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Existence of Trajectories for Bohmian Mechanics

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We discuss the problem of global existence and uniqueness of Bohmian mechanics, focusing on the role played by the quantum probability flux. The relation to the self-adjointness of the Hamiltonian is alluded to.

Bohmian mechanics is a non-Newtonian theory for the motion of point particles which is Galilean and time-reversal invariant. The state of an N-particle system is given by the configuration $Q = (\mathbf{Q}_1, \ldots, \mathbf{Q}_N) \in \mathbb{R}^{3N}$ and the wave function ψ on configuration space $\mathbb{R}^{3N}$. Here $\mathbf{Q}_k \in \mathbb{R}^3$ is the position of the kth particle. On the subset of $\mathbb{R}^{3N}$ where $\psi \neq 0$ and differentiable, ψ induces a velocity field $v^\psi = (\mathbf{v}_1^\psi, \ldots, \mathbf{v}_N^\psi)$ via

$$\mathbf{v}_k^\psi(q) = \frac{\hbar}{m_k} \operatorname{Im} \frac{\nabla_k \psi(q)}{\psi(q)} = \frac{\hbar}{2im_k}\left(\frac{\psi^*\nabla_k\psi - \psi\nabla_k\psi^*}{\psi^*\psi}\right)(q) \tag{1}$$

determining the motion of particles with masses $m_1, \ldots, m_N$. The time evolution of the state (Q_t, ψ_t) is given by a first-order differential equation for the configuration Q_t,

$$\frac{dQ_t}{dt} = v^{\psi_t}(Q_t) \tag{2}$$

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and by Schrödinger's equation for the wave function ψ_t

$$i\hbar \frac{\partial \psi_t(q)}{\partial t} = \left[-\sum_{k=1}^{N} \frac{\hbar^2}{2m_k} \Delta_k + V(q) \right] \psi_t(q) \qquad (3)$$

It is by now well established that Bohmian mechanics resolves all problems associated with the measurement problem in nonrelativistic quantum mechanics (Bohm, 1952; Bohm and Hiley, 1992; Bell, 1987; Dürr *et al.*, 1992). It accounts for quantum randomness, absolute uncertainty, the concept of the wave function of a subsystem, collapse of the wave function, and familiar (macroscopic) reality. For a thorough analysis of the physics entailed by Bohmian mechanics see (Bohm and Hiley, 1992; Dürr *et al.*, 1992; Daumer *et al.*, 1993).

We report here on our work on the problem of the existence and uniqueness of Bohmian mechanics (Berndl *et al.*, 1993). To establish global existence and uniqueness means: given Q_0 and ψ_0 at some "initial" time t_0 ($t_0 = 0$), show unique existence of solutions of (2) for Q_t and of (3) for ψ_t on arbitrary finite time intervals such that $Q_{t_0} = Q_0$ and $\psi_{t_0} = \psi_0$.

In orthodox quantum theory the time evolution of the state ψ_t is given by a one-parameter unitary group U_t on a Hilbert space $\mathscr{H}$. U_t is generated by a self-adjoint operator H, which on smooth wave functions in $\mathscr{H} = L^2(\mathbb{R}^{3N})$ is given by

$$H = -\sum_{k=1}^{N} \frac{\hbar^2}{2m_k} \Delta_k + V$$

i.e., Schrödinger's equation is regarded as the "generator equation" for U_t. Hence the "problem of the existence of dynamics" is reduced to showing that the relevant Hamiltonian H (given by the particular choice of the potential V) is self-adjoint. This has been done in great generality, independent of the number of particles and for a large class of potentials, including singular potentials such as the Coulomb potential, which is of primary physical interest.[5] However, these highly developed rigorous results concerning the unitarity of the time evolution have a curious status within orthodox quantum theory: that theory is mainly concerned with measurements, i.e., with situations where the unitary evolution is interrupted by the dubious procedure of "collapse."

In Bohmian mechanics we have not only Schrödinger's equation (3) to consider, but also the differential equation (2) for the motion of the particles. *Local* existence and uniqueness of Bohmian trajectories is guaran-

[5]We remark here that in the case of systems with more than four particles, the "analogous" problem in Newtonian mechanics, namely gravitational interaction, has not been solved yet.

teed only if the velocity field v^{ψ} is continuously differentiable. Therefore we need more regularity properties than merely requiring that the wave function ψ be in $L^2(\mathbb{R}^{3N})$. For a large class of potentials, including Coulomb-type potentials, the regularity properties we wish to demand are satisfied on the set of C^{∞}-vectors of the self-adjoint Hamiltonian H, a set which is a dense [in $L^2(\mathbb{R}^{3N})$] and invariant (under $e^{-itH/\hbar}$ for $t \in \mathbb{R}$) subset of the domain of H.

