymbol{r}_1+\tfrac{1}{2}\boldsymbol{y}_1)\cdots\hat{\psi}^\dagger(\boldsymbol{r}_N+\tfrac{1}{2}\boldsymbol{y}_N))$$
$$=\left(\frac{1}{2\pi\hbar}\right)^{3N}\frac{1}{N!}\int \mathrm{d}^3\boldsymbol{y}_1\cdots\int \mathrm{d}^3\boldsymbol{y}_N\,\exp\{(\mathrm{i}/\hbar)(\boldsymbol{p}_1\cdot\boldsymbol{y}_1+\cdots+\boldsymbol{p}_N\cdot\boldsymbol{y}_N)\}$$
$$\times\,\mathrm{Tr}(\hat{\rho}_N\,\hat{\psi}^\dagger(\boldsymbol{r}_1+\tfrac{1}{2}\boldsymbol{y}_1)\cdots\hat{\psi}^\dagger(\boldsymbol{r}_N+\tfrac{1}{2}\boldsymbol{y}_N)\,\hat{\psi}(\boldsymbol{r}_N-\tfrac{1}{2}\boldsymbol{y}_N)\cdots\hat{\psi}(\boldsymbol{r}_1-\tfrac{1}{2}\boldsymbol{y}_1))\,. \quad (2.134)$$

This is the desired expression for the Wigner function in second-quantized form (Brittin and Chappell [1962]; Imre, Ozizmir, Rosenbaum and Zweifel [1967]).

It is also possible to derive expressions for the reduced distribution functions in terms of the quantized field operators (Brittin and Chappell [1962]; Imre, Ozizmir, Rosenbaum and Zweifel [1967]). The distribution function of order N, reduced to the jth order, is defined as

$$P_j(\boldsymbol{r}_1,\ldots\boldsymbol{r}_j;\boldsymbol{p}_1,\ldots\boldsymbol{p}_j)=\int \mathrm{d}^3\boldsymbol{r}_{j+1}\cdots\int \mathrm{d}^3\boldsymbol{r}_N\int \mathrm{d}^3\boldsymbol{p}_{j+1}\cdots\int \mathrm{d}^3\boldsymbol{p}_N\,P(\boldsymbol{r}_1,\ldots\boldsymbol{r}_N;\boldsymbol{p}_1,\ldots\boldsymbol{p}_N) \quad (2.135)$$

and this definition will be used for the rest of this section. This can also be expressed, by making use of eq. (2.134), as

$$P_j(\boldsymbol{r}_1,\ldots\boldsymbol{r}_j;\boldsymbol{p}_1,\ldots\boldsymbol{p}_j)=\left(\frac{1}{2\pi\hbar}\right)^{3N}\frac{1}{N!}\int \mathrm{d}^3\boldsymbol{r}_{j+1}\cdots\int \mathrm{d}^3\boldsymbol{r}_N\int \mathrm{d}^3\boldsymbol{p}_{j+1}\cdots\int \mathrm{d}^3\boldsymbol{p}_N\int \mathrm{d}^3\boldsymbol{y}_1\cdots\int \mathrm{d}^3\boldsymbol{y}_N$$
$$\times\,\exp\{\mathrm{i}(\boldsymbol{p}_1\cdot\boldsymbol{y}_1+\cdots+\boldsymbol{p}_N\cdot\boldsymbol{y}_N)/\hbar\}\,\mathrm{Tr}(\hat{\rho}_N\hat{\psi}^\dagger(\boldsymbol{r}_1+\tfrac{1}{2}\boldsymbol{y}_1)\cdots\hat{\psi}^\dagger(\boldsymbol{r}_N+\tfrac{1}{2}\boldsymbol{y}_N)\,\hat{\psi}(\boldsymbol{r}_N-\tfrac{1}{2}\boldsymbol{y}_N)\cdots\hat{\psi}(\boldsymbol{r}_1-\tfrac{1}{2}\boldsymbol{y}_1))$$
$$=\left(\frac{1}{2\pi\hbar}\right)^{3j}\frac{1}{N!}\int \mathrm{d}^3\boldsymbol{r}_{j+1}\cdots\int \mathrm{d}^3\boldsymbol{r}_N\int \mathrm{d}^3\boldsymbol{y}_1\cdots\int \mathrm{d}^3\boldsymbol{y}_j\,\exp\{\mathrm{i}(\boldsymbol{p}_1\cdot\boldsymbol{y}_1+\cdots+\boldsymbol{p}_j\cdot\boldsymbol{y}_j)/\hbar\}\,\mathrm{Tr}(\hat{\rho}_N\,\hat{\psi}^\dagger(\boldsymbol{r}_1+\tfrac{1}{2}\boldsymbol{y}_1)$$
$$\cdots\hat{\psi}^\dagger(\boldsymbol{r}_j+\tfrac{1}{2}\boldsymbol{y}_j)\,\hat{\psi}^\dagger(\boldsymbol{r}_{j+1})\cdots\hat{\psi}^\dagger(\boldsymbol{r}_N)\,\hat{\psi}(\boldsymbol{r}_N)\cdots\hat{\psi}(\boldsymbol{r}_{j+1})\,\hat{\psi}(\boldsymbol{r}_j-\tfrac{1}{2}\boldsymbol{y}_j)\cdots\hat{\psi}(\boldsymbol{r}_1-\tfrac{1}{2}\boldsymbol{y}_1))\,. \quad (2.136)$$

In order to analyze this expression further we first note that

$$\int \mathrm{d}^3\boldsymbol{r}\,\hat{\psi}^\dagger(\boldsymbol{r})\,\hat{\psi}(\boldsymbol{r})=\hat{N}\,, \quad (2.137)$$

where $\hat{N}$ is just the number operator. We then have that, for both bosons and fermions

$$[\hat{\psi}(\boldsymbol{r}),\hat{N}]=\hat{\psi}(\boldsymbol{r})\,. \quad (2.138)$$

Therefore,

$$\int \mathrm{d}^3\boldsymbol{r}_{N-1}\,\hat{\psi}^\dagger(\boldsymbol{r}_{N-1})\,\hat{N}\,\hat{\psi}(\boldsymbol{r}_{N-1})=\hat{N}\,(\hat{N}-1) \quad (2.139)$$

and

$$\int d^3r_{j+1}\cdots\int d^3r_{N-1}\,\hat{\psi}^\dagger(r_{j+1})\cdots\hat{\psi}^\dagger(r_{N-1})\,\hat{N}\,\hat{\psi}(r_{N-1})\cdots\hat{\psi}(r_{j+1})=\hat{N}\,(\hat{N}-1)\cdots(\hat{N}-N+j+1)\,. \tag{2.140}$$

Eq. (2.136) becomes

$$P_j(r_1,\ldots r_j;p_1,\ldots p_j)=\left(\frac{1}{2\pi\hbar}\right)^{3j}\frac{1}{N!}\int d^3y_1\cdots\int d^3y_j\,\exp\{i(p_1\cdot y_1+\cdots+p_j\cdot y_j)/\hbar\}$$
$$\times\,\mathrm{Tr}(\hat{\rho}_N\hat{\psi}^\dagger(r_1+\tfrac{1}{2}y_1)\cdots\hat{\psi}^\dagger(r_j+\tfrac{1}{2}y_j)\,\hat{N}\,(\hat{N}-1)\cdots(\hat{N}-N+j+1)\,\hat{\psi}(r_j-\tfrac{1}{2}y_j)\cdots\hat{\psi}(r_1-\tfrac{1}{2}y_1))\,. \tag{2.141}$$

Because $\hat{\rho}_N$ is an N-particle density matrix we have that

$$\hat{N}(\hat{N}-1)\cdots(\hat{N}-N+j+1)\,\hat{\psi}(r_j-\tfrac{1}{2}y_j)\cdots\hat{\psi}(r_1-\tfrac{1}{2}y_1)\,\hat{\rho}_N=(N-j)!\,\hat{\psi}(r_j-\tfrac{1}{2}y_j)\cdots\hat{\psi}(r_1-\tfrac{1}{2}y_1)\,\hat{\rho}_N\,, \tag{2.142}$$

so that our final expression for the reduced Wigner function is

$$P_j(r_1,\ldots r_j;p_1,\ldots p_j)=\left(\frac{1}{2\pi\hbar}\right)^{3j}\frac{(N-j)!}{N!}\int d^3y_1\cdots\int d^3y_j\,\exp\{i(p_1\cdot y_1+\cdots+p_j\cdot y_j)/\hbar\}$$
$$\times\,\mathrm{Tr}(\hat{\rho}_N\,\hat{\psi}^\dagger(r_1+\tfrac{1}{2}y_1)\cdots\hat{\psi}^\dagger(r_j+\tfrac{1}{2}y_j)\,\hat{\psi}(r_j-\tfrac{1}{2}y_j)\cdots\hat{\psi}(r_1-\tfrac{1}{2}y_1))\,. \tag{2.143}$$

