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Hamiltonian theory of wave and particle in quantum mechanics I. Liouville's theorem and the interpretation of the de Broglie-Bohm theory

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Summary. — This paper and a following one develop a Hamiltonian formulation of the de Broglie-Bohm (deBB) interpretation of quantum mechanics. Drawing upon a unified Hamiltonian treatment of a classical particle and its associated ensemble, it is shown how the interaction of a particle and a spin-0 quantum wave can be consistently expressed in a canonical framework. A formulation is found in which the particle is acted upon by a force determined by the quantum potential but the particle does not react on the Schrödinger field. This requires the introduction of an additional field which the particle does act upon, and allows the deBB theory to be expressed in Hamiltonian terms. An ensemble theory for the wave-particle system based on Liouville's equation is developed, and it is shown that for a pure quantum state the particle obeys its own Liouville equation. The general particle phase space distribution that is compatible with $|\psi|^2$ is derived. A special case of this corresponds to the relation $p = \partial S/\partial q$ (and thus the guidance law of the deBB theory) but more general distributions, and hence non-deBB motions, are possible. This relation is interpreted as a constraint on the phase space of the composite system. Using the theory of Hamiltonian constraints it is shown that the first-order guidance law and Hamilton's second-order particle equations are dynamically equivalent.

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1. – Introduction

1˙1. *The problem.* – The Hamiltonian approach is generally regarded as the deepest formulation of dynamics, and most physically important theories of particles and fields can be treated according to its methods. A problem that has not been fully addressed in the literature is whether theories of quantum mechanics which employ the trajectory concept, in particular the de Broglie-Bohm (hereafter deBB) theory of motion [1], can be couched in these terms. In the deBB theory a quantum system comprises a wave

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aspect whose evolution is described by Schrödinger's equation, and a particle whose motion is determined by a specific deterministic law involving the wavefunction. It is not established that this theory admits a Hamiltonian formulation.

As it exists at present the deBB proposal formally works in the sense that, for an ensemble of trajectories, the flow generates the quantum-statistical predictions. As a result it reproduces the empirical content of quantum mechanics while providing a causally connected account of individual processes. Yet, while the deBB theory has been successfully applied to a variety of problems and some of its general ramifications explored [1], the law of motion on which it is based is an unexplained postulate. If S is the phase of the wavefunction obeying the (spin 0) Schrödinger equation for a particle of mass m (see the *mathematical note* below),

$$i\hbar\frac{\partial\psi}{\partial t} = -\frac{\hbar^2}{2m}\frac{\partial^2\psi}{\partial q_i^2} + V\psi, \tag{1.1}$$

where $\psi = \sqrt{\rho}\exp[iS/\hbar]$, the particle track is the solution $q_i = q_i(t)$ to the differential equation (the "guidance law")

$$m\frac{\mathrm{d}q_i(t)}{\mathrm{d}t} = \left.\frac{\partial S(q_i,t)}{\partial q_i}\right|_{q_i=q_i(t)}, \quad i = 1,2,3. \tag{1.2}$$

The phase obeys the equation

$$\frac{\partial S}{\partial t} + \frac{1}{2m}\frac{\partial S}{\partial q_i}\frac{\partial S}{\partial q_i} + Q + V = 0, \tag{1.3}$$

where

$$Q(q,t) = -\frac{\hbar^2}{2m\sqrt{\rho}}\frac{\partial^2\sqrt{\rho}}{\partial q_i^2} = \frac{\hbar^2}{4m\rho}\left(\frac{1}{2\rho}\left(\frac{\partial\rho}{\partial q_i}\right)^2 - \frac{\partial^2\rho}{\partial q_i^2}\right) \tag{1.4}$$

is what Bohm called the quantum potential. To compute an individual trajectory we need only specify the initial position q_0. As far as is known the resulting theory is consistent yet, viewed from the perspective of the general dynamical theory of individual systems, (1.2) is something of an enigma. This equation is reminiscent of the sort of relation implied in classical Hamilton-Jacobi (HJ) theory, and indeed it was the latter that de Broglie [2] and Bohm [3] drew upon as justification for their proposed law. Thus, (1.3) looks like the classical HJ equation modified by an additional quantum potential term, and this led to the appellation "the quantum Hamilton-Jacobi equation" (*e.g.*, [4]). However, simply postulating the validity of (1.2) without further justification is analogous in classical mechanics to being presented with one half of the canonical transformation equations which trivialize the motion (*i.e.*, which effect a transformation to a set of constant (in time) phase space coordinates), together with the HJ equation, and being given no further explanation as to the meaning or origin of the equations. Our understanding would be enhanced if we could derive (1.2) from, for example, some Hamiltonian theory, much as happens in the classical case, or at least if we could establish its connection with such a description.

In fact, the reason the deBB theory works in the first instance is not because of the putative HJ analogy but because of the second equation implied by the Schrödinger equation:

$$\frac{\partial \rho}{\partial t} + \frac{1}{m}\frac{\partial}{\partial q_i}\left(\rho \frac{\partial S}{\partial q_i}\right) = 0. \tag{1.5}$$

If the initial values q_0 are distributed according to $|\psi_0|^2$, (1.5) ensures that the flow defined by (1.2) generates the quantal distribution for all time. Indeed, there are good reasons to question whether (1.2) really is a HJ-type relation, with (1.3) as the associated HJ equation. To begin with, the quantum phase is not in general a function of a set of non-additive constants and hence cannot generate a transformation which trivializes the motion (for an early discussion of this point see [5]). Moreover, (1.3) does not seem to be a HJ-like equation at all—as noted, it contains the quantum potential, and this, by virtue of (1.5), depends on S. The equation thus has a complicated dependence on S quite different from that of any classical HJ equation. This is evident, for example, in cases where we may use (1.5) to eliminate ρ from (1.3) to leave just an equation for S [6]. It is found that the "quantum HJ equation" involves derivatives of S higher than the first—what kind of Hamiltonian theory could have such a relation as its associated HJ equation?

Two questions are addressed here. First, can the quantum trajectory theory indeed be formulated as a brand of Hamiltonian mechanics? Second, is there a relationship between the law of motion (1.2) and some HJ theory of the system—can the quantum phase be regarded as the generator of a canonical transformation which trivializes the motion, for instance?

A possible starting point in seeking a Hamiltonian theory of the particle is, for this purpose at least, to treat the quantum potential as if it were an external field function of q on a par with V. Then, assuming by analogy with classical HJ theory that the relation

$$p_i = \frac{\partial S(q,t)}{\partial q_i} \tag{1.6}$$

holds, we may propose that (1.3) is representative of the Hamiltonian (*e.g.*, [7])

$$H(q,p,t) = \frac{1}{2m}p_i p_i + Q(q,t) + V(q,t) \tag{1.7}$$

when the substitution (1.6) is made. Hamilton's equations imply

$$p_i = m\dot{q}_i, \qquad \dot{p}_i = -\frac{\partial}{\partial q_i}(V+Q), \tag{1.8}$$

so that the particle moves in response to a force determined by the classical and quantum potentials, as expected from (1.3). It is this proposal that we are going to investigate in this paper. However, in itself, the idea is not satisfactory, being open to the following three objections.

First, we have just pointed out that Q depends on S, and this in turn is connected to p via (1.6). It is therefore arbitrary to suppose that in the phase space formulation Q is a function of q alone and not of p—maybe it should be expressed as a function of both so that it becomes a function of just q only in the HJ representation, say.

Second, in such a theory the initial position and momentum coordinates can be chosen freely and there is no guarantee that the ensemble of q-projected motions will generate the quantal distribution. There are potentially "too many" possible motions and these must be restricted somehow, *e.g.*, by imposing the deBB law (1.2) or something like it as a subsidiary condition on the initial coordinates. A way of seeing this is to consider the HJ equation implied by (1.7):

$$\frac{\partial \sigma}{\partial t} + \frac{1}{2m}\frac{\partial \sigma}{\partial q_i}\frac{\partial \sigma}{\partial q_i} + Q + V = 0. \tag{1.9}$$

Although it has the same form, this equation admits many more solutions than (1.3) and in general the HJ function σ does not coincide with the quantum phase S [8].

The final and most serious objection to the use of (1.7) is that it is not clear whether this Hamiltonian is compatible with the wave equation and *its* Hamiltonian description. The particle is, after all, acted upon by the wave and we have to ensure that the interaction can be formulated in a way that does not give rise to a back-reaction which would disturb the Schrödinger evolution of the wave, and hence alter the usual predictions of quantum mechanics.

It is the latter problem in particular that is addressed in this paper. We shall explore the use of (1.7), and the associated Lagrangian, but in the context of a fully interacting wave-particle system which includes the field Hamiltonian. In the course of our analysis we shall see that the first objection mentioned above, although reasonable, is not an impediment to the development of a consistent phase space theory. In addition, we show how to accommodate the second objection by imposing suitable restrictions on the phase space of the total system. In this way we answer the two questions posed above. We find that we can indeed formulate the deBB theory in Hamiltonian terms, in the context of an interacting wave-particle system, and that it does have an interpretation in HJ theory.

In this first paper we shall concentrate on establishing the Hamiltonian theory, proving its consistency with quantum mechanics, and showing how the deBB theory is to be interpreted in Hamiltonian terms. Our method is based on a generalization of a particular canonical treatment of a classical particle and its associated ensemble (sects. **2**, **3**), and necessitates the introduction of an additional (complex) field of which the particle is a source (sect. **4**). Within this scheme equations (1.3) and (1.5), supplemented by equations determining the evolution of the particle and additional-field variables, come out as Hamilton equations. The consistency of the Hamiltonian theory with quantum mechanics is demonstrated through a thorough examination of Liouville ensemble theory for the total system (sect. **5**), and it is shown that for a pure quantum state the particle obeys its own Liouville equation. The general expression for the particle phase space distribution that is compatible with quantum statistics is found. A special case of this corresponds to the relation (1.6) (and thus the guidance law of the deBB theory) but more general distributions, and hence non-deBB motions, are possible. The relation (1.6) is interpreted as a constraint on the phase space coordinates of the total wave-particle system (sect. **6**). It is shown how this can be consistently regarded as a constraint on Hamilton's equations for the particle and, using the theory of Hamiltonian constraints, that the first-order guidance law and Hamilton's second-order particle equations are dynamically equivalent. The HJ theory of the system and an examination of alternative forms for the Hamiltonian are presented in the following paper. There we shall also give an explicit solution for the additional field which includes a particle back-reaction term, and discuss the conservation of energy and momentum in the model.

