Self-adjointness and the Existence of Deterministic Trajectories in Quantum Theory

November 30, 1993

K. Berndl[1], D. Dürr[1], S. Goldstein[2] and N. Zanghì[3]

1. Mathematisches Institut der Universität München, Theresienstraße 39, 80333 München, Germany

2. Department of Mathematics, Rutgers University, New Brunswick, NJ 08903, USA

3. Dipartimento di Fisica, Università di Genova, Sezione INFN Genova, Via Dodecaneso 33, 16146 Genova, Italy

1 Abstract

We show that the particle motion in Bohmian mechanics as the solution of an ordinary differential equation exists globally, i.e., the singularities of the velocity field and infinity will not be reached in finite time for typical initial configurations and a large class of potentials, including the physically most relevant potential of N-particle Coulomb interaction with arbitrary charges and masses. The analysis is based on the probabilistic significance of the quantum flux. We point to the connection between the global existence of Bohmian mechanics and the self-adjointness of the Schrödinger Hamiltonian.

2 Introduction

The title alludes to two of the tenets of orthodox quantum theory: 1) the self-adjointness of observables, especially of the Hamiltonian

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

and 2) the impossibility of understanding quantum phenomena on the basis of an underlying theory with deterministic trajectories, with quantum randomness arising "classically" from randomness in the initial conditions.

David Bohm [1] showed several decades ago that the second tenet is false: His theory, *Bohmian mechanics*, does precisely what has been held impossible. Bohmian mechanics is a Galilean and time-reversal invariant theory for the motion of point particles. 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 $\mathbb{R}^{3N}$. $\mathbf{Q}_k \in \mathbb{R}^3$ is the position of the

k-th particle. On the subset of $\mathbb{R}^{3N}$ where $\psi \neq 0$ and is differentiable, ψ generates a velocity field $v^\psi = (\mathbf{v}_1^\psi, \ldots, \mathbf{v}_N^\psi)$

$$\mathbf{v}_k^\psi = \frac{\hbar}{m_k} \mathrm{Im} \frac{\nabla_k \psi}{\psi} \tag{2}$$

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

$$\frac{dQ_t}{dt} = v^{\psi_t}(Q_t) \tag{3}$$

and Schrödinger's equation for the wave function ψ_t

$$i\hbar \frac{\partial \psi_t(q)}{\partial t} = \left(-\sum_{k=1}^N \frac{\hbar^2}{2m_k} \Delta_k + V(q) \right) \psi_t(q). \tag{4}$$

We shall assume that the potential V is a C^∞-function on an open set $\Omega \subset \mathbb{R}^{3N}$, and the set of singularities $\mathcal{S}(= \mathbb{R}^{3N} \setminus \Omega)$ of the potential is a set of Lebesgue measure zero.

Bohmian mechanics can be regarded as a (completion of) nonrelativistic quantum theory. It resolves all problems associated with the measurement problem in nonrelativistic quantum mechanics [1, 2]. It accounts for the "collapse" of the wave function, for the quantum randomness as expressed by Born's law $\rho = |\psi|^2$, and familiar (macroscopic) reality. Moreover, the usual quantum measurement formalism involving self-adjoint operators as observables emerges from Bohmian mechanics as a phenomenological description. (See [2, 3], and the contribution of M. Daumer et al. in this volume.)

Here we are concerned with the mathematical problem of existence and uniqueness of the motion in Bohmian mechanics, i.e., with establishing that for given Q_0 and ψ_0 at some "initial" time t_0 ($t_0 = 0$), solutions (Q_t, ψ_t) of (3, 4) with $Q_{t_0} = Q_0$ and $\psi_{t_0} = \psi_0$ exist uniquely and globally in time. This problem initiates further analysis on the status of the self-adjointness of the Hamiltonian.

3 Global existence of Bohmian mechanics

The solution of the problem of the existence of dynamics for Schrödinger's equation (4) (which is independent of the solution of equation (3), i.e., the actual motion of the configuration) is, of course, well known: if the Hamiltonian is self-adjoint (on a domain $\mathcal{D}(H)$), there exists a unitary one parameter group $U_t = e^{-itH/\hbar}$, and, for all $\psi_0 \in \mathcal{D}(H)$, $\psi_t := U_t \psi_0$ is a solution of Schrödinger's equation in the L^2-sense.

