

Phase-space dynamics and quantum mechanics

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Summary. An n -dimensional system with a classical Hamiltonian $H(\mathbf{p}, \mathbf{q}, t)$ may be described by a phase-space distribution function $\mathcal{D}(\mathbf{q}, \mathbf{p}, t)$. The dynamical equation for $\mathcal{D}(\mathbf{q}, \mathbf{p}, t)$ is postulated to be

$$\mathcal{D}(\mathbf{q}, \mathbf{p}, t + \delta t) = h^{-n} \iint e^{i2\pi S/h} \mathcal{D}^*(\mathbf{q}_0, \mathbf{p}_0, t) d\mathbf{q}_0 d\mathbf{p}_0$$

where δt is small and the phase angle $2\pi S/h$ is defined by

$$S = -\Delta H \delta t + \Delta \mathbf{q} \cdot \Delta \mathbf{p},$$

with

$$\Delta H = H(\mathbf{p}, \mathbf{q}_0, t) - H(\mathbf{p}_0, \mathbf{q}, t); \quad \Delta \mathbf{q} = \mathbf{q} - \mathbf{q}_0; \quad \Delta \mathbf{p} = \mathbf{p} - \mathbf{p}_0$$

The dynamical equation follows from a simple conceptual picture for propagation of the distribution function in phase space. This equation leads to (1) solutions of the form $\mathcal{D}(\mathbf{q}, \mathbf{p}, t) = h^{-n/2} \psi^*(\mathbf{q}, t) a(\mathbf{p}, t) e^{i2\pi \mathbf{q} \cdot \mathbf{p}/h}$ where $\psi(\mathbf{q}, t)$ and $a(\mathbf{p}, t)$ are related as Fourier transforms, and (2) the time-dependent Schrödinger equation.

Key words: Phase-space dynamics — Quantum theory — Schrödinger equation

1. Introduction

The principles of quantum mechanics form the basis for our current description of physical phenomena. The conventional presentation of these principles (see texts such as [1, 2]) typically involves the following postulates:

1. A physical system at time t can be completely described by a normalized wave

function $\psi(\mathbf{q}, t)$ whose absolute square gives the probability per unit volume that the system is found at position \mathbf{q} (the Born postulate).

2. The wave function $\psi(\mathbf{q}, t)$ evolves in time according to a dynamical equation—the Schrödinger equation. The Schrödinger equation for the standard case of a spinless non-relativistic particle with mass m and charge e is given by

$$i\hbar \frac{\partial \psi}{\partial t} = \left(-\frac{\hbar^2}{2m} \nabla^2 + \frac{ie\hbar}{mc} \mathbf{A} \cdot \nabla + W \right) \psi \quad (1)$$

where

$$W = \frac{e^2 A^2}{2mc^2} + e\phi + V. \quad (2)$$

Here V is the potential energy (e.g., the Coulomb potential for an electron in a hydrogen atom) and the Coulomb-gauge electromagnetic field [3] is characterized by a scalar potential ϕ and a vector potential \mathbf{A} ($\nabla \cdot \mathbf{A} = 0$). (The arguments of functions such as $\phi(\mathbf{q}, t)$, $\mathbf{A}(\mathbf{q}, t)$, etc. will be omitted unless required for clarity.)

3. For every classical physical quantity F , there is a corresponding linear Hermitian operator \hat{F} (e.g., the conjugate momentum $\hat{p} = -i\hbar \nabla$); with a proper choice of the order of operators corresponding to the product of the momentum and the vector potential, the Schrödinger equation above can be written in the usual form:

$$i\hbar \frac{\partial \psi}{\partial t} = \hat{H} \psi$$

where \hat{H} is the operator corresponding to the classical Hamiltonian

$$H(\mathbf{p}, \mathbf{q}, t) = \frac{1}{2m} \left(\mathbf{p} - \frac{e}{c} \mathbf{A} \right)^2 + e\phi + V. \quad (3)$$

4. The average value of the physical quantity $F(\mathbf{q}, \mathbf{p})$ is given by the expectation value

$$\bar{F} = \int \psi^* \hat{F} \psi d\mathbf{q}.$$

(Integrals are over all possible values of the coordinates, usually from $-\infty$ to $+\infty$.)

Needless to say, each of these postulates is not perceived on initial exposure to be a self-evident or even reasonable statement about the nature of physical reality (although one becomes more comfortable with these statements as one becomes more familiar with them and, probably more important, comes to realize their success in accounting for physical phenomena). Perhaps in consequence, many workers have tried to develop alternative formulations which both lead to quantum mechanics and involve more familiar ideas, simpler equations, and/or fewer postulates. A sampling of approaches is provided by [4–17]; a bibliography which includes criticisms of some of these is to be found in [18].

One important alternative approach to quantum mechanics is the path-integral formulation of Feynman [4, 5], in which the first postulate is preserved but the second is replaced by a sum-over-paths equation which gives the time development of the wave function. Neither the derivatives in the Schrödinger equation nor the operator-replacement postulates are needed in this formulation, and the picture is thus somewhat more pleasing. However, both postulate 1 and a postulated dynamical equation are required. In addition, the conceptual picture underlying the path-integral formulation involves accepting the notion that the amplitude (wave function) at a point in space depends on all the paths by which a particle *might* reach that point from some other point.

