Hamiltonian Theory of Wave and Particle in Quantum Mechanics II: Hamilton-Jacobi Theory and Particle Back-Reaction

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Abstract

Pursuing the Hamiltonian formulation of the de Broglie-Bohm (deBB) theory presented in the preceding paper [1], the Hamilton-Jacobi (HJ) theory of the wave-particle system is developed. It is shown how to derive a HJ equation for the particle, which enables trajectories to be computed algebraically using Jacobi's method. Using Liouville's equation in the HJ representation we find the restriction on the Jacobi solutions which implies the quantal distribution. This gives a first method for interpreting the deBB theory in HJ terms. A second method proceeds via an explicit solution of the field+particle HJ equation. Both methods imply that the quantum phase may be interpreted as an incomplete integral. Using these results and those of the first paper it is shown how Schrödinger's equation can be represented in Liouvillian terms, and vice versa. The general theory of canonical transformations that represent quantum unitary transformations is given, and it is shown in principle how the trajectory theory may be expressed in other quantum representations. Using the solution found for the total HJ equation, an explicit solution for the additional field containing a term representing the particle back-reaction is found. The conservation of energy and momentum in the model is established, and a weak form of the action-reaction principle is shown to hold. Alternative forms for the Hamiltonian are explored and it is shown that, within this theoretical context, the deBB theory is not unique. The theory potentially provides an alternative way of obtaining the classical limit.

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1. Introduction

In the preceding paper [1] we have developed a Hamiltonian formalism describing the interaction of a particle with the Schrödinger field and an additional (complex) field. Representing the system by the phase space coordinates $\left(q, \rho(q'), S(q'), p, \pi_\rho(q'), \pi_S(q')\right)$, the total Hamiltonian is given by the expression

$$H_{tot} = H + \int \left\{ -\pi_\rho \left(\frac{1}{m} \frac{\partial}{\partial q_i'} \left(\rho \frac{\partial S}{\partial q_i'} \right) \right) - \pi_S \left(\frac{1}{2m} \frac{\partial S}{\partial q_i'} \frac{\partial S}{\partial q_i'} + Q + V \right) \right\} d^3 q' \tag{1.1}$$

where

$$H(\rho, q, p, t) = \frac{1}{2m} p_i p_i + V(q,t) + Q(\rho(q)) \tag{1.2}$$

and

$$Q(q,t) = -\frac{\hbar^2}{2m\sqrt{\rho}} \frac{\partial^2 \sqrt{\rho}}{\partial q_i^2} = \frac{\hbar^2}{4m\rho} \left(\frac{1}{2\rho} \left(\frac{\partial \rho}{\partial q_i} \right)^2 - \frac{\partial^2 \rho}{\partial q_i^2} \right) \tag{1.3}$$

is the quantum potential. Hamilton's particle equations are

$$\dot{q}_i = \frac{1}{m} p_i \tag{1.4}$$

$$\dot{p}_i = -\frac{\partial}{\partial q_i} \left[V(q,t) + Q(\rho(q)) \right] \tag{1.5}$$

and the field equations are

$$\dot{\rho}(q', t) = -\frac{1}{m} \frac{\partial}{\partial q_i'} \left(\rho(q') \frac{\partial S(q')}{\partial q_i'} \right) \tag{1.6}$$

$$\dot{S}(q',t) = -\frac{1}{2m}\frac{\partial S(q')}{\partial q'_i}\frac{\partial S(q')}{\partial q'_i} - V(q',t) - Q(\rho(q')) \quad (1.7)$$

$$\dot{\pi}_\rho(q',t) = -\frac{1}{m}\frac{\partial \pi_\rho(q')}{\partial q'_i}\frac{\partial S(q')}{\partial q'_i} + \frac{\delta}{\delta\rho(q')}\int \pi_S(q'')Q(\rho(q''))d^3q'' - \frac{\delta Q(\rho(q))}{\delta\rho(q')} \quad (1.8)$$

$$\dot{\pi}_S(q',t) = \frac{1}{m}\frac{\partial}{\partial q'_i}\left(\rho(q')\frac{\partial \pi_\rho(q')}{\partial q'_i} - \pi_S(q')\frac{\partial S(q')}{\partial q'_i}\right). \quad (1.9)$$

Equations (1.6) and (1.7) are equivalent to Schrödinger's equation. Equations (1.4) and (1.5) exhibit the influence of the wave on the particle through the quantum potential, and the last two coupled equations contain a particle source term in (1.8). We showed in §5.1(I) (numbers of sections and equations in the first paper will be followed by (I)) that for a pure quantum state the particle obeys its own Liouville equation,

$$\frac{\partial f}{\partial t} + \frac{\partial H}{\partial p_i}\frac{\partial f}{\partial q_i} - \frac{\partial H}{\partial q_i}\frac{\partial f}{\partial p_i} = 0, \quad (1.10)$$

which with (1.2) gives

$$\frac{\partial f}{\partial t} + \frac{p_i}{m}\frac{\partial f}{\partial q_i} - \frac{\partial\left(V(q,t) + Q(\rho(q,t))\right)}{\partial q_i}\frac{\partial f}{\partial p_i} = 0. \quad (1.11)$$

The general solution of this equation compatible with the q-projected distribution ρ is given by

$$f(q,p,t) = f_\delta(q,p,t) + \theta(q,p,t) \quad (1.12)$$

where

$$f_\delta(q,p,t) = \rho(q,t)\delta\left(p - \frac{\partial S(q,t)}{\partial q}\right) \quad (1.13)$$

and θ is subject to a series of conditions. The solution (1.13) implies the following constraint on the system phase space:

$$p_i = \frac{\partial S(q,t)}{\partial q_i}. \tag{1.14}$$

In conjunction with Hamilton's equation (1.4), (1.14) gives the de Broglie-Bohm (deBB) guidance equation

$$m\frac{dq_i(t)}{dt} = \left.\frac{\partial S(q_i,t)}{\partial q_i}\right|_{q_i=q_i(t)}, \quad i=1,2,3. \tag{1.15}$$

The particle trajectory may be computed from (1.15) or from Hamilton's equations (1.4) and (1.5) subject to the constraint (1.14) on the initial coordinates.

The principal aims of the present paper are to examine the second question posed in Paper I, that is, the relation of the deBB theory to Hamilton-Jacobi (HJ) theory, to give an explicit solution for the additional field which includes the particle back-reaction term, and to explore further the issue of the uniqueness of the particle law of motion within the Hamiltonian framework. We start by establishing the HJ theory for the total system, and derive a HJ equation just for the particle (which comes out as (1.9)(I)) (§2). This enables trajectories to be computed algebraically using Jacobi's method. Using Liouville's equation (1.11) in the HJ representation we find the restriction on the Jacobi solutions which implies the quantal distribution. This gives a first method for interpreting the deBB theory in HJ terms. A second method proceeds via an explicit solution of the field+particle HJ equation. Both methods imply that the quantum phase may be interpreted as a component of an (incomplete) integral of the HJ equation for the total system. Using these results and those of the first paper it is shown how Schrödinger's equation can be represented in Liouvillian terms, and vice versa (§3). The general theory of canonical transformations that represent quantum unitary transformations is given (§4), and it is shown in principle how the trajectory theory may be expressed in other quantum representations. Using the solution found for the total HJ equation, an explicit solution for the additional field containing a term representing the particle back-reaction is found (§5). The conservation of energy and momentum in the model is established, and a weak form of the action-reaction principle is shown to hold. Alternative forms for the Hamiltonian are explored and it is shown that, within the theoretical context discussed here, the deBB theory is not a unique solution to the problem of formulating a deterministic substructure for quantum mechanics (§6). The paper concludes with a discussion of the results obtained, and it is pointed out that the theory potentially provides an alternative way of obtaining the classical limit (§7).

2. The Hamilton-Jacobi theory for the wave-particle system

2.1 Jacobi's laws of motion

We consider canonical transformations on the total phase space, generalizing the canonical theory of fields [e.g., 2] to include the particle variables. The quantity $W\left[q,\rho,S,\bar{p},\pi'_\rho,\pi'_S,t\right]$, which is a function of the particle coordinates and a functional of the fields, generates a canonical transformation from the set of phase space coordinates $\left(q,\rho,S,p,\pi_\rho,\pi_S\right)$ to a new set $\left(\bar{q},\rho',S',\bar{p},\pi'_\rho,\pi'_S\right)$ if

$$\begin{aligned} p_i dq_i &+ \int \left(\pi_\rho(q')\delta\rho(q') + \pi_S(q')\delta S(q')\right) d^3q' - H_{tot}\,dt \\ &= -\bar{q}_i d\bar{p}_i - \int \left(\rho'(q')\delta\pi'_\rho(q') + S'(q')\delta\pi'_S(q')\right) d^3q' - H'_{tot}dt + dW \end{aligned} \tag{2.1}$$

where H'_{tot} is the transformed Hamiltonian. Here

$$\begin{aligned} dW = \frac{\partial W}{\partial t}dt + \frac{\partial W}{\partial q_i}dq_i + \frac{\partial W}{\partial \bar{p}_i}d\bar{p}_i &+ \int \left(\frac{\delta W}{\delta\rho(q')}\delta\rho(q') + \frac{\delta W}{\delta S(q')}\delta S(q')\right) d^3q' \\ &+ \int \left(\frac{\delta W}{\delta\pi'_\rho(q')}\delta\pi'_\rho(q') + \frac{\delta W}{\delta\pi'_S(q')}\delta\pi'_S(q')\right) d^3q' \end{aligned} \tag{2.2}$$

which, on comparing with (2.1), gives

$$
\left.\begin{aligned}
&\bar{q}_i = \frac{\partial W}{\partial \bar{p}_i}, \quad \rho'(q') = \frac{\delta W}{\delta \pi'_\rho(q')}, \quad S'(q') = \frac{\delta W}{\delta \pi'_S(q')}, \\
&p_i = \frac{\partial W}{\partial q_i}, \quad \pi_\rho(q') = \frac{\delta W}{\delta \rho(q')}, \quad \pi_S(q') = \frac{\delta W}{\delta S(q')}, \\
&H'_{tot} = H_{tot} + \frac{\partial W}{\partial t}.
\end{aligned}\right\} \tag{2.3}
$$

The first two rows in (2.3) are the equations of motion in Jacobi's form. We have chosen the generating function W to be a function of the old coordinates and the new momenta (a generalization of the function F_2 of Goldstein [3]) because of the requirements of unitary invariance to be examined later (see §4). Choosing $H'_{tot} = 0$, Hamilton's equations imply that the new variables are constant in time. Then W generates a transformation that trivializes the motion, and from the last relation in (2.3) and (1.1) it obeys the HJ equation:

$$
\begin{aligned}
&\frac{\partial W}{\partial t} + \frac{1}{2m}\frac{\partial W}{\partial q_i}\frac{\partial W}{\partial q_i} + V(q,t) + Q(\rho(q)) + \int \left\{ -\frac{\delta W}{\delta \rho(q')}\left(\frac{1}{m}\frac{\partial}{\partial q'_i}\left(\rho(q')\frac{\partial S(q')}{\partial q'_i}\right)\right)\right. \\
&\qquad \left. -\frac{\delta W}{\delta S(q')}\left(\frac{1}{2m}\frac{\partial S(q')}{\partial q'_i}\frac{\partial S(q')}{\partial q'_i} + Q(\rho(q')) + V(q',t)\right)\right\} d^3q' = 0.
\end{aligned} \tag{2.4}
$$

The total energy of the system is now represented by $(-\partial W/\partial t)$.