1˙2. *Role of the quantum potential.* – In the approach developed here we shall be giving a central physical role to the quantum potential. There are three principal reasons for this.

One reason is that, as we shall see, it allows a consistent Hamiltonian formulation of the theory. In a previous attempt to give a Lagrangian description of this system, Squires [9] found a field + particle Lagrangian from which one can derive the guidance law (1.2) directly, but in that approach the Schrödinger equation becomes modified by an extraneous nonlinear term. An important aspect of our demonstration based on (1.7) is that we can formulate the particle-field interaction in a way that maintains the exact validity of the Schrödinger equation.

The second reason for giving a central role to the quantum potential has to do with the problem of which variables associated with the wavefunction should be afforded ontological status. It may be argued that this cannot be the wavefunction itself since the phase is defined only up to an additive constant. One idea then might be to define the physical object as the equivalence class of wavefunctions, analogous to the idea of a geometric object in general relativity [10]. However, unlike the latter case where we have some notion of the physical meaning of the different coordinate systems, there does not seem to be a comparable interpretation of the "coordinate systems" with respect to which the phase takes different values (in the related case of the (gauge-dependent) electromagnetic potentials we do not attribute the physical content of the potentials to an equivalence class). Hence, it seems reasonable to seek to define the physical content of ψ through individual functions which do not display the phase freedom. We might choose $\partial S/\partial q$, and indeed this quantity will play a central role in what follows. However, this quantity gives a meaningful description of the physical content of ψ only in the case of an external scalar potential. More generally, we have to contend with even greater arbitrariness in the phase than that just cited—when external electromagnetic fields are present a gauge transformation of the potentials is accompanied by a local phase transformation of the wavefunction which modifies $\partial S/\partial q$. Now, the gauge freedom in the electromagnetic potentials is usually adduced as an argument against their physical reality, the physical fields being gauge invariant functions of the potentials. It seems that a similar argument should apply to the wavefunction—the local gauge freedom in the phase mitigates against it or its derivatives having a direct physical significance, and hence against the wavefunction as a whole. What we should do then is treat the wavefunction as analogous to a potential field (for further discussion of this in the context of nonlinear theories see [11]), the corresponding physical field being described by gauge invariant functions of this potential. The amplitude $\sqrt{\rho}$ of the wavefunction is one such function, and the quantum potential Q (an unfortunate name in this context) is another. One of the insights of Bohm's version of the trajectory theory is that it is precisely Q that captures those features of ψ that are relevant to the guidance of a particle, and contributes to an explanation of the difference between quantum and classical behaviour. When considering the particle motion, then, it is natural to regard Q as the physical field, an assumption that applies in all cases.

The final reason for emphasizing the quantum potential is that it has explanatory power in situations where other basic aspects of the theory, such as the guidance law (1.2), are silent. There are many such cases—in the extension of the deBB approach to quantized fields, for instance, where the field variables obey a guidance law analogous to (1.2), the Casimir effect is due to the force exerted by the quantum potential [12].

Along these lines, an example of a macroscopic effect which is relevant to the particle case is the explanation the theory provides for the pressure exerted by a non-interacting quantum gas. If we suppose the gas is in a real stationary state the guidance law (1.2) generalized to a many-body system [13] implies that all the gas particles are at rest. Hence, in this case the pressure cannot come from particle motions and the guidance law provides no insight. The usual expression for the pressure of a gas is

$$p = -Z^{-1} \sum_n e^{-E_n/kT} \frac{\partial E_n}{\partial \Sigma}, \quad Z = \sum_n e^{-E_n/kT}, \quad \Sigma = \text{volume}, \tag{1.10}$$

where E_n is the energy of the gas in the n-th stationary state. Noting that the Schrödinger equation for the gas reduces to $E_n = Q_n$, this expression becomes

$$p = -Z^{-1} \sum_n e^{-Q_n/kT} \frac{\partial Q_n}{\partial \Sigma} \tag{1.11}$$

which locates the quantum potential as the origin of pressure.

Mathematical note.

Repeated discrete indices are summed over, with $i, j, k = 1, 2, 3$. Let L be a functional of a field function $g(x, t)$ and its derivatives with respect to the arguments t (up to the first order) and x_μ, $\mu = 1, \ldots, n$ (up to the second order), and $\mathcal{L}$ its associated density:

$$L\big[g, \dot{g}, \partial_x g, \partial_x^2 g\big] = \int \mathcal{L}\big(g, \dot{g}, \partial_x g, \partial_x^2 g\big)\, \mathrm{d}^n x. \tag{1.12}$$

The variational derivative of L with respect to g is given by

$$\frac{\delta L}{\delta g} = \frac{\partial \mathcal{L}}{\partial g} - \frac{\partial}{\partial x_\mu} \frac{\partial \mathcal{L}}{\partial(\partial g/\partial x_\mu)} + \frac{\partial^2}{\partial x_\mu \partial x_\nu} \frac{\partial \mathcal{L}}{\partial\big(\partial^2 g/\partial x_\mu \partial x_\nu\big)}, \quad \mu, \nu = 1, \ldots, n. \tag{1.13}$$

In the case that L is a Lagrangian, the Euler-Lagrange equations are

$$\frac{\mathrm{d}}{\mathrm{d}t} \frac{\delta L}{\delta \dot{g}} - \frac{\delta L}{\delta g} = 0. \tag{1.14}$$

Quantities are assumed to have units so that the Lagrangian has the dimension of energy. Applying the formula (1.13) to the density in (1.12) gives for its functional derivative

$$\begin{aligned} \frac{\delta \mathcal{L}(x)}{\delta g(x')} = \frac{\partial \mathcal{L}(x')}{\partial g(x')} \delta\big(x - x'\big) - \frac{\partial}{\partial x'_\mu} \left(\frac{\partial \mathcal{L}(x')}{\partial(\partial g/\partial x'_\mu)} \delta\big(x - x'\big) \right) + \\ + \frac{\partial^2}{\partial x'_\mu \partial x'_\nu} \left(\frac{\partial \mathcal{L}(x')}{\partial\big(\partial^2 g/\partial x'_\mu \partial x'_\nu\big)} \delta\big(x - x'\big) \right). \end{aligned} \tag{1.15}$$

When integrating by parts it is assumed that all surface integrals at infinity vanish, whatever the nature of the variable x. For two functionals L, M of g partial functional integration may then be performed using the usual exchange rule:

$$\int M \frac{\delta L}{\delta g} \prod_{x'} \mathrm{d}g(x')\, \mathrm{d}^n x = -\int L \frac{\delta M}{\delta g} \prod_{x'} \mathrm{d}g(x')\, \mathrm{d}^n x. \tag{1.16}$$

2. – Hamiltonian theory of individual and ensemble in classical dynamics

To motivate the treatment of quantum systems we give below we start by looking at a particular formulation of classical ensemble theory as defined by an appropriate Lagrangian for Liouville's equation. This is useful also because, as we shall see, the Liouville equation is central to our quantum treatment.

Liouville's theorem asserts that, for an ensemble of identical systems obeying the same Hamilton equations in the phase space labelled by (q, p), their density $f(q, p, t)$ is conserved along each phase space path:

$$\frac{\mathrm{d}f}{\mathrm{d}t} = 0, \tag{2.1}$$

where

$$\frac{\mathrm{d}}{\mathrm{d}t} = \frac{\partial}{\partial t} + \dot{q}_i \frac{\partial}{\partial q_i} + \dot{p}_i \frac{\partial}{\partial p_i}. \tag{2.2}$$

Employing Hamilton's equations

$$\dot{q}_i = \frac{\partial H}{\partial p_i}, \qquad \dot{p}_i = -\frac{\partial H}{\partial q_i}, \tag{2.3}$$

Liouville's theorem may be written in field-theoretic form:

$$\frac{\partial f}{\partial t} + \frac{\partial H}{\partial p_i}\frac{\partial f}{\partial q_i} - \frac{\partial H}{\partial q_i}\frac{\partial f}{\partial p_i} = 0. \tag{2.4}$$

This is the fundamental equation describing the flow of ensembles in classical mechanics. There are several interpretations that may be given to f [14] but here and subsequently we shall assume that f represents a probability density (and that it is normalized).

Liouville's theorem is proved [15] by considering an ensemble whose boundary is defined by the moving phase space points. Each point evolves by a canonical transformation in accordance with Hamilton's equations, and hence so does the volume of points. Phase space volume is a canonical invariant and so, since the number of points in the volume is fixed, the density of points is also constant. But, instead of thinking of (2.4) as a deduction from Hamilton's equations, we may regard it as an independent field equation and seek to derive it from a variational principle (we shall refer to f as a "field").

We shall consider functions on the phase space (q, p) and introduce a Lagrangian density $\mathcal{L}_f(q, p, t)$ in this space that implies a Lagrangian functional:

$$L_f = \int \mathcal{L}_f\big(q', p', t\big)\, \mathrm{d}^3q'\, \mathrm{d}^3p'. \tag{2.5}$$

Throughout this paper we shall attach primes to field arguments to distinguish them from the particle coordinates, except where we evaluate the fields in the particle subspace (*e.g.*, (2.4) and sect. **5**). We desire to obtain Liouville's equation as the Euler-Lagrange equation corresponding to a suitably chosen Lagrangian. To achieve this we employ the technique of introducing an independent auxiliary function (*e.g.*, [16]) on the phase space, $g(q,p,t)$, and define the Lagrangian to be

$$L_f = \int g\left(\dot{f} + \frac{\partial H}{\partial p_i'}\frac{\partial f}{\partial q_i'} - \frac{\partial H}{\partial q_i'}\frac{\partial f}{\partial p_i'}\right) \mathrm{d}^3q'\,\mathrm{d}^3p'. \tag{2.6}$$

This is a functional of f and g (H is a prescribed function of q and p).