It is now possible to formulate the dynamics of this theory in a way which is independent of the number of particles. We first go to the Heisenberg picture in which the field operators become time dependent. We then consider the operators

$$\hat{F}_j(r_1,\ldots r_j;p_1,\ldots p_j)=\left(\frac{1}{2\pi\hbar}\right)^{3j}\int d^3y_1\cdots\int d^3y_j\,\exp\{i(p_1\cdot y_1+\cdots+p_j\cdot y_j)/\hbar\}$$
$$\times\,\hat{\psi}^\dagger(r_1+\tfrac{1}{2}y_1;t)\cdots\hat{\psi}^\dagger(r_j+\tfrac{1}{2}y_j;t)\cdots\hat{\psi}(r_j-\tfrac{1}{2}y_j;t)\cdots\hat{\psi}(r_1-\tfrac{1}{2}y_1;t)\,. \tag{2.144}$$

The distribution functions for an N-particle theory are then just

$$\hat{P}_j(r_1,\ldots r_j;p_1,\ldots p_j)=\frac{(N-j)!}{N!}\,\mathrm{Tr}(\hat{\rho}_N\hat{F}_j(r_1,\ldots r_j;p_1,\ldots p_j)) \tag{2.145}$$

We see that in this formulation all of the dynamical information is contained in the operators $\hat{F}_j$ which contain no reference to a specific particle number and also contain the information about the statistics of the particles. Thus, in principle, the second-quantized formalism should be a useful starting-point for the incorporation of statistics into problems involving a system of identical particles. However, it must be admitted that – to our knowledge – no application has been made along these lines.

3. Other distribution functions

We now want to examine certain other distributions besides the one considered so far. These may arise out of a desire to make use of an operator ordering scheme other than that proposed by Weyl or a desire to have a distribution function with certain properties. For example, we may want to make use of

symmetric ordering

$$q^m p^n \to \tfrac{1}{2}(\hat{q}^m \hat{p}^n + \hat{p}^n \hat{q}^m)\,, \tag{3.1}$$

in which case we would use the distribution function (Margenau and Hill [1961]; Mehta [1964])

$$P_s(q,p) = \frac{1}{4\pi\hbar}\,\mathrm{Re}\left\{\psi(q)\int_{\infty}^{\infty} \mathrm{d}y\; \mathrm{e}^{-(\mathrm{i}/\hbar)py}\,\psi^*(q-y)\right\}. \tag{3.2}$$

On the other hand, we may want to consider a distribution which is always greater than or equal to zero. We will discuss a distribution which has this property shortly.

A scheme for generating distribution functions was proposed by Cohen [1966] and further examined by Summerfield and Zweifel [1969]. They give the rather general expression

$$P_g(q,p) = \left(\frac{1}{2\pi\hbar}\right)^2 \int \mathrm{d}\sigma \int \mathrm{d}\tau \int \mathrm{d}u\, \exp\{-(\mathrm{i}/\hbar)\,[\sigma(q-u)+\tau p]\}\, g(\sigma,\tau)\,\psi^*\!\left(u-\frac{\tau}{2}\right)\psi\!\left(u+\frac{\tau}{2}\right) \tag{3.3a}$$

$$= \int \mathrm{d}q' \int \mathrm{d}p'\, \tilde{g}(q-q', p-p')\, P_w(q',p') \tag{3.3b}$$

for the distribution function of the pure state $\psi(q)$, where

$$\tilde{g}(q,p) = \int \mathrm{d}\sigma \int \mathrm{d}\tau\, \exp\{-(\mathrm{i}/\hbar)(\sigma q + \tau p)\}\, g(\sigma,\tau)\,. \tag{3.4}$$

Thus the function P is simply the original function P_w smeared with another function g. The basic requirement which leads to eq. (3.3) is that P transform correctly with respect to space displacement, $\psi(q) \to \psi(q-a)$, and transition to a uniformly moving coordinate system, $\psi(q) \to \exp(-\mathrm{i}mvq)\,\psi(q)$. These requirements were formulated in giving the form eq. (3.3a) to P_g – and the satisfaction of the requirements can easily be verified; eq. (3.3b) then follows.

Cohen also pointed out that it is possible to obtain distributions whose dependence upon the wave function of the system is other than bilinear simply by choosing $g(\sigma,\tau)$ to depend upon $\psi(q)$. For example, one can choose

$$g(\sigma,\tau) = \int \mathrm{d}q\, \psi\!\left(q - q_0\frac{\sigma\tau}{\hbar}\right)\psi^*\!\left(q + q_0\frac{\sigma\tau}{\hbar}\right), \tag{3.5}$$

where q_0 is an arbitrary value of q. This choice for $g(\sigma,\tau)$ satisfies $g(0,\tau) = g(\sigma,0) = 1$ so that the correct marginal distributions are obtained. On the other hand, we now have the rather awkward situation that the function-operator correspondence depends upon the wave function. An even simpler choice is, of course

$$P_g(q,p) = (\pi\hbar)^{-1}\,|\psi(q)|^2\,|\phi(p)|^2\,, \tag{3.6}$$

where $\phi(p)$, the Fourier transform of $\psi(q)$ is defined by eq. (2.14). The conditions on $\tilde{g}(q,p)$ which must be satisfied so that the correct marginal distributions are obtained are

$$\int \mathrm{d}q\, \tilde{g}(q,p) = (2\pi\hbar)^2\, \delta(p) \tag{3.7a}$$

$$\int \mathrm{d}p\, \tilde{g}(q,p) = (2\pi\hbar)^2\, \delta(q)\,. \tag{3.7b}$$

One choice of $\tilde{g}(q,p)$ which does not satisfy eqs. (3.7) but which is interesting nonetheless is given by

$$\tilde{g}(q,p;\alpha) = \left(\frac{1}{\pi\hbar}\right) \mathrm{e}^{-q^2/\alpha}\, \mathrm{e}^{-\alpha p^2/\hbar^2}\,. \tag{3.8}$$

The use of this smearing function was first proposed by Husimi [1940] and has been investigated by a number of authors since (Bopp [1956]; Kano [1965]; McKenna and Frisch [1966]; Cartwright [1976]; Prugovecki [1978]; O'Connell and Wigner [1981b]). It leads to a distribution function, $P_{\mathrm{H}}(q,p)$, where the subscript H denotes Husimi, which is non-negative for all p and q. One can see this by noting that $\tilde{g}(q-q', p-p'; \alpha)$ is just the Wigner distribution function which one obtains from the displaced (in both position and momentum) harmonic oscillator ground state wave function

$$\psi_{q,p}(q';\alpha) = (\pi\alpha)^{-1/4}\, \mathrm{e}^{-(q'-q)^2/2\alpha}\, \mathrm{e}^{\mathrm{i}pq'/\hbar}\,, \tag{3.9}$$

which we will call $P_{q,p}$ (O'Connell and Wigner [1981b]). If the Wigner distribution in question, P_ϕ, corresponds to a wave function $\phi(q)$ we have

$$P_{\mathrm{H}}(q,p) = \int \mathrm{d}q' \int \mathrm{d}p'\, P_{q,p}(q',p')\, P_\phi(q',p') = \left(\frac{1}{2\pi\hbar}\right) \left| \int \mathrm{d}q'\, \psi^*_{q,p}(q')\, \phi(q') \right|^2 \geq 0\,, \tag{3.10}$$

where we have used eq. (2.8). Note that in order to get a positive distribution function we had to violate condition (ii) on our list of properties of the Wigner function. Property (vi) is also violated as was shown by Prugovecki [1978] and by O'Connell and Wigner [1981a].