More generally, we shall treat W as a complete integral that is a function of a set of arbitrary non-additive constants: $W[q_i, \rho(q'), S(q'), \alpha_i, A_\rho(q'), A_S(q'), t]$. The Jacobi equations of motion from which we may calculate the time dependence of the coordinates are then

$$
\beta_i = \frac{\partial W}{\partial \alpha_i}, \quad B_\rho(q') = \frac{\delta W}{\delta A_\rho(q')}, \quad B_S(q') = \frac{\delta W}{\delta A_S(q')}. \tag{2.5}
$$

In order to invert these relations to find explicit expressions for the coordinates, we must assume that the Hessian matrix,

$$h_{ij}(q,q',q'',q''') = \begin{pmatrix} \dfrac{\partial^2 W}{\partial q_i \partial \alpha_j} & \dfrac{\delta^2 W}{\partial q_i \delta A_\rho(q)} & \dfrac{\delta^2 W}{\partial q_i \delta A_S(q')} \\ \dfrac{\delta^2 W}{\delta\rho(q'')\partial\alpha_j} & \dfrac{\delta^2 W}{\delta\rho(q'')\delta A_\rho(q)} & \dfrac{\delta^2 W}{\delta\rho(q'')\delta A_S(q')} \\ \dfrac{\delta^2 W}{\delta S(q''')\partial\alpha_j} & \dfrac{\delta^2 W}{\delta S(q''')\delta A_\rho(q)} & \dfrac{\delta^2 W}{\delta S(q''')\delta A_S(q')} \end{pmatrix}, \tag{2.6}$$

is invertible: $\det h \neq 0$ (h is a square matrix; if we think for a moment of the argument of each field as having n values, there are 3+2n rows and columns). Having solved (2.5) for the coordinates, the momenta may be found by substituting into the three relations in the second row of (2.3).

The Hamilton equations (1.6) and (1.7) for the fields ρ and S are independent of the particle variables and the conjugate field momenta. Hence we must be able to derive from the transformation equations (2.5) a closed solution for the field coordinates. This will happen since, as we shall see in §4, when we restrict to transformations corresponding to quantum unitary transformations W is linear in π'_ρ $(= A_\rho)$ and π'_S $(= A_S)$. The last two equations in (2.5) are thus equivalent to the Schrödinger equation. This closure of ρ and S is preserved under canonical transformations which correspond to unitary transformations (see §4).

To check the validity of Jacobi's equations, we now derive Hamilton's equations from them by extending the well known techniques of particle mechanics [4] to include the fields. To obtain Hamilton's equations for the coordinates, we differentiate each of the Jacobi equations (2.5) in turn with respect to time. For the first (particle) equation, say, we obtain,

$$\begin{aligned} 0 = \dot\beta_j &= \left(\frac{\partial}{\partial t} + \dot q_i \frac{\partial}{\partial q_i} + \int d^3q' \left(\dot\rho(q') \frac{\delta}{\delta\rho(q')} + \dot S(q') \frac{\delta}{\delta S(q')} \right) \right) \frac{\partial W}{\partial \alpha_j} \\ &= \left(-\frac{1}{m} p_i + \dot q_i \right) \frac{\partial^2 W}{\partial q_i \partial \alpha_j} + \int \left(\dot\rho + \frac{1}{m} \frac{\partial}{\partial q''_i} \left(\rho \frac{\partial S}{\partial q''_i} \right) \right) \frac{\delta^2 W}{\delta\rho(q'')\partial\alpha_j} d^3q'' \\ &\quad + \int \left(\dot S + \frac{1}{2m} \frac{\partial S}{\partial q'''_i} \frac{\partial S}{\partial q'''_i} + Q + V \right) \frac{\delta^2 W}{\delta S(q''')\partial\alpha_j} d^3q''' \end{aligned} \tag{2.7}$$

where we have substituted for $\partial W/\partial t$ from (2.4) and replaced $\partial W/\partial q_i$ by p_i. Doing the same for the other (field) Jacobi equations (2.5) we can employ the Hessian (2.6) to write the complete set of time-differentiated Jacobi equations in matrix form as follows:

$$\left(-\frac{1}{m}p_i+\dot{q}_i \quad \int d^3q''\left(\dot{\rho}+\frac{1}{m}\frac{\partial}{\partial q_i''}\left(\rho\frac{\partial S}{\partial q_i''}\right)\right) \quad \int d^3q'''\left(\dot{S}+\frac{1}{2m}\frac{\partial S}{\partial q_i''}\frac{\partial S}{\partial q_i'''}+Q+V\right)\right)$$
$$\times h_{ij}(q,q',q'',q''')=0. \tag{2.8}$$

Post-multiplying this equation by $h^{-1}_{jk}(\tilde{q},\tilde{q}',q,q')$ and summing over (j,q,q') we deduce that the row vector vanishes; Hamilton's equations then follow. Likewise, we can differentiate the momentum relations (the second row in (2.3)) with respect to time and recover the second (momentum) set of Hamilton's equations (for examples see §§2.3 and 2.4).

We saw in §5(I) that the ensemble of particle motions implied by Hamilton's equations (corresponding to varying the initial values) is too broad to give the quantal distribution. We now show how this *largesse* is represented in the HJ formalism, and see how the ensemble may be suitably restricted to give the correct distribution. In the process, we shall confirm the result of §§5(I) and 6(I) that more general laws than that of deBB are possible. We will describe two ways in which the latter may be regarded as fitting into the HJ description.

2.2 Hamilton-Jacobi equation for the particle

When computing a single system trajectory using the HJ method we are employing a description that involves the entire ensemble of potential trajectories, i.e., the lines orthogonal to the surfaces of constant *W*. Here, in order to examine compatibility with the quantum distribution, we want to restrict attention to just the particle component of the ensemble. To arrive at this description, we use the fact that the ρ, *S* fields form a closed system whose dynamics is independent of the particle. Hence, if we suppose that we have available a solution for the fields (by directly solving Hamilton's equations, say), so that they are fixed as explicit functions of *q* and *t*,

$$\rho = \rho(q, t, \rho_0(q)) \quad S = S(q, t, S_0(q)), \tag{2.9}$$

we may consistently insert these in the HJ equation to leave an equation whose variables pertain solely to the particle. Another way of saying this is that the non-additive constants $(A_\rho, A_S, B_\rho, B_S)$, which correspond to the initial actual values that are assumed for the wavefunction and the field momenta, are fixed once and for all. This is analogous to the insertion of a field solution in Liouville's equation in §5.1(I). The remaining (particle) degrees of freedom are contained in the function

$$\sigma(q, \alpha, t) = W\left[q, \rho(q', t), S(q', t), \alpha, A_\rho(q'), A_S(q'), t\right] \tag{2.10}$$

We have

$$\frac{\partial \sigma}{\partial t} = \frac{\partial W}{\partial t} + \int d^3q' \left(\dot{\rho}(q') \frac{\delta W}{\delta \rho(q')} + \dot{S}(q') \frac{\delta W}{\delta S(q')} \right), \quad \frac{\partial \sigma}{\partial q} = \frac{\partial W}{\partial q}. \tag{2.11}$$

Substituting for the time derivatives of the fields from Hamilton's equations (1.6) and (1.7), the HJ equation (2.4) therefore becomes

$$\frac{\partial \sigma}{\partial t} + \frac{1}{2m} \frac{\partial \sigma}{\partial q_i} \frac{\partial \sigma}{\partial q_i} + Q(q, t) + V(q, t) = 0. \tag{2.12}$$

The canonical equations of motion ((2.5) and the second row of (2.3)) are now

$$p_i = \frac{\partial \sigma(q, \alpha, t)}{\partial q_i}, \quad \beta_i = \frac{\partial \sigma(q, \alpha, t)}{\partial \alpha_i}. \tag{2.13}$$

We thus recover from our theory of the interacting wave-particle system the HJ equation (1.9)(I) associated with the putative particle Hamiltonian (1.7)(I) (i.e., (1.2)). However, whereas (1.9)(I) was simply postulated, we have derived it here in a way that takes full account of the interaction of the particle with the wave, and thus have demonstrated its consistency. Moreover, we understand how the equation is to be interpreted: it is a reduced form of the HJ equation for the total wave-particle system. The function σ is Hamilton's principal function which generates a transformation trivializing the particle motion. The equations (2.12) and (2.13) therefore constitute a genuine HJ theory of the particle, where the possible particle paths are orthogonal to the surfaces σ = constant. The particle energy is given by $(-\partial\sigma/\partial t)$, as expected from the first relation in (2.11).

Given a solution to (2.12), we can solve for the particle motion using (2.13) by algebraic means, just as in classical HJ theory. There may be circumstances where it is easier to solve (2.12) if the quantum effects are expressed through the phase rather than the quantum potential. To obtain this form, it proves convenient to write

$$\sigma(q,\alpha,t) = S(q,t) + \sigma'(q,\alpha,t). \tag{2.14}$$

Subtracting (2.12) from Hamilton's equation (1.7) for S we then get

$$\frac{\partial\sigma'}{\partial t} + \frac{1}{2m}\frac{\partial\sigma'}{\partial q_i}\frac{\partial\sigma'}{\partial q_i} + \frac{1}{m}\frac{\partial S}{\partial q_i}\frac{\partial\sigma'}{\partial q_i} = 0 \tag{2.15}$$

and the quantum effects are contained in the last term.

2.3 Ensembles compatible with the quantum distribution - the de Broglie-Bohm theory

The equation (2.12) has the form of the Hamilton equation (1.7) for S but it admits more general solutions, including multivalued ones. Since this theory is just the HJ version of Hamilton's particle equations (1.4) and (1.5), we know from §5(I) that the Jacobi equations (2.13) imply an ensemble of motions that is generally incompatible with the distribution ρ. We now examine the nature of the restriction that must be imposed on the solutions to ensure compatibility.

To see that the ensemble of motions implied by (2.13) for arbitrary HJ functions σ is in general too broad, we return to Liouville's equation (1.11) which we express in the HJ language (see the Appendix). We are working now in the space of the mixed coordinates (q,α) which link the two phase space coordinate systems (q,p) and (α,β). In this space, (1.11) becomes (see (A13))

$$\frac{\partial \Gamma}{\partial t}+\frac{1}{m}\frac{\partial}{\partial q_i}\left(\Gamma\frac{\partial \sigma}{\partial q_i}\right)=0 \tag{2.16}$$

where Γ is the probability density in the space (q,α). Equation (2.16) together with the HJ equation (2.12) are equivalent to Liouville's equation in the form (1.10) together with Hamilton's particle equations (1.4) and (1.5). Clearly, the q-projected density will not generally reproduce ρ, and we must restrict it in some way.