Another approach to quantum mechanics which has been developed in various forms involves phase-space dynamics, in which a system is described in terms of a time-dependent distribution in position and momentum analogous to the usual phase-space distribution function of classical statistical mechanics [19]. A distribution function constructed to be consistent with the basic elements of quantum mechanics was first introduced by Wigner [20]. However, the standard Wigner distribution is not fully compatible with quantum mechanics; for example, it does not yield the square of the eigenvalue of the Hamiltonian operator as the average value of the square of the energy when the system is in an eigenstate [21].

Properties of the Wigner distribution and other phase-space distribution functions have been developed over the years by Moyal [6], Cohen [21–24], Mehta [25], and others (e.g., [26–28]). Recent discussions from different perspectives are to be found in [16, 17, 29].

The approach to be taken here will be based on the description of a physical system by a phase-space distribution function, with a postulated dynamical equation for the distribution. That is, the only non-self-evident statement will be the proposition (in Einstein's term [30]) of the dynamical equation. The nature of the distribution functions and the Schrödinger equation will follow from the dynamical equation. With this approach, it will be seen that there is no need to invoke any of the usual postulates of quantum mechanics.

It is notable that the conceptual picture underlying quantum mechanics has been and continues to be of both great interest and considerable controversy. The continuing appearance of books and articles on the subject (for recent discussions, see [10, 15, 17, 31–37]) over sixty years after introduction of the Schrödinger equation attests to the interest. The controversy essentially revolves around the question of the distinction between metaphysics and physical science; for a discussion of this issue which is still germane, see the editorial preface to Ballentine's 1970 paper [28]. Whether or not predictions of new physical phenomena will emerge from consideration of possible physical pictures which may underly quantum mechanics remains to be seen. The point of view here is that it is worthwhile to look for equations based on what appear to be reasonable conceptual pictures which are consistent with conventional quantum mechanics and which have a minimum number of assumptions or postulates; that is, to pursue the goal described by Einstein [30] of seeking as complete as possible a comprehension of experimental results through the use of a minimum number of primary concepts and relations.

2. Phase-space distribution functions

The dynamics of a physical system (e.g., a particle with kinetic and potential energies) is determined by functions of the variables \mathbf{q} and \mathbf{p} , which are interpreted in classical mechanics as the position and conjugate momentum [38]. One way of describing the dynamics is in terms of a phase-space distribution function $\mathcal{D}(\mathbf{q}, \mathbf{p}, t)$. Such distribution functions have the following properties [22]:

Property 1. The distribution function is normalized; that is, the total probability of finding the particle, the integral of the distribution function over phase space, is equal to unity:

$$\int \int \mathcal{D}(\mathbf{q}, \mathbf{p}, t) d\mathbf{q} d\mathbf{p} = 1. \quad (4)$$

Property 2. The probability per unit volume that the particle is found at position \mathbf{q}_0 at time t is equal to $\int \mathcal{D}(\mathbf{q}_0, \mathbf{p}, t) d\mathbf{p}$; i.e., the integral of the distribution function over all values of \mathbf{p} corresponding to the position \mathbf{q}_0 .

Similarly, the probability the particle is found to have momentum \mathbf{p}_0 at time t is determined by the integral $\int \mathcal{D}(\mathbf{q}, \mathbf{p}_0, t) d\mathbf{q}$.

Property 3. The average value at time t of any physically-observable property $F(\mathbf{q}, \mathbf{p})$ is equal to

$$\bar{F} = \int \int F(\mathbf{q}, \mathbf{p}) \mathcal{D}(\mathbf{q}, \mathbf{p}, t) d\mathbf{q} d\mathbf{p}.$$

As a trivial example, the distribution function for a single classical particle moving in one spatial dimension and characterized by a classical Hamiltonian $H(p, q)$ can be written as a product of Dirac delta functions:

$$\mathcal{D}(q, p, t) = \delta(q - q_{cl})\delta(p - p_{cl})$$

where q_{cl} and p_{cl} represent the classical path determined by Hamilton's equations.

Even for a non-classical system, the dynamics are characterized by functions of the variables \mathbf{q} and \mathbf{p} ; and it may be taken as axiomatic that the system at time t may be completely characterized by a (distribution) function $\mathcal{D}(\mathbf{q}, \mathbf{p}, t)$ of these variables.

In classical mechanics, a distribution function is most commonly interpreted as the probability of finding specific \mathbf{q}, \mathbf{p} values for a multiparticle system, and consequently must take on only positive real values. Here the distribution function is regarded merely as a function which can be used to characterize the dynamics of the system, and there is no need for such a restriction. In addition, at present (and most likely forever) for a quantum system it is impossible to observe the value of $\mathcal{D}(\mathbf{q}, \mathbf{p}, t)$ at a single point \mathbf{q}, \mathbf{p} (this is one way of looking at the Heisenberg uncertainty principle). Consequently, it is not necessary that $\mathcal{D}(\mathbf{q}, \mathbf{p}, t)$ be positive or even real as long as Properties 1–3 are satisfied.