Varying with respect to g, the Euler-Lagrange equation (1.14) with x_μ replaced by (q_i, p_i) yields the Liouville equation (2.4). Varying with respect to f, the Euler-Lagrange equation (with f in place of g) implies that g also obeys Liouville's equation:

$$\dot{g} + \frac{\partial H}{\partial p_i}\frac{\partial g}{\partial q_i} - \frac{\partial H}{\partial q_i}\frac{\partial g}{\partial p_i} = 0. \tag{2.7}$$

A key point about the Lagrangian (2.6) is that the Euler-Lagrange equation for f is independent of g. The nature of the latter will be left unspecified—in particular, it need not have a probability interpretation (note that it has different units to f).

It is straightforward now to write down a Lagrangian from which we may obtain both the individual orbit and the evolution of the ensemble. To this end, we consider a configuration space labelled by the numbers $(q, f(q', p'), g(q', p'))$ and the Lagrangian

$$L_{\mathrm{tot}}\big(q, \dot{q}, f, \dot{f}, g, \dot{g}, t\big) = L\big(q, \dot{q}, t\big) + L_f\big[f, \dot{f}, g, \dot{g}, t\big]. \tag{2.8}$$

In the following we shall be concerned particularly with the particle Lagrangian

$$L\big(q, \dot{q}, t\big) = \frac{1}{2}m\dot{q}_i\dot{q}_i - V(q,t) \tag{2.9}$$

although much of the formalism is independent of this specific form. Here V is of course independent of f and g. The Euler-Lagrange equations for the total system then yield Newton's second law

$$m\ddot{q}_i = -\left.\frac{\partial V(q,t)}{\partial q_i}\right|_{q=q(t)} \tag{2.10}$$

together with the field equations (2.4) and (2.7).

The Hamiltonian version of this theory is easy to derive. We define the momenta conjugate to the particle (q) and field (f) coordinates, respectively, as

$$p_i = \frac{\partial L_{\mathrm{tot}}}{\partial \dot{q}_i} = m\dot{q}_i, \qquad \pi(q,p) = \frac{\delta L_{\mathrm{tot}}}{\delta \dot{f}(q,p)} = g(q,p). \tag{2.11}$$

The momentum conjugate to the coordinate g is zero and hence the Poisson brackets (PBs) between the coordinate and the momentum cannot be satisfied. This variable must therefore be eliminated from the Hamiltonian (this is similar to the situation in the usual canonical treatments of Schrödinger's equation and Maxwell's equations [17]).

Then a Legendre transformation gives for the total Hamiltonian

$$
\begin{aligned}
(2.12)\qquad H_{\mathrm{tot}} &= p_i\dot{q}_i + \int \pi\big(q',p'\big)\dot{f}\big(q',p'\big)\,\mathrm{d}^3q'\,\mathrm{d}^3p' - L_{\mathrm{tot}} \\
&= H - \int \pi\left(\frac{\partial H}{\partial p'_i}\frac{\partial f}{\partial q'_i} - \frac{\partial H}{\partial q'_i}\frac{\partial f}{\partial p'_i}\right)\mathrm{d}^3q'\,\mathrm{d}^3p',
\end{aligned}
$$

where

$$
(2.13)\qquad H(q,p,t) = p_i\dot{q}_i - L = \frac{1}{2m}p_ip_i + V(q,t).
$$

Thus,

$$
(2.14)\qquad H_{\mathrm{tot}} = \frac{1}{2m}p_ip_i + V - \int \pi\left(\frac{p'_i}{m}\frac{\partial f}{\partial q'_i} - \frac{\partial V}{\partial q'_i}\frac{\partial f}{\partial p'_i}\right)\mathrm{d}^3q'\,\mathrm{d}^3p'.
$$

Hamilton's equations for the total system,

$$
(2.15)\qquad \dot{q}_i = \frac{\partial H_{\mathrm{tot}}}{\partial p_i},\qquad \dot{p}_i = -\frac{\partial H_{\mathrm{tot}}}{\partial q_i},\qquad \dot{f} = \frac{\delta H_{\mathrm{tot}}}{\delta \pi},\qquad \dot{\pi} = -\frac{\delta H_{\mathrm{tot}}}{\delta f},
$$

give the particle and field equations (2.3), (2.4) and (2.7) (with g replaced by π).

3. – Generalization to an interacting system

Although in the theory just described the particle and the fields enter into a single Hamiltonian, they evolve independently in the sense that neither is a physical source of the other. We now consider how the theory can be generalized to provide a model of an interacting field-particle system in which the particle and the fields act on one another, so that in particular the particle motion is modified, in such a way that the evolution of one of the fields is undisturbed. The purpose of this is to illustrate the kind of idea we shall use in our treatment of quantum systems.

Suppose, then, we modify the Hamiltonian (2.14) by introducing an interaction term into the particle component:

$$
(3.1)\quad H_{\mathrm{tot}} = \frac{1}{2m}p_ip_i + V(q,t) + U\big(q,p,f(q,p),t\big) - \int \pi\left(\frac{p'_i}{m}\frac{\partial f}{\partial q'_i} - \frac{\partial V}{\partial q'_i}\frac{\partial f}{\partial p'_i}\right)\mathrm{d}^3q'\,\mathrm{d}^3p'.
$$

The most general form that will be assumed for U is that it is a function of the particle phase space coordinates, and a local function of f. This dependence implies that the particle Hamilton equations (2.3) and eq. (2.7) for the conjugate field momentum will be modified, but not Liouville's equation (2.4) for f. From the point of view of physics this move is illegitimate as it makes the behaviour of an individual particle depend on a fictitious ensemble (described by f) of which it is a representative. Suppose, however, that we attribute to f a new primary property that it is descriptive of a physical field, and that only as a secondary property it has a (additional) statistical interpretation. Then such action on the particle would be meaningful. In the context of the classical ensemble theory we are using to illustrate the general idea the proposed generalization would not be a particularly appealing or well-motivated thing to do, but as a point of principle such a theory would be consistent. In this connection, consistency requires that the new term does not affect the (now secondary) statistical interpretation of f in the sense that its presence in the Hamiltonian should not alter Liouville's equation when the variation is made, and that is why U is assumed to be independent of π. Although f is not affected, this does not mean that there is no reciprocal action of the particle. Rather, this exists but is confined to the equation obeyed by π which is modified by a source term. We shall not write this down since we shall examine an equation of this type below in the analogous quantum case.

Mathematically, our proposal is similar to the conventional description of any interacting field-particle system, with the novel element here that one component of the total system—one of the fields (f)—forms a closed system (it is independent of the conjugate momentum and the particle variables).

4. – Canonical treatment of wave and particle in quantum mechanics

The method we have used to treat in a single canonical formalism the dynamics of a classical particle and an associated field which also has an ensemble interpretation provides a clue as to how to proceed in the quantum case. Actually, the connection between the classical and quantum cases is deeper than just an analogy for, as we shall see later, the Liouville equation plays a key role in selecting a consistent set of admissible quantum particle motions (sect. **5**), and indeed the quantum formalism can be written in a Liouvillian language of the type just described in sect. **3** (see sect. **3** of the following paper). To establish the precise form of the latter that corresponds to quantum mechanics, we begin with a Lagrangian defined directly in terms of the Schrödinger field variables, taking as our cue the method of auxiliary functions used for the classical Liouville function.

It is convenient, in particular for the HJ theory to be developed later, to represent the field $\psi(q,t)$ by the two real fields ρ and S defined in sect. **1**. Introducing two independent auxiliary real fields $g_1(q,t)$ and $g_2(q,t)$ the field Lagrangian is

$$L_\psi = \int \left\{ g_1\left(\dot\rho + \frac{1}{m}\frac{\partial}{\partial q_i'}\left(\rho\frac{\partial S}{\partial q_i'}\right)\right) + g_2\left(\dot S + \frac{1}{2m}\frac{\partial S}{\partial q_i'}\frac{\partial S}{\partial q_i'} + Q + V\right)\right\} \mathrm{d}^3 q', \tag{4.1}$$

where in the integrand $\dot\rho = \partial\rho(q',t)/\partial t$, etc.

Including the particle variables, the total Lagrangian will be

$$L_{\text{tot}} = L_\psi + L \tag{4.2}$$

with

$$L\big(\rho(q,t), q, \dot q, t\big) = \frac{1}{2}m\dot q_i^2 - V(q,t) - Q\big(\rho(q,t)\big), \tag{4.3}$$

where we represent the quantum effects through the quantum potential. The total physical system now comprises the fields ρ, S, g_1 and g_2, and the particle. We shall refer to this as a "wave-particle" system with the understanding that this includes the auxiliary fields as well as the wavefunction.