Following the argument of §5.2(I), the q-projected equations implied by (2.16) must yield just implications of the Schrödinger equation. We can follow the method of that section to find the general form of Γ consistent with this requirement. As before, our basic requirement is that the spatial density is the quantum expression:

$$\rho(q,t)=\int f(q,p,t)\,d^3p=\int \Gamma(q,\alpha,t)\,d^3\alpha. \tag{2.17}$$

The momentum moments (5.36)(I) become

$$\overline{p_{i_1}\cdots p_{i_n}}(q,t)=\int \frac{\partial \sigma}{\partial q_{i_1}}\cdots\frac{\partial \sigma}{\partial q_{i_n}}\Gamma d^3\alpha \Big/ \rho. \tag{2.18}$$

Repeating the analysis of §5.2(I), the result for Γ will be (1.12) rewritten in the HJ formalism. Hence, only a Γ so restricted will reproduce the ρ-distribution.

We shall give the form of Γ that corresponds to the special solution f_δ, (1.13). Substituting (1.13) into (A3) and using (A11) we obtain

$$\Gamma_\delta(q,\alpha,t)=D(q,\alpha,t)\rho(q,t)\delta\left(\frac{\partial \sigma(q,\alpha,t)}{\partial q}-\frac{\partial S(q,t)}{\partial q}\right) \tag{2.19}$$

where D is the modulus of the determinant of the Hessian (see (A10)). Here σ is regarded as a prescribed function (as are ρ and S) obtained as a solution of (2.12). This expression implies that the motion as represented in (q,α)-space is confined to the moving curve defined by the equations

$$\frac{\partial\sigma(q,\alpha,t)}{\partial q_i}-\frac{\partial S(q,t)}{\partial q_i}=0, \quad i=1,2,3. \tag{2.20}$$

This equation is to be interpreted as a relation specifying the range of admissible values of α as functions of q and t (determined by the q-turning points of the function $\sigma - S$). To find this explicitly, we note that we can invert the first Jacobi equation (2.13) to get $\alpha = \alpha(q,p,t)$ which is a single-valued function of q and p (the condition for this is $D \neq 0$ for all q, α). Substituting $p = \partial S/\partial q$ in this expression we obtain the solution of (2.20):

$$\alpha = \alpha(q, p = \partial S/\partial q, t) = \alpha_0(q,t) \tag{2.21}$$

which, because p is uniquely fixed by q, is a single-valued function of q. This is the HJ analogue of the relation $p = \partial S/\partial q$ in the phase space coordinates, which gives the admissible values of p corresponding to q. And, just as we solve Hamilton's particle equations for independent q and p and then restrict to the subset of initial conditions obeying $p = \partial S/\partial q$, so here we solve Jacobi's equation $\beta = \partial\sigma/\partial q$ and restrict to the subset of initial qs obeying $\partial\sigma/\partial q = \partial S/\partial q$.

Using the formula

$$\delta^3(g_i(\alpha)) = \sum_n d_n^{-1}\delta^3(\alpha_i - \alpha_{ni}), \quad g_i(\alpha_n) = 0, \quad d_n = \left|\det\frac{\partial g_i}{\partial\alpha_j}\right|_{\alpha=\alpha_n} \neq 0 \tag{2.22}$$

the dependence of Γ_δ on α may be expressed more simply. Since the equations (2.20) have only a single root α_0, we obtain using (2.22)

$$\Gamma_\delta(q,\alpha,t) = \rho(q,t)D(q,\alpha,t)D^{-1}(q,\alpha,t)\big|_{\alpha=\alpha_0(q,t)}\delta(\alpha-\alpha_0(q,t)) \tag{2.23}$$

since by assumption $D \neq 0$. This is the HJ representation of f_δ. Clearly, (2.23) implies the relation (2.17).

We may instead regard (2.20) as defining q as a (generally multivalued) function of α and t. We can under certain circumstances (namely, when the relevant determinants corresponding to the d_ns in (2.22) are non-zero) then write (2.19) in terms of a sum of delta-functions of q (a similar procedure may be applied to the phase space function (1.13) when $\det\left(\partial^2 S / \partial q_i \partial q_j\right) \neq 0$).

It is readily checked that, via (2.18), (2.19) gives the correct momentum moments (5.41)(I) with all X-tensors zero. In particular, substituting in (2.16) and integrating over α we obtain Hamilton's equation (1.6) for ρ. Similarly, multiplying (2.16) by $\partial\sigma/\partial q_i$, integrating over α, using (2.12), and dividing by ρ, we get the q-derivative of Hamilton's equation for S. Hence, when we assume a distribution Γ_δ, Liouville's equation (2.16) and the HJ equation (2.12) together imply results consistent with Schrödinger's equation. Just as in the original phase space representation (see §3), we do not get more than this from the HJ theory of course. For example, multiplying (2.12) by Γ_δ, integrating, and dividing by ρ, we might hope to derive Hamilton's equation for S rather than just its derivative, so that the q-projections of (2.12) and (2.16) together would be equivalent to the Schrödinger equation. In fact, we obtain

$$\frac{\partial S}{\partial t} + \frac{1}{2m}\frac{\partial S}{\partial q_i}\frac{\partial S}{\partial q_i} + Q + V + c(t) = 0 \qquad (2.24)$$

where $c(t)$ is undetermined, and this just restates that the q-derivative of Hamilton's equation for S vanishes.

To prove that the constraint (2.20) is consistent, we show that we indeed obtain the deBB theory from Jacobi's equations (2.13) when (2.20) holds, using the technique of §2.1. First, we differentiate the second Jacobi relation with respect to time to obtain

$$0 = \dot{\beta}_i = \left(\frac{\partial}{\partial t} + \dot{q}_j \frac{\partial}{\partial q_j}\right)\frac{\partial \sigma}{\partial \alpha_i} = \left(-\frac{1}{m}\frac{\partial \sigma}{\partial q_j} + \dot{q}_j\right)\frac{\partial^2 \sigma}{\partial q_j \partial \alpha_i} \qquad (2.25)$$

where we have substituted from (2.12). Since the determinant of the Hessian is non-zero, we deduce that

$$m\dot{q}_i = \left.\frac{\partial \sigma(q,\alpha,t)}{\partial q_i}\right|_{q=q(t)}. \qquad (2.26)$$

Using the first Jacobi equation, (2.26) becomes

$$m\dot{q}_i = p_i. \tag{2.27}$$

Next, we differentiate the first Jacobi relation with respect to time:

$$\dot{p}_i = \left(\frac{\partial}{\partial t} + \dot{q}_j \frac{\partial}{\partial q_j}\right)\frac{\partial \sigma}{\partial q_i} = \left(-\frac{1}{m}\frac{\partial \sigma}{\partial q_j} + \dot{q}_j\right)\frac{\partial^2 \sigma}{\partial q_j \partial q_i} - \frac{\partial (V+Q)}{\partial q_i} \tag{2.28}$$

where again we have used (2.12). Employing the relation (2.26) then gives

$$\dot{p}_i = -\left.\frac{\partial (V+Q)}{\partial q_i}\right|_{q=q(t)}. \tag{2.29}$$

Thus, we recover in (2.27) and (2.29) Hamilton's particle equations. Finally, combining (2.26) with (2.20) we obtain the deBB law (1.15), and from (2.27) the constraint in the form $p = \partial S / \partial q$.

We are now in a position to clarify the relation between the deBB theory and HJ theory. To begin with, we see that $\partial \sigma / \partial q = \partial S / \partial q$, being a rewording of the relation $p = \partial S / \partial q$, has the interpretation we gave in §6(I), namely, it is a relation between the field coordinate S and the particle variables (here α and q). And as in §6(I), it may also be viewed as a relation between just the particle variables. We are thus able to interpret the phase space constraint in HJ theory. However, we have an additional possibility of interpretation here. For, instead of seeking a complete integral of (2.12), suppose all we have available is an incomplete integral so that σ does not depend on any non-additive constants: $\sigma = \sigma(q,t)$. Then, of course, we cannot develop the ensemble theory we have given above or use Jacobi's equations to solve for the motion. The latter reduce just to the first relation in (2.13),

$$p_i = \frac{\partial \sigma(q,t)}{\partial q_i}, \tag{2.30}$$

and we must invoke Hamilton's equation $p_i = m\dot{q}_i$ to find the particle motion using (2.30). Introducing the constraint $p = \partial S / \partial q$ of the deBB theory, (2.30) implies that

$$\frac{\partial \sigma(q,t)}{\partial q_i} - \frac{\partial S(q,t)}{\partial q_i} = 0. \tag{2.31}$$

Since q is arbitrary we must have

$$\sigma(q,t) = S(q,t) + c. \tag{2.32}$$

Hence, up to a constant c, the choice of incomplete solution is uniquely fixed to be S. Conversely, we may use (2.32) to interpret S: the quantum phase may be regarded as a (incomplete) integral of a HJ equation, namely (2.12), the latter coinciding with part of Schrödinger's equation. Since, using (2.32), the Jacobi equation (2.30) is just the deBB constraint $p = \partial S / \partial q$, we see that it is legitimate to regard the latter as a genuine HJ relation in the sense just stated. This answers the second of the questions posed in §1(I): S may be regarded as a HJ function, but it is incomplete so does not generate a canonical transformation. In particular, the independence of S from a set of non-additive constants is not evidence of its non-HJ nature. Moreover, this interpretation is consistent with the partial dependence of Q in the HJ equation on S. One of the field Hamilton equations thus coincides with the HJ equation for the particle.

So far in this sub-section we have considered the implications of Γ_δ. We observe that, if we could construct non-trivial solutions for Γ involving the X-tensors, the constraint (2.20) will be replaced by some other condition and the particle equations (2.13) determining motions that are compatible with ρ will generally differ from that of deBB. We thus recover in a different way the result of §§5(I) and 6(I) that the deBB theory is not unique. In this more general case, because the constants α appear in (2.13), solving for the motion generally requires specifying both q_o and p_o.

2.4 A second method of deriving the deBB theory

There is an alternative method of arriving at the deBB theory from the HJ theory which uses in a different way the technique of inserting a solution to Schrödinger's equation. This starts from a particular solution of the total HJ equation which reduces the latter to the HJ equation for just the field. The method thus complements that of §§2.2 and 2.3 where the total HJ equation reduced to the HJ equation for just the particle. The solution used turns out to have great significance as it enables us to find a solution of Hamilton's equations for the conjugate field momenta, which involve the particle source term (see §5).

Instead of seeking a complete integral of (2.4) and solving for the system trajectory algebraically using Jacobi's method, we can solve for the motion using an incomplete solution if we appeal to Hamilton's equations to supply the necessary differential equation(s) corresponding to the missing constants (as has already been illustrated in §2.3). To this end, let us suppose that the constants α do not appear in W, and let us separate out the q-dependence and attribute it to just the coordinate S:

$$W\left[q_i,\rho(q'),S(q'),A_\rho(q'),A_S(q'),t\right]=w\left[\rho(q'),S(q'),A_\rho(q'),A_S(q'),t\right]+S(q). \tag{2.33}$$

Then

$$\frac{\partial W}{\partial q_i}=\frac{\partial S(q)}{\partial q_i},\quad \frac{\delta W}{\delta\rho(q')}=\frac{\delta w}{\delta\rho(q')},\quad \frac{\delta W}{\delta S(q')}=\frac{\delta w}{\delta S(q')}+\delta(q-q') \tag{2.34}$$

and the transformation equations (2.3) and (2.5) become

$$\left.\begin{aligned} &p_i=\frac{\partial S(q)}{\partial q_i},\quad \pi_\rho(q')=\frac{\delta w}{\delta\rho(q')},\quad \pi_S(q')=\frac{\delta w}{\delta S(q')}+\delta(q-q'),\\ &B_\rho(q')=\frac{\delta w}{\delta A_\rho(q')},\quad B_S(q)=\frac{\delta w}{\delta A_S(q)}. \end{aligned}\right\} \tag{2.35}$$

Note that the determinant of the Hessian (2.6) vanishes so this transformation is not canonical according to the usual definition [5]. However, with respect to transformations of just the field variables the relevant Hessian (the lower right-hand square matrix in (2.6)) has non-vanishing determinant (this will be demonstrated in §4 where the explicit form for a w which generates unitary transformations is given). This means that we may invert the field Jacobi equations in (2.35) to solve for the field coordinates as functions of time.