The question of so-called “negative probabilities” has been of concern beginning with the earliest discussions of quantum mechanics in terms of phase-space dynamics [6, 27]; and a number of years ago Cohen [22] showed

that quantum mechanics is not consistent with restriction of $\mathcal{D}(\mathbf{q}, \mathbf{p}, t)$ to positive real values. Feynman [39] noted that the issue may not be of concern since the measurements which would give physically unreasonable results perhaps cannot be made.

The possibility of having physically unreasonable results is, of course, implicit in quantum mechanics. As a simple example, consider the operator $\frac{1}{2}(\hat{p}^2\hat{q}^2 + \hat{q}^2\hat{p}^2)$, a Hermitian operator corresponding to the physical quantity q^2p^2 . For a one-dimensional harmonic oscillator in the ground state, the expectation value of this operator is $-\hbar^2/4$. That is, the product of q^2 and p^2 (both of which as squares can take on only positive values) has a negative expectation value for this system. This physically unreasonable result is readily achieved by allowing “negative probabilities” for sets of values q, p ; i.e., by allowing negative values of $\mathcal{D}(q, p)$. (There is also an unresolved question as to the proper form for the operator which corresponds to the quantity q^2p^2 [40, 41]; and whether or not expectation values of such quantities can be measured remains another open question.)

3. The dynamical equation for $\mathcal{D}(\mathbf{q}, \mathbf{p}, t)$

For simplicity, discussion will be restricted to the distribution function for a single non-relativistic particle in n spatial dimensions with the classical Hamiltonian $H(\mathbf{p}, \mathbf{q}, t)$ given by Eq. (3). Also, for clarity mathematical details in the discussion will be kept to a minimum.

There are several acceptable forms for the dynamical equation for the distribution function; that is, several forms are both consistent with quantum mechanics and lead to the Schrödinger equation. Again for simplicity, discussion will be restricted to one of these. The relationship between this choice and other possibilities will be discussed, as will possible ways of distinguishing among them.

Proposition. *A physical system can be characterized by a normalized distribution function $\mathcal{D}(\mathbf{q}, \mathbf{p}, t)$ which evolves in time according to*

$$\mathcal{D}(\mathbf{q}, \mathbf{p}, t + \delta t) = \frac{1}{h^n} \int \int e^{i2\pi S/\hbar} \mathcal{D}^*(\mathbf{q}_0, \mathbf{p}_0, t) d\mathbf{q}_0 d\mathbf{p}_0 \quad (5)$$

where δt must be small enough that $\mathcal{D}(\mathbf{q}, \mathbf{p}, t)$ changes only slightly in the time interval (otherwise, an integration or a successive set of calculations is to be made) and for the classical Hamiltonian of Eq. (3) the phase angle $2\pi S/\hbar$ is defined by

$$S = -\Delta H \delta t + \Delta \mathbf{q} \cdot \Delta \mathbf{p} \quad (6)$$

with

$$\Delta H = H(\mathbf{p}, \mathbf{q}_0, t) - H(\mathbf{p}_0, \mathbf{q}, t) \quad (7)$$

$$\Delta \mathbf{q} = \mathbf{q} - \mathbf{q}_0; \quad \Delta \mathbf{p} = \mathbf{p} - \mathbf{p}_0.$$

Equation (5) initially appears no more reasonable or self-evident than the

usual set of postulates of quantum mechanics (although it has the advantage of being more compact). Actually, as shown below, the form of Eq. (5) follows from a simple conceptual picture for the propagation of the distribution function in phase space. Before this picture is described, it may be useful to note that (a) the $\delta t \rightarrow 0$ limit for Eq. (5) will be used in Sect. 4 to determine the form of $\mathcal{D}(\mathbf{q}, \mathbf{p}, t)$ and (b) expansion of Eq. (5) to first order in δt will be shown in Sect. 5 to lead to the Schrödinger equation (note that the right-hand side of Eq. (5) includes the factor $e^{-i2\pi \Delta H \delta t/h} = 1 - i2\pi \Delta H \delta t/h - \dots$).

Although the dynamical equation (5) can stand alone as a formal alternative to the usual postulates of quantum mechanics, its form becomes plausible on the basis of the following conceptual picture. Consider a point $\mathbf{q}_0, \mathbf{p}_0$ in phase space with a value for the distribution function $\mathcal{D}(\mathbf{q}_0, \mathbf{p}_0, t) = R_0 e^{i\theta_0}$ at time t , where R_0 is the magnitude of $\mathcal{D}(\mathbf{q}_0, \mathbf{p}_0, t)$. At the slightly later time $t + \delta t$, it is postulated that the magnitude R_0 of the distribution function has propagated equally to all points in phase space. However, the phase angle θ at different points is given by

$$\theta = \frac{2\pi S}{h} - \theta_0. \quad (8)$$

That is, the contribution of point $\mathbf{q}_0, \mathbf{p}_0$ at time t to the distribution function at point \mathbf{q}, \mathbf{p} at time $t + \delta t$ will be proportional to $R_0 e^{i\theta}$.