Variation of (4.2) with respect to g_1 and g_2 yields, respectively, eqs. (1.5) and (1.3):

$$\frac{\partial\rho(q',t)}{\partial t}+\frac{1}{m}\frac{\partial}{\partial q'_i}\left(\rho(q',t)\frac{\partial S(q',t)}{\partial q'_i}\right)=0, \tag{4.4}$$

$$\frac{\partial S(q',t)}{\partial t}+\frac{1}{m}\frac{\partial S(q',t)}{\partial q'_i}\frac{\partial S(q',t)}{\partial q'_i}+Q(q',t)+V(q',t)=0. \tag{4.5}$$

These equations are equivalent to the Schrödinger equation for ψ if the fields obey conditions corresponding to those imposed on the wavefunction (single-valuedness, boundedness, etc.). Next, varying with respect to ρ and S gives, in turn,

$$\begin{aligned}&\frac{\partial g_1(q',t)}{\partial t}+\frac{1}{m}\frac{\partial g_1(q',t)}{\partial q'_i}\frac{\partial S(q',t)}{\partial q'_i}=\\ &\frac{\delta}{\delta\rho(q')}\int g_2(q'',t)Q\big(\rho(q'',t)\big)\,\mathrm{d}^3q''-\frac{\delta Q\big(\rho(q(t),t)\big)}{\delta\rho(q')},\end{aligned} \tag{4.6}$$

$$\frac{\partial g_2(q',t)}{\partial t}-\frac{1}{m}\frac{\partial}{\partial q'_i}\left(\rho(q',t)\frac{\partial g_1(q',t)}{\partial q'_i}-g_2(q',t)\frac{\partial S(q',t)}{\partial q'_i}\right)=0. \tag{4.7}$$

The external potential V is absent in these equations, its effect being carried by ρ and S. We can evaluate the integral term in (4.6) in terms of local derivatives of ρ and g_2 but it will prove useful to leave it in this form. It will be noted that in (4.6) the second term on the right-hand side involves the delta-function $\delta(q(t)-q')$ and its derivatives, and represents a particle source term. Finally, varying the variables q, we obtain

$$m\ddot{q}_i=-\frac{\partial}{\partial q_i}(V+Q)\bigg|_{q=q(t)}. \tag{4.8}$$

In passing to the Hamiltonian version of this theory we note that in our approach ρ and S have been treated as coordinates and not as canonically conjugate variables as is usually assumed (where one or other of these fields, or equivalently ψ or ψ^*, is regarded as a momentum variable [17]). As discussed previously, we have developed the theory in this way so that the field equations (*i.e.*, Schrödinger's equation) are not modified by the inclusion of the field in the particle component of the total Lagrangian and Hamiltonian. In the conventional approach this inclusion would introduce a (singular) particle source term in the Schrödinger equation. Our approach necessitates the introduction of additional field variables g_1 and g_2 whose coupled equations of motion do, as we have seen, include a source term.

The momenta corresponding to the variables g_1 and g_2 are zero and hence, as in sect. **2**, these variables must be eliminated from the Hamiltonian. Points in the phase space of the total system are then labelled just by the coordinates $(q,\rho(q'),S(q'),p,\pi_\rho(q'),\pi_S(q'))$. Here the canonical momenta are given by

$$p_i=\frac{\partial L_{\rm tot}}{\partial\dot{q}_i}=m\dot{q}_i,\qquad \pi_\rho(q')=\frac{\delta L_{\rm tot}}{\delta\dot{\rho}(q')}=g_1(q'),\qquad \pi_S(q')=\frac{\delta L_{\rm tot}}{\delta\dot{S}(q')}=g_2(q'). \tag{4.9}$$

Generally in Hamiltonian theory the canonical momenta do not have direct physical significance but in this theory the relations (4.9) imply that we may equivalently treat

π_ρ and π_S as the additional physical fields, and p as the physical momentum. Making a Legendre transformation, the Hamiltonian will be

$$H_{\text{tot}} = H + \int \Big\{ -\pi_\rho \Big(\frac{1}{m} \frac{\partial}{\partial q'_i} \Big(\rho \frac{\partial S}{\partial q'_i} \Big) \Big) - \pi_S \Big(\frac{1}{2m} \frac{\partial S}{\partial q'_i} \frac{\partial S}{\partial q'_i} + Q + V \Big) \Big\} \, \mathrm{d}^3 q' \tag{4.10}$$

with

$$H(\rho, q, p, t) = p_i \dot{q}_i - L = \frac{1}{2m} p_i p_i + V(q,t) + Q\big(\rho(q)\big). \tag{4.11}$$

Although the field component is here defined only on q-space, the theory is of the type described in sect. **3**.

In this phase space the PB between two functionals A and B is defined by

$$\begin{aligned} \{A, B\} = {} & \frac{\partial A}{\partial q_i} \frac{\partial B}{\partial p_i} - \frac{\partial A}{\partial p_i} \frac{\partial B}{\partial q_i} + \\ & + \int \Big(\frac{\delta A}{\delta \rho(q')} \frac{\delta B}{\delta \pi_\rho(q')} + \frac{\delta A}{\delta S(q')} \frac{\delta B}{\delta \pi_S(q')} - \frac{\delta A}{\delta \pi_\rho(q')} \frac{\delta B}{\delta \rho(q')} - \frac{\delta A}{\delta \pi_S(q')} \frac{\delta B}{\delta S(q')} \Big) \, \mathrm{d}^3 q'. \end{aligned} \tag{4.12}$$

The basic PBs are

$$\big\{ q_i, p_j \big\} = \delta_{ij}, \quad \big\{ \rho(q'), \pi_\rho(q'') \big\} = \delta(q' - q''), \quad \big\{ S(q'), \pi_S(q'') \big\} = \delta(q' - q'') \tag{4.13}$$

with all others zero. Hamilton's equations now give,

$$\dot{q}_i = \big\{ q_i, H_{\text{tot}} \big\} = \frac{\partial H_{\text{tot}}}{\partial p_i} = \frac{1}{m} p_i, \tag{4.14}$$

$$\dot{p}_i = \big\{ p_i, H_{\text{tot}} \big\} = -\frac{\partial H_{\text{tot}}}{\partial q_i} = -\frac{\partial}{\partial q_i} \big[V(q,t) + Q\big(\rho(q)\big) \big], \tag{4.15}$$

$$\dot{\rho}(q', t) = \big\{ \rho, H_{\text{tot}} \big\} = \frac{\delta H_{\text{tot}}}{\delta \pi_\rho(q')} = -\frac{1}{m} \frac{\partial}{\partial q'_i} \Big(\rho(q') \frac{\partial S(q')}{\partial q'_i} \Big), \tag{4.16}$$

$$\dot{S}(q', t) = \big\{ S, H_{\text{tot}} \big\} = \frac{\delta H_{\text{tot}}}{\delta \pi_S(q')} = -\frac{1}{2m} \frac{\partial S(q')}{\partial q'_i} \frac{\partial S(q')}{\partial q'_i} - V(q', t) - Q\big(\rho(q')\big), \tag{4.17}$$

$$\begin{aligned} \dot{\pi}_\rho(q', t) = \big\{ \pi_\rho, H_{\text{tot}} \big\} = {} & -\frac{\delta H_{\text{tot}}}{\delta \rho(q')} \\ = {} & -\frac{1}{m} \frac{\partial \pi_\rho(q')}{\partial q'_i} \frac{\partial S(q')}{\partial q'_i} + \frac{\delta}{\delta \rho(q')} \int \pi_S(q'') Q\big(\rho(q'')\big) \, \mathrm{d}^3 q'' - \frac{\delta Q\big(\rho(q)\big)}{\delta \rho(q')}, \end{aligned} \tag{4.18}$$

$$\dot{\pi}_S(q', t) = \big\{ \pi_S, H_{\text{tot}} \big\} = -\frac{\delta H_{\text{tot}}}{\delta S(q')} = \frac{1}{m} \frac{\partial}{\partial q'_i} \Big(\rho(q') \frac{\partial \pi_\rho(q')}{\partial q'_i} - \pi_S(q') \frac{\partial S(q')}{\partial q'_i} \Big), \tag{4.19}$$

where on the right-hand sides of these equations we write

$$\begin{aligned} & \rho(q') = \rho(q', t), \qquad S(q') = S(q', t), \qquad \pi_\rho(q') = \pi_\rho(q', t), \\ & \pi_S(q') = \pi_S(q', t), \qquad q_i = q_i(t), \qquad p_i = p_i(t). \end{aligned} \tag{4.20}$$

The motion of the composite system is thus represented as a single moving point in the total phase space. As discussed in sect. **3**, the coupled fields ρ and S have a dual interpretation: they define a physical field (represented by Q) and, as a secondary property, have a statistical interpretation (ρ represents the probability distribution of the particle—see sect. **5**).

To clarify the meaning of the time derivatives in these equations, note that "dot" represents the total time derivative:

$$\frac{\mathrm{d}}{\mathrm{d}t} = \frac{\partial}{\partial t} + \dot{q}_i \frac{\partial}{\partial q_i} + \dot{p}_i \frac{\partial}{\partial p_i} + \\ + \int \mathrm{d}^3 q' \left(\dot{\rho}(q') \frac{\delta}{\delta \rho(q')} + \dot{S}(q') \frac{\delta}{\delta S(q')} + \dot{\pi}_\rho(q') \frac{\delta}{\delta \pi_\rho(q')} + \dot{\pi}_S(q') \frac{\delta}{\delta \pi_S(q')} \right). \tag{4.21}$$

The term $\partial/\partial t$ applies to time dependence at a fixed point in the phase space, *i.e.*, to change other than that due to the natural evolution of the system. Thus, for example, when we write $\partial S/\partial t$ for $\dot{S}$ this is to be interpreted as the total time derivative and is represented by the fifth term on the right-hand side of (4.21).

As required, the field equations for ρ and S are unmodified by the particle variables, but the equations for the conjugate momenta are. We can see the effect of the source term in a more transparent way by a redefinition of variables. Writing the canonical momenta in terms of the momenta conjugate to ψ and ψ^*, the latter obey the complex conjugate Schrödinger equation and the Schrödinger equation, respectively, modified by additional source terms (see eq. (4.5) of the following paper), and eqs. (4.18) and (4.19) (and (4.6) and (4.7) for g_1 and g_2) are equivalent to these. (It follows that for the pure field case the equations for the conjugate momenta are equivalent to the Schrödinger equation.) The presence of the particle source term in the momentum field equations implies that the additional fields cannot generally be combined so that they obey the linear superposition principle.

We can solve for the particle motion by first solving (4.16) and (4.17) for the fields ρ and S and then computing Q from (1.4). Inserting this in (4.14) and (4.15) we can solve for

$$q = q\big(q_0, p_0, t\big), \qquad p = p\big(q_0, p_0, t\big). \tag{4.22}$$

In the theory presented so far there is no restriction on the initial coordinates q_0 and p_0. The particle Hamilton equations are those suggested by the deBB theory, (1.8), but we have not yet considered the role of the deBB law (1.2).

The formal generalization of the above theory to a system of N bodies, including an external electromagnetic field, proceeds in an obvious way. Specifically, in (4.10) we make the replacements

$$p_i \longrightarrow p_i - eA_i(q), \qquad \frac{\partial S}{\partial q'_i} \longrightarrow \frac{\partial S}{\partial q'_i} - eA_i(q') \tag{4.23}$$

and extend the range of the index to $i = 1, \ldots, 3N$. With this extension it becomes possible to apply the theory to a typical measurement process. Using analogous techniques the theory may in principle also be extended to describe systems with spin, relativistic matter systems, and quantum fields. These extensions will be discussed in detail elsewhere.