We will encounter $P_{\mathrm{H}}(q,p)$ again in the next section in a somewhat different form. It is the "Q" or "anti-normally-ordered" distribution function of quantum optics. It is one of a number of distributions which are useful in the description of harmonic oscillators, and, hence, modes of the electromagnetic field. We now proceed to examine these distribution functions.

4. Distribution functions in terms of creation and annihilation operators

The harmonic oscillator is a system that is ubiquitous in physics, so that it is not surprising that quantum distribution functions have been developed which are tailored to its description. It is in the description of the modes of the electromagnetic field that these distribution functions have found their widest application.

It should be emphasized that many problems in quantum optics require a fully quantized treatment not only of the atoms but also of the field. For example, an analysis of experiments dealing with photon counting or a derivation of the fluctuations in intensity of a laser near threshold both require the quantum theory of radiation (Scully and Lamb [1967]; De Giorgio and Scully [1970]; Graham and Haken

[1970]). The latter is developed within the framework of annihilation and creation operators for bosons (see below) but it is then possible to go to a description in terms of c-numbers (while fully retaining the quantum aspects of the situation) by means of distribution functions. In most cases, this greatly facilitates the calculation while, at the same time, it contributes to a better understanding of the connection between the quantum and classical descriptions of the electromagnetic field.

A number of studies of these distribution functions have been done (Mehta and Sudarshan [1965]; Lax and Louisell [1967]; Lax [1968]; Cahill and Glauber [1969]; Agarwal and Wolf [1970]; Louisell [1973]). We will rely most heavily upon the papers by Cahill and Glauber [1969] in our treatment. Their discussion considers a continuum of possible operator ordering schemes, and hence distributions (an even larger class is considered in Agarwal and Wolf [1970]) but we will consider only three of these. A final section will discuss distributions defined on a 4-dimensional, rather than a 2-dimensional, phase space.

We will describe the system in terms of its annihilation and creation operators

$$\hat{a} = \left(\frac{1}{2\hbar}\right)^{1/2} \left(\lambda \hat{q} + \frac{\mathrm{i}}{\lambda} \hat{p}\right) \tag{4.1a}$$

$$a^{+} = \left(\frac{1}{2\hbar}\right)^{1/2} \left(\lambda \hat{q} - \frac{\mathrm{i}}{\lambda} \hat{p}\right), \tag{4.1b}$$

satisfying

$$[\hat{a}, \hat{a}^{+}] = 1 . \tag{4.2}$$

As mentioned before, it is assumed that the field operators we consider obey Bose statistics. Each pair of $\hat{a}$, $\hat{a}^{+}$ refers to a certain function of position. These functions form an orthonormal set which is countable if the basic domain is assumed to be finite, and continuous if infinite. We deal with a very large, but finite, system so that the system is only approximately relativistically invariant (exact invariance is achieved for an infinitely large system, but this would make the calculation in other ways difficult).

The various functions of $\hat{a}$ and $\hat{a}^{+}$ are investigated individually because the corresponding $\hat{a}$ and $\hat{a}^{+}$ do not interact with the $\hat{a}$ and $\hat{a}^{+}$ of another member of the set. They interact with the matter which is in the basic domain. Thus, for example, when we apply this formalism to the case of the electromagnetic field, we investigate each mode (corresponding to a definite momentum and definite direction of polarization) separately, and the operators associated with different modes commute (no interaction between modes). In addition, there will be a distribution function corresponding to each mode.

The $\hat{a}$ and $\hat{a}^{+}$ operators act on the basis vectors $|n\rangle$, the so-called "particle number states", and have the properties:

$$\hat{a}\,|n\rangle = \sqrt{n}\,|n-1\rangle \tag{4.2a}$$

$$\hat{a}^{+}\,|n\rangle = \sqrt{n+1}\,|n+1\rangle \tag{4.2b}$$

$$\hat{a}^{+} a\,|n\rangle = n\,|n\rangle \tag{4.2c}$$

$$\hat{a}\,|0\rangle = 0 . \tag{4.2d}$$

In addition, one can prove that

$$[\hat{a}, (\hat{a}^+)^n] = n(\hat{a}^+)^{n-1} . \tag{4.2e}$$

If we are considering an oscillator of mass m and angular frequency ω we take $\lambda = (m\omega)^{1/2}$ and if we are considering a mode of the electromagnetic field of angular frequency ω we set $\lambda = (\hbar^{1/2}\omega/c)$.

We also want to consider a special class of states known as coherent states (Schrödinger [1926]; Glauber [1963a]; Glauber [1963b]; Sudarshan [1963]; Glauber [1965]). To define these we first define for each complex number α the unitary displacement operator:

$$\hat{D}(\alpha) = \mathrm{e}^{(\alpha\hat{a}^+ - \alpha^*\hat{a})} = \mathrm{e}^{-|\alpha|^2/2}\, \mathrm{e}^{\alpha\hat{a}^+}\, \mathrm{e}^{-\alpha^*\hat{a}} , \tag{4.3}$$

where the last expression is obtained by use of the Baker–Hausdorff theorem (eq. (2.35a)) and the commutation relation given by eq. (4.2). The operator $\hat{D}(\alpha)$ has the property that

$$\hat{D}^{-1}(\alpha)\, \hat{a}\, \hat{D}(\alpha) = \hat{a} + \alpha \tag{4.4a}$$

$$\hat{D}^{-1}(\alpha)\, \hat{a}^+\, \hat{D}(\alpha) = \hat{a}^+ + \alpha^* . \tag{4.4b}$$

The proof of eq. (4.4) readily follows from eqs. (4.2e) and (4.3). We now define the coherent state (Glauber [1963a]; Glauber [1963b]; Sudarshan [1963]), which we denote by $|\alpha\rangle$, as

$$|\alpha\rangle \equiv \hat{D}(\alpha)\,|0\rangle = \mathrm{e}^{-|\alpha|^2/2} \sum_{n=0}^{\infty} \frac{\alpha^n}{n!} (\hat{a}^+)^n\, |0\rangle = \mathrm{e}^{-|\alpha|^2/2} \sum_{n=0}^{\infty} \frac{\alpha^n}{(n!)^{1/2}} |n\rangle , \tag{4.5}$$

where $|0\rangle$ is the ground state of the oscillator. This state has the property that it is an eigenstate of the annihilation operators with eigenvalue α. Again, this can be verified by using eq. (4.2e). Perhaps it should be emphasized that the symbol α always refers to a complex eigenvalue whereas $|\alpha\rangle$ always denotes a state, just as n denotes a real eigenvalue and $|n\rangle$ a state, the so-called "number state". Also, just as $|n\rangle$ refers to a definite state of excitation of a system of *one* mode, $|\alpha\rangle$ also refers to a state of *one* mode.

The $|\alpha\rangle$ states are not orthogonal but they are complete (in fact overcomplete). Explicitly,

$$\langle\beta|\alpha\rangle = \exp[-\tfrac{1}{2}(|\alpha|^2 + |\beta|^2) + \beta^*\alpha] , \tag{4.6}$$

which follows immediately from eq. (4.5) and the fact that the number states are orthonormal. Furthermore, it is possible to express the identity operator as

$$I = \frac{1}{\pi} \int \mathrm{d}^2\alpha\, |\alpha\rangle\langle\alpha| , \tag{4.7a}$$

where $\mathrm{d}^2\alpha = \mathrm{d}(\mathrm{Re}\,\alpha)\,\mathrm{d}(\mathrm{Im}\,\alpha) = \frac{1}{2}\mathrm{d}\alpha\, \mathrm{d}\alpha^*$. The proof of eq. (4.7a) follows by setting $\alpha = r\,\mathrm{e}^{\mathrm{i}\theta}$, so that $\mathrm{d}^2\alpha = r\,\mathrm{d}r\,\mathrm{d}\theta$, and then using eq. (4.5) to get

$$\frac{1}{\pi} \int \mathrm{d}^2\alpha\, |\alpha\rangle\langle\alpha| = \frac{1}{\pi} \sum_{m=0}^{\infty} \sum_{n=0} \frac{|m\rangle\langle n|}{(m!)^{1/2}(n!)^{1/2}} \int_0^{\infty} \mathrm{d}r\, \mathrm{e}^{-r^2} r^{m+n+1} \int_0^{2\pi} \mathrm{e}^{\mathrm{i}(m-n)\theta}\, \mathrm{d}\theta = 2 \sum_n \frac{|n\rangle\langle n|}{n!} \int_0^{\infty} \mathrm{d}r\, \mathrm{e}^{-r^2} r^{2n+1} , \tag{4.7b}$$

where we have used the fact that the angular integral simply equals $2\pi\delta_{mn}$. The latter radial integral equals $n!/2$, so that using the fact that $\Sigma_n |n\rangle\langle n| = 1$, eq. (4.7a) readily follows. A direct consequence of eq. (4.7a) is that the trace of any operator $\hat{A}$ is just

$$\mathrm{Tr}(\hat{A}) = \frac{1}{\pi}\int \mathrm{d}^2\alpha\, \langle\alpha|\hat{A}|\alpha\rangle\,. \tag{4.8}$$