Roughly speaking, the hypothesis is that the initial point $\mathbf{q}_0, \mathbf{p}_0$ acts as the source of a wave in phase space. The phase "received" by other points depends on the phase of the initial point and a quantity which depends on the time interval and the positions of the two points in phase space. The quantity S has units of action and is to be divided by a unit of action h (which will turn out to be Planck's constant in order to be consistent with experiment; i.e., with the Schrödinger equation).

The complex conjugate $\mathcal{D}^*(\mathbf{q}_0, \mathbf{p}_0, t)$ appears in Eq. (5) because the initial phase θ_0 is reversed in Eq. (8) in order to obtain time-reversal symmetry. The term S defined by Eq. (6) is unchanged if the roles of $\mathbf{q}_0, \mathbf{p}_0$ and \mathbf{q}, \mathbf{p} are reversed and the sign of δt is changed. Thus reversal of the initial phase results in consistency between the phase ($\theta = 2\pi S/h - \theta_0$) of the contribution of point $\mathbf{q}_0, \mathbf{p}_0$ to \mathbf{q}, \mathbf{p} in the time interval $t \rightarrow t + \delta t$ and the phase ($\theta_0 = 2\pi S/h - \theta$) of the contribution of \mathbf{q}, \mathbf{p} to $\mathbf{q}_0, \mathbf{p}_0$ in the time interval $t + \delta t \rightarrow t$.

It is interesting to note that for several common cases the quantity S reduces to even simpler forms:

(a) For a free particle for which the Hamiltonian is simply the kinetic energy, S is given by

$$S = \Delta \tilde{\mathbf{q}} \cdot \Delta \tilde{\mathbf{p}}$$

that is, the scalar product of the changes in the four-position $\tilde{\mathbf{q}} = (\mathbf{q}, ict)$ and in the four-momentum $\tilde{\mathbf{p}} = (\mathbf{p}, iE/c)$ between the two points [42].

(b) For a particle with no electromagnetic field and a potential energy $V(\mathbf{q})$, S is given by

$$S = -\Delta L \delta t + \Delta \mathbf{q} \cdot \Delta \mathbf{p}$$

$$\Delta L = L(\mathbf{p}, \mathbf{q}) - L(\mathbf{p}_0, \mathbf{q}_0)$$

where $L(\mathbf{p}, \mathbf{q})$ is the Lagrangian

$$L(\mathbf{p}, \mathbf{q}) = \frac{1}{2m} p^2 - V(\mathbf{q}).$$

If we now switch to the viewpoint of a point \mathbf{q}, \mathbf{p} in the phase space at time $t + \delta t$, its distribution function $\mathcal{D}(\mathbf{q}, \mathbf{p}, t + \delta t)$ will be the integrated sum of the contributions as described above from all points in phase space, each with its appropriate magnitude and phase. This integration, with the inclusion of a normalization factor, yields Eq. (5).

4. The form of $\mathcal{D}(\mathbf{q}, \mathbf{p}, t)$

In the limit $\delta t \rightarrow 0$, Eq. (5) yields the identity

$$\mathcal{D}(\mathbf{q}, \mathbf{p}, t) = \frac{1}{h^n} \iint e^{i2\pi \Delta \mathbf{q} \cdot \Delta \mathbf{p}/h} \mathcal{D}^*(\mathbf{q}_0, \mathbf{p}_0, t) d\mathbf{q}_0 d\mathbf{p}_0. \quad (9)$$

One now tries to find functions $\mathcal{D}(\mathbf{q}, \mathbf{p}, t)$ consistent with Eq. (9). Consider the trial function in which the variables \mathbf{q} and \mathbf{p} are in effect separated as follows:

$$\mathcal{D}(\mathbf{q}, \mathbf{p}, t) = h^{-n/2} \psi^*(\mathbf{q}, t) a(\mathbf{p}, t) e^{i2\pi \mathbf{q} \cdot \mathbf{p}/h}. \quad (10)$$

To avoid confusion in the discussion to come, the notation anticipates the result in the next section that $\psi(\mathbf{q}, t)$ and $a(\mathbf{p}, t)$ will be identified as the normalized coordinate-space and momentum-space wave functions, respectively; and the powers of h in Eqs. (5) and (10) anticipate the factors required for consistency with the normalization condition of Eq. (4). However, at this point these functions are regarded as arbitrary functions whose properties are defined by the requirement that $\mathcal{D}(\mathbf{q}, \mathbf{p}, t)$ be consistent with Eqs. (4) and (5).