5. – Liouville's theorem for the wave-particle system

5˙1. *Derivation of Liouville's equation for the particle*. – So far we have presented a canonical formalism which treats together the Schrödinger field and the particle moving in the quantum and external potentials. For the reason given in sect. **1** this theory is not yet complete if it is our aim that an ensemble of particle motions should reproduce the quantum distribution ρ—there are "too many" potential motions. To see that the ensemble associated with the theory presented so far is more general than that desired, we examine the probability distributions implied by Liouville's theorem for the combined system, and derive the equation obeyed by the partial distribution in the reduced phase space of the particle.

Consider an ensemble of composite systems with distribution $P[q,p,\rho(q'),S(q'),\pi_\rho(q'),\pi_S(q'),t]$ (in general P will depend on the derivatives of the fields; see, *e.g.*, (5.46)). Since the motion of each ensemble element is governed by Hamilton's equations, this distribution will obey Liouville's equation in the total phase space:

$$\frac{\mathrm{d}P}{\mathrm{d}t}=0, \tag{5.1}$$

where the total time derivative is defined by (4.21). That is

$$\begin{aligned}\frac{\partial P}{\partial t}+\frac{\partial H_{\text{tot}}}{\partial p_i}\frac{\partial P}{\partial q_i}-\frac{\partial H_{\text{tot}}}{\partial q_i}\frac{\partial P}{\partial p_i}+\\ +\int\left(\frac{\delta H_{\text{tot}}}{\delta\pi_\rho}\frac{\delta P}{\delta\rho}+\frac{\delta H_{\text{tot}}}{\delta\pi_S}\frac{\delta P}{\delta S}-\frac{\delta H_{\text{tot}}}{\delta\rho}\frac{\delta P}{\delta\pi_\rho}-\frac{\delta H_{\text{tot}}}{\delta S}\frac{\delta P}{\delta\pi_S}\right)\mathrm{d}^3q'=0.\end{aligned} \tag{5.2}$$

The functional P is assumed to be normalized:

$$\int P\big[q,p,\rho(q'),S(q'),\pi_\rho(q'),\pi_S(q'),t\big]\,\mathrm{d}^3q\,\mathrm{d}^3p\prod_{q'}\mathrm{d}\rho(q')\,\mathrm{d}S(q')\,\mathrm{d}\pi_\rho(q')\,\mathrm{d}\pi_S(q')=1, \tag{5.3}$$

a condition that is preserved by (5.2). The particle phase space distribution function is defined by the projection of P on the (q,p)-coordinates:

$$f(q,p,t)=\int P\big[q,p,\rho(q'),S(q'),\pi_\rho(q'),\pi_S(q'),t\big]\prod_{q'}\mathrm{d}\rho(q')\,\mathrm{d}S(q')\,\mathrm{d}\pi_\rho(q')\,\mathrm{d}\pi_S(q'). \tag{5.4}$$

The normalization (5.3) then becomes

$$\int f(q,p,t)\,\mathrm{d}^3q\,\mathrm{d}^3p=1. \tag{5.5}$$

The evolution of f is obtained by integrating (5.2) over the field variables. It is easy to see that the final (integral) term in (5.2) will vanish if we perform a functional partial integration and assume that $P\to 0$ when the fields$\to\infty$ (see (1.16)). We obtain finally

$$\frac{\partial f}{\partial t}+\frac{\partial H}{\partial p_i}\frac{\partial f}{\partial q_i}-\int\frac{\partial H}{\partial q_i}\frac{\partial P}{\partial p_i}\prod_{q'}\mathrm{d}\rho(q')\,\mathrm{d}S(q')\,\mathrm{d}\pi_\rho(q')\,\mathrm{d}\pi_S(q')=0. \tag{5.6}$$

For general P the final term in (5.6) cannot be evaluated in terms of just f because the quantum potential in H depends on ρ. We now show how this term can be evaluated in terms of just f when P describes a quantum-mechanical pure state.

We first use the usual probability formula to write P in the form

$$P = \Omega\big[q, p, \pi_\rho(q'), \pi_S(q'), t \mid \rho(q'), S(q')\big] P_\psi\big[\rho(q'), S(q'), t\big], \tag{5.7}$$

where Ω is the conditional probability density of the variables q, p, π_ρ, π_S given ρ, S and P_ψ is the marginal distribution of the wavefunction:

$$\begin{aligned} &P_\psi\big[\rho(q'), S(q'), t\big] = \\ &\int P\big[q, p, \rho(q'), S(q'), \pi_\rho(q'), \pi_S(q'), t\big]\, \mathrm{d}^3q\, \mathrm{d}^3p \prod_{q'} \mathrm{d}\pi_\rho(q')\, \mathrm{d}\pi_S(q'). \end{aligned} \tag{5.8}$$

The functional P_ψ is the probability distribution of wavefunctions appearing in the usual quantum-mechanical density matrix. Integrating (5.2), doing some partial integrations, and using the fact that H_{tot} is linear in the field momenta, P_ψ obeys its own Liouville equation:

$$\frac{\mathrm{d}P_\psi}{\mathrm{d}t} = \frac{\partial P_\psi}{\partial t} + \int \left(\frac{\delta H_{\mathrm{tot}}}{\delta \pi_\rho} \frac{\delta P_\psi}{\delta \rho} + \frac{\delta H_{\mathrm{tot}}}{\delta \pi_S} \frac{\delta P_\psi}{\delta S} \right) \mathrm{d}^3q' = 0. \tag{5.9}$$

This equation depends only on the variables ρ, S which is expected since these quantities are dynamically independent of all the others. This means that we can freely choose an appropriate form for P_ψ. Here we shall only consider pure states (mixed states will be discussed in another paper) so that P_ψ is a delta-function in the ρ, S variables. Thus

$$P_\psi = \prod_{q'} \delta\big(\rho(q') - \rho(q', t)\big) \delta\big(S(q') - S(q', t)\big) \tag{5.10}$$

and the total distribution function has the form

$$\begin{aligned} P = \Omega\big[q, p, \pi_\rho(q'), \pi_S(q'), t \mid \rho(q'), S(q')\big] \cdot \\ \cdot \prod_{q'} \delta\big(\rho(q') - \rho(q', t)\big) \delta\big(S(q') - S(q', t)\big). \end{aligned} \tag{5.11}$$

In this connection, note that we could not assume that P is also a delta-function in the fields π_ρ and π_S since fixed solutions for these depend on the particle variables (through the source term in the coupled equations (4.18) and (4.19)) and the latter are distributed. Thus, we evaluate P for a fixed solution of Schrödinger's equation so that the distribution is restricted to lie on the Schrödinger phase space trajectory, but for each such trajectory the particle phase space coordinates (and the field momenta) are distributed. The connection between the particle distribution f and Ω will be established below.

To show that (5.11) is a solution of the Liouville equation we substitute it into the left-hand side of (5.1):

$$\frac{\mathrm{d}P}{\mathrm{d}t} = \Omega \frac{\mathrm{d}\prod_{q'} \delta_\rho \delta_S}{\mathrm{d}t} + \frac{\mathrm{d}\Omega}{\mathrm{d}t} \prod_{q'} \delta_\rho \delta_S, \tag{5.12}$$

where the deltas correspond to those in (5.11), in an obvious notation. The first term on the right-hand side of (5.12) is zero (or equivalently, (5.10) obeys (5.9)) since, when applied to the δ_ρ-factor, for example, the total time derivative is

$$\frac{\mathrm{d}}{\mathrm{d}t} \prod_{q'} \delta_\rho = \left(\frac{\partial}{\partial t} + \int \mathrm{d}^3 q \left(\dot{\rho}(q) \frac{\delta}{\delta \rho(q)} \right) \right) \prod_{q'} \delta_\rho \tag{5.13}$$

and evaluating the partial time derivative gives

$$\frac{\partial}{\partial t} \prod_{q'} \delta_\rho = - \int \mathrm{d}^3 q \left(\dot{\rho}(q) \frac{\delta}{\delta \rho(q)} \right) \prod_{q'} \delta_\rho . \tag{5.14}$$

The same result holds for δ_S, which establishes that the pure state is preserved by Liouville's equation. Hence, (5.11) is a solution of Liouville's equation (5.2) if the functional Ω obeys the equation

$$\frac{\mathrm{d}\Omega}{\mathrm{d}t} \prod_{q'} \delta_\rho \delta_S = 0, \tag{5.15}$$

or, integrating over the field coordinates,

$$\begin{aligned} &\left.\frac{\partial \Omega}{\partial t}\right|_{\substack{\rho=\rho(t)\\ S=S(t)}} + \frac{\partial H}{\partial p_i}\frac{\partial \Omega}{\partial q_i} - \frac{\partial H}{\partial q_i}\frac{\partial \Omega}{\partial p_i} + \\ &+ \int \left(\frac{\delta H_{\mathrm{tot}}}{\delta \pi_\rho}\frac{\partial \Omega}{\delta \rho(t)} + \frac{\delta H_{\mathrm{tot}}}{\delta \pi_S}\frac{\delta \Omega}{\delta S(t)} - \frac{\delta H_{\mathrm{tot}}}{\delta \rho(t)}\frac{\delta \Omega}{\delta \pi_\rho} - \frac{\delta H_{\mathrm{tot}}}{\delta S(t)}\frac{\delta \Omega}{\delta \pi_S} \right) \mathrm{d}^3 q' = 0. \end{aligned} \tag{5.16}$$

We now show that the assumption of a pure state, (5.11), reduces (5.6) to an equation in just f. Substituting (5.11) into (5.4) gives

$$f(q,p,t) = \int \Omega\big[q, p, \pi_\rho(q'), \pi_S(q'), t \mid \rho(q',t), S(q',t)\big] \prod_{q'} \mathrm{d}\pi_\rho(q')\, \mathrm{d}\pi_S(q'). \tag{5.17}$$

That is, the particle distribution function is the functional Ω evaluated along the field trajectory and integrated over the field momenta. Note that f depends on the fields ρ and S (an explicit expression is given in subsect. **5**˙2). Then, substituting (5.11) into (5.6) and using (5.17) gives the desired result:

$$\frac{\partial f}{\partial t} + \frac{\partial H}{\partial p_i}\frac{\partial f}{\partial q_i} - \frac{\partial H}{\partial q_i}\frac{\partial f}{\partial p_i} = 0. \tag{5.18}$$

Here ρ in the quantum potential is now time-dependent.