Inserting the relations (2.34) in the HJ equation (2.4) we see that the particle variables cancel to leave an equation involving just the field variables (recall that in this context the function *S* is simply a coordinate and so independent of time):

$$\frac{\partial w}{\partial t}+\int\left\{-\frac{\delta w}{\delta\rho(q')}\left(\frac{1}{m}\frac{\partial}{\partial q'_i}\left(\rho\frac{\partial S}{\partial q'_i}\right)\right)-\frac{\delta w}{\delta S(q')}\left(\frac{1}{2m}\frac{\partial S}{\partial q'_i}\frac{\partial S}{\partial q'_i}+Q+V\right)\right\}d^3q'=0. \qquad (2.36)$$

This is the HJ equation of the pure Schrödinger field, corresponding to the field part of the Hamiltonian (1.1). An interesting property of (2.36) is that it is linear in the functional *w*. We may therefore construct a general solution to (2.36) by linearly superposing complete solutions *w* corresponding to different values of the non-additive constants A_ρ and A_S.

Since the solution (2.33) is incomplete in the constants α the first Jacobi equation in (2.5) can no longer be used to solve for the particle motion and is replaced by Hamilton's equation (1.4):

$$p_i = m\dot{q}_i. \qquad (2.37)$$

To find the particle path we proceed as follows. We insert in the last two relations in (2.35) a complete integral obeying (2.36) and solve for the field coordinates as functions of the time. This gives us a solution of Schrödinger's equation. We then substitute the $S(q,t)$ so found into the first relation. This establishes the relation between *p* and *S* discussed in §6(I). Combining this with (2.37) then allows us to find the particle trajectory by solving the differential equation

$$\frac{\partial S}{\partial q_i} = m\dot{q}_i. \qquad (2.38)$$

We thus recover once again the deBB equation of motion (1.15). This method thus implies a similar interpretation to that found in §2.3: the relation $p=\partial S/\partial q$ is one of Jacobi's equations evaluated for a given field solution *S* corresponding to an incomplete integral of the total HJ equation (in §2.3 *S* corresponds to an incomplete integral of the particle HJ equation).

We have one final task to perform: to prove that (2.33) is a valid solution by showing that the transformation equations (2.35) and the field HJ equation (2.36) imply Hamilton's equations for the particle and field (apart from (2.37) which, as noted, must be assumed). We do this by following the method of §2.1. To begin with, we differentiate the last two equations in (2.35) with respect to time and find an equation analogous to (2.8) where only the last two terms in the row matrix are present and the Hessian is just the (invertible) lower right-hand square matrix in (2.6). Hamilton's equations for the fields ρ and S then follow. Next, we differentiate the first three equations in (2.35) with respect to time. For the particle momentum:

$$\dot{p}_i = \left(\dot{q}_j \frac{\partial}{\partial q_j} + \int d^3q' \dot{S}(q') \frac{\delta}{\delta S(q')}\right) \frac{\partial S(q)}{\partial q_i} = \dot{q}_j \frac{\partial^2 S}{\partial q_j \partial q_i} + \frac{\partial}{\partial q_i} \dot{S}(q). \tag{2.39}$$

Substituting for $\dot{S}$ from Hamilton's equation (1.7) and using (2.38) we obtain Hamilton's equation (1.5) for the particle momentum. For the field momentum π_ρ we get

$$\begin{aligned}\dot{\pi}_\rho(q') &= \left(\frac{\partial}{\partial t} + \int d^3q'' \left(\dot{\rho}(q'') \frac{\delta}{\delta \rho(q'')} + \dot{S}(q'') \frac{\delta}{\delta S(q'')}\right)\right) \frac{\delta w}{\delta \rho(q')} \\ &= \int d^3q'' \left(\frac{\delta w}{\delta \rho(q'')} \frac{\delta}{\delta \rho(q')} \frac{1}{m} \frac{\partial}{\partial q_i''}\left(\rho \frac{\partial S}{\partial q_i''}\right) + \frac{\delta w}{\delta S(q'')} \frac{\delta Q(\rho(q''))}{\delta \rho(q')}\right)\end{aligned} \tag{2.40}$$

where we have substituted for $\partial w / \partial t$ from (2.36) and for $\dot{\rho}$ and $\dot{S}$ from Hamilton's equations. Replacing the derivatives of w from the second and third relations in (2.35) then gives

$$\dot{\pi}_\rho(q') = -\frac{1}{m} \frac{\partial \pi_\rho(q')}{\partial q_i'} \frac{\partial S(q')}{\partial q_i'} + \int \pi_S(q'') \frac{\delta Q(\rho(q''))}{\delta \rho(q')} d^3q'' - \frac{\delta Q(\rho(q))}{\delta \rho(q')} \tag{2.41}$$

which is Hamilton's equation (1.8). Finally, for the field momentum π_S we find using the same substitutions

$$
\dot{\pi}_S(q') = \left(\frac{\partial}{\partial t} + \dot{q}_j \frac{\partial}{\partial q_j} + \int d^3q'' \left(\dot{\rho}(q'') \frac{\delta}{\delta\rho(q'')} + \dot{S}(q'') \frac{\delta}{\delta S(q'')} \right)\right)\left(\frac{\delta w}{\delta S(q')} + \delta(q-q') \right)
$$

$$
= \int d^3q'' \left(\frac{\delta w}{\delta\rho(q'')} \frac{\delta}{\delta S(q')} \frac{1}{m} \frac{\partial}{\partial q_i''}\left(\rho \frac{\partial S}{\partial q_i''}\right) + \frac{\delta w}{\delta S(q'')} \frac{\delta}{\delta S(q')} \left(\frac{1}{2m} \frac{\partial S}{\partial q_i''} \frac{\partial S}{\partial q_i''} \right)\right) + \dot{q}_j \frac{\partial}{\partial q_j} \delta(q-q')
$$

$$
= \frac{1}{m} \frac{\partial}{\partial q_i'}\left(\rho(q') \frac{\partial \pi_\rho(q')}{\partial q_i'} - \pi_S(q') \frac{\partial S(q')}{\partial q_i'} \right) + \frac{1}{m} \frac{\partial}{\partial q_i'}\left(\delta(q-q') \frac{\partial S(q')}{\partial q_i'} \right) + \dot{q}_j \frac{\partial}{\partial q_j} \delta(q-q') \tag{2.42}
$$

The q-dependent terms cancel (multiply by a test function $\mu(q')$ and integrate over q') and we get Hamilton's equation (1.9). We conclude that the solution (2.33) is consistent with Hamilton's equations for the combined system.

3. Liouville's equation and Schrödinger's equation

3.1 Liouvillian form of the Schrödinger equation

The analysis of §5(I) indicates that there is an intimate connection between the Schrödinger and Liouville equations. Indeed, as we now briefly describe, up to an undetermined factor the former can be expressed in the form of the latter. In principle this provides an alternative method of calculating the wavefunction (up to a time-dependent addition to the phase).

To begin with, we note that we have shown in §5(I) that the Schrödinger equation implies that the function (1.13),

$$
f(q,p,t) = f_\delta(q,p,t) = \rho(q,t)\delta\left(p - \frac{\partial S(q,t)}{\partial q}\right), \tag{3.1}
$$

obeys Liouville's equation (1.11),

$$
\frac{\partial f}{\partial t} + \frac{p_i}{m}\frac{\partial f}{\partial q_i} - \frac{\partial(V+Q)}{\partial q_i}\frac{\partial f}{\partial p_i} = 0. \tag{3.2}
$$

We may assert a partial converse of this result: assuming f has the form (3.1), we may deduce from (3.2) Hamilton's equation (1.4) for ρ and the derivative of Hamilton's equation (1.5) for S. Hence, if the distribution function has the form (3.1) initially, we can construct from the solution to Liouville's equation a solution to Schrödinger's equation, up to a time-dependent factor, using the following formulas:

$$\rho(q,t)=\int f(q,p,t)\,d^3p \tag{3.3}$$

$$S(q,t)=\int^q \left(\frac{\int p_i f(q',p,t)\,d^3p}{\int f(q',p,t)\,d^3p} \right) dq_i' + c(t) \tag{3.4}$$

where $c(t)$ is an undetermined function of t. To solve Liouville's equation we first substitute (3.3) into the quantum potential (1.3) so that (3.2) is expressed purely in terms of f. It is evident that this is a highly nonlinear integro-differential equation in f so this method is unlikely to be a practical aid to finding solutions to the wave equation. To complete the solution we can fix the function $c(t)$ by substituting (3.3) and (3.4) into Hamilton's equation for S, as pointed out by Takabayasi [6] in a similar context (see [7] for the analogous reconstruction of ψ from the Wigner function).

3.2 Liouville's equation in Schrödinger form

Using the HJ representation developed in §2 we can go in the opposite direction and write Liouville's equation in a form closer to Schrödinger's equation. Defining the complex function

$$\phi(q,\alpha,t)=\sqrt{\Gamma(q,\alpha,t)}\exp\left(i\sigma(q,\alpha,t)/\hbar\right) \tag{3.5}$$

Liouville's equation in the form (2.16) and the associated HJ equation (2.12) can be combined into a single Schrödinger-like equation:

$$i\hbar\frac{\partial\phi}{\partial t} = -\frac{\hbar^2}{2m}\frac{\partial^2\phi}{\partial q_i^2} + V\phi + \left(Q-\tilde{Q}\right)\phi. \tag{3.6}$$

Here

$$\tilde{Q}(q,\alpha,t) = -\frac{\hbar^2}{2m\sqrt{\Gamma}}\frac{\partial^2\sqrt{\Gamma}}{\partial q_i^2} \tag{3.7}$$

is a 'quantum potential' constructed from the distribution function (2.19),

$$\Gamma(q,\alpha,t) = \Gamma_\delta(q,\alpha,t) = D(q,\alpha,t)\rho(q,t)\delta\left(\frac{\partial\sigma(q,\alpha,t)}{\partial q} - \frac{\partial S(q,t)}{\partial q}\right). \tag{3.8}$$

As in §3.1, equation (3.6) subject to (3.8) implies Schrödinger's equation up to a factor. Since we can express ρ in Q in terms of Γ via the relation (2.17),

$$\rho = \int \Gamma(q,\alpha,t)\, d^3\alpha, \tag{3.9}$$

(3.6) may be expressed purely in terms of Γ and σ (the analogue of expressing (3.2) in terms of f). Solving (3.6) for ϕ and extracting Γ and σ, we can then construct the wavefunction, up to a factor, via the formulas (3.9) and

$$S(q,t) = \int^q \left(\frac{\int \frac{\partial\sigma(q',\alpha,t)}{\partial q_i}\Gamma(q',\alpha,t)\, d^3\alpha}{\int \Gamma(q',\alpha,t) d^3\alpha} \right) dq_i' + c(t). \tag{3.10}$$

4. Canonical and unitary transformations

So far we have worked in a set of phase space coordinates in which the Hamiltonian takes the form (1.1). In that frame we have supplemented the Hamiltonian with a constraint which ensures that the flow of the particle component of the wave-particle system coincides with the density ρ. In §2 we considered a canonical transformation which maps into constant coordinates in this frame. We now develop the general theory of canonical transformations to arbitrary frames on the phase space, and explore the connection between these and quantum unitary transformations. An eventual aim of this work is to allow computation of the particle trajectories in other representations (so far we have worked in the position representation), but here we shall confine attention to developing the general formalism with some simple applications, and only indicate in principle how to pass to other representations. It will be shown within this formalism how a transformation can be chosen so that the particle component of the Hamiltonian is transformed away (as was shown in §2.4; the solution of the HJ equation which is used in this demonstration will be of use in §5). In addition, we throw further light on our HJ treatment of §2.