Substituting Eq. (10) into Eq. (9) gives

$$\begin{aligned} & \psi^*(\mathbf{q}, t) a(\mathbf{p}, t) e^{i2\pi \mathbf{q} \cdot \mathbf{p}/h} \\ &= \frac{1}{h^n} \iint e^{i2\pi(\mathbf{q} - \mathbf{q}_0) \cdot (\mathbf{p} - \mathbf{p}_0)/h} [\psi(\mathbf{q}_0, t) a^*(\mathbf{p}_0, t) e^{-i2\pi \mathbf{q}_0 \cdot \mathbf{p}_0/h}] d\mathbf{q}_0 d\mathbf{p}_0. \end{aligned}$$

Collecting terms and separating the integrals yields

$$\frac{\psi^*(\mathbf{q}, t)}{h^{-n/2} \int a^*(\mathbf{p}_0, t) e^{-i2\pi \mathbf{q} \cdot \mathbf{p}_0/h} d\mathbf{p}_0} = \frac{h^{-n/2} \int \psi(\mathbf{q}_0, t) e^{-i2\pi \mathbf{q}_0 \cdot \mathbf{p}/h} d\mathbf{q}_0}{a(\mathbf{p}, t)}. \quad (11)$$

The left-hand side of Eq. (11) is a function of only \mathbf{q} and t , and the right-hand side is a function of only \mathbf{p} and t . Hence both sides must be functions

of only t ; i.e., a function $f(t)$ constant with respect to \mathbf{q} and \mathbf{p} for each value of t . One then has

$$\psi^*(\mathbf{q}, t) = \frac{f(t)}{h^{n/2}} \int a^*(\mathbf{p}_0, t) e^{-i2\pi\mathbf{q} \cdot \mathbf{p}_0/h} d\mathbf{p}_0$$

$$a(\mathbf{p}, t) = \frac{1}{f(t)h^{n/2}} \int \psi(\mathbf{q}_0, t) e^{-i2\pi\mathbf{q}_0 \cdot \mathbf{p}/h} d\mathbf{q}_0.$$

The function $f(t)$ is arbitrary since it does not affect $\mathcal{D}(\mathbf{q}, \mathbf{p}, t)$, and may be chosen simply to be 1. Thus the trial function of Eq. (10) is consistent with Eq. (5) if $\psi(\mathbf{q}, t)$ and $a(\mathbf{p}, t)$ are related as Fourier transforms [43]:

$$\psi(\mathbf{q}, t) = h^{-n/2} \int a(\mathbf{p}, t) e^{i2\pi\mathbf{q} \cdot \mathbf{p}/h} d\mathbf{p} \quad (12)$$

$$a(\mathbf{p}, t) = h^{-n/2} \int \psi(\mathbf{q}, t) e^{-i2\pi\mathbf{q} \cdot \mathbf{p}/h} d\mathbf{q}. \quad (13)$$

The normalization requirement Eq. (4) results in

$$\int \int h^{-n/2} \psi^*(\mathbf{q}, t) a(\mathbf{p}, t) e^{i2\pi\mathbf{q} \cdot \mathbf{p}/h} d\mathbf{q} d\mathbf{p} = \int \psi^* \psi d\mathbf{q} = 1$$

and, similarly, if the integration with respect to \mathbf{q} is performed first:

$$\int a^* a d\mathbf{p} = 1.$$

That is, conventional normalization of $\psi(\mathbf{q}, t)$ and $a(\mathbf{p}, t)$ ensures consistency with Eq. (4).

The function of Eq. (10) (or its complex conjugate or its real part), with $\psi(\mathbf{q}, t)$ satisfying the Schrödinger equation, been considered as a quantum-mechanical phase-space distribution function by several workers [23, 25, 27], usually as a consequence of the standard postulates of quantum mechanics. As another approach, Pitowsky [15] and Gudder [17] have postulated that this form represents the physically allowed form of the distribution function. The approach here has been to show that the form of Eq. (10) follows from the postulated dynamical equation (5).

5. Time evolution of $\mathcal{D}(\mathbf{q}, \mathbf{p}, t)$; the Schrödinger equation

To determine how $\mathcal{D}(\mathbf{q}, \mathbf{p}, t)$ evolves in time, one could begin with a distribution function consistent with Eq. (10) at an initial time t , use Eq. (5) to find each value of the distribution function at a slightly later time $t + \delta t$, and carry out a successive set of calculations. A familiar result is obtained by taking an infinitesimal time interval $\delta t \rightarrow dt$, in which case Eq. (5) becomes

$$\mathcal{D}(\mathbf{q}, \mathbf{p}, t + dt) = \frac{1}{h^n} \iint \left[1 - \frac{i2\pi \Delta H dt}{h} \right] e^{i2\pi \Delta \mathbf{q} \cdot \Delta \mathbf{p}/h} \mathcal{D}^*(\mathbf{q}_0, \mathbf{p}_0, t) d\mathbf{q}_0 d\mathbf{p}_0.$$