To clarify the meaning of the time derivative in (5.18) we derive the latter from (5.16) by integrating over the field momenta. By partial functional integration the last two terms in the integral in (5.16) vanish and, because H_{tot} is linear in the field momenta, we find

$$\left.\frac{\partial f}{\partial t}\right|_{\substack{\rho=\rho(t)\\ S=S(t)}} + \frac{\partial H}{\partial p_i}\frac{\partial f}{\partial q_i} - \frac{\partial H}{\partial q_i}\frac{\partial f}{\partial p_i} + \int\left(\frac{\delta H_{\mathrm{tot}}}{\delta\pi_\rho}\frac{\delta f}{\delta\rho(t)} + \frac{\delta H_{\mathrm{tot}}}{\delta\pi_S}\frac{\delta f}{\delta S(t)}\right)\mathrm{d}^3q' = 0. \tag{5.19}$$

This equation is the same as (5.18) if we take note of (5.17) which shows that the time dependence of f has two sources—the explicit dependence of Ω on t and its implicit dependence through the fields. That is,

$$\frac{\partial f}{\partial t} = \left.\frac{\partial f}{\partial t}\right|_{\rho,S} + \int\left(\dot\rho\frac{\delta f}{\delta\rho} + \dot S\frac{\delta f}{\delta S}\right)\mathrm{d}^3q'. \tag{5.20}$$

It is therefore the "total" partial time derivative which appears in (5.18).

Inserting the explicit form of H from (4.11) we obtain finally the following equation of evolution for the particle distribution function:

$$\frac{\partial f}{\partial t} + \frac{p_i}{m}\frac{\partial f}{\partial q_i} - \frac{\partial\big(V(q,t)+Q\big(\rho(q,t)\big)\big)}{\partial q_i}\frac{\partial f}{\partial p_i} = 0. \tag{5.21}$$

Thus, under the assumption of a pure state, we may restrict attention to the subspace (q,p) of the total phase space, the total potential $V+Q$ in (5.16) being treated as a prescribed function of space and time. This is Liouville's equation for the particle which we may evidently write as

$$\frac{\mathrm{d}f}{\mathrm{d}t} = \frac{\partial f}{\partial t} + \dot q_i\frac{\partial f}{\partial q_i} + \dot p_i\frac{\partial f}{p_i} = 0, \tag{5.22}$$

where the partial time derivative is given by (5.20). We may thus treat f as a constant of the motion in the usual way.

To see that the flow implied by (5.21) does not generally reproduce the quantal particle distribution ρ, consider the space- (q-) projection. Defining the spatial distribution to be

$$n(q,t) = \int f(q,p,t)\,\mathrm{d}^3p, \tag{5.23}$$

we have

$$\frac{\partial n}{\partial t} + \frac{1}{m}\frac{\partial\big(n\bar p_i\big)}{\partial q_i} = 0, \tag{5.24}$$

where

$$\bar p_i(q,t) = \int p_i f\,\mathrm{d}^3p/n \tag{5.25}$$

is the local mean momentum. If the particle is distributed according to ρ, (5.24) should coincide with the field equation (1.5) but clearly in general it does not. Even if $n(q, t = 0) = \rho(q, t = 0)$, $n \neq \rho$ for other times since the mean momentum is arbitrary. As an example of a distribution that is incompatible with the quantum distribution we note that a possible solution of (5.21) is a "pure state" for the particle:

$$f(q, p, t) = \delta\big(q - q(t)\big)\delta\big(p - p(t)\big). \tag{5.26}$$

The q-projection of this function is a δ-function for all time and we know that a quantal distribution cannot have this form.

5˙2. *Constraints giving the quantal distribution: general form of the phase space distribution function.* – To ensure that the ensemble of particles is distributed as required we have to restrict the flow of permissible motions in some way. Our basic constraint will be to require that the space-projected density n coincides with ρ for all time. Then from (5.23) and (5.24)

$$\rho(q, t) = \int f(q, p, t)\, \mathrm{d}^3 p\,, \tag{5.27}$$

$$\frac{\partial \rho}{\partial t} + \frac{1}{m}\frac{\partial\big(\rho \bar{p}_i\big)}{\partial q_i} = 0\,, \tag{5.28}$$

so that the current is given by $\rho\bar{p}_i$. We now examine the implications of this assumption for the flow, taking into account that (5.21) must be consistent with Hamilton's equations (4.16) and (4.17) for the fields ρ and S, *i.e.*, Schrödinger's equation. In this way we shall exhibit the most general particle phase space distribution that is compatible with the quantal spatial distribution, for particles moving according to Hamilton's equations (4.14) and (4.15). As envisaged in sect. **3** the field coordinate ρ is now playing two roles: it is a component of a physical field which contributes to the force acting on the particle and, as we shall see, it is a component of the particle distribution function; there is no conceptual inconsistency between these two roles. This dual role has the effect of making Liouville's equation (5.21) highly nonlinear.

Comparing (4.16) with (5.28) shows that the local mean momentum must be restricted by the condition

$$\bar{p}_i = \frac{\partial S}{\partial q_i} + \frac{1}{\rho}X_i, \tag{5.29}$$

$$\frac{\partial X_i}{\partial q_i} = 0, \tag{5.30}$$

where the vector field $X_i(q, t)$ may depend on the fields. The evolution equation (5.28) is then the same as the Hamilton equation for ρ. The divergenceless of X_i gives a second constraint on the flow.

Multiplying (5.21) by p_i and integrating over p we get an equation of evolution for the local mean momentum:

$$\frac{\partial}{\partial t}\big(\rho\bar{p}_i\big) + \frac{1}{m}\frac{\partial}{\partial q_j}\big(\rho\overline{p_i p_j}\big) = -\rho\frac{\partial(V + Q)}{\partial q_i}, \tag{5.31}$$

where

$$\overline{p_i p_j}(q,t) = \int p_i p_j f \, \mathrm{d}^3 p/\rho \tag{5.32}$$

is the local mean momentum stress tensor. Now, using the Hamilton equation (4.16) for ρ, the q-derivative of the Hamilton equation (4.17) for S may be brought to the form

$$\frac{\partial}{\partial t}\left(\rho \frac{\partial S}{\partial q_i}\right) + \frac{1}{m}\frac{\partial}{\partial q_j}\left(\rho \frac{\partial S}{\partial q_i}\frac{\partial S}{\partial q_j}\right) = -\rho \frac{\partial (V+Q)}{\partial q_i}. \tag{5.33}$$

Subtracting (5.33) from (5.32) and using (5.29), then gives

$$\frac{\partial X_i}{\partial t} + \frac{1}{m}\frac{\partial X_{ij}}{\partial q_j} = 0, \tag{5.34}$$

where

$$\overline{p_i p_j} = \frac{\partial S}{\partial q_i}\frac{\partial S}{\partial q_j} + \frac{1}{\rho} X_{ij} \tag{5.35}$$

and the tensor field $X_{ij}(q,t)$ is symmetric. Equation (5.34) is a third constraint on the flow, analogous to (5.30). If the condition (5.34) is obeyed, eq. (5.31) for the mean momentum coincides with eq. (5.33) derived from the Schrödinger equation.

Now, ρ is uniquely fixed by the two coupled Hamilton equations (4.16) and (4.17) so the information contained in the Liouville equation pertaining to ρ should at most reproduce the implications of these two equations. Hence eq. (5.28) for ρ and eq. (5.31) for $\bar{p}_i$, which can in principle be solved together to give ρ, must already exhaust the independent morsels of information on ρ implied by the Liouville equation, and must be equivalent to deductions from the Schrödinger equation (these two equations are independent since, for example, the latter involves V). This means that the equations for all the higher momentum moments deducible from (5.21), which are functions of q and t, must simply reproduce the information on ρ contained in these first two moment equations, or equivalently in the Schrödinger equation. This requirement imposes constraints on the higher moments, and consequently on the distribution function, as we now see. (Actually, all possible space-projected equations must reproduce just implications of Schrödinger's equation. For polynomial functions of p with (q,t)-dependent coefficients this will be ensured by conditions on the momentum moments, and we may confine attention to the latter as they give sufficient information to determine the distribution f as a function of p, as shown below).

The trend implicit in eqs. (5.28)-(5.35) is clear. Defining the n-th momentum moment as

$$\overline{p_{i_1} \cdots p_{i_n}}(q,t) = \int p_{i_1} \cdots p_{i_n} f \, \mathrm{d}^3 p/\rho, \tag{5.36}$$

we deduce from (5.21)

$$\frac{\partial}{\partial t}\left(\rho \overline{p_{i_1} \cdots p_{i_{n-1}}}\right) + \frac{1}{m}\frac{\partial}{\partial q_{i_n}}\left(\rho \overline{p_{i_1} \cdots p_{i_n}}\right) = -\rho \sum_{\mathbf{P}} \overline{p_{i_1} \cdots p_{i_{n-2}}} \frac{\partial (V+Q)}{\partial q_{i_{n-1}}}, \tag{5.37}$$

where $\mathbf{P}$ denotes permutation of the indices and $n = 1, \ldots, \infty$ with the convention that

$$\overline{p_{i_0}} = 1, \qquad \overline{p_{i_r}} = 0, \quad r < 0. \tag{5.38}$$

Likewise, the field Hamilton equations (4.16) and (4.17) imply, with the same convention,

$$\begin{aligned}\frac{\partial}{\partial t}\left(\rho\frac{\partial S}{\partial q_{i_1}}\cdots\frac{\partial S}{\partial_{i_{n-1}}}\right) + \frac{1}{m}\frac{\partial}{\partial q_{i_n}}\left(\rho\frac{\partial S}{\partial q_{i_1}}\cdots\frac{\partial S}{\partial q_{i_n}}\right) &= \\ = -\rho\sum_{\mathbf{P}}\frac{\partial S}{\partial q_{i_1}}\cdots\frac{\partial S}{\partial q_{i_{n-2}}}\frac{\partial(V+Q)}{\partial q_{i_{n-1}}}&.\end{aligned} \tag{5.39}$$

Subtracting these relations, we get

$$\frac{\partial X_{i_1\cdots i_{n-1}}}{\partial t} + \frac{1}{m}\frac{\partial X_{i_1\cdots i_n}}{\partial q_{i_n}} = -\sum_{\mathbf{P}} X_{i_1\cdots i_{n-2}}\frac{\partial(V+Q)}{\partial q_{i_{n-1}}}, \tag{5.40}$$

where

$$\overline{p_{i_1}\cdots p_{i_n}} = \frac{\partial S}{\partial q_{i_1}}\cdots\frac{\partial S}{\partial q_{i_n}} + \frac{1}{\rho}X_{i_1\cdots i_n}, \qquad X_{i_r} = 0, \quad r \leq 0 \tag{5.41}$$

and the tensor field $X_{i_1\cdots i_n}$ is totally symmetric. We shall call the latter the "X-tensor". The set of X-tensors are connected by (5.40), a set of relations which generalize (5.30) and (5.34), and they generally depend on the fields. Under these circumstances the equations obeyed by the space projections of polynomial functions of p simply reproduce implications of the Schrödinger equation. Note that each X-tensor generally appears in three equations in the set (5.40).