Thus we assume, as usual, the Hamiltonian to be a self-adjoint extension of $H|_{C_0^\infty(\Omega)}$. (Under the above assumptions on the potential V, the set $C_0^\infty(\Omega)$ is dense in $L^2(\mathbb{R}^{3N})$, and the Hamiltonian as defined by (1) is symmetric on this set. Since the Hamiltonian commutes with complex conjugation, there always exist self-adjoint extensions of $H|_{C_0^\infty(\Omega)}$.)

In order for equation (3) to be well-defined we need the wave function to be smooth. A particular suitable set of wave functions is the set $C^\infty(H)$ of C^∞-vectors of H.[1] This set of wave functions is dense in $L^2(\mathbb{R}^{3N})$ and invariant under the time evolution $e^{-itH/\hbar}$ (and is hence a core, i.e., a domain of essential self-adjointness for H).

[1] $C^\infty(H) = \bigcap_{n=1}^\infty \mathcal{D}(H^n)$, where $\mathcal{D}(H^n)$ is the domain of H^n. Special C^∞-vectors are eigenfunctions and "wave packets" $\psi \in \mathrm{Ran}(P_{[a,b]})$, where $P_{[a,b]}$ denotes the spectral projection of H to the finite energy interval $[a, b]$.

We shall therefore assume that the initial wave function $\psi_0 \in C^\infty(H)$. Then $\psi_t = e^{-itH/\hbar}\psi_0$ may be regarded as an element of $C^\infty(\Omega \times \mathbb{R})$ and thus also as a classical solution of Schrödinger's equation [4]. The velocity field v^ψ is thus C^∞ on the complement of the set $\mathcal{N} := \{(q,t) \in \Omega \times \mathbb{R} : \psi_t(q) = 0\}$ of nodes of ψ, and the (space-time) set of singularities $\mathcal{S} \times \mathbb{R}$, i.e., on the set of "good" points $\mathcal{G} := (\Omega \times \mathbb{R}) \setminus \mathcal{N}$, which is an open subset of configuration-space-time $\mathbb{R}^{3N} \times \mathbb{R}$. Let $\mathcal{G}_t$ denote the slice of $\mathcal{G}$ at a fixed time t: $\mathcal{G}_t := \Omega \setminus \mathcal{N}_t$, where $\mathcal{N}_t := \{q \in \Omega : \psi_t(q) = 0\}$. Then by a standard theorem of existence and uniqueness of ordinary differential equations, for any initial value q_0 in $\mathcal{G}_0$ there exists a unique right maximal (non-extendible in positive time direction[2]) solution Q_t of (3) on a time interval $0 \le t < \tau(q_0)$. The problem is to exclude that $\tau(q_0) < \infty$, in which case the solution Q_t as $t \nearrow \tau$ reaches infinity or points in the boundary of $\mathcal{G}$, i.e., singularities of the velocity field v^ψ.

For large classes of potentials, we shall show that for typical q_0 we have that $\tau(q_0) = \infty$, i.e., that the solution exists globally in time P^{ψ_0}-almost surely,

$$P^{\psi_0}(\tau < \infty) = 0,$$

where P^{ψ_0} denotes the probability measure on configuration space $\mathbb{R}^{3N}$ (supported on $\mathcal{G}_0$) given by the density $|\psi_0|^2$. (We assume the initial wave function ψ_0 to be normalized.) This measure is the natural measure associated with the dynamical system defined by "Bohmian mechanics:" it plays the role of the "equilibrium measure" and defines our notion of "typicality" [2]. Moreover, *given* the existence of the dynamics for configurations Q_t—the result we report on here—the notion of typicality is time independent by "equivariance" [2]:

$$\rho_0 = |\psi_0|^2 \Longrightarrow \rho_t = |\psi_t|^2 \;\text{ for all }\; t \in \mathbb{R},$$

where ρ_t denotes the probability density on configuration space $\mathbb{R}^{3N}$ at time t—the image density of ρ_0 under the process Q_t.