Invoking Eq. (9) yields

$$\mathcal{D}(\mathbf{q}, \mathbf{p}, t + dt) = \mathcal{D}(\mathbf{q}, \mathbf{p}, t) - \frac{i2\pi dt}{h^{n+1}} \iint \Delta H e^{i2\pi \Delta \mathbf{q} \cdot \Delta \mathbf{p}/h} \mathcal{D}^*(\mathbf{q}_0, \mathbf{p}_0, t) d\mathbf{q}_0 d\mathbf{p}_0.$$

or

$$\frac{i\hbar}{2\pi} \frac{\partial \mathcal{D}}{\partial t}(\mathbf{q}, \mathbf{p}, t) = \frac{1}{h^n} \iint \Delta H e^{i2\pi \Delta \mathbf{q} \cdot \Delta \mathbf{p}/h} \mathcal{D}^*(\mathbf{q}_0, \mathbf{p}_0, t) d\mathbf{q}_0 d\mathbf{p}_0. \quad (14)$$

The time dependence of the functions $\psi(\mathbf{q}, t)$ and $a(\mathbf{p}, t)$ can be obtained by substituting Eq. (10) and the form of the Hamiltonian for the specific system under consideration. The result will be obtained here for the single-particle Hamiltonian of Eq. (3). For this case, ΔH defined by Eq. (7) can be written as

$$\Delta H = \left[\frac{1}{2m} p^2 - W(\mathbf{q}) \right] - \left[\frac{1}{2m} p_0^2 - W(\mathbf{q}_0) \right] - \frac{e}{mc} [\mathbf{p} \cdot \mathbf{A}(\mathbf{q}_0, t) - \mathbf{p}_0 \cdot \mathbf{A}(\mathbf{q}, t)] \quad (15)$$

where $W(\mathbf{q})$ is defined by Eq. (2). Substitution of Eq. (10) into Eq. (14) yields

$$\begin{aligned} & \frac{i\hbar}{2\pi} \frac{\partial}{\partial t} [\psi^*(\mathbf{q}, t) a(\mathbf{p}, t) e^{i2\pi \mathbf{q} \cdot \mathbf{p}/h}] \\ &= \frac{1}{h^n} \iint \Delta H e^{i2\pi(\mathbf{q} - \mathbf{q}_0) \cdot (\mathbf{p} - \mathbf{p}_0)/h} [\psi(\mathbf{q}_0, t) a^*(\mathbf{p}_0, t) e^{-i2\pi \mathbf{q}_0 \cdot \mathbf{p}_0/h}] d\mathbf{q}_0 d\mathbf{p}_0. \end{aligned}$$

Making use of the identity

$$\int x^n f(x) e^{-i2\pi xy/h} dx = \left(\frac{i\hbar}{2\pi} \right)^n \frac{\partial^n}{\partial y^n} \int f(x) e^{-i2\pi xy/h} dx \quad (16)$$

and Eqs. (12)–(13), and rearranging leads to

$$\begin{aligned} \frac{i\hbar}{\psi^*} \frac{\partial \psi^*}{\partial t} + \frac{1}{\psi^*} \left[-\frac{\hbar^2}{2m} \nabla^2 \psi^* - \frac{ie\hbar}{mc} \mathbf{A} \cdot \nabla \psi^* + W\psi^* \right] \\ = -\frac{i\hbar}{a} \frac{\partial a}{\partial t} + \frac{1}{a} \left[\frac{p^2}{2m} a + \tau - \frac{e}{mc} \mathbf{p} \cdot \mathbf{T} \right] \quad (17) \end{aligned}$$

where

$$\begin{aligned} \tau &= h^{-n/2} \int W(\mathbf{q}_0, t) \psi(\mathbf{q}_0, t) e^{-i2\pi \mathbf{q}_0 \cdot \mathbf{p}/h} d\mathbf{q}_0 \\ \mathbf{T} &= h^{-n/2} \int \mathbf{A}(\mathbf{q}_0, t) \psi(\mathbf{q}_0, t) e^{-i2\pi \mathbf{q}_0 \cdot \mathbf{p}/h} d\mathbf{q}_0. \end{aligned}$$

The left-hand side of Eq. (17) is a function of only \mathbf{q} and t , and the right-hand side is a function of only \mathbf{p} and t . Hence each side must be a function of only t , say $g(t)$. It is simplest to set $g(t)$ equal to zero, in which case one obtains

$$-i\hbar \frac{\partial \psi^*}{\partial t} = -\frac{\hbar^2}{2m} \nabla^2 \psi^* - \frac{ie\hbar}{mc} \mathbf{A} \cdot \nabla \psi^* + W\psi^*$$

or

$$i\hbar \frac{\partial \psi}{\partial t} = -\frac{\hbar^2}{2m} \nabla^2 \psi + \frac{ie\hbar}{mc} \mathbf{A} \cdot \nabla \psi + W\psi \quad (18)$$

$$i\hbar \frac{\partial a}{\partial t} = \frac{p^2}{2m} a + \tau - \frac{e}{mc} \mathbf{p} \cdot \mathbf{T}. \quad (19)$$

If the constant \hbar is set equal to Planck's constant, Eqs. (18) and (19) become the standard configuration-space and momentum-space time-dependent Schrödinger equations for a particle in a potential and an electromagnetic field (Eq. (1) and its Fourier transform).