Does a distribution f having these properties exist? This is a difficult question to answer in general but we can at least exhibit its explicit form, given that it does exist, by using the method of moments [18]. The method we use fixes the p-dependence of f. Then, as we shall see, it is possible to prove the existence of at least one solution, and in the process fix the q-dependence of f in terms of known functions as well.

The (complex) momentum characteristic function is defined as

$$M(\lambda, q, t) = \int e^{i\lambda_j p_j} f(q,p,t)\,\mathrm{d}^3p \tag{5.42}$$

$$= \rho\left(1 + \sum_{n=1}^{\infty}\frac{i^n}{n!}\lambda_{i_1}\cdots\lambda_{i_n}\overline{p_{i_1}\cdots p_{i_n}}\right), \tag{5.43}$$

using the definition (5.36). Here λ_i is real and we integrate over all p. Inserting (5.41) in (5.43) gives

$$M(\lambda, q, t) = \rho e^{i\lambda_j(\partial S/\partial q_j)} + \sum_{n=1}^{\infty}\frac{i^n}{n!}\lambda_{i_1}\cdots\lambda_{i_n}X_{i_1\cdots i_n}. \tag{5.44}$$

Inverting (5.42) we get for the particle distribution

$$f(q,p,t) = (2\pi)^{-3} \int e^{-i\lambda_j p_j} M(\lambda, q, t)\,\mathrm{d}^3\lambda \tag{5.45}$$

which, with (5.44), gives finally

$$f(q,p,t) = f_\delta(q,p,t) + \theta(q,p,t), \tag{5.46}$$

where

$$f_\delta(q,p,t) = \rho(q,t)\delta\left(p - \frac{\partial S(q,t)}{\partial q}\right) \tag{5.47}$$

and

$$\theta(q,p,t) = (2\pi)^{-3} \int e^{-i\lambda_j p_j} \sum_{n=1}^{\infty} \frac{i^n}{n!} \lambda_{i_1} \cdots \lambda_{i_n} X_{i_1 \cdots i_n}(q,t)\,\mathrm{d}^3\lambda. \tag{5.48}$$

The function (5.46), subject to the constraints that the component θ obeys the relations

$$\int \theta(q,p,t)\,\mathrm{d}^3 p = 0, \qquad \int p_{i_1} \cdots p_{i_n} \theta\,\mathrm{d}^3 p = X_{i_1 \cdots i_n} \tag{5.49}$$

(the first condition comes from (5.27)) where the X-tensors satisfy (5.40), is the most general solution of (5.21) which ensures that the space-projected equations obeyed by polynomial functions of p (with (q,t)-dependent coefficients) will be consistent with the Schrödinger equation. An ensemble of particles moving in accordance with Hamilton's equations (4.14) and (4.15) will generate the quantal distribution ρ if their phase space distribution is (5.46). The dependence of f on the fields will be observed. Note that we have ignored mathematical issues here, such as whether the series that defines θ converges.

To check the validity of (5.46) we can compute its momentum moments and confirm that it obeys (5.21). In fact, the functions f_δ and θ are independent solutions. To check this it is easier (*e.g.*, to avoid the δ-function) to use the evolution equation obeyed by the characteristic function. Inserting (5.42) in (5.21) this is

$$\frac{\partial M}{\partial t} - \frac{i}{m}\frac{\partial^2 M}{\partial \lambda_j \partial q_j} + i\lambda_j \frac{\partial (V+Q)}{\partial q_j} M = 0. \tag{5.50}$$

Using the relations (5.39) and (5.40) it is readily confirmed that each of the components in (5.44) corresponding to f_δ and θ is a solution. Although (5.21) is nonlinear in f we see that it obeys a limited form of the superposition principle. A caveat to this result is that, although it obeys the differential equation, θ cannot be an acceptable solution on its own since it does not give the correct momentum moments (5.27) and (5.36) when integrated over p. Likewise f_δ is not individually acceptable as it does not imply the moments (5.36) (however, f_δ is acceptable if $\theta = 0$ for all q, p).

While the function (5.46) is compatible with the (non-negative) quantal spatial distribution, we have not required so far that it be non-negative everywhere in the particle phase space (q, p), which would justify the appellation "distribution". In analogous studies of phase space functions in quantum mechanics, such as the Wigner function, it is accepted that the functions may have no particular sign since they are not supposed to be representative of an underlying physical motion of an ensemble of particles. Here in contrast f is precisely such a descriptor, and hence we require that it be non-negative: $f \geq 0$. The function f_δ already obeys this condition but it imposes further constraints on θ. The first relation in (5.49) shows that, if finite, θ must be negative for some values of p, for each q. Consider the case where $p \neq \partial S/\partial q$. Then from (5.46) $f = \theta$ so that θ must be positive for those p's for which it is finite, for all q. Hence, θ must be strictly negative for some $p = \partial S/\partial q$, and only there. (If θ is zero for all $p = \partial S/\partial q$ it will be zero everywhere since it must be negative somewhere). Thus, if θ is finite,

$$\theta(q,p,t) \begin{cases} < 0, & \text{for some } p = \partial S/\partial q, \\ \geq 0, & p \neq \partial S/\partial q. \end{cases} \tag{5.51}$$

5˙3. *A special solution.* – We do not enter into the general question of whether a finite function θ can be found that obeys all the conditions (5.40), (5.49), and (5.51) in order that it contributes to a genuine distribution function f. For, as hinted at above, it is clear that there exists at least one solution that satisfies all our criteria: $\theta = 0$ for all q, p and t. This is ensured if we assume that all the X-tensors vanish, which is obviously a possible solution of (5.40). In fact, by virtue of the fact that a solution (here, $f = \theta$) to Liouville's equation (5.22) is a constant of the motion we need merely assume that θ vanishes for all q, p at one instant, for this condition will be preserved for all t. Making this assumption, we have then the solution

$$f(q,p,t) = f_\delta(q,p,t) = \rho(q,t)\delta\left(p - \frac{\partial S(q,t)}{\partial q}\right). \tag{5.52}$$

This solution has the property that no arbitrary functions appear—both the p- and the q-dependences are uniquely fixed in terms of known functions. We conclude that a distribution that obeys Liouville's equation, that is non-negative everywhere in the phase space, and that generates the quantal distribution, is given by (5.52).

However, although (5.52) is a valid solution, the possible existence of finite-θ solutions implies that the conditions we have imposed on solutions to Liouville's equation to ensure compatibility with the Schrödinger equation do not result in a unique distribution. In fact, these conditions do not exhaust those that we may reasonably impose. For example, we may require that the momentum moments have some connection with the quantum-mechanical mean values of the corresponding momentum operators, or there may be natural conditions to be imposed on the q-moments of f. Connected with this, we may, for instance, require that the mean momentum density $\rho\bar{p}_i$ (obeying (5.28)) coincides with the usual expression for the quantum-mechanical current. From (5.29) this implies that $X_i = 0$ and amounts to the assertion that the usual expression for the current is unique. Schrödinger's equation *per se* does not imply this uniqueness for we can add to the usual expression a divergenceless vector to obtain a total current that is consistent with the same spatial distribution, as in (5.29) (an argument may be advanced for the uniqueness of the spin-(1/2) current starting from relativistic considerations and it is possible a similar demonstration could be given for the spin-0 current [19]). However, even if we could demonstrate uniqueness of the current, the single condition $X_i = 0$ will not imply a unique expression for θ (it does not, for example, imply that all the other X-tensors vanish) and other assumptions must be made. And in any case, if our concern is to demonstrate, for example, the uniqueness of the deBB theory (which as we shall see in sect. **6** is connected with f_δ) such a result will be of no assistance for we shall show later using other arguments that this theory is not unique (see the following paper).

6. – Interpretation of the phase space constraint $p = \partial S(q,t)/\partial q$. The de Broglie-Bohm theory

The dependence of the distribution (5.52) on the particle coordinates q and p is expressed through the (q- and t-dependent) field coordinates ρ and S. This function thus pertains not just to the particle subspace (where it is a distribution function) but also to a wider subspace of the phase space of the composite system. To emphasize this dependence we may express the distribution as a functional:

$$f_\delta(q,p,t) \equiv f_\delta\left[q,p,\rho(q',t),S(q',t)\right] = \int \rho(q',t)\delta\left(p - \frac{\partial S(q',t)}{\partial q'}\right)\delta(q-q')\,\mathrm{d}^3q'. \tag{6.1}$$

It is finite only in the region of the total phase space defined by the following relation:

$$p = \frac{\partial S(q,t)}{\partial q}. \tag{6.2}$$

The relation (6.2) makes p a q- and t-dependent function. This is not yet an equation determining the time dependence of p along a particle path, *i.e.*, it is not a solution to Hamilton's equations. It is rather the sought-for constraint on the full set of Hamilton's equations which is sufficient to ensure that the particle phase space flow reproduces the quantal distribution.