We now state the **Theorem** we have established in [4]: *If i) the potential V is a C^∞-function on an open set $\Omega \subset \mathbb{R}^{3N}$, and the set of singularities $\mathcal{S} (= \mathbb{R}^{3N} \setminus \Omega)$ of the potential is contained in a finite union of $(3N-3)$-dimensional hyperplanes $\mathcal{S}_l$, $\mathcal{S} \subset \bigcup_{l=1}^m \mathcal{S}_l$, ii) the Hamiltonian H is a self-adjoint extension of $H|_{C_0^\infty(\Omega)}$, iii) the initial wave function ψ_0 is a C^∞-vector of H and normalized, and iv) for all $T > 0$ $\int_0^T \|\nabla\psi_t\|^2 dt < \infty$, then $P^{\psi_0}(\tau < \infty) = 0$, i.e., Bohmian mechanics exists uniquely and globally in time P^{ψ_0}-almost surely.*

We comment on the conditions in the theorem: The condition i) on the shape of $\mathcal{S}$ is very natural from a physical point of view, as it includes pair potentials and central potentials. The condition iv) of "finite integrated kinetic energy" is automatically satisfied for all $\psi \in \mathcal{Q}(H) (\supset C^\infty(H))$, the form domain of H, provided the quadratic form $(\nabla\psi_t, \nabla\psi_t) (\le M(\psi_t, H_0\psi_t)$ with $M = (2/\hbar^2)\max(m_1, \ldots, m_N))$ can be bounded in terms of the form $(\psi_t, H\psi_t)$, which is finite and independent of t. Such a bound follows from various bounds on the potential: (a) Potentials which are bounded below, a class which includes, for example, harmonic and anharmonic potentials, and arbitrarily strong positive repulsive potentials. (b) H_0-form bounded potentials with relative bound $a < 1$. This class, with arbitrarily small relative bound a, includes for example $R + L^\infty$

[2]From time reversal invariance, $P^{\psi_0}(\tau < \infty) = 0$ implies $P^{\psi_0}(\tau^- < \infty) = 0$, when (τ^-, τ) denotes the existence interval of the maximal solution. Therefore it is sufficient to consider the positive time direction.

or $L^{3/2} + L^\infty$ on $\mathbb{R}^3$, where R is the Rollnik class. (For details, see for example [5].) Therefore H_0-form bounded potentials include power law interaction $1/r^\alpha$ with $\alpha < 2$ and thus the physically most relevant potential of N-particle Coulomb interaction with arbitrary charges and masses. (The class of H_0-form bounded potentials contains the more familiar class of H_0-operator bounded potentials, which already includes the N-particle Coulomb interaction.)

We remark that also from the point of view of establishing only self-adjointness of the Hamiltonian, these classes of potentials are particularly well understood, in the sense that much is known about cores, lower bounds, etc. [5].

At this point we shall emphasize that on the one hand, this result of global existence of Bohmian mechanics should not be too surprising because the "bad sets" are either very small—the set of nodes has "generically" codimension 2, and the set of singularities has codimension at least 3—or infinitely far away. But on the other hand, especially when compared with the N-body problem in Newtonian mechanics, where general results for systems of more than 4 particles are still missing, the generality of the result of existence of dynamics for Bohmian mechanics and also the essential simplicity of the proof should be quite surprising. Taking now this result for Bohmian mechanics and also the general emergence of the quantum formalism [2, 3] into account, we maintain that the failure of Newtonian mechanics both to describe the physics in the nonrelativistic domain correctly and to be mathematically well understood on the most basic level of existence and uniqueness is not due to its having point particles as fundamental elements; rather it is due to its having the "wrong" dynamics.

4 Basic idea of the proof: flux estimates

Consider the random trajectory $(\mathcal{G}_0, P = P^{\psi_0}, \tilde{Q}_t)$, where for $t \geq 0, q_0 \in \mathcal{G}_0$, the process $\tilde{Q}_t(q_0) = Q_t(q_0)$ for $t < \tau(q_0)$ and $\tilde{Q}_t(q_0) = \dagger$ for $t \geq \tau(q_0)$. The image density of $\tilde{Q}_t$ on $\mathcal{B}_t := \mathrm{Ran}\tilde{Q}_t \cap \mathcal{G}_t$ will be denoted by ρ_t. ρ_t is bounded by $|\psi_t|^2$ on $\mathcal{G}_t, t \geq 0$ [4].