It is also of use to compare the expression for the displacement operator $\hat{D}(\alpha)$ to our previous results and use this comparison to derive an expansion for a general operator $\hat{A}$ in terms of $\hat{D}^{-1}(\alpha)$. This will be of use later. First we note that if we set $\alpha = (2\hbar)^{-1/2}(\lambda\tau + \mathrm{i}\lambda^{-1}\sigma)$ then (see eq. (4.1))

$$\hat{D}(\alpha) = \exp\{(\mathrm{i}/\hbar)(\sigma\hat{q} + \tau\hat{p})\} = \hat{C}(\sigma, \tau)\,, \tag{4.9}$$

where $\hat{C}$ was defined earlier by eq. (2.43). Thus from eqs. (2.42) and (4.9) it is clear that the characteristic function is the expectation value of the displacement operator. This in conjunction with eqs. (4.5), (4.6) and (4.8) gives

$$\mathrm{Tr}(\hat{D}(\alpha)\,\hat{D}^{-1}(\beta)) = \pi\,\delta^{(2)}(\alpha - \beta)\,, \tag{4.10}$$

where the δ function here is $\delta^2(\xi) = \delta(\mathrm{Re}\,\xi)\,\delta(\mathrm{Im}\,\xi)$. Suppose that we can expand the operator $\hat{A}(\hat{a}, \hat{a}^+)$ as

$$\hat{A} = \frac{1}{\pi}\int \mathrm{d}^2\xi\, g(\xi)\,\hat{D}^{-1}(\xi)\,. \tag{4.11}$$

Using eq. (4.10) we find that

$$g(\xi) = \mathrm{Tr}(\hat{A}\,\hat{D}(\xi))\,. \tag{4.12}$$

It can be shown (Cahill and Glauber [1969]) that if $\hat{A}$ is Hilbert–Schmidt (i.e. $\mathrm{Tr}(\hat{A}^+\hat{A}) < \infty$) then the function $g(\xi)$ is square integrable.

The three types of ordering of the operators $\hat{a}$ and $\hat{a}^+$ which we wish to consider are defined as follows:

(i) Normal ordering – A product of m annihilation operators and n creation operators is normally ordered if all of the annihilation operators are on the right, i.e. if it is in the form $(\hat{a}^+)^n\,\hat{a}^m$.

(ii) Symmetric ordering – A product of m annihilation operators and n creation operators can be ordered in $(n+m)!/n!\,m!$ ways. The symmetrically ordered product of these operators, denoted by $\{(\hat{a}^+)^n\,\hat{a}^m\}$, is just the average of all of these differently ordered products. For example

$$\{\hat{a}^+\hat{a}\} = \tfrac{1}{2}(\hat{a}^+\hat{a} + \hat{a}\hat{a}^+) \tag{4.13a}$$

$$\{\hat{a}^+\hat{a}^2\} = \tfrac{1}{3}(\hat{a}^+\hat{a}^2 + \hat{a}\hat{a}^+\hat{a} + \hat{a}^2\hat{a}^+) \tag{4.13b}$$

$$\{\hat{a}^{+2}\hat{a}^2\} = \tfrac{1}{6}(\hat{a}^{+2}\hat{a}^2 + \hat{a}^+\hat{a}\hat{a}^+\hat{a} + \hat{a}^+\hat{a}^2\hat{a}^+ + \hat{a}\hat{a}^{+2}\hat{a} + \hat{a}\hat{a}^+\hat{a}\hat{a}^+ + \hat{a}^2\hat{a}^{+2})\,. \tag{4.13c}$$

(iii) Anti-normal ordering – A product of m annihilation operators and n creation operators is

anti-normally ordered if all of the annihilation operators are on the left, i.e. if it is of the form $\hat{a}^m(\hat{a}^+)^n$.

For each operator ordering we have a rule which associates a function of α and α^* with a given operator. The rule is as follows: for any operator ordering scheme the product of m annihilation and n creation operators, ordered according to that scheme, is associated with the function $(\alpha^*)^n\alpha^m$. For example, if we are considering normal ordering the product $(\hat{a}^n)^n\hat{a}^m$ is associated with $(\alpha^*)^n\alpha^m$; if anti-normal ordering is being considered then $\hat{a}^m(\hat{a}^+)^n$ is associated with $\alpha^m(\alpha^*)^n$. We will now make the meaning of our rule more explicit by considering each of these orderings and its associated distribution function.

4.1. Normal ordering

Let us suppose that we can expand a given operator $\hat{A}(\hat{a}, \hat{a}^+)$ in a normally ordered power series

$$\hat{A} = \sum_{n,m=0}^{\infty} c_{nm}(\hat{a}^+)^n\hat{a}^m . \tag{4.14}$$

Let us further suppose that we can express the density matrix as

$$\hat{\rho} = \int \mathrm{d}^2\alpha\, P(\alpha)|\alpha\rangle\langle\alpha| \tag{4.15}$$

where $P(\alpha)$ is a c-number and the state $|\alpha\rangle$ is given by eq. (4.5). $P(\alpha)$ is called the P-representation of the density matrix (or the distribution function representing the density matrix) of the *particular* mode under study. It should be emphasized that both the real and imaginary parts of α are used as the variables of the distribution function. Also, it is probably worthwhile mentioning again that our discussion is restricted to a system of bosons and thus the distribution functions under study are not applicable to, for instance, a gas of neutrinos. Also, we are dealing with a very large but countable set since we assumed that the basic domain is finite.

From eqs. (4.10) and (4.7a) and because $\langle\alpha|\hat{a}^{+n}\hat{a}^m|\alpha\rangle = \alpha^{*n}\alpha^m$, it follows that

$$\begin{aligned}\mathrm{Tr}(\hat{A}\hat{\rho}) &= \frac{1}{\pi}\int \mathrm{d}^2\beta \int \mathrm{d}^2\alpha\, P(\alpha)\langle\beta|\hat{A}|\alpha\rangle\langle\alpha|\beta\rangle = \int \mathrm{d}^2\alpha\, P(\alpha)\langle\alpha|\hat{A}|\alpha\rangle \\ &= \int \mathrm{d}^2\alpha\, P(\alpha)\left[\sum_{n,m=0}^{\infty} c_{nm}(\alpha^*)^n\alpha^m\right] \equiv \int \mathrm{d}^2\alpha\, P(\alpha)\, A_{\mathrm{N}}(\alpha, \alpha^*) ,\end{aligned} \tag{4.16}$$

with

$$A_{\mathrm{N}}(\alpha, \alpha^*) = \langle\alpha|\hat{A}|\alpha\rangle = \sum_{n,m=0}^{\infty} c_{nm}(\alpha^*)^n\alpha^m . \tag{4.17}$$

Therefore, we associate the operator $\hat{A}(\hat{a}, \hat{a}^+)$ with the function $A_{\mathrm{N}}(\alpha, \alpha^*)$ in the evaluation of expectation values with the P-representation.

We now want to derive two expressions for $P(\alpha)$ in terms of the density matrix. It is not always possible to find a useful representation of $\hat{\rho}$ of the form given by eq. (4.15). For some density matrices $P(\alpha)$ would have to be so singular that it would not even be a tempered distribution (Cahill [1965]; Klauder and Sudarshan [1968]). This difficulty will be apparent in our formal expression for $P(\alpha)$.