If one had chosen $g(t)$ to be a non-zero function, solutions of Eq. (17) would have been of the form

$$\begin{aligned} \psi^*(\mathbf{q}, t) &= \chi^*(\mathbf{q}, t) e^{-i2\pi \int g(t) dt/\hbar} \\ a(\mathbf{p}, t) &= b(\mathbf{p}, t) e^{i2\pi \int g(t) dt/\hbar} \end{aligned}$$

where the functions $\chi(\mathbf{q}, t)$ and $b(\mathbf{p}, t)$ would satisfy the configuration-space and momentum-space Schrödinger equation, respectively. The distribution function $\mathcal{D}(\mathbf{q}, \mathbf{p}, t)$, average values, and consistency with quantum mechanics are unchanged by the choice of $g(t)$.

6. Properties of $\mathcal{D}(\mathbf{q}, \mathbf{p}, t)$

It is instructive to illustrate that the properties of the distribution function $\mathcal{D}(\mathbf{q}, \mathbf{p}, t)$ are consistent with standard quantum mechanics. For simplicity, consider a one-dimensional system.

Property 2. The probability per unit length a particle is found at position q_0 is given by

$$\begin{aligned} \int \mathcal{D}(q_0, p, t) dp &= \int h^{-1/2} \psi^*(q_0, t) a(p, t) e^{i2\pi q_0 p/\hbar} dp \\ &= \psi^*(q_0, t) \psi(q_0, t) \end{aligned}$$

the usual quantum-mechanical result.

Property 3. Let us examine several average values to show that the usual quantum-mechanical results are obtained.

(a) The average value of q^n .

$$\begin{aligned} \overline{q^n} &= \iint q^n \mathcal{D}(q, p, t) dq dp = \iint q^n [h^{-1/2} \psi^* a e^{i2\pi q_0 p/\hbar}] dq dp \\ &= \int q^n \psi^* \psi dq. \end{aligned}$$

Alternatively, making use of Eq. (16) yields

$$\overline{q^n} = \int a \left(\frac{\hbar}{i} \frac{\partial}{\partial p} \right)^n a^* dp.$$

(b) The average value of p^n .

$$\begin{aligned}\overline{p^n} &= \iint p^n \mathcal{D}(q, p, t) dq dp = \iint p^n [h^{-1/2} \psi^* a e^{i2\pi qp/h}] dq dp \\ &= \int p^n a^* a dp \\ &= \int \psi^* \left(\frac{\hbar}{i} \frac{\partial}{\partial q} \right)^n \psi dq.\end{aligned}$$

(c) The average value of $H^2(p, q)$, with

$$H = \frac{p^2}{2m} + V$$

and where $\psi(q, t)$ is an eigenfunction of \hat{H} ,

$$-\frac{\hbar^2}{2m} \frac{\partial^2 \psi}{\partial q^2} = (E - V)\psi \quad (20)$$

$$\overline{H^2} = \iint \left(\frac{p^2}{2m} + V \right)^2 [h^{-1/2} \psi^* a e^{i2\pi qp/h}] dq dp.$$

Making use of Eqs. (16) and (20) yields

$$\overline{H^2} = \int \psi^* \left[\frac{\hbar^4}{4m^2} \frac{\partial^4}{\partial q^4} - \frac{\hbar^2 V}{m} \frac{\partial^2}{\partial q^2} + V^2 \right] \psi dq$$

and after integrating by parts one obtains

$$\overline{H^2} = \int \psi^* [(E - V)^2 + 2V(E - V) + V^2] \psi dq = E^2.$$

It is also worth noting that the distribution function $\mathcal{D}(q, p, t)$ is consistent with the uncertainty principle; as shown by Cohen [22], one can readily find the relationship

$$\iint (q - \bar{q})^2 (p - \bar{p})^2 \mathcal{D}(q, p, t) dq dp \geq \left(\frac{\hbar}{2} \right)^2.$$

7. Discussion

Several comments should be made about the conceptual picture presented here and its consequences. First, the essence of the postulated dynamical equation (5) is that the distribution function at a point q_0, p_0 propagates in time with equal magnitude but different phases to all points in phase space. This hypothesis uncouples momentum from its classical interpretation as mass times velocity, since a classical distribution function at q_0, p_0 would propagate in a small time δt only to $q_0 + p_0 \delta t/m, p_0 - \nabla V \delta t$. However, this hypothesis is compatible with the form of the Hamiltonian as simply a function of two independent variables, with their interdependence, if any, resulting from the dynamical equations of motion. In the present picture, the interdependence may be regained through average values according to the usual quantum-mechanical result.