Consider now a smooth surface Σ in $\mathcal{G}$. Reflecting on the probabilistic significance of the flux $J_t(q) := (\rho_t(q) v^{\psi_t}(q), \rho_t(q))$, we obtain that the expected number of crossings of Σ by the random trajectory $\tilde{Q}_t$ is given by

$$\int_\Sigma |J_t(q) \cdot U| \, d\sigma,$$

where U denotes the local unit normal vector. ($\int_\Sigma J \cdot U \, d\sigma$ is the expected number of *signed* crossings of Σ.) The probability of crossing Σ (at least once) is hence bounded by $\int_\Sigma |J_t(q) \cdot U| \, d\sigma$, which in turn from

$$|J_t(q) \cdot U| \leq |(|\psi_t(q)|^2 v^{\psi_t}(q), |\psi_t(q)|^2) \cdot U| = |(j^{\psi_t}, |\psi_t|^2) \cdot U| = |J^{\psi_t} \cdot U|$$

is bounded by

$$P^{\psi_0}(\tilde{Q}_t \text{ crosses } \Sigma) \leq \int_\Sigma |J^{\psi_t}(q) \cdot U| \, d\sigma.$$

This insight can be applied to prove (almost sure) global existence by choosing a sequence of surfaces around the "bad points:" consider the surface of $\mathcal{G}^{\epsilon\delta n}$, the set of "$\epsilon$-$\delta$-$n$-good" points in configuration-space-time:

$$\mathcal{G}^{\epsilon\delta n} := (\mathcal{K}^n \times \mathbb{R}) \setminus (\mathcal{N}^\epsilon \cup (\mathcal{S}^\delta \times \mathbb{R})),$$

where $(\mathcal{K}^n)_{n\in\mathbb{N}}$ is a sequence of balls with radius n in configuration space (that serves as cutoff at infinity), $\mathcal{N}^\epsilon$ and $\mathcal{S}^\delta$ are neighborhoods of $\mathcal{N}$ (in configuration-space-time) resp. $\mathcal{S}$ (in configuration space) (that take care of the nodes resp. the singularities). We further denote $\mathcal{G}_0^{\epsilon\delta n} := \mathcal{K}^n \setminus (\mathcal{N}_0^\epsilon \cup \mathcal{S}^\delta)$.

Then we arrive at: for all $T > 0, \epsilon > 0, \delta > 0, n < \infty$

$$\begin{aligned} P^{\psi_0}(\tau < T) &\leq P^{\psi_0}(\mathcal{G}_0 \setminus \mathcal{G}_0^{\epsilon\delta n}) + P^{\psi_0}(\tilde{Q}_t \text{ crosses } \partial\mathcal{G}^{\epsilon\delta n} \cap (\mathbb{R}^{3N} \times (0,T))) \\ &\leq P^{\psi_0}(\mathcal{G}_0 \setminus \mathcal{G}_0^{\epsilon\delta n}) + \int_{\partial\mathcal{N}^\epsilon \cap ((\mathcal{K}^n \setminus \mathcal{S}^\delta)\times(0,T))} |J^{\psi_t}(q) \cdot U|\, d\sigma + \\ &\quad \int_{\partial\mathcal{S}^\delta \times (0,T)} |J^{\psi_t}(q) \cdot U|\, d\sigma + \int_{(\partial\mathcal{K}^n \cap \Omega)\times(0,T)} |J^{\psi_t}(q) \cdot U|\, d\sigma \\ &= P^{\psi_0}(\mathcal{G}_0 \setminus \mathcal{G}_0^{\epsilon\delta n}) + \mathbf{N} + \mathbf{S} + \mathbf{I}. \end{aligned}$$

Moreover, (almost sure) global existence follows if the right hand side goes to 0. It is heuristically now rather clear that all the flux integrals should vanish as the limit $\epsilon \to 0, \delta \to 0$, and $n \to \infty$ is suitably approached: For the "nodal integral" $\mathbf{N}$ it seems fairly obvious that this term vanishes as $\epsilon \to 0$ because J^{ψ_t} is zero at the nodes, and, moreover, one expects that $\mathcal{N}$ has codimension 2, so $\partial\mathcal{N}^\epsilon$ should have small area. The "singularity integral" $\mathbf{S}$ should vanish in the limit $\delta \to 0$ since the set $\mathcal{S}$ of singular points of the potential has codimension greater than 1 for potentials that are normally considered. Finally, the "infinity integral" $\mathbf{I}$ should tend to zero as $n \to \infty$ since $\psi_t(q)$ and hence $J^{\psi_t}(q)$ should rapidly go to zero as $|q| \to \infty$.

