QUANTUM-MECHANICAL DISTRIBUTION FUNCTIONS: CONDITIONS FOR UNIQUENESS

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We add to the postulate, that the distribution function give the proper probabilities for the position and momentum variables (actually only the former is needed) and that its connection with the wave function which it represents have the natural invariances, another one. This is that the integral of the product of two distribution functions be equal, except for a universal constant (which turns out to be $2\pi\hbar$), to the transition probability between the two states they represent. We then show that it follows from these conditions that the distribution function is the one defined earlier by one of us (E.W.).

Quantum-mechanical distribution functions provide a framework for an exact reformulation of non-relativistic quantum mechanics in terms of classical concepts [1,2]. This has led to various discussions of their properties (refs. [3–6], and references therein, provide a representative sample of recent papers on this subject) and to their application to a variety of problems in physics [7] [‡1].

The distribution functions $P(q,p)$ are functions of positional and momentum coordinates q and p, and various definitions for P appear in the literature. Thus the question arises as to what conditions are necessary for providing a unique definition for P. One of us has previously examined this question and provided one such set of conditions [2]. In addition to those listed below – (a) to (e) – the relevant new condition was that, for free particles, the time dependence of P becomes the non-relativistic classical one. It is our purpose here to replace this by a perhaps more general criterion.

As in ref. [2], we list as our basic constraints on P:

(a) that it be a hermitian, that is bilinear, form of the wave function ψ, and

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

Next, on grounds of simplicity and naturalness, it was required

(c) that the correspondence between P and the wave function ψ be Galilei invariant, i.e. invariant with respect to displacements and non-relativistic transitions, to moving coordinate systems;

(d) that P be real for all ψ.

These conditions led to the result that [2, eq. (4.12)]

$$P(q,p) = \iint K^0(2q - x - x', x - x')\, \mathrm{e}^{\mathrm{i}p(x-x')/\hbar}\, \psi(x)^* \psi(x')\, \mathrm{d}x\, \mathrm{d}x' , \tag{1}$$

the explicit form of K^0 to be determined by further conditions. Our considerations here will be restricted to one dimension but it will be clear that they can be generalized to higher dimensions.

For our present deliberations, it turns out to be more convenient to replace K^0 by a more symmetric-looking function f, as follows:

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[‡1] See, for example, the various papers cited in ref. [1] of ref. [2] above. Some more recent applications are discussed in refs. [8–10].

$$P(q,p)=\iint f(q-x,q-x')\,e^{ip(x-x')/\hbar}\,\psi(x)^*\psi(x')\,dx\,dx'\,. \tag{2}$$

As in ref. [2], we next introduce the requirement:

(e) that the correspondence given by eq. (2) be invariant with respect to space and time reflections.

This leads to the result that

$$f(\alpha,\beta)=f(\beta,\alpha)^*=f(\beta,\alpha)=f(-\alpha,-\beta)=f(-\beta,-\alpha)\,. \tag{3}$$

A new requirement – which will turn out to be the only other condition necessary to determine P uniquely – is:

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

$$\left|\int\psi(x)^*\phi(x)\,dx\right|^2=k\iint P_\psi(q,p)P_\phi(q,p)\,dq\,dp\,, \tag{4}$$

where k is an arbitrary constant, the same for all ψ and ϕ, which is determined by the condition that the total integral of P be unity. As we will see below, k turns out to be $2\pi\hbar$.

We will now show that we have enough information to determine the function f uniquely.

Using eqs. (2) and (4) we obtain

$$\int\psi(u)^*\phi(u)\,\psi(v)\phi(v)^*\,du\,dv=k\int dp\,dq\,e^{ip(x-x')/\hbar}f(q-x,q-x')\,\psi(x)^*\psi(x')$$

$$\times\,e^{ip(y-y')/\hbar}f(q-y,q-y')\,\phi(y)^*\phi(y')\,dx\,dx'\,dy\,dy'\,. \tag{5}$$

Carrying out the p integration introduces a $2\pi\hbar\delta[(x-x')+(y-y')]$ factor, which prompts us to introduce a new variable ξ such that $x'=x-\xi$, $y'=y+\xi$, so that the right side of eq. (5) becomes

$$2\pi\hbar k\int dq\,f(q-x,q-x+\xi)\,f(q-y,q-y-\xi)\,\psi(x)^*\psi(x-\xi)\phi(y)^*\phi(y+\xi)\,dx\,dy\,d\xi\,.$$