Second, the goal here has been to show that solutions of the postulated

dynamical equation (5) are consistent with quantum mechanics; that is, to reproduce the results of quantum mechanics using a minimum number of assumptions or postulates (“primary concepts and relations” [30]). As noted earlier, the standard results of quantum mechanics are both consistent with and follow from several alternative forms for the dynamical equation and the distribution function. For example, changing the sign of the phase angle $2\pi S/h \rightarrow -2\pi S/h$ in Eqs. (5) and (8) leads to solutions of the form

$$h^{-n/2} \psi(\mathbf{q}, t) a^*(\mathbf{p}, t) e^{-i2\pi \mathbf{q} \cdot \mathbf{p}/h}$$

with no changes in the properties ($\overline{q^n}$, $\overline{p^n}$, etc.) discussed in the preceding section. In fact, none of these properties is affected if the distribution function is any normalized linear combination of $\mathcal{D}(\mathbf{q}, \mathbf{p}, t)$ and its complex conjugate. In particular, the distribution function and hence average values do not take on complex values if it has the form $(\text{Re } \mathcal{D} + \alpha \text{ Im } \mathcal{D})$, where α is any real constant and \mathcal{D} satisfies Eqs. (4) and (5).

There is no need to propose which of these alternatives is correct, since there appears to be no current experimental test of such a hypothesis. On the other hand, predicted average values of quantities such as qp , q^2p^2 , ... (“mixed moments” of the distribution) do depend on the choice among these alternatives. Development of methods for determining average values for such quantities would lead to a choice among the alternatives and a test of the hypotheses of Eqs. (5) and (8).

References

1. Blinder SM (1974) Foundations of quantum dynamics. Academic Press, New York, pp 49–77
2. McQuarrie DA (1983) Quantum chemistry. University Science Books, Mill Valley, CA
3. Jackson JD (1962) Classical electrodynamics. Wiley, New York, p 181
4. Feynman RP (1948) Rev Mod Phys 20:367
5. Feynman RP, Hibbs AR (1965) Quantum mechanics and path integrals. McGraw-Hill, New York, pp 25–81
6. Moyal IE (1949) Proc Cambridge Phil Soc 45:99
7. Bohm D (1952) Phys Rev 85:166
8. Bohm D (1952) Phys Rev 85:180
9. Nelson E (1966) Phys Rev 150:1079
10. Nelson E (1985) Quantum fluctuations. Princeton University Press, Princeton, NJ
11. De La Peña-Auerbach L (1967) Phys Lett 24A:603
12. Kuryshkin VV (1977) In: Price WC, Shissick SS (eds) The uncertainty principle and foundations of quantum mechanics. Wiley, New York, pp 61–83
13. Young RH (1980) Found Phys 10:33
14. Guerra F (1981) Phys Reports 77:263
15. Pitowsky I (1984) In: Roth LM, Inomata A (eds) Fundamental questions in quantum mechanics conference proceedings. CUNY, Albany, NY, pp 241–252
16. Gudder SP (1985) Int J Theor Phys 24:243
17. Gudder SP (1988) Quantum probability. Academic Press, New York
18. Namsrai K (1986) Nonlocal quantum field theory and stochastic quantum mechanics. Reidel, Boston
19. Eyring H, Henderson D, Stover BJ, Eyring EM (1982) Statistical mechanics and dynamics. Wiley, New York, pp 165–175

20. Wigner EP (1932) *Phys Rev* 40:749
21. Cohen L (1966) *J Math Phys* 7:781
22. Cohen L (1966) *Philos Sci* 33:317
23. Cohen L (1970) *J Math Phys* 11:3296
24. Cohen L, Zaparovanny YI (1980) *J Math Phys* 21:794
25. Mehta CL (1964) *J Math Phys* 5:677
26. Bopp F (1956) *Ann L'Inst Henri Poincaré* 15:81
27. Margenau H, Hill RN (1961) *Progr Theoret Phys* 26:722
28. Ballentine IL (1970) *Rev Mod Phys* 42:358
29. Wang L, O'Connell RF (1988) *Found Phys* 18:1023
30. Einstein A (1954) *Ideas and opinions*. Crown, New York, p 293
31. Price WC, Chissick SS (eds) (1977) *The uncertainty principle and foundations of quantum mechanics*. Wiley, New York
32. Tarozzi G, van der Merwe A (1985) *Open questions in quantum physics*. Reidel, Boston
33. Greenberg D (ed) (1987) *New techniques and ideas in quantum measurement theory*. NY Acad Sci
34. Hiley BJ, Peat FD (eds) (1987) *Quantum implications*. Routledge and Kegan Paul, New York
35. Honig WM, Kraft DW, Panarella E (eds) (1986) *Quantum uncertainties*. Plenum Press, New York
36. Ghirardi GC, Rimini A, Weber T (1988) *Found Phys* 18:1
37. Wignall JWG (1988) *Found Phys* 18:591
38. Goldstein H (1950) *Classical mechanics*. Addison-Wesley, Reading, MA, pp 215–218
39. Feynman RP (1987) In: Hiley BJ, Peat FD (eds) *Quantum implications*. Routledge and Kegan Paul, New York, pp. 235–248
40. Shewell JR (1959) *Am J Phys* 27:16
41. Kerner EH, Sutcliffe WG (1970) *J Math Phys* 11:391
42. Sard RD (1970) *Relativistic mechanics*. Benjamin, New York, pp 112, 160
43. Bracewell RN (1978) *The Fourier transform and its applications*. McGraw-Hill, New York, p 7