In order to connect the formalism with the linear unitary transformations it will be convenient to use ψ and ψ^* as independent field coordinates in place of ρ and *S,* for it is in terms of these that the linearity is most naturally expressed. We introduce in addition corresponding canonical field momenta π_ψ and π_{ψ^*}. This replacement is a time-independent canonical transformation with respect to which the Hamiltonian is a scalar, given by

$$\left.\begin{aligned} &\rho = \psi^* \psi, \quad S = \frac{\hbar}{2i}\log\frac{\psi}{\psi^*}, \\ &\pi_\rho = \frac{1}{2\psi^*\psi}\left(\psi\pi_\psi + \psi^*\pi_{\psi^*}\right) \quad \pi_S = \frac{1}{i\hbar}\left(\psi^*\pi_{\psi^*} - \psi\pi_\psi\right) \\ &q = \bar{q}, \quad p = \bar{p}. \end{aligned}\right\} \tag{4.1}$$

It is readily checked using the formulas for a canonical transformation,

$$\psi = \frac{\delta W}{\delta \pi_\psi}, \quad \psi^* = \frac{\delta W}{\delta \pi_{\psi^*}}, \quad \pi_\rho = \frac{\delta W}{\delta \rho}, \quad \pi_S = \frac{\delta W}{\delta S}, \quad \bar{q} = \frac{\partial W}{\partial \bar{p}}, \quad p = \frac{\partial W}{\partial q}, \tag{4.2}$$

that the substitution is generated by the functional

$$W\left[q, \rho, S, \bar{p}, \pi_\psi, \pi_{\psi^*}\right] = q_i \bar{p}_i + \int \left(\pi_\psi \sqrt{\rho}\exp(iS/\hbar) + \pi_{\psi^*}\sqrt{\rho}\exp(-iS/\hbar)\right) d^3q'. \tag{4.3}$$

Using the new variables the Hamiltonian (1.1) is

$$H_{tot} = H\left(q, p, \psi, \psi^*\right) + \int \left\{ \frac{\pi_\psi(q')}{i\hbar}\left(-\frac{\hbar^2}{2m}\frac{\partial^2 \psi(q')}{\partial q_i'^2} + V(q')\psi(q') \right) \right.$$

$$\left. - \frac{\pi_{\psi^*}(q')}{i\hbar}\left(-\frac{\hbar^2}{2m}\frac{\partial^2 \psi^*(q')}{\partial q_i'^2} + V(q')\psi^*(q') \right) \right\} d^3 q'. \qquad (4.4)$$

Hamilton's equations yield the Schrödinger equation (1.1)(I) for ψ and, as anticipated in §4(I), the canonical momentum π_ψ satisfies the complex conjugate Schrödinger equation modified by an additional source term:

$$-i\hbar \frac{\partial \pi_\psi(q')}{\partial t} = \left(-\frac{\hbar^2}{2m}\frac{\partial^2}{\partial q_i'^2} + V(q') \right) \pi_\psi(q') + i\hbar \left. \frac{\delta Q\left(\psi(q), \psi^*(q)\right)}{\delta \psi(q')} \right|_{q=q(t)}. \qquad (4.5)$$

The fields ψ^* and π_{ψ^*} obey the complex conjugate equations. It will be useful to write the Hamiltonian in the form

$$H_{tot} = H\left(q, p, \psi, \psi^*\right) + (i\hbar)^{-1} \int \left(\pi_\psi(q')\hat{H}(q', q'')\psi(q'') - \pi_{\psi^*}(q')\hat{H}^*(q', q'')\psi^*(q'') \right) d^3q'\, d^3q'' \qquad (4.6)$$

where

$$\hat{H}(q', q'') = \left(-\frac{\hbar^2}{2m}\frac{\partial^2}{\partial q_i'^2} + V(q') \right) \delta(q' - q''). \qquad (4.7)$$

It is well known that unitary transformations in quantum mechanics can be represented as canonical transformations in the phase space defined by the wavefunction coefficients [8]. Translating this construction into our phase space, and generalizing to include the particle variables, we consider a transformation between two sets of phase space coordinates $\left(q, p, \psi(q'), \psi^*(q'), \pi_\psi(q'), \pi_{\psi^*}(q')\right)$ and $\left(\bar{q}, \bar{p}, \psi'(a), \psi'^*(a), \pi_{\psi'}(a), \pi_{\psi'^*}(a)\right)$. Here we allow for the possibility that the argument (a) of the transformed field phase space functions does not coincide with the space of the particle coordinates ($\bar{q}$). A unitary transformation $U(a,q)$ establishes a (linear) relation between the old and new field coordinates (we assume that the arguments q and a of the functions are both 3-d continuous variables):

$$\psi'(a) = \int U(a,q')\psi(q')\, d^3q' \tag{4.8}$$

where

$$\int U(a,q')U^*(a,q'')\, d^3a = \delta(q'-q''),\ \int U(a,q')U^*(a',q')\, d^3q' = \delta(a-a') \tag{4.9}$$

and likewise for the complex conjugate coordinate. Hence, because the old and new coordinates are functionally related we shall assume that the canonical transformation which generates the unitary transformation is a function of the old coordinates and the new momenta [9]. Considering the field coordinates alone, a unitary transformation is generated by the functional

$$w\left[\psi,\psi^*,\pi_{\psi'},\pi_{\psi'^*},t\right] = \int \left(\pi_{\psi'}(a)U(a,q')\psi(q') + \pi_{\psi'^*}(a)U^*(a,q')\psi^*(q')\right) d^3a\, d^3q' \tag{4.10}$$

where the possible time dependence of w comes from U. Including the particle variables the complete generator will be

$$W\left[q,\psi,\psi^*,\bar{p},\pi_{\psi'},\pi_{\psi'^*},t\right] = w\left[\psi,\psi^*,\pi_{\psi'},\pi_{\psi'^*},t\right] + F\left(q,\psi,\psi^*,\bar{p},t\right) \tag{4.11}$$

where it is allowed that F may depend on (local functions of) the old field coordinates but not on the new field momenta since this would modify the relation (4.8). For, by the equations of a canonical transformation, we have

$$\psi'(a) = \frac{\delta W}{\delta \pi_{\psi'}(a)} = \int U(a,q')\psi(q')\, d^3q' \tag{4.12}$$

$$\psi'^*(a) = \frac{\delta W}{\delta \pi_{\psi'^*}(a)} = \int U^*(a,q')\psi^*(q')\, d^3q' \tag{4.13}$$

$$\pi_\psi(q') = \frac{\delta W}{\delta \psi(q')} = \int \pi_{\psi'}(a) U(a,q')\, d^3a + \frac{\delta F}{\delta \psi(q')} \tag{4.14}$$

$$\pi_{\psi^*}(q') = \frac{\delta W}{\delta \psi^*(q')} = \int \pi_{\psi'^*}(a) U^*(a,q')\, d^3a + \frac{\delta F}{\delta \psi^*(q')} \tag{4.15}$$

$$p_i = \frac{\partial W}{\partial q_i} = \frac{\partial F}{\partial q_i} \tag{4.16}$$

$$\bar{q}_i = \frac{\partial W}{\partial \bar{p}_i} = \frac{\partial F}{\partial \bar{p}_i} \tag{4.17}$$

and so the relation (4.8) is recovered. The mapping (4.11) is the most general possible in this theory that is compatible with quantum unitary transformations. We have not yet specified F but we expect this will generally depend on U. Adapting the definition (2.6) to the new variables and using the transformation equations (4.12) – (4.17), the Hessian matrix is

$$h_{ij}(a,a',q'',q''') = \begin{pmatrix} \dfrac{\partial^2 F}{\partial q_i \partial \bar{p}_j} & 0 & 0 \\ \dfrac{\delta^2 F}{\delta \psi(q'')\partial \bar{p}_j} & U(a,q'') & 0 \\ \dfrac{\delta^2 F}{\delta \psi^*(q''')\partial \bar{p}_j} & 0 & U^*(a',q''') \end{pmatrix}. \tag{4.18}$$

The condition for the transformation to be canonical, $\det h \neq 0$, will be obeyed if the determinant of the upper left-hand term is non-zero.

Let us apply this transformation to the Hamiltonian (4.6). The transformed Hamiltonian is given by

$$H'_{tot} = H_{tot} + \frac{\partial W}{\partial t} \tag{4.19}$$

which we must express in terms of the new variables. Substituting (4.12) – (4.15) we get

$$H'_{tot} = H' + (i\hbar)^{-1}\int\Big(\pi_{\psi'}(a)\hat{H}'(a,a')\psi'(a') - \pi_{\psi'^*}(a)\hat{H}'^*(a,a')\psi'^*(a')\Big)d^3a\, d^3a' \tag{4.20}$$

where

$$\hat{H}'(a,a') = \int U(a,q')\left(\hat{H}(q',q'')U^*(a',q'') - i\hbar\frac{\partial U^*(a',q'')}{\partial t}\delta(q'-q'')\right)d^3q'\, d^3q'' \tag{4.21}$$

is the usual transformed Hamiltonian operator, and

$$H' = H + (i\hbar)^{-1}\int\left\{\frac{\delta F}{\delta\psi(q')}\hat{H}(q',q'')\psi(q'') - \frac{\delta F}{\delta\psi^*(q')}\hat{H}^*(q',q'')\psi^*(q'')\right\}d^3q'\, d^3q'' + \frac{\partial F}{\partial t} \tag{4.22}$$

where we must substitute the new coordinates for ψ, ψ^*, q and p using (4.12), (4.13), (4.16) and (4.17).

As a first application of these formulas we show that a judicious choice of F reduces the transformed total Hamiltonian to just the field component. Substituting for p from (4.16) and introducing the function $\Psi = \sqrt{\rho}\exp(iF/\hbar)$ we can express the original particle component H as

$$\begin{aligned} H &= \frac{1}{2m}\frac{\partial F}{\partial q_i}\frac{\partial F}{\partial q_i} + Q + V \\ &= \frac{1}{2\Psi^*(q)\Psi(q)}\int\Big(\Psi^*(q)\hat{H}(q,q'')\Psi(q'') + \Psi(q)\hat{H}^*(q,q'')\Psi^*(q'')\Big)d^3q''. \end{aligned} \tag{4.23}$$

Choosing F to have the (time-independent) form

$$F(q) = (\hbar/2i)\log\big(\psi/\psi^*\big)(= S), \tag{4.24}$$

so that $\Psi = \psi$, and substituting into (4.22), then implies that $H' = 0$ which proves the assertion. Thus we rederive the result of §2.4. Note that this transformation is not canonical according to the usual definition [5] as *F* is independent of $\bar{p}$.