Let us now choose for the operator A

$$\hat{A} = e^{\xi \hat{a}^+} e^{-\xi^* \hat{a}} . \tag{4.18}$$

The corresponding function is then $A_N(\alpha, \alpha^*) = \exp(\xi\alpha^* - \xi^*\alpha)$. Inserting these expressions into eq. (4.16) we find that

$$\chi_N(\xi) \equiv \mathrm{Tr}(\hat{\rho}\, e^{\xi \hat{a}^+} e^{-\xi^* \hat{a}}) = \int d^2\alpha\, P(\alpha)\, e^{\xi\alpha^* - \xi^*\alpha} . \tag{4.19}$$

The function $\chi_N(\xi)$ is known as the normally ordered characteristic function. The right-hand side of eq. (4.19) is just a Fourier transform in a somewhat disguised form. In fact one has that if

$$f(\alpha) = \frac{1}{\pi} \int d^2\xi\, e^{\alpha\xi^* - \alpha^*\xi} \tilde{f}(\xi) \tag{4.20a}$$

then

$$\tilde{f}(\xi) = \frac{1}{\pi} \int d^2\alpha\, e^{\xi\alpha^* - \xi^*\alpha} f(\alpha) , \tag{4.20b}$$

and vice versa. Therefore, we have for $P(\alpha)$

$$P(\alpha) = \frac{1}{\pi^2} \int d^2\xi\, e^{\alpha\xi^* - \alpha^*\xi} \chi_N(\xi) . \tag{4.21}$$

The problem with this expression is that $\chi_N(\xi)$ can grow rather rapidly. In fact we have that because $\exp(\xi\hat{a}^+ - \xi^*\hat{a})$ is unitary

$$|\chi_N(\xi)| = e^{|\xi|^2/2} |\mathrm{Tr}(\hat{\rho}\, e^{\xi\hat{a}^+ - \xi^*\hat{a}})| \le e^{|\xi|^2/2} , \tag{4.22}$$

which suggests the type of behavior which is possible. For example, if $\hat{\rho} = |n\rangle\langle n|$, where $|n\rangle$ is the eigenstate of the number operator with eigenvalue n, then for large $|\xi|$ we have $|\chi_N(\xi)| \sim |\xi|^{2n}$. This representation, then, is not appropriate for all density matrices, but, nonetheless, is useful in many of the cases of interest.

Finally, we will derive an expression for $P(\alpha)$ in terms of a series expansion for the density matrix. Let us suppose that we can express the density matrix as an *anti-normally* ordered series

$$\hat{\rho} = \sum_{n,m=0}^{\infty} \rho_{nm} \hat{a}^m (\hat{a}^+)^n . \tag{4.23}$$

If we again consider the expression for $\hat{A}(\hat{a}, \hat{a}^+)$ given by eq. (4.14) we find that

$$\mathrm{Tr}(\hat{\rho}\hat{A}) = \sum_{n,m=0}^{\infty} \sum_{r,s=0}^{\infty} \rho_{nm} c_{rs}\, \mathrm{Tr}(\hat{a}^m (\hat{a}^+)^n (\hat{a}^+)^r \hat{a}^s) . \tag{4.24}$$

The trace in eq. (4.24) can be expressed as

$$\mathrm{Tr}(\hat{a}^m(\hat{a}^+)^{n+r}\hat{a}^s) = \mathrm{Tr}((\hat{a}^+)^{n+r}\hat{a}^{s+m})$$

so that

$$\mathrm{Tr}(\hat{\rho}\hat{A}) = \frac{1}{\pi}\int \mathrm{d}^2\alpha \sum_{n,m=0}^{\infty}\sum_{r,s=0}^{\infty} \rho_{nm}c_{rs}\alpha^{*n}\alpha^m\alpha^{*r}\alpha^s . \tag{4.25}$$

Comparing this with eq. (4.16) we see that

$$P(\alpha) = \frac{1}{\pi}\sum_{n,m=0}^{\infty} \rho_{nm}\alpha^{*n}\alpha^m . \tag{4.26}$$

The difficulties which we had when considering eq. (4.21) suggest that we will have similar problems with eq. (4.26). In fact the problem goes back to eq. (4.23). The class of operators for which a meaningful anti-normally ordered expansion exists is highly restricted. One can see this by considering the representation for an operator given by eq. (4.11). Expand $\hat{D}^{-1}(\xi) = \exp(\xi^*\hat{a})\exp(-\xi\hat{a}^+)\exp(\frac{1}{2}|\xi|^2)$ in an anti-normally ordered power series and insert it back into eq. (4.11). This gives us an anti-normally-ordered power series for $\hat{A}$:

$$\hat{A} = \sum_{n,m=0}^{\infty} d_{nm}\hat{a}^m(\hat{a}^+)^n , \tag{4.27}$$

with the coefficients given by

$$d_{nm} = \frac{1}{n!\,m!}\frac{1}{\pi}\int \mathrm{d}^2\xi\, \mathrm{Tr}(\hat{A}\hat{D}(\xi))\, \mathrm{e}^{|\xi|^2/2}(-\xi)^n(\xi^*)^m . \tag{4.28}$$

For these coefficients to exist $\mathrm{Tr}(\hat{A}\hat{D}(\xi))$ must be a very rapidly decreasing function of $|\xi|$. Our previous remarks indicate that this will not be true in general for Hilbert–Schmidt operators and, in fact, will not be true in general for operators of trace class (operators, $\hat{A}$, for which $\mathrm{Tr}([\hat{A}^\dagger\hat{A}]^{1/2}) < \infty$) such as density matrices.

It should be mentioned that normally-ordered power series expansions are far better behaved. A derivation similar to the one above gives for the coefficients c_{nm} in eq. (4.14)

$$c_{nm} = \frac{1}{n!\,m!}\frac{1}{\pi}\int \mathrm{d}^2\xi\, \mathrm{Tr}(\hat{A}\hat{D}(\xi))\, \mathrm{e}^{-|\xi|^2/2}(-\xi)^n(\xi^*)^m . \tag{4.29}$$

This clearly exists for a much wider class of operators than does d_{nm}. The c_{nm}'s exist, in fact, for all Hilbert–Schmidt operators and the series converges in the sense that if one takes its matrix element between two coherent states, $\langle\alpha|$ on the left and $|\beta\rangle$ on the right, the resulting series converges to $\langle\alpha|A|\beta\rangle$.

4.2. Symmetric ordering

Before proceeding with a discussion of the distribution function for this case we would like to consider a few properties of the ordering scheme itself. We first note that

$$(\xi_1\hat{a}^+ + \xi_2\hat{a})^n = \sum_{l=0}^{n} \xi_1^{(n-l)}\,\xi_2^l \binom{n}{l} \{(\hat{a}^+)^{n-l}\,\hat{a}^l\}\,, \tag{4.30}$$

which implies that

$$\mathrm{e}^{(\xi_1\hat{a}^+ + \xi_2\hat{a})} = \sum_{l,m=0}^{\infty} \frac{1}{l!\,m!}\,\xi_1^m\,\xi_2^l\,\{(\hat{a}^+)^m\,\hat{a}^l\}\,. \tag{4.31}$$

Our operator-function correspondence is now done in a way analogous to that of the preceding section. Expand an operator $\hat{A}(\hat{a}, \hat{a}^+)$ in a symmetrically ordered power series

$$\hat{A} = \sum_{n,m=0}^{\infty} b_{nm}\,\{(\hat{a}^+)^n\,\hat{a}^m\}\,. \tag{4.32}$$

The function corresponding to the operator is then

$$A_s(\alpha, \alpha^*) = \sum_{n,m=0}^{\infty} b_{nm}\,(\alpha^*)^n\,\alpha^m\,. \tag{4.33}$$

Under this correspondence we see from eq. (4.30) that the function $\hat{D}(\xi)$ goes to

$$\hat{D}(\xi) = \mathrm{e}^{\xi\hat{a}^+ - \xi^*\hat{a}} \to \mathrm{e}^{\xi\alpha^* - \xi^*\alpha}\,. \tag{4.34}$$