Global existence for the solution of (2) is more delicate. It may be obstructed by the points where the velocity field (1) is not defined. This is the case (i) at $\mathcal{N}$, the set of nodes of ψ: $\mathcal{N} := \{(q, t) \in \mathbb{R}^{3N} \times \mathbb{R}\colon \psi_t(q) = 0\}$ and (ii) at the points where ψ is not differentiable. For a large class of potentials, including those of Coulomb type, the latter set is contained in the set $\mathcal{S}$ of singularities of the potential for wave functions which are C^{∞}-vectors of H. Furthermore, the solution of (2) may explode, i.e., it may reach infinity in a finite amount of time.

The problem we have addressed can now be stated as follows: Suppose that at some *arbitrary* "initial time" ($t = 0$) the N-particle configuration Q_0 lies in the complement of the nodal set of ψ_0 and of $\mathcal{S}$. Does the configuration develop in a finite amount of time into a singular point, i.e., a point in $\mathcal{N}$ or $\mathcal{S} \times \mathbb{R}$, or does it reach infinity in finite time? We shall argue that the answer is negative for "typical" Q_0 and "sufficiently regular" ψ_0. By "typicality" we mean that this holds for almost all Q_0 with respect to P^{ψ_0}, the probability measure on configuration space $\mathbb{R}^{3N}$ with the density $|\psi_0|^2$. "Sufficient regularity" pertains to a set of wave functions ψ_0 which is dense in $L^2(\mathbb{R}^{3N})$ and invariant under $e^{-itH/\hbar}$ for $t \in \mathbb{R}$ such as, for example, the set of C^{∞}-vectors of the self-adjoint Hamiltonian H.

We first give a simple intuitive argument as to why nodes are typically missed by the particles. A "generic" wave function ψ is complex: it has "independent" real and imaginary parts. Therefore the equation $\psi_t(q) = 0$ [$\Leftrightarrow \operatorname{Re} \psi_t(q) = 0, \operatorname{Im} \psi_t(q) = 0$] will "generically" require (q, t) to lie in a manifold of codimension 2 in configuration-space-time $\mathbb{R}^{3N} \times \mathbb{R}$, like, e.g., isolated points in $(1 + 1)$-dimensional space-time. Then it is reasonable to expect that most likely the trajectory will miss this small set, or in other words: the set of exceptional initial positions which develop into nodes should have (P^{ψ_0}-) measure zero.

Note that this "argument" applied to N spin-1/2 particles, i.e., "to the real world situation," shows that a "generic" N-particle spinor wave function has no zeros: Since it consists of 2^{N+1} real components, the 2^{N+1} equations for a node overdetermine grossly the $3N$ variables.[6] In the following we shall discuss the "worst case" of spinless particles.

[6]"Spin" can easily be incorporated in Bohmian mechanics by a straightforward generalization to spinor wave functions.

We use notions of sufficient regularity and typicality which are time independent because Bohmian mechanics, as given by equations (2) and (3), is time-translation invariant. Note in particular that therefore the set of sufficiently regular wave functions depends upon the Hamiltonian H. *Given* the existence of the dynamics for configurations Q_t, the result we wish to establish here, the notion of typicality is time independent by equivariance (Dürr *et al.*, 1992):

$$\rho_0 = |\psi_0|^2 \Rightarrow \rho_t = |\psi_t|^2 \qquad \text{for all} \quad t \in \mathbb{R}$$

where ρ_t denotes the probability density on configuration space $\mathbb{R}^{3N}$, which is the image density of ρ_0 under Q_t. This follows from comparing the continuity equation for an ensemble density ρ_t

$$\frac{\partial \rho_t(q)}{\partial t} + \sum_{k=1}^{N} \nabla_k \cdot [\mathbf{v}_k^{\psi_t}(q)\rho_t(q)] = 0 \tag{4}$$

with the quantum "continuity equation"

$$\frac{\partial |\psi_t(q)|^2}{\partial t} + \sum_{k=1}^{N} \nabla_k \cdot \mathbf{j}_k^{\psi_t}(q) = 0 \tag{5}$$

and noting that the quantum "probability current" $j^{\psi} = (\mathbf{j}_1^{\psi}, \ldots, \mathbf{j}_N^{\psi})$ is given by

$$\mathbf{j}_k^{\psi} = \mathbf{v}_k^{\psi} |\psi|^2 = \frac{\hbar}{2im_k} (\psi^* \nabla_k \psi - \psi \nabla_k \psi^*)$$