Next, we consider the case where the unitary transformation is the time evolution of the system, with ψ' being constant in time and $a = q'$. Then U^* obeys the Schrödinger equation so that from (4.21) $\hat{H}' = 0$. Choosing *F* as in (4.24) then implies from (4.20) that $H'_{tot} = 0$ and from (4.19) we recover the HJ equation (2.4). The generator of time evolution for the total system is then

$$W = w + (\hbar/2i)\log(\psi/\psi^*) \tag{4.25}$$

where *w* obeys the field HJ equation (2.36).

The formalism developed here allows us, in principle, to determine the particle trajectories in any representation connected with the original *q*-representation by the continuous relation (4.8). We can compute the trajectories in the transformed frame in two ways. First, by solving the transformed Hamilton equations which must then be supplemented with constraints which ensure that the flow of the particle component of the wave-particle system coincides with the quantal distribution in the relevant representation. Second, by inserting a trajectory that is already known in the (*q,p*) coordinates into the transformation equations (4.16) and (4.17) and inverting. Both methods require knowing *F* (in particular as a function of $\bar{p}$). The determination of this will be considered elsewhere.

5. Particle back-reaction and the action-reaction principle

5.1 Explicit solution for the particle back-reaction

In §2.4 we found a solution of the total HJ equation, (2.33), which implies the deBB law of motion. We showed that the field canonical momenta implied by this function satisfy Hamilton's equations (1.8) and (1.9), the latter exhibiting a particle source term. The second and third equations in (2.35) give this solution as

$$\pi_\rho(q',t) = \bar{\pi}_\rho(q',t), \quad \pi_S(q',t) = \bar{\pi}_S(q',t) + \delta(q(t) - q') \tag{5.1}$$

where $\bar{\pi}_\rho$ and $\bar{\pi}_S$ obey the pure field equations ((1.8) and (1.9) without the source term). It is easy to check by direct substitution that (5.1) indeed obeys (1.8) and (1.9). Using the transformation equations (4.1) this solution may be written in terms of the ψ variables as

$$\pi_\psi(q',t) = \bar{\pi}_\psi(q',t) - \frac{i\hbar}{2\psi(q',t)}\delta(q(t) - q') \tag{5.2}$$

where $\bar{\pi}_\psi$ obeys the complex conjugate Schrödinger equation. Again, it is readily checked that this function satisfies the field equation (4.5). Note that in (5.2) the δ-function term is indeterminate at nodes ($\psi = 0$), for the trajectory does not pass there. To complete the solution we have to specify $\bar{\pi}_\psi$ and insert an explicit solution $q = q(q_0, t)$ of the deBB law as determined by ψ. The initial function $\bar{\pi}_{\psi 0}$ is arbitrary so we can in principle choose for $\bar{\pi}_\psi$ any solution of the complex conjugate Schrödinger equation in the given potential V.

Of all possible functions, we can choose $\bar{\pi}_\psi$ proportional to ψ^*. In fact, it will be shown below that this choice, together with a certain choice of proportionality constant, is a natural one. Specifically, we choose the solution

$$\pi_\psi(q',t) = \frac{i\hbar}{2}\left(\psi^*(q',t) - \frac{1}{\psi(q',t)}\delta(q(t,q_0) - q')\right). \tag{5.3}$$

The additional field π_ψ may thus be represented up to a proportionality factor as the complex conjugate wavefunction ψ^* superposed with a δ-function singularity which follows one (fixed by q_0) of the particle orbits determined by ψ via the deBB law, modulated by the inverse of ψ. In this case the field π_ψ is no longer an independent degree of freedom and the system consists of just the wavefunction together with the particle.

5.2 Energy and momentum of the field-particle system

Our total physical system comprises two complex fields (ψ and π_ψ) and a particle (q). This is what we mean in this theory by 'a quantum system'. In order to justify this appellation we have to ensure that certain basic properties of the composite system coincide with key ones that are relevant to the conventional concept of a quantum system. Up to now we have concentrated on ensuring concordance for one such property, the probability distribution of the particle component. We now examine the energy and momentum. We shall be concerned with establishing the conservation laws obeyed by these quantities, and their connection with the corresponding quantum mechanical values.

We consider first the rate of change of energy. Since the PB of H_{tot} with itself vanishes we have, using (1.1),

$$\frac{dH_{tot}}{dt} = \frac{\partial H_{tot}}{\partial t} = \frac{\partial V(q,t)}{\partial t} - \int \pi_S(q')\frac{\partial V(q',t)}{\partial t} d^3q'. \tag{5.4}$$

We immediately conclude that the total energy is conserved when the external potential is time-independent, the usual condition for conservation in quantum mechanics.

We pass now to the momentum. Returning to the Lagrangian (4.2)(I) the total momentum of the composite system is given by

$$\begin{aligned} p_{tot\,i} &= \frac{\partial L_{tot}}{\partial \dot{q}_i} - \int \left(\frac{\delta L_{tot}}{\delta \dot{\rho}} \frac{\partial \rho}{\partial q'_i} + \frac{\delta L_{tot}}{\delta \dot{S}} \frac{\partial S}{\partial q'_i} + \frac{\delta L_{tot}}{\delta \dot{g}_\rho} \frac{\partial g_\rho}{\partial q'_i} + \frac{\delta L_{tot}}{\delta \dot{g}_S} \frac{\partial g_S}{\partial q'_i} \right) d^3q' \\ &= m\dot{q}_i - \int \left(g_\rho \frac{\partial \rho}{\partial q'_i} + g_S \frac{\partial S}{\partial q'_i} \right) d^3q'. \end{aligned} \tag{5.5}$$

Converting to phase space variables we have

$$p_{tot\,i} = p_i - \int \left(\pi_\rho \frac{\partial \rho}{\partial q'_i} + \pi_S \frac{\partial S}{\partial q'_i} \right) d^3q' = p_i - \int \left(\pi_{\psi^*} \frac{\partial \psi^*}{\partial q'_i} + \pi_\psi \frac{\partial \psi}{\partial q'_i} \right) d^3q' \tag{5.6}$$

using the transformation equations (4.1). Using Schrödinger's equation for ψ, the field equation (4.5) for π_ψ, and Hamilton's equation (1.5) for p, it is straightforward to calculate the rate of change of the momentum:

$$\frac{dp_{tot\,i}}{dt} = -\frac{\partial V(q,t)}{\partial q_i} + \int \frac{1}{i\hbar}\left(\psi^* \pi_{\psi^*} - \psi \pi_\psi\right)\frac{\partial V(q',t)}{\partial q_i} d^3q'$$

$$= -\frac{\partial V(q,t)}{\partial q_i} + \int \pi_S(q')\frac{\partial V(q',t)}{\partial q_i} d^3q'. \tag{5.7}$$

We therefore see that the total momentum is conserved when the external potential is space-independent, once again the usual condition for conservation in quantum mechanics.

We have thus established agreement between the theory of the composite system and quantum mechanics as regards the conditions under which energy and momentum are conserved. These results hold for the unconstrained Hamiltonian system and are obviously valid also when the constraint $p = \partial S/\partial q$ is imposed. We now consider the additional implications of the latter condition.

While agreeing with quantum mechanics in their conservation properties, the (unconstrained) values of the total energy and momentum are arbitrary and do not generally coincide with the corresponding quantum values. A natural constraint on our 'quantum system' is that the total energy and momentum be just those which quantum mechanics defines as the total energy and momentum of a physical system. In the latter all we have is the ψ-field and the total energy and momentum of the field are given by (equal to the mean values)

$$\langle \hat{H} \rangle = \int \psi^*(q')\hat{H}(q',q'')\psi(q'')d^3q'\, d^3q'' \tag{5.8}$$

$$\langle \hat{p}_i \rangle = -i\hbar \int \psi^*(q')\frac{\partial}{\partial q'_i}\psi(q')d^3q' . \tag{5.9}$$

Consider the case where $p = \partial S/\partial q$ and the independent components of our quantum system reduce to just ψ and the particle, with π_ψ given by (5.3). Then it is easy to see that in the expression (4.4) for the total energy the particle component cancels out and the resulting field energy is the quantum expression (5.8). Likewise, the particle contribution to the total momentum (5.6) drops out and what remains is the total quantum field momentum (5.9). Thus, under these conditions,

$$H_{tot} = \langle \hat{H} \rangle, \; p_{tot\,i} = \langle \hat{p}_i \rangle. \tag{5.10}$$

The constraint $p = \partial S/\partial q$ characterizing the deBB theory therefore implies not only the quantum mechanical distribution for the particle, but also agreement with the quantum values for energy and momentum. This may be regarded as a justification for adopting the solution (5.3), in which definite choices were made for $\overline{\pi}_\psi$ and the proportionality constant.

5.3 The action-reaction principle

One of the distinctive aspects of the deBB theory in its conventional presentation is that, in acting on the particle, the quantum wave suffers no back-reaction. This is not a logical problem as there is no principle of physics which requires such reaction in all cases (and there are other examples in science where it is not obeyed, e.g., catalysis) but in this regard it is quite unlike other theories of field-particle interaction. By placing the theory of quantum particle motion in a wider Hamiltonian framework we have seen that the absence of reaction is only apparent due to the incompleteness of the usual description of the deBB theory. To be sure, the Schrödinger field itself continues to suffer no reaction – we constructed the theory with this aim in mind in order to preserve the usual predictions of quantum mechanics - but the equations obeyed by the additional field π_ψ, whose presence is necessitated by this construction, do include action by the particle. The question then is whether this two-way action is of such a kind that we can claim the action-reaction principle is obeyed.

While the independence of ψ precludes implementation of a full version of the action-reaction principle, which requires mutual action of all interacting entities [10], we can establish the validity of a weaker form. Making precise the notion of an equal action between two qualitatively dissimilar systems is a subtle affair, e.g., deciding at what level the mutual actions should be analysed, or quantifying their relative strengths. It may be argued that a key component of the action-reaction principle is that the total energy and momentum of an isolated coupled system are conserved [10]. Within these terms, the demonstration above that the total energy and momentum of our composite quantum system are conserved when the external potential is suitably restricted establishes the validity of at least this component of the principle in this theory. In the conventional presentation of the deBB theory this component is violated because the particle simply responds to the field, through the quantum potential, as if the latter were just an additional external potential. The energy and momentum of the particle in isolation are not conserved when the external potential obeys the usual conditions for conservation. In contrast, when the particle is treated as a component of an interacting field-particle system of the kind we have described, the trade-off between the mutual actions is of just the right measure to ensure conservation.

In fact, the description introduced here has the potential for modification so as to include a reaction of the particle on ψ as well if we so desired, thus allowing a fuller implementation of the action-reaction principle. In the analogous model described in §3(I) this would be effected by changing the functional dependence of U in (3.1)(I). This possibility will be discussed elsewhere.