Comparison with eq. (4.9) shows us that this is nothing other than Weyl ordering expressed in a different form. The distribution function, therefore, should be the Wigner function. As before we define this as the Fourier transform of the characteristic function $\chi(\xi)$ (see eqs. (2.42)–(2.45)) and we use the real and imaginary parts of $\alpha = \alpha_r + \mathrm{i}\alpha_i$ as the variables of the distribution function, so that, analogous to eq. (4.1), $\alpha = (2\hbar)^{-1/2}(\lambda q + (\mathrm{i}/\lambda)p)$, where $\lambda = (m\omega)^{1/2}$. Thus

$$\begin{aligned} W(\alpha) &= \frac{1}{\pi}\int \mathrm{d}^2\xi\,\mathrm{e}^{(\alpha\xi^* - \alpha^*\xi)}\,\chi(\xi) = \frac{1}{\pi}\int\int \mathrm{d}\xi_r\,\mathrm{d}\xi_i\,\mathrm{e}^{2\mathrm{i}(\alpha_i\xi_r - \alpha_r\xi_i)}\,\mathrm{Tr}[\hat{\rho}\,\mathrm{e}^{\xi\hat{a}^+ - \xi^*\hat{a}}] \\ &= \frac{1}{\pi}\int\int \mathrm{d}\xi_r\,\mathrm{d}\xi_i\,\mathrm{Tr}\left[\hat{\rho}\,\exp\left\{2\mathrm{i}\xi_r\left(\alpha_i - \frac{\hat{p}}{(2\hbar)^{1/2}\lambda}\right) - 2\mathrm{i}\xi_i\left(\alpha_r - \frac{\lambda\hat{q}}{(2\hbar)^{1/2}}\right)\right\}\right], \end{aligned} \tag{4.35}$$

where

$$\chi(\xi) = \mathrm{Tr}(\hat{\rho}\,\hat{D}(\xi))\,. \tag{4.36}$$

It may be verified, using eqs. (2.42), (2.45) and (4.35) that

$$\begin{aligned} W(\alpha) &= (2\pi\hbar)\,P_w(q,p) = 2\int_{-\infty}^{\infty} \mathrm{d}y \sum_n \sum_m \langle q-y|n\rangle\,\langle n|\hat{\rho}|m\rangle\,\langle m|q+y\rangle\,\mathrm{e}^{2\mathrm{i}py/\hbar} \\ &= \beta\int_{-\infty}^{\infty} \mathrm{d}y \sum_n \sum_m \left(\frac{1}{2^n n!}\right)^{1/2}\left(\frac{1}{2^m m!}\right)^{1/2} \mathrm{e}^{-\beta^2(q^2+y^2)}\,\mathrm{e}^{2\mathrm{i}py/\hbar}\,H_n(\beta(q+y))\,H_m(\beta(q-y))\,\psi_n^*\,\psi_m\,, \end{aligned} \tag{4.37}$$

where, in the derivation of the last line from the previous line, we have used eq. (2.90) and where $\beta = (m\omega/\hbar)^{1/2}$ and $\langle n|\hat{\rho}|m\rangle = \psi_n^* \psi_n$.

Examination of eqs. (4.11) and (4.34) shows us that the function A_s which corresponds, by eqs. (4.32) and (4.33), to the operator $\hat{A}(\hat{a}, \hat{a}^+)$ can also be represented as

$$A_s(\alpha, \alpha^*) = \frac{1}{\pi} \int \mathrm{d}^2\xi \, \mathrm{Tr}(\hat{A}\hat{D}(\xi)) \, \mathrm{e}^{\xi^*\alpha - \xi\alpha^*} . \tag{4.38}$$

We would now like to use this to show that

$$\mathrm{Tr}(\hat{\rho}\hat{A}) = \frac{1}{\pi} \int \mathrm{d}^2\alpha \, A_s(\alpha, \alpha^*) \, W(\alpha) . \tag{4.39}$$

Evaluating the right-hand side we see that

$$\frac{1}{\pi} \int \mathrm{d}^2\alpha \, A_s(\alpha, \alpha^*) \, W(\alpha) = \frac{1}{\pi^2} \int \mathrm{d}^2\alpha \int \mathrm{d}^2\xi \, \mathrm{Tr}(\hat{A}\hat{D}(\xi)) \, \mathrm{e}^{\xi^*\alpha - \xi\alpha^*} \, W(\alpha) . \tag{4.40}$$

Making use of the relation

$$\delta^{(2)}(\alpha) = \frac{1}{\pi^2} \int \mathrm{d}^2\xi \, \mathrm{e}^{\alpha\xi^* - \alpha^*\xi} , \tag{4.41}$$

we find that

$$\frac{1}{\pi} \int \mathrm{d}^2\alpha \, \mathrm{e}^{\xi^*\alpha - \xi\alpha^*} \, W(\alpha) = \chi(-\xi) . \tag{4.42}$$

We also have from eqs. (4.11) and (4.36)

$$\frac{1}{\pi} \int \mathrm{d}^2\xi \, \chi(-\xi) \, \hat{D}(\xi) = \frac{1}{\pi} \int \mathrm{d}^2\xi \, \chi(\xi) \, \hat{D}^{-1}(\xi) = \hat{\rho} , \tag{4.43}$$

so that

$$\frac{1}{\pi} \int \mathrm{d}^2\alpha \, A_s(\alpha, \alpha^*) \, W(\alpha) = \frac{1}{\pi} \int \mathrm{d}^2\xi \, \mathrm{Tr}(\hat{A}\hat{D}(\xi)) \, \chi(-\xi) = \mathrm{Tr}(\hat{A}\hat{\rho}) , \tag{4.44}$$

which proves eq. (4.39) and shows that $A_s(\alpha, \alpha^*)$ and $W(\alpha)$ can be used to calculate the expectation values of symmetrically ordered operators.

We would also like to say a word about symmetrically ordered power series. Comparison of eqs. (4.11) and (4.31) allows us to calculate the coefficients appearing in eq. (4.32)

$$b_{nm} = \frac{1}{n!\, m!} \frac{1}{\pi} \int \mathrm{d}^2\xi \, \mathrm{Tr}(\hat{A}\hat{D}(\xi)) \, (-\xi)^n \, (\xi^*)^m . \tag{4.45}$$

These coefficients, then, will exist for all operators which have the property that all moments of $\mathrm{Tr}(\hat{A}\hat{D}(\xi))$ are finite. While this behavior is not as good as that for a normally ordered power series it is certainly better than that of anti-normally ordered series.

It is also of interest to examine the behavior of $W(\alpha)$. First we note that

$$\frac{1}{\pi}\int \mathrm{d}^2\xi\, |\chi(\xi)|^2 = \frac{1}{\pi}\int \mathrm{d}^2\xi\, \mathrm{Tr}[\mathrm{Tr}(\hat{\rho}\hat{D}(\xi))\, \hat{D}^{-1}(\xi)\hat{\rho}] = \mathrm{Tr}\,\hat{\rho}^2 \leq 1 \tag{4.46}$$

so that $\chi(\xi)$ is a square integrable function. As $W(\alpha)$ is just the Fourier transform of $\chi(\xi)$ it too is square integrable. Therefore, $W(\alpha)$ is far better behaved than $P(\alpha)$ and will exist for all density matrices.

It is also possible to express the Wigner distribution in terms of the P representation. If we can represent the density matrix as in eq. (4.15) we then have that

$$\chi(\xi) = \int \mathrm{d}^2\beta\, P(\beta)\, \langle\beta|\, \mathrm{e}^{\xi\hat{a}^+ - \xi^*\hat{a}}\, |\beta\rangle = \int \mathrm{d}^2\beta\, P(\beta)\, \mathrm{e}^{\xi\beta^* - \xi^*\beta - |\xi|^2/2}\,. \tag{4.47}$$

Taking the Fourier transform of $\chi(\xi)$ gives us, with the use of eqs. (4.35) and (4.37),

$$\begin{aligned} W(\alpha) &= \frac{1}{\pi}\int \mathrm{d}^2\xi \int \mathrm{d}^2\beta\, P(\beta)\, \mathrm{e}^{\alpha\xi^* - \alpha^*\xi}\, \mathrm{e}^{\xi\beta^* - \xi^*\beta}\, \mathrm{e}^{-|\xi|^2/2} \\ &= \frac{1}{\pi}\int \mathrm{d}^2\beta \int \mathrm{d}^2\xi\, P(\beta)\, \mathrm{e}^{(\alpha-\beta)\xi^* - (\alpha^*-\beta^*)\xi - |\xi|^2/2} \\ &= 2\int \mathrm{d}^2\beta\, P(\beta)\, \mathrm{e}^{-2|\alpha-\beta|^2}\,. \end{aligned} \tag{4.48}$$