We would like to stress the conceptual difference between equations (4) and (5). Equation (5) is an identity for every ψ_t which satisfies Schrödinger's equation, but, without having established global existence of the particle motion, it is not a continuity equation in the classical sense—despite its name. By establishing global existence, we simultaneously show that the quantum "probability current" j^{ψ_t} is indeed a classical probability current, propagating the ensemble density $|\psi_t|^2$ along the integral curves of the velocity field v^{ψ_t}.

The continuity equation (4), even without global existence of trajectories Q_t, holds "locally" on the complement of the nodal set $\mathcal{N}$ and the set of singularities $\mathcal{S} \times \mathbb{R}$, with ρ_t suitably interpreted. This will be used in the following argument for global existence.

Recall that a probability current $j_t(q) = \rho_t(q) v_t(q)$ of an ensemble density ρ_t along a vector field v_t has the following probabilistic significance:

$$|J_t(q) \cdot n| \, d\sigma \quad \text{with the flux} \quad J_t(q) := (j_t(q), \rho_t(q))$$

is the expected number of crossings, by the random trajectory defined by ρ and v and hence by J, of the $3N$-dimensional hypersurface element $d\sigma$ in configuration-space-time $\mathbb{R}^{3N} \times \mathbb{R}$ at a point (q, t), where n denotes the local normal vector. [$(J \cdot n)\, d\sigma$ is the expected number of *signed* crossings of the surface element $d\sigma$.]

Given then an arbitrary hypersurface $\mathscr{T}$ in configuration-space-time $\mathbb{R}^{3N} \times \mathbb{R}$, we have (by linearity of the expectation) that

$$\int_{\mathscr{T}} |J_t(q) \cdot n|\, d\sigma = \text{expected total number of crossings of } \mathscr{T}$$

Now we wish to apply this insight to establish global existence for the particle motion in Bohmian mechanics, i.e., to argue that none of the singular points of v^{ψ_t} are reached in finite time. Roughly speaking, the idea is this: "If there is no flux into the singular points, the singular points are unproblematic." The set of singular points in configuration-space-time $\mathbb{R}^{3N} \times \mathbb{R}$ is formed by $\mathscr{N} \cup (\mathscr{S} \times \mathbb{R})$. We introduce $\mathscr{N}' := \mathscr{N} \setminus (\mathscr{S} \times \mathbb{R})$. (On $\mathscr{N}'$, J^{ψ_t} is continuous, which is needed below.) However, v^{ψ_t} is not defined on $\mathscr{N}'$ and on $\mathscr{S}$. This may be taken care of by considering for $\epsilon > 0$, $\delta > 0$ an ϵ-neighborhood (in $\mathbb{R}^{3N} \times \mathbb{R}$) of $\mathscr{N}'$ and a δ-neighborhood (in $\mathbb{R}^{3N}$) of $\mathscr{S}$:

$$\mathscr{N}'^{\epsilon} := \bigcup_{z \in \mathscr{N}'} \{(q, t) \in \mathbb{R}^{3N} \times \mathbb{R} : |(q, t) - z| \le \epsilon\}$$

$$\mathscr{S}^{\delta} := \bigcup_{y \in \mathscr{S}} \{q \in \mathbb{R}^{3N} : |q - y| \le \delta\}$$