6. Alternative choices for the Hamiltonian

We started by assuming a Hamiltonian (1.1) which expresses the quantum effects on a particle through the quantum potential Q, and have shown how the flow it generates will be consistent with ρ if it is supplemented by the condition $p = \partial S / \partial q$ which implies the deBB equation of motion (1.15). In view of what we already knew about the deBB theory, in particular the key role it implies for the quantum potential, this result is not surprising. Indeed, the choice of the quantum potential as the agent of quantum actions on the particle was suggested in the first place by the deBB law. However, given that the latter is simply a postulate, representing the quantum effects through the quantum potential is somewhat arbitrary. Would other choices for the Hamiltonian imply flows that are compatible with the ρ spatial distribution? And if so, what is their relation to the deBB theory? We shall investigate these questions for two classes of Hamiltonian, the second a generalization of the first. We find that we may indeed adopt other Hamiltonian descriptions, and that the accompanying laws of motion generally differ from that of deBB.

First, we show that Hamiltonians of the type

$$H = \frac{1}{2m} p^2 + V(q,t) + Q'(q,t), \tag{6.1}$$

where $Q' \neq Q$, can in principle be compatible with the quantal distribution, and that the only admissible potentials for which the distribution is f_δ, i.e., (1.13) (and hence the deBB equation holds), are those that differ from Q by at most an undetermined additive function of time (in accord with the discussion in §3). Here it is assumed that Q' may be some function of q, ρ and S but not of p or the conjugate field momenta. This ensures that Hamilton's equation (1.4) for the particle, and Schrödinger's equation, are unmodified. This H is to be inserted into the total Hamiltonian (1.1), and we may repeat the analysis of §5.1(I) to arrive at the Liouville equation (1.10) for the particle distribution. Hamilton's equations (1.4)-(1.9) for the combined system are the same except that $Q \to Q'$ and both field momentum equations now have source terms.

To establish the first result, we examine the momentum moments defined in §5.2(I). For the Hamiltonian (6.1) the particle Liouville equation (1.10) becomes

$$\frac{\partial f}{\partial t} + \frac{p_i}{m}\frac{\partial f}{\partial q_i} - \frac{\partial (V + Q')}{\partial q_i}\frac{\partial f}{\partial p_i} = 0. \tag{6.2}$$

In this case, the evolution equations for the momentum moments are (5.37)(I) with Q replaced by Q', while the equations (5.39)(I) deduced from the Schrödinger equation remain the same. Subtracting these two sets of equations, the equations (5.40)(I) for the X-tensors (defined as before by (5.51)(I)) are replaced by

$$\frac{\partial X_{i_1 \dots i_{n-1}}}{\partial t} + \frac{1}{m}\frac{\partial X_{i_1 \dots i_n}}{\partial q_{i_n}} = -\sum_{\mathbf{P}} X_{i_1 \dots i_{n-2}}\frac{\partial (V + Q')}{\partial q_{i_{n-1}}} - \rho \sum_{\mathbf{P}} \frac{\partial S}{\partial q_{i_1}} \dots \frac{\partial S}{\partial q_{i_{n-2}}}\frac{\partial (Q' - Q)}{\partial q_{i_{n-1}}}. \tag{6.3}$$

The distribution function will have the same form (1.12) as before,

$$f(q, p, t) = f_\delta(q, p, t) + \theta(q, p, t) \tag{6.4}$$

except that it is now subject to (6.3). To see whether this satisfies (6.2) we substitute the characteristic function M from (5.44)(I) (also unchanged) into the left-hand side of the modified characteristic function equation (5.50)(I), where Q is replaced by Q'. Using (5.39)(I) and (6.3) the result is

$$lhs = i\rho e^{i\lambda_i(\partial S/\partial q_i)}\lambda_j \frac{\partial(Q'-Q)}{\partial q_j} - \rho\sum_{n=1}^{\infty}\frac{i^n}{n!}\lambda_{i_1}\ldots\lambda_{i_n}\sum_{\mathbf{P}}\frac{\partial S}{\partial q_{i_1}}\cdots\frac{\partial S}{\partial q_{i_{n-1}}}\frac{\partial(Q'-Q)}{\partial q_{i_n}}. \tag{6.5}$$

Expanding the exponential and gathering terms this expression is zero, and hence (6.4) is a solution of (6.2) (and is indeed the most general solution compatible with the Schrödinger equation). However, unlike the case originally considered in §5.2(I) (where $Q' = Q$) the functions f_δ and θ are not solutions separately. Here, if $Q' \neq Q$, only the total f is a solution. It may appear odd that we have managed to find the general solution to Liouville's equation without needing to specify Q' but it must be borne in mind that this solution is valid only to the extent that we can construct solutions for the X-tensors that obey (6.3), and that imply a non-negative f, and these requirements will impose constraints on Q'. To the extent that this construction is possible, an ensemble of (non-deBB) motions obeying Hamilton's particle equations (1.4) and (1.5) (with $Q \to Q'$) will reproduce the quantum flow if the coordinates are distributed according to (6.4).

An example which apparently supports this result is a non-negative solution to (6.2) (for a particular choice of Q') presented by Sutherland [11] which is not of the form f_δ and for which the zeroth and first momentum moments are the quantum expressions (so that $X_i = 0$). However, if one calculates X_{ij} by computing the second momentum moment of this solution, this does not obey (6.3) when $n = 2$. Hence this solution is not consistent with the Schrödinger equation.

If we insist on f_δ being a solution to (6.2), this means that the first term in (6.5) is zero so that

$$\frac{\partial(Q'-Q)}{\partial q_i} = 0 \text{ or } Q'(q,t) = Q(q,t) + \varepsilon(t) \tag{6.6}$$

where $\varepsilon(t)$ is arbitrary, which proves our second assertion regarding the Hamiltonian (6.1).

We pass now to the second class of Hamiltonians and show that the distribution f_δ can be valid even though the deBB law of motion is not. This we do by generalizing the Hamiltonian (6.1) to include a vector potential A:

$$H = \frac{1}{2m}(p - A(q,t))^2 + V(q,t) + Q'(q,t). \tag{6.7}$$

Here Q' and A may depend on ρ and S but not on π_ρ or π_S. The particle Hamilton equations are now

$$m\dot{q}_i = p_i - A_i(q,t) \tag{6.8}$$

$$\dot{p}_i = -\frac{\partial}{\partial q_i}(V + Q') + \frac{1}{m}(p_j - A_j)\frac{\partial A_j}{\partial q_i}. \tag{6.9}$$

The Liouville equation (1.10) holds with this H. In this case we shall not derive the most general distribution that is compatible with the Hamiltonian but only enquire whether (6.7) is compatible with the distribution f_δ (which we know generates the correct q-projected flow). The particle equations (6.8) and (6.9) are then subject to the subsidiary condition $p = \partial S/\partial q$ so that

$$m\dot{q}_i = \left.\left(\frac{\partial S}{\partial q_i} - A_i\right)\right|_{q=q(t)}. \tag{6.10}$$

Hence, if f_δ is indeed a solution, the law (6.10) implies motions different from that of deBB.

To show that f_δ is a solution if the free functions appearing in (6.7) obey certain constraints, we use the characteristic equation which is now

$$\frac{\partial M}{\partial t} - \frac{1}{m}\left(i\frac{\partial}{\partial \lambda_j} + A_j\right)\frac{\partial M}{\partial q_j} + \frac{1}{m}\frac{\partial A_j}{\partial q_k}\left(i\frac{\partial}{\partial \lambda_j} + A_j\right)(i\lambda_k M) + i\lambda_j\frac{\partial (V + Q')}{\partial q_j}M = 0. \tag{6.11}$$

Substituting the characteristic function corresponding to f_δ, $M = \rho e^{i\lambda_j(\partial S/\partial q_j)}$, this obeys (6.11) if the following four (real) conditions hold:

$$\frac{\partial}{\partial q_i}(\rho A_i) = 0 \tag{6.12}$$

$$\frac{1}{m}A_j\left(\frac{1}{2}A_j-\frac{\partial S}{\partial q_j}\right)+Q'-Q=\varepsilon(t) \qquad (6.13)$$

where $\varepsilon(t)$ is arbitrary. If we can construct a solution for A obeying the first equation, the second equation defines Q'. When these relations are obeyed, we can write the Schrödinger equation (1.4) and (1.5) as

$$\frac{\partial\rho}{\partial t}+\frac{1}{m}\frac{\partial}{\partial q_i}\left(\rho\left(\frac{\partial S}{\partial q_i}-A_i\right)\right)=0 \qquad (6.14)$$

$$\frac{\partial S}{\partial t}+\frac{1}{2m}\left(\frac{\partial S}{\partial q_i}-A_i\right)\left(\frac{\partial S}{\partial q_i}-A_i\right)+V+Q'+\varepsilon=0. \qquad (6.15)$$

Given that we can find a suitable solution for *A*, the law (6.10) then implies non-deBB motions.

As pointed out in §5.3(I) the non-relativistic quantum mechanical current is determined only up to a divergenceless vector field, and the law of motion (6.10) with the condition (6.12) is an expression of this non-uniqueness. We thus bring within the scope of our analysis previous discussions of the latitude in choices for the particle law of motion that exploit the underdetermination in the current [12,13] (possible forms for *A* have been examined by Deotto and Ghirardi [13]). Hamiltonians of the type (6.7) have also been considered by Roy and Singh [14] who have developed a trajectory theory in which the phase space distribution (which differs from f_δ) has position and momentum partial distributions which both coincide with the quantal expressions.

One could continue this investigation and consider yet more general (particle) Hamiltonians but there does not seem to be much virtue in the effort. It does not seem that this is a useful method if our aim is to limit the possibilities for theoretically valid particle laws of motion since these seem to proliferate the more complex the Hamiltonian gets, and there does not seem to be any principle limiting the possible forms of the latter (it is possible that requiring the energy to coincide with the mean quantum energy as in §5.2 may be useful in this regard). A more oblique attack on this problem may be fruitful. As mentioned in §5.3(I) it has been shown that relativistic considerations fix uniquely the form of the non-relativistic quantum mechanical current for a spin $\frac{1}{2}$ particle [15] (this differs from the deBB equation). Although that particular argument does not apply directly to the spin 0 case considered here, it may be possible to develop similar arguments to restrict the *X*-tensors.

7. Discussion

The conventional presentation of the deBB theory implies several novel features in the theory of quantum waves and particles in comparison with classical theories of interacting fields and particles. The question arises whether these features are genuinely new insights in physics or just artefacts of the original description of the deBB theory, in particular its possible incompleteness. For example, we have shown in §5 that the action-reaction principle, disobeyed according to the usual approach, is in fact obeyed, at least in a weak form, in the wider Hamiltonian framework.