4.3. Anti-normal ordering

Let us suppose that we have an operator given by an anti-normally ordered power series as in eq. (4.27). The function corresponding to the $\hat{A}$ of eq. (4.27) is then

$$A_{\mathrm{a}}(\alpha, \alpha^*) = \sum_{n,m=0} d_{nm}\, \alpha^m\, (\alpha^*)^m\,. \tag{4.49}$$

By analogy with our discussion of the P representation (eq. (4.26)) we can then express $\hat{A}(\hat{a}, \hat{a}^+)$ as

$$\hat{A}(\hat{a}, \hat{a}^+) = \frac{1}{\pi}\int \mathrm{d}^2\alpha\, A_{\mathrm{a}}(\alpha, \alpha^*)\, |\alpha\rangle\langle\alpha|\,. \tag{4.50}$$

We then have that

$$\mathrm{Tr}(\hat{\rho}\hat{A}) = \frac{1}{\pi}\int \mathrm{d}^2\alpha\, A_{\mathrm{a}}(\alpha, \alpha^*)\, \mathrm{Tr}(\hat{\rho}|\alpha\rangle\langle\alpha|) = \int \mathrm{d}^2\alpha\, A_{\mathrm{a}}(\alpha, \alpha^*)\, Q(\alpha)\,, \tag{4.51}$$

where we have set (Kano [1965])

$$Q(\alpha) = \frac{1}{\pi} \langle \alpha | \hat{\rho} | \alpha \rangle . \tag{4.52}$$

This distribution can also be expressed in terms of a characteristic function

$$\chi_{\mathrm{A}}(\xi) = \mathrm{Tr}(\hat{\rho}\, \mathrm{e}^{-\xi^* \hat{a}}\, \mathrm{e}^{\xi \hat{a}^+}) . \tag{4.53}$$

We have that

$$\chi_{\mathrm{A}}(\xi) = \frac{1}{\pi} \int \mathrm{d}^2\alpha\, \langle \alpha |\, \mathrm{e}^{\xi \hat{a}^+}\, \hat{\rho}\, \mathrm{e}^{-\xi^* \hat{a}} | \alpha \rangle = \frac{1}{\pi} \int \mathrm{d}^2\alpha\, \mathrm{e}^{\xi \alpha^* - \xi^* \alpha}\, \langle \alpha | \hat{\rho} | \alpha \rangle \tag{4.54}$$

so that

$$\begin{aligned} Q(\alpha) &= \frac{1}{\pi^2} \int \mathrm{d}^2\xi\, \mathrm{e}^{\alpha \xi^* - \alpha^* \xi}\, \chi_{\mathrm{A}}(\xi) \\ &= \frac{1}{\pi^3} \int \int \mathrm{d}^2\xi\, \mathrm{d}^2\beta\, \mathrm{e}^{\alpha \xi^* - \alpha^* \xi}\, \mathrm{e}^{\beta^* \xi - \beta \xi^*}\, \langle \beta | \hat{\rho} | \beta \rangle = \frac{1}{\pi} \langle \alpha | \hat{\rho} | \alpha \rangle . \end{aligned} \tag{4.55}$$

Again by considering our derivation of the P representation we can derive an alternate expression for $A_{\mathrm{a}}(\alpha, \alpha^*)$. Examining eq. (4.21) we see that

$$A_{\mathrm{a}}(\alpha, \alpha^*) = \frac{1}{\pi} \int \mathrm{d}^2\xi\, \mathrm{e}^{\alpha \xi^* - \alpha^* \xi}\, \mathrm{Tr}(\hat{A}\, \mathrm{e}^{\xi \hat{a}^+}\, \mathrm{e}^{-\xi^* \hat{a}}) . \tag{4.56}$$

The "function" $A_{\mathrm{a}}(\alpha, \alpha^*)$ has, of course, all of the singularity problems of the P representation.

The distribution function, $Q(\alpha)$, has, on the other hand, no singularity problems at all. It exists for all density matrixes, is bounded, and is even greater than or equal to zero for all α. The problems in this ordering scheme arise in the representation of the operators.

As a final remark, we note that all of the distribution functions can be written in terms of the Wigner distribution function (McKenna and Frisch [1966]; Agarwal and Wolf [1970]; Haken [1975]; O'Connell [1983b]), by use of integrals or derivatives.

4.4. Examples

We would now like to calculate $Q(\alpha)$ and $P(\alpha)$ for a single mode of the radiation field of angular frequency ω. The system which we will consider will be a canonical ensemble at temperature $T \equiv (k\beta)^{-1}$. Our discussion will follow that given in Nussenzveig [1973].

We first consider the anti-normal distribution function $Q(\alpha)$. The density matrix for this system is

$$\hat{\rho} = (1 - \mathrm{e}^{-\beta \hbar \omega}) \sum_{n=0}^{\infty} \mathrm{e}^{-n \beta \hbar \omega}\, |n\rangle \langle n| . \tag{4.57}$$

For $Q(\alpha)$ we than have from eq. (4.52)

$$\begin{aligned} Q(\alpha) &= \frac{1}{\pi}(1-\mathrm{e}^{-\beta\hbar\omega}) \sum_{n=0}^{\infty} \mathrm{e}^{-n\beta\hbar\omega} \langle\alpha|n\rangle\langle n|\alpha\rangle \\ &= \frac{1}{\pi}(1-\mathrm{e}^{-\beta\hbar\omega}) \sum_{n=0}^{\infty} \mathrm{e}^{-n\beta\hbar\omega} \mathrm{e}^{-|\alpha|^2} \frac{|\alpha|^{2n}}{n!} \\ &= \frac{1}{\pi}(1-\mathrm{e}^{-\beta\hbar\omega}) \exp[-|\alpha|^2(1-\mathrm{e}^{-\beta\hbar\omega})] . \end{aligned} \tag{4.58}$$

To obtain $P(\alpha)$ we make use of our result for $Q(\alpha)$. We first find $\chi_{\mathrm{A}}(\xi)$ from eq. (4.54). If we set

$$s = (1-\mathrm{e}^{-\beta\hbar\omega}), \qquad \xi = x + \mathrm{i}y, \qquad \alpha = r + \mathrm{i}k \tag{4.59}$$

then

$$\begin{aligned} \chi_{\mathrm{A}}(\xi) &= \frac{s}{\pi}\int \mathrm{d}^2\alpha\, \mathrm{e}^{\xi\alpha^*-\xi^*\alpha}\, \mathrm{e}^{-s|\alpha|^2} = \frac{s}{\pi}\int \mathrm{d}r \int \mathrm{d}k\, \exp\{-2\mathrm{i}(kx-ry) - s(r^2+k^2)\} \\ &= \frac{s}{\pi}\int \mathrm{d}r \int \mathrm{d}k\, \exp\{-s(r-\mathrm{i}y/s)^2 - s(k+\mathrm{i}x/s)^2\} \exp\{-(x^2+y^2)/s\} = \mathrm{e}^{-|\xi|^2/s} . \end{aligned} \tag{4.60}$$

To calculate $\chi_{\mathrm{N}}(\xi)$, given by eq. (4.19), we now use the general relation

$$\chi_{\mathrm{N}}(\xi) = \mathrm{Tr}(\hat{\rho}\, \mathrm{e}^{\xi\hat{a}^+}\, \mathrm{e}^{-\xi^*\hat{a}}) = \mathrm{Tr}(\hat{\rho}\, \mathrm{e}^{-\xi^*\hat{a}}\, \mathrm{e}^{\xi\hat{a}^+})\, \mathrm{e}^{|\xi|^2} = \mathrm{e}^{|\xi|^2} \chi_{\mathrm{A}}(\xi) . \tag{4.61}$$

Therefore, we see that

$$\chi_{\mathrm{N}}(\xi) = \exp\{-|\xi|^2(1-s)/s\} . \tag{4.62}$$

If we set $\lambda = (1-s)/s = (\mathrm{e}^{\beta\hbar\omega}-1)^{-1}$ then from eq. (4.21) we have

$$\begin{aligned} P(\alpha) &= \frac{1}{\pi^2}\int \mathrm{d}^2\xi\, \mathrm{e}^{\alpha\xi^*-\alpha^*\xi}\, \mathrm{e}^{-\lambda|\xi|^2} = \frac{1}{\pi^2}\int \mathrm{d}x \int \mathrm{d}y\, \exp\{2\mathrm{i}(kx-ry) - \lambda(x^2+y^2)\} \\ &= \frac{1}{\pi\lambda}\, \mathrm{e}^{-|\alpha|^2/\lambda} = \frac{1}{\pi}(\mathrm{e}^{\beta\hbar\omega}-1) \exp[-|\alpha|^2(\mathrm{e}^{\beta\hbar\omega}-1)] . \end{aligned} \tag{4.63}$$

For this system $P(\alpha)$ is a well-behaved function, a Gaussian in fact, and has no singularities. It is even positive definite. $Q(\alpha)$ is also well behaved, but this comes as no surprise. Our general discussion had ensured that this would be the case.