This constraint on the available phase space has two interpretations. First, it asserts a relation between the particle position and momentum coordinates q and p and the field coordinate S (where the latter is evaluated along a field trajectory). However, regarded as a constraint, this relation restricts only the particle coordinates and not S. Hence we have a second interpretation: regarding S as a given "external" function, (6.2) implies a relation just between the particle momentum and position coordinates which defines a moving curve in the particle subspace to which the particle motion is confined. The value of p is uniquely fixed when we specify the particle position q. Conversely, given the momentum, we can in principle invert (6.2) to obtain the associated position although in general this is not unique (indeed, there can be an infinite number of q's associated with a single momentum value; *e.g.*, for a real stationary state, $p = 0$ for all q (outside nodes where the right-hand side of (6.2) is undefined)). Our statistical argument of sect. **5** has therefore resulted in a condition that limits the motion of individual members of the ensemble of particles.

Although (6.2) is not a restriction on S, it can be used to construct possible initial phase functions. Thus, if

$$p_{i0} = \mu_i(q_0)\,, \tag{6.3}$$

where $\mu_i(q)$ is a given single-valued function, we can define

$$S_0(q_0) = \int^{q_0} \mu_i(q)\, \mathrm{d}^3 q_i. \tag{6.4}$$

The consistency of the constraint (6.2) may be demonstrated by establishing its compatibility with Hamilton's equations. We note first that (6.2) is automatically consistent with the field Hamilton equations (4.16)-(4.19) since these are independent of p. Next, we may demonstrate that (6.2) is consistent with Hamilton's equation for p by showing that the latter follows from the other Hamilton equations when we assert the validity of (6.2). To this end, we insert the position $q(t)$ in (6.2):

$$p(t) = \frac{\partial S\big(q(t), t\big)}{\partial q}. \tag{6.5}$$

Then

$$\dot{p}_i = \left(\dot{q}_j \frac{\partial}{\partial q_j} + \int \mathrm{d}^3 q' \dot{S}(q') \frac{\delta}{\delta S(q')}\right) \frac{\partial S}{\partial q_i} = \dot{q}_j \frac{\partial^2 S}{\partial q_j \partial q_i} + \frac{\partial}{\partial q_i} \dot{S}(q). \tag{6.6}$$

Taking the q-derivative of (4.17) we get

$$\left(\frac{\partial}{\partial t} + \frac{1}{m} \frac{\partial S}{\partial q_j} \frac{\partial}{\partial q_j}\right) \frac{\partial S}{\partial q_i} = -\frac{\partial (V+Q)}{\partial q_i}. \tag{6.7}$$

Using Hamilton's equation (4.14) we obtain from (6.5) the law of motion:

$$m\dot{q}_i(t) = \left.\frac{\partial S\big(q_i, t\big)}{\partial q_i}\right|_{q_i = q_i(t)}, \quad i = 1, 2, 3. \tag{6.8}$$

Inserting (6.8) and (6.7) in (6.6) then gives Hamilton's equation (4.15), and the consistency is proved.

In the course of deriving a constraint on the solutions of Hamilton's equations we have given a condition which in the form (6.8) can itself be used to solve for the particle motion. This of course is the deBB law (1.2). We see that the deBB equation arises through a particular solution of Liouville's equation, f_δ, whose form is fixed by the requirement that the phase space evolution is compatible with the implications of Schrödinger's equation. It is to be interpreted as arising from a relation between the phase space coordinates of the total wave-particle system, one which also implies a relation between the particle phase space coordinates. Although it has the form of a HJ-type relation it has been derived here without reference to HJ theory. The role of the latter is discussed in the following paper.

We have shown that the force law follows from the constraint (6.2) (in conjunction with Hamilton's equations for q and S) so this condition encodes information on the forces acting on the particle (a similar situation obtains in classical HJ theory). To examine whether the constraint implies forces additional to those already contained in Hamilton's particle equations, we set it within the context of the usual theory of constraints in

Hamiltonian systems [20]. Suppose for a moment that the phase space were subject to a general set of (primary) constraints

$$\phi_\mu\big(q_i, p_i, \rho(q'), S(q'), \pi_\rho(q'), \pi_S(q'), t\big) = 0, \tag{6.9}$$

where μ is less than the number of freedoms in the system. Then Hamilton's equations are to be evaluated using the modified Hamiltonian

$$\bar{H}_{\text{tot}} = H_{\text{tot}} + \sum_\mu u_\mu \phi_\mu, \tag{6.10}$$

where u_μ is an undetermined multiplier (independent of the phase space coordinates). In the present case we have three primary constraints since, writing

$$\phi_i \equiv p_i - \int \frac{\partial S(q', t)}{\partial q'_i}\delta(q - q')\,\mathrm{d}^3 q' = 0, \tag{6.11}$$

q' is a dummy index. Using the modified Hamiltonian (6.10) in Hamilton's particle equations gives

$$\dot{q}_i = \frac{\partial H_{\text{tot}}}{\partial p_i} + u_j \frac{\partial \phi_j}{\partial p_i} = \frac{1}{m} p_i + u_i, \tag{6.12}$$

$$\dot{p}_i = -\frac{\partial H_{\text{tot}}}{\partial q_i} - u_j \frac{\partial \phi_j}{\partial q_i} = -\frac{\partial}{\partial q_i}(V + Q) + u_j \frac{\partial^2 S}{\partial q_j \partial q_i}. \tag{6.13}$$

Hamilton's equations for the fields computed using the modified Hamiltonian are unchanged except for eq. (4.19) for π_S which picks up an additional δ-function term multiplied by u_i. This shows, as stated above, that (6.11) is not a constraint on the Schrödinger field. To ensure that eq. (6.11) is obeyed for all time we require that $\dot{\phi}_i = 0$ (so that ϕ_i is a constant of the motion). In general such a condition implies identities, secondary constraints, or further conditions on u_i. Using the definition (4.21) of the total time derivative, Hamilton's equations (6.12) and (6.13), and Hamilton's equation for S, we find

$$\frac{\mathrm{d}\phi_i}{\mathrm{d}t} = \frac{\mathrm{d}}{\mathrm{d}t}\left(p_i - \frac{\partial S(q,t)}{\partial q_i}\right) = -\frac{1}{m}\left(p_j - \frac{\partial S}{\partial q_j}\right)\frac{\partial^2 S}{\partial q_j \partial q_i}, \tag{6.14}$$

which vanishes in virtue of the constraint (6.11). Thus, ϕ_i is a constant of the motion automatically and we do not obtain any extra useful conditions.

To fix u_i we appeal to Liouville's equation (5.22). The flow implied by (6.12) and (6.13) must be compatible with the distribution f_δ (since we are assuming the constraint (6.11) implied by the latter) and hence, inserting $\dot{q}$ and $\dot{p}$ into (5.22) and noting that f_δ is a solution when $u_i = 0$, we must have

$$u_i \frac{\partial f_\delta}{\partial q_i} + u_j \frac{\partial^2 S}{\partial q_j \partial q_i}\frac{\partial f_\delta}{\partial p_i} = 0. \tag{6.15}$$

This equation reduces to

$$u_i \frac{\partial \rho}{\partial q_i} \delta\left(p - \frac{\partial S}{\partial q}\right) = 0 \tag{6.16}$$

and, integrating over p, we deduce that $u_i = 0$. The complete set of Hamilton's equations is therefore unmodified by the constraint (6.11) and we conclude in particular that the latter does not introduce any forces additional to those implied by $V + Q$.

If we use Hamilton's particle equations to solve for the motion (rather than deBB) the role of the constraint is then to restrict the admissible initial conditions. This follows since, if the constraint is obeyed at an instant, Hamilton's equations guarantee its validity for all time by virtue of Liouville's equation (5.22):

$$\frac{\mathrm{d}}{\mathrm{d}t}\left(\rho(q,t)\delta\left(p - \frac{\partial S(q,t)}{\partial q}\right)\right) = 0. \tag{6.17}$$

Thus, if the initial coordinates obey the constraint evaluated at $t = 0$,

$$p_0 = \left.\frac{\partial S_0(q)}{\partial q}\right|_{q=q_0}, \tag{6.18}$$

where S_0 is a prescribed function, we may solve for the ensemble of admissible motions using the particle Hamilton equations (4.14) and (4.15), and the flow so obtained will coincide with that obtained by directly integrating (6.8). This result was asserted by Bohm [3,5] starting from the second-order equation for q (obtained by substituting (4.14) in (4.15)) but he did not prove it explicitly.

We have thus shown that we can solve for the particle motion in two dynamically equivalent ways: solve Hamilton's equations subject to the constraint (6.18) on the initial coordinates, or solve (6.8). The deBB theory can therefore be formulated as a brand of Hamiltonian mechanics in a way that preserves its statistical harmony with quantum mechanics. This answers the first of the questions posed in sect. **1** which motivated this investigation.

We have seen in subsect. **5**˙2, however, that, while the assumption of the deBB law (6.8) implies that the quantum potential is the appropriate quantity with which to describe quantum actions on the particle, the converse is not true: the Hamiltonian theory based on the quantum potential does not uniquely result in the deBB law if our only concern is compatibility of Liouville's equation with Schrödinger's. Thus, we could have laws other than deBB (*i.e.*, we could restrict the solutions to Hamilton's equations (4.14) and (4.15) in a different way) so long as the coordinates are distributed according to the general expression (5.46). The momentum need not then be restricted to a unique value when the position is specified.

That the function f_δ is the distribution appropriate to the deBB theory was first shown by Takabayasi [21]. We shall see in sect. **6** of the following paper, however, that it has more general validity in that it can be valid in cases where the particle law of motion is different from that of deBB. Note that the argument resulting in f_δ applies in a phase space frame in which H has the form (4.10). The relations (6.1) and (6.2) are not canonically invariant and will take different forms in other frames. How to effect this transformation is discussed in sect. **4** of the following paper. There we shall also discuss further the significance of the results obtained here.

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