To treat the problem of possible explosion, we introduce an increasing sequence of compact sets $(\mathscr{K}_l)_{l \in \mathbb{N}}$ exhausting $\mathbb{R}^{3N}$: $\mathscr{K}_l \nearrow \mathbb{R}^{3N}$. Then the set of "good" points is $\mathscr{G}_{\epsilon,\delta,l} := (\mathscr{K}_l \times \mathbb{R}) \setminus (\mathscr{N}'^{\epsilon} \cup (\mathscr{S}^{\delta} \times \mathbb{R}))$. Let the configuration Q start in $\mathscr{G}_{\epsilon,\delta,l}$ at $t = 0$ [i.e., $(Q_0, 0) \in \mathscr{G}_{\epsilon,\delta,l}$] with a density $|\psi_0|^2$. We construct the trajectory Q_t by integrating v^{ψ_t} until Q_t hits the boundary of $\mathscr{G}_{\epsilon,\delta,l}$, at which time the configuration is put into a cemetary, i.e., it is taken out of the ensemble. We now infer—by comparing the continuity equation (4) for this process with (5) on $\mathscr{G}_{\epsilon,\delta,l}$—that the density of hittings of the surface $\partial\mathscr{G}_{\epsilon,\delta,l}$ at the point (q, t) is bounded by $|J^{\psi_t}(q) \cdot n|$ (Berndl *et al.*, 1993). But the probability for a first hitting of $\partial\mathscr{G}_{\epsilon,\delta,l}$ within a time interval $[0, T]$ is bounded by the expected total number of hittings of $\mathscr{T} := \partial\mathscr{G}_{\epsilon,\delta,l} \cap (\mathbb{R}^{3N} \times [0, T])$. Hence for all ϵ, δ, and l:

Probability of reaching a node, a singularity or infinity within $[0, T]$

$$\le \int_{\mathscr{T}} |J^{\psi_t}(q) \cdot n|\, d\sigma \le \mathbf{N} + \mathbf{S} + \mathbf{I} \tag{6}$$

where

$$\mathbf{N} := \int_{\partial \mathcal{N}'^{\epsilon} \cap \mathcal{T}} |J^{\psi_t}(q) \cdot n| \, d\sigma$$

$$\mathbf{S} := \int_{(\partial \mathcal{S}^{\delta} \times [0, T]) \cap \mathcal{T}} |J^{\psi_t}(q) \cdot n| \, d\sigma$$

$$\mathbf{I} := \int_{(\partial \mathcal{K}_l \times [0, T]) \cap \mathcal{T}} |J^{\psi_t}(q) \cdot n| \, d\sigma$$

Under the condition that the integrals **N**, **S**, and **I** vanish in the limit $\epsilon \to 0$, $\delta \to 0$, and $l \to \infty$, Bohmian mechanics exists globally. We now explain why this should be so.

1. The "nodal integral" **N**: As $\epsilon \to 0$, there are two reasons why **N** should vanish: (i) J^{ψ_t} is zero at the nodes, and hence is small on $\partial \mathcal{N}'^{\epsilon}$. (ii) $\partial \mathcal{N}'^{\epsilon} \to \partial \mathcal{N}'$ as $\epsilon \to 0$ and, as argued above, one expects that $\mathcal{N}$ and hence also $\mathcal{N}'$ has codimension 2. Thus $\partial \mathcal{N}'^{\epsilon}$ should have small surface area.

2. The "singularity integral" **S**: This term should vanish as $\delta \to 0$ since the set $\mathcal{S}$ of singular points of the potential has codimension greater than 1 for the class of potentials that are normally considered, for example, the Coulomb pair interaction of the atomic Hamiltonian.

3. The "infinity integral" **I** should tend to zero as $l \to \infty$, since $\psi_t(q)$ and hence $J^{\psi_t}(q)$ should rapidly go to 0 as $|q| \to \infty$.

To make argument 1 rigorous, very mild control on the surface area of the *boundary* of the nodal set $\mathcal{N}$ would suffice. In fact we would need only that the boundary of $\mathcal{N}$ be a countable union of pieces with finite area. As natural as this may appear [wave functions having pathological nodal sets—for example, of (uncountably) infinite area—should be pathological as well], it is nonetheless even unclear whether this condition is valid for a suitable class of wave functions. However, this problem can be bypassed: We show (Berndl *et al.*, 1993) how, by a more delicate analysis, the nodal integral can be controlled along the lines suggested by 1.

To make the arguments in 2 and 3 rigorous, one needs regularity and boundary conditions on ψ which are satisfied by those C^{∞}-vectors of the self-adjoint Hamiltonian H having "finite integrated kinetic energy," a condition automatically satisfied for several large classes of potentials V—remarkably, precisely the classes defined by the standard conditions for the self-adjointness of the Hamiltonian (Berndl *et al.*, 1993), i.e., for the existence of the wave function dynamics alone. For details, as well as some simple illuminating examples and a more thorough discussion of this connection between the global existence of the particle motion and the self-adjointness of the Hamiltonian, see Berndl *et al.* (1993).

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