4.5. Distribution functions on four-dimensional phase space

We would now like to briefly discuss some distribution functions which are functions on a four- rather than a two-dimensional phase space. The first of these, the R representation, was discussed by

Glauber in his 1963 paper. It is very well behaved but has found little use in applications. More recently a new class of these distributions, the generalized P representations, has been used to study the photon statistics of various non-linear optical devices [Walls, Drummond and McNeil [1981]; Drummond and Gardiner [1980]; Drummond, Gardiner and Walls [1981]).

The R representation of the density matrix is obtained by using the coherent state resolution of the identity twice. One has

$$\hat{\rho} = \frac{1}{\pi^2} \int d^2\alpha \int d^2\beta \exp\{-\tfrac{1}{2}(|\alpha|^2 + |\beta|^2)\} R(\alpha^*, \beta) |\alpha\rangle \langle\beta| , \tag{4.64}$$

where $|\alpha\rangle$ is defined in eq. (4.5) and $|\beta\rangle$ has the corresponding meaning, and

$$R(\alpha^*, \beta) = \exp\{\tfrac{1}{2}(|\alpha|^2 + |\beta|^2)\} \langle\alpha|\hat{\rho}|\beta\rangle . \tag{4.65}$$

This representation has no singularity problems. Also it exists and is unique for all density matrices provided that $R(\alpha^*, \beta)$ is an analytic function of α^* and β (Glauber [1963b]). It can be used to evaluate normally ordered products. One has

$$\langle(\hat{a}^+)^n \hat{a}^m\rangle = \mathrm{Tr}[\hat{\rho}\, (\hat{a}^+)^n \hat{a}^m] = \frac{1}{\pi^2} \int d^2\alpha \int d^2\beta \exp\{-(|\alpha|^2 + |\beta|^2) + \beta^*\alpha\} R(\alpha^*, \beta)\, \alpha^m\, (\beta^*)^n . \tag{4.66}$$

The generalized P representations (Drummond and Gardiner [1980]; Drummond, Gardiner and Walls [1981]) are again functions of two complex variables but are not necessarily defined for all values of these variables. To define these representations we define the operator

$$\hat{\Lambda}(\alpha, \beta) = |\alpha\rangle \langle\beta^*| / \langle\beta^*|\alpha\rangle \tag{4.67}$$

and an integration measure $d\mu(\alpha, \beta)$. It is the choice of this measure which determines the distribution function. We will consider two different choices. The density matrix is then

$$\hat{\rho} = \int_{\mathrm{D}} d\mu(\alpha, \beta)\, P(\alpha, \beta)\, \hat{\Lambda}(\alpha, \beta) , \tag{4.68}$$

where D is the domain of integration. Normally ordered products are then given by

$$\langle(\hat{a}^+)^n (\hat{a})^m\rangle = \int d\mu(\alpha, \beta)\, P(\alpha, \beta)\, \beta^n \alpha^m . \tag{4.69}$$

Our first integration measure is $d\mu(\alpha, \beta) = d\alpha\, d\beta$ where α and β are to be integrated on some contours C and C′ respectively. This gives rise to what is called the complex P representation. Let us consider the case in which C and C′ are contours which enclose the origin. One can then show (Drummond and Gardiner [1980]) that if the density matrix is of the form

$$\hat{\rho} = \sum_n \sum_m c_{nm} |n\rangle \langle m| , \tag{4.70}$$

where both sums are finite then $P(\alpha, \beta)$ exists and is analytic when neither α nor β is 0. Whether $P(\alpha, \beta)$ exists for a general density matrix is not known. The complex P representation is also not unique; if one complex P representation exists for a given density matrix, then an infinite number of representation exist.

The second measure which we wish to consider is $\mathrm{d}\mu(\alpha, \beta) = \mathrm{d}\alpha^2\, \mathrm{d}\beta^2$. Because the coherent states are linearly dependent such a representation is not unique. In fact we have encountered one representation of this type already, the R representation. It is possible to choose $P(\alpha, \beta)$ so that it is real and non-negative (Drummond and Gardiner [1980]), i.e.

$$P(\alpha, \beta) = (1/4\pi^2) \exp\{-\tfrac{1}{4}|\alpha - \beta^*|^2\} \langle \tfrac{1}{2}(\alpha + \beta^*)|\hat{\rho}|\tfrac{1}{2}(\alpha + \beta^*)\rangle . \tag{4.71}$$

This representation, the positive P representation, is defined for all density matrices.

These two distributions have been used in problems in which non-classical photon states (states which are more like number states than coherent states) are produced. Under these conditions the above defined generalized P representations are better behaved than the original P representation. For example, the P representation corresponding to a density matrix $\hat{\rho} = |n\rangle\langle n|$ contains derivatives of delta functions up to order $2n$. On the other hand, the complex P representation for this state (again defined on two contours C and C′ encircling the origin) is just (Drummond and Gardiner [1980])

$$P(\alpha, \beta) = -(1/4\pi^2)\, n!\, \mathrm{e}^{\alpha\beta}\, (1/\alpha\beta)^{n+1} \tag{4.72}$$

while the positive P representation is, from eq. (4.70)

$$P(\alpha, \beta) = (1/4\pi^2)\,(1/n!) \exp\{-\tfrac{1}{4}|\alpha - \beta^*|^2\} \exp\{-\tfrac{1}{2}|\alpha + \beta^*|^2\}\, |\tfrac{1}{2}(\alpha + \beta^*)|^{2n} . \tag{4.73}$$

Both of these functions are far less singular than the original P representation.

The original motivation for the introduction of these generalized P distributions was connected with their practical applicability to the solution of quantum mechanical master equations (Drummond and Gardiner [1980]; Drummond, Gardiner and Walls [1981]). In general, using a coherent state basis, it is possible to develop phase-space Fokker–Planck equations that correspond to quantum master equations for the density operator (Haken [1970]; Louisell [1973]). From this equation observables are obtained in terms of moments of the P function. However, for various problems, as for example the analysis of recent experiments on atomic fluorescence (Kimble, Dagenais and Mandel [1978]) where we are dealing with non-classical photon statistics (Carmichael and Walls [1976]), the Glauber–Sudarshan P function is singular whereas the generalized P function discussed above is not. Also, use of the latter leads to Fokker–Planck equations with positive semi-definite diffusion coefficients whereas the former gives rise to non-positive-definite diffusion coefficients. In particular, the generalized P representations were applied successfully to non-linear problems in quantum optics (two-photon absorption; dispersive bistability; degenerate parametric amplifier) and chemical reaction theory (Drummond and Gardiner [1980]; Drummond, Gardiner and Walls [1981]; Walls and Milburn [1982]). On the other hand, the usefulness of the Wigner distribution in quantum optics has been demonstrated in a paper by Lugiato, Casagrande and Pizzuto [1982] who consider a system of N two-level atoms interacting with a resonant mode radiation field and coupled to suitable reservoirs. The presence of an external CW coherent field injected into the cavity is also included, which allows for the possibility of treating optical bistability (which occurs when a non-linear optical medium, interacting with a coherent driving field, has more than one stable steady state) as well as a laser with injected signal.

5. Conclusion

We have given what we hope is a useful summary of some of the formalism surrounding the use of quantum mechanical quasiprobability distribution functions. To be of use, however, the formalism should either provide insight or convenient methods of calculation. In our next paper dealing with applications we hope to show that this particular formalism does both in that it has proven to be a tool of great effectiveness in many areas of physics.

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