In this, we replace the variable x by u and ξ by $u-v$. Hence, we obtain, instead of eq. (5),

$$\int\psi(u)^*\,\psi(v)\,\phi(u)\,\phi(v)^*\,du\,dv$$

$$=2\pi\hbar k\int dq\,f(q-u,q-v)\,f(q-y,q-y-u+v)\psi(u)^*\psi(v)\phi(y)^*\phi(y+u-v)\,du\,dv\,dy\,. \tag{6}$$

Since this is valid for any function ψ, one can conclude rather easily that the factors of $\psi(u)^*\psi(v)$ in the two integrals must be equal, i.e.

$$\phi(u)\,\phi(v)^*=2\pi\hbar k\iint dq\,dy\,f(q-u,q-v)\,f(q-y,q-y-u+v)\phi(y)^*\phi(y+u-v)\,. \tag{7}$$

To proceed further, we replace the integration variable y by $y+v$ to obtain

$$\phi(u)\,\phi(v)^*=2\pi\hbar k\int dq\,dy\,f(q-u,q-v)\,f(q-v-y,q-u-y)\,\phi(u+y)\,\phi(v+y)^*\,, \tag{8}$$

from which we conclude that

$$2\pi\hbar k\int dq\,f(q-u,q-v)\,f(q-u-y,q-v-y)=\delta(y)\,. \tag{9}$$

Using eq. (3), we have interchanged the variables in the second f of eq. (8).

We can, finally, regard f as a function of the sum and the difference of its variables,

$$f(\alpha,\beta) = \kappa(\tfrac{1}{2}(\alpha+\beta), \alpha-\beta). \tag{10}$$

In terms of this κ, if we substitute w for $q - \frac{1}{2}(u+v)$ and z for $v-u$, eq. (9) reads

$$2\pi\hbar k \int \kappa(w,z)\kappa(w-y,z)\,\mathrm{d}w = \delta(y)\,, \tag{11}$$

from which it follows that κ is a δ function of its first variable. Hence

$$f(\alpha,\beta) = g(\alpha-\beta)\delta(\alpha+\beta-c)\,. \tag{12}$$

It follows from eq. (3), $f(\alpha,\beta) = f(-\beta,-\alpha)$, that

$$g(\alpha-\beta)\delta(\alpha+\beta-c) = g(-\beta+\alpha)\,\delta(-\alpha-\beta-c)\,, \tag{12a}$$

i.e. that $c = 0$. But the function g remains to be determined.

From requirement (b), we have

$$\int P(q,p)\,\mathrm{d}p = |\psi(q)|^2\,. \tag{13}$$

Hence, from eqs. (2), (12) and (13) we obtain $g(q) = (\pi\hbar)^{-1}$. Thus

$$f(\alpha,\beta) = (\pi\hbar)^{-1}\,\delta(\alpha+\beta)\,, \tag{14}$$

which, when substituted in eq. (2), leads to the result

$$P(q,p) = (\pi\hbar)^{-1} \iint \psi(x)^*\psi(x')\,\delta(2q-x-x')\,\mathrm{e}^{\mathrm{i}p(x-x')/\hbar}\,\mathrm{d}x\,\mathrm{d}x'$$

$$= (\pi\hbar)^{-1}\int \psi(x)^*\,\psi(2q-x)\,\mathrm{e}^{\mathrm{i}p(2x-2q)/\hbar}\,\mathrm{d}x\,. \tag{15}$$

Thus, if we set $x = q + y$, we finally obtain

$$P(q,p) = (\pi\hbar)^{-1}\int \psi(q+y)^*\psi(q-y)\,\mathrm{e}^{2\mathrm{i}py/\hbar}\mathrm{d}y\,. \tag{16}$$

Using this result in eq. (4) leads to the result that $k = 2\pi\hbar$ [‡2].

In summary, we have shown that, if in addition to the postulates (a) to (e), already discussed in ref. [2], we add the postulate that the integral of the product of two distribution functions gives, up to a universal constant (which turned out to be $2\pi\hbar$), the transition probability between the corresponding two states, we are led uniquely to the distribution function given by eq. (16) – which is the original distribution function given in ref. [1].

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[‡2] Hence eq. (4) is equivalent to eq. (4.34) of ref. [2], except that the latter equation – and also eq. (4.33a) of ref. [2] – has the $2\pi\hbar$ factor in the wrong side of the equation, as is evident from dimensionality considerations.

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