Another example of a possibly misleading implication is the notion, fostered by the conventional presentation based on (1.15), that the deBB theory (fundamentally) differs from classical dynamics in being essentially a 'first-order' (in time) theory [e.g., 16]. By placing the theory in a Hamiltonian environment we have shown that this distinction is not compelling - the particle Hamilton equations (1.4) and (1.5) imply a second-order expression for the position. To be sure, we have imposed on the solutions to Hamilton's equations the relation $p = \partial S/\partial q$ but this merely selects a set of admissible initial coordinates (see §6(I)) and in this regard at least does not imply a qualitatively new notion of dynamics. The first-order law $m\dot{q} = \partial S/\partial q$ can certainly be employed as an alternative way of calculating the paths but, as shown in §6(I), it is dynamically equivalent to Hamilton's equations. Moreover, the first-order law can be employed in classical theory as well; given the classical HJ function as a function of position, all we need to solve for the trajectories is the initial position. Finally, as we have shown, in the Hamiltonian theory (using both the original Hamiltonian (1.1) and for more general Hamiltonians) laws other than that of deBB can be used and it is, in general, Hamilton's equations that must be solved in the first instance (see below) (and indeed, in the case of spin $\frac{1}{2}$ particles, the deBB law is incorrect if it is to be regarded as the limit of the relativistic theory [15]).

In connection with this point, it is not suggested that bringing the deBB theory within the orbit of Hamiltonian theory gives a 'classical' theory of a quantum system. Rather, our aim is to complete the deBB theory, thereby removing some of its artificial features and bringing out more sharply how the quantum and classical theories differ. And indeed the new model does exhibit highly nonclassical features, the principal one being that the description of the state of a matter system is not exhausted by the state of the particles but includes something (ψ) which has its own independent dynamics (and which gives rise in particular to nonlocality in the extension of the theory to many bodies).

A further question that touches the issue of which features displayed by the deBB theory constitute new insights rather than artefacts is its uniqueness. The problem that motivated this investigation is the rather arbitrary way in which the deBB law has been traditionally appended to quantum mechanics, without any theoretical justification other than its compatibility with the $|\psi|^2$ distribution. The aim was to remove some of this arbitrariness by embedding the theory in a consistent Hamiltonian approach, thus giving it an interpretation therein, and also clarifying its connection with HJ theory. These aims have been achieved but in the process we have discovered that Hamiltonian theories can be formulated that admit particle laws of motion different from that of deBB. Two types of non-uniqueness in the particle law have been found. The first source of underdetermination is that, given the Hamiltonian (1.1) in which quantum effects on the particle are attributed to the quantum potential, the most general particle phase space distribution that generates $|\psi|^2$, (1.12), is compatible with motions derived from Hamilton's particle equations that differ from those implied by the deBB equation. The latter corresponds to the case where the momentum p at each point q is fixed. Given the latter restriction we can solve for the motion using the deBB law or, imposing the restriction on the initial conditions, by solving Hamilton's equations. For the general distribution on the other hand we may have many ps associated with each q and we must use Hamilton's equations to find the paths. The resulting trajectories generally differ from those of deBB. The second source of underdetermination in the particle law of motion is that we may choose a different particle component for the Hamiltonian of the total system (§6). Again, we may have a distribution of momenta at each space point (e.g., (6.4)) and hence non-deBB motions.

The possibility of having non-deBB Hamiltonian flows may have a bearing on the problem of deriving (the valid part of) classical physics as a limiting case of quantum mechanics. As has been discussed elsewhere [17] this is problematic in the deBB theory because of the stringent restriction implied by a single-valued momentum, which persists in any limit (a version of a deBB-type theory with crossing q-projected trajectories has been proposed [18] but there the wave propagates in the particle phase space which implies a more abstract interpretation). In contrast, as just pointed out, in the case of the more general phase space distributions considered here this restriction is relaxed and we generally obtain an ensemble of trajectories whose q-projections cross. An advantage of the present approach over the original deBB theory is that we may carry out the limiting process for these trajectories at the level of Hamilton's equations. In the case of the theory based on the Hamiltonian (1.1) the appropriate criterion for the classical limit is that the quantum force is negligible compared to he classical force:

$$\left|\frac{\partial Q}{\partial q_i}\right| << \left|\frac{\partial V}{\partial q_i}\right|. \tag{7.1}$$

When this condition is obeyed the particle is fully decoupled dynamically from the wave ψ and is subject to just the classical equations. Apart from satisfying the condition (7.1), the limiting wavefunction remains essentially quantum mechanical in its properties. Note that this criterion is not sufficient to decouple the quantum system (as we have defined it) entirely from the particle since the latter still enters as a source term in the field equation (4.5) for the conjugate field momentum π_ψ. Some additional condition on the functional derivative of Q is required to ensure a full decoupling, which then implies that the field momentum obeys the Schrödinger equation (note that this condition is not necessary to achieve classical motion for the particle). Note that these limiting results cannot be obtained merely by assuming that Q is numerically small in comparison with the other energies in H_{tot}, for such a condition has no bearing on the magnitude of the derivatives of Q. However, although this procedure implies classical motion for individual particles, we will not recover from this approach the general theory of classical ensembles since in the latter the distribution function is arbitrary while here we obtain only a limiting form of the distribution (1.12).

Similar results may be obtained for the classical limit of the more general Hamiltonians considered in §6. In this connection, the Hamiltonian theory may provide an alternative approach to the treatment of chaos in the quantum particle motions. It may also imply a technique to treat 'hybrid quantum-classical systems', where a classical particle that acts on a quantum system is subject to a quantum back-reaction (see, e.g., [19]). Indeed, it is conceivable that some variant of this approach could provide a means to answer another related problem [17], that of transcending the classical and quantum theories so that each is a special case of a wider enveloping theory. These questions will be investigated elsewhere.

We have seen that, within the framework of Hamiltonian theories, the deBB theory is but one of a wide class of trajectory interpretations. Actually, the underdetermination problem is even deeper for there exists at least one other deterministic trajectory theory [12] which does not fall within the class considered here (a Hamiltonian formulation of this is yet to be investigated). The essential problem is that the basic condition of compatibility of these theories with quantum mechanics, that the space-projection of the Hamiltonian flow generates $|\psi|^2$, is too weak. What is needed now are some physical principles to underpin the mathematical speculation.

Appendix: Liouville's equation in the Hamilton-Jacobi representation

We derive here the form of Liouville's equation (1.11) for the particle,

$$\frac{\partial f}{\partial t}+\frac{p_i}{m}\frac{\partial f}{\partial q_i}-\frac{\partial(V+Q)}{\partial q_i}\frac{\partial f}{\partial p_i}=0, \tag{A1}$$

when we transform from the phase space (q,p) to the mixed system of coordinates (q,α) using the first transformation equation (2.13):

$$p_i=\frac{\partial\sigma(q,\alpha,t)}{\partial q_i}. \tag{A2}$$

The phase space distribution becomes a function of the mixed coordinates:

$$F(q,\alpha,t)=f\left(q,p=\frac{\partial\sigma(q,\alpha,t)}{\partial q_i},t\right). \tag{A3}$$

We have

$$\frac{\partial F}{\partial t}=\left.\frac{\partial f}{\partial t}\right|_{q,p}+\left.\frac{\partial p_i}{\partial t}\right|_{q,\alpha}\left.\frac{\partial f}{\partial p_i}\right|_{q,t},\quad \frac{\partial F}{\partial q_i}=\left.\frac{\partial f}{\partial q_i}\right|_{p,t}+\left.\frac{\partial p_j}{\partial q_i}\right|_{\alpha,t}\left.\frac{\partial f}{\partial p_j}\right|_{q,t} \tag{A4}$$

where we substitute (A2). Substituting (A2), and for the derivatives of f from (A4), in (A1), we get

$$\frac{\partial F}{\partial t}+\frac{1}{m}\frac{\partial \sigma}{\partial q_i}\frac{\partial F}{\partial q_i}-\left(\frac{\partial^2 \sigma}{\partial t \partial q_i}+\frac{1}{m}\frac{\partial \sigma}{\partial q_j}\frac{\partial^2 \sigma}{\partial q_j \partial q_i}+\frac{\partial (V+Q)}{\partial q_i}\right)\left.\frac{\partial f}{\partial p_i}\right|_{q,t}=0. \tag{A5}$$

Taking the q-derivative of the particle HJ equation (2.12),

$$\frac{\partial \sigma}{\partial t}+\frac{1}{2m}\frac{\partial \sigma}{\partial q_i}\frac{\partial \sigma}{\partial q_i}+Q(q,t)+V(q,t)=0, \tag{A6}$$

we see that the term in brackets in (A5) vanishes and hence Liouville's equation becomes

$$\frac{\partial F}{\partial t}+\frac{1}{m}\frac{\partial \sigma}{\partial q_i}\frac{\partial F}{\partial q_i}=0. \tag{A7}$$

This is not yet the final desired form, for F is not the probability density in (q,α)-space. To obtain the latter, we use the relation (A2) for fixed q to change variables from p to α in the normalization condition. Then

$$dp_i=\frac{\partial^2 \sigma}{\partial q_i \partial \alpha_j}d\alpha_j \tag{A8}$$

and the normalization condition becomes

$$1=\int f(q,p,t)\,d^3q\,d^3p=\int F(q,\alpha,t)D\,d^3q\,d^3\alpha \tag{A9}$$

where

$$D(q,\alpha,t) = \left|\det \frac{\partial^2 \sigma}{\partial q_i \partial \alpha_j}\right| \tag{A10}$$

is the modulus of the Jacobian of the transformation, which is here the determinant of the Hessian matrix (the latter is the Van Vleck determinant in the analogous classical case (where $Q = 0$)). By assumption $D \neq 0$. The domain of integration of α_i corresponding to $p_i \in (-\infty, \infty)$ is determined by (A2). The probability density in (q,α)-space is therefore given by the function

$$\Gamma(q,\alpha,t) = F(q,\alpha,t) D(q,\alpha,t). \tag{A11}$$

To obtain the law of evolution obeyed by this function, we need to know the equation satisfied by D. Remarkably, the HJ equation (A6) implies that D obeys the conservation equation

$$\frac{\partial D}{\partial t} + \frac{1}{m}\frac{\partial}{\partial q_i}\left(D \frac{\partial \sigma}{\partial q_i}\right) = 0 \tag{A12}$$

(this has been shown for the classical HJ equation [20] and the inclusion of Q in (A6) does not alter the proof). Multiplying (A12) by F and (A7) by D and adding, we obtain finally the equation satisfied by the distribution Γ:

$$\frac{\partial \Gamma}{\partial t} + \frac{1}{m}\frac{\partial}{\partial q_i}\left(\Gamma \frac{\partial \sigma}{\partial q_i}\right) = 0. \tag{A13}$$

Equation (A13) is Liouville's equation written in the HJ language. It is equivalent to (A1) since, assuming (A6), we may start from (A13) and retrace our steps to derive (A1). Since in addition we may derive the particle Hamilton equations from the HJ equation (A6) (see §2.3), we conclude that the set of Liouville's and Hamilton's equations (A1), (1.4) and (1.5) is equivalent to the set of equations (A13) and (A6), and we may use the latter to study the behaviour of ensembles. The two descriptions are linked by Jacobi's equations (2.13). In particular, the partial q-distribution has the two expressions

$$\rho(q,t) = \int f(q,p,t)\, d^3p = \int \Gamma(q,\alpha,t)\, d^3\alpha. \tag{A14}$$

Two points about (A13) are noteworthy: First, the external potential $V + Q$ does not appear explicitly – information on this is carried by the HJ function σ (obeying (A6)) which we must first obtain in order to solve for Γ. Second, no derivatives of the non-additive constants α appear so that, for each choice of the αs, (A13) is a conservation equation in q-space.

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