The main difficulty in making these considerations rigorous lies in controlling the area of the surface of the nodal set and the behavior of the flux at the singularities and at infinity. This is done in [4].

5 Summary and perspective: Bohmian mechanics and self-adjointness of the Hamiltonian

In this final section we shall comment on the connection between the global existence of Bohmian mechanics and the self-adjointness of the Hamiltonian, as mediated by the quantum flux $J = (j, |\psi|^2)$:

Bohmian mechanics $\overset{1}{\longleftrightarrow}$ J—the quantum flux $\overset{2}{\longleftrightarrow}$ self-adjointness of H

"$\overset{1}{\longrightarrow}$" Bohmian mechanics gives meaning to the quantum flux as a flux of particles. Indeed, the quantum current j is a current of particles moving along deterministic trajectories with a velocity given by a functional of the wave function ψ.

"$\overset{2}{\longrightarrow}$" In standard quantum theory, the unitarity of the time evolution U_t of ψ or equivalently the self-adjointness of its generator H is taken as one of the *axioms*. For a concrete physical problem, the generator is given by (1). There is, however, no general rule yielding the *domain* on which this operator should be considered. One first has to find a dense set of vectors where the Hamiltonian is definable by (1) and is symmetric. $C_0^\infty(\mathbb{R}^{3N})$, $C_0^\infty(\Omega)$, or Schwartz space are good and usual candidates. Then one has to analyse whether the Hamiltonian is essentially self-adjoint on that domain, so that the unitary time evolution is uniquely determined. If this is not the case, there are (infinitely many) different self-adjoint extensions, giving rise to different unitary evolutions. It is now a matter of the physics of the system being described to choose the right one. As an example, consider a free particle on $(0,\infty)$: there is a one-parameter family of self-adjoint extensions H^a of $H_0|_{C_0^\infty(0,\infty)}$, characterized by the boundary condition $\psi'(0) = a\psi(0)$ with $a \in \mathbb{R}$ or $\psi(0) = 0$ ("$a = \infty$") defining the respective domain. a determines the law of reflection of the ψ-function at 0 [5].

In Bohmian mechanics, there is *a priori* no reason to demand self-adjointness of the Hamiltonian: Any solution ψ of Schrödinger's equation (4) for which global trajectories Q_t solving (3) exist is fine. Rather, the axiom of self-adjointness experiences an a posteriori justification in Bohmian mechanics. Consider the above mentioned example of a free particle on $(0, \infty)$: To have the Bohmian particle motion well defined on $(0, \infty)$ it seems inevitable to demand $j_t(0) = 0$, i.e., $\psi_t(0) = 0$ or $v^{\psi_t}(0) = 0$ which in view of (2) yields $\frac{\nabla\psi_t(0)}{\psi_t(0)} \in \mathbb{R}$. In this way, by immediately suggesting $j(0) = 0$, Bohmian mechanics leads directly to the necessary boundary condition for self-adjointness in terms of the current. For a more detailed discussion see [4].

"$\stackrel{2}{\longleftarrow}$" We have proven that self-adjointness of the Hamiltonian (together with "finite integrated kinetic energy") guarantees the right behavior of the quantum flux at the bad points—"No flux into the bad points"—and thereby

"$\stackrel{1}{\longleftarrow}$" global existence of Bohmian mechanics.

Acknowledgments: This work was partially supported by DFG, by NSF Grant No. DMS-9105661 and No. DMS-9305930, and by INFN.

References:

1. D. Bohm, A suggested interpretation of the quantum theory in terms of "hidden" variables, I and II, *Phys. Rev.* **85**, 166 and 180 (1952).

2. D. Dürr, S. Goldstein, and N. Zanghì, Quantum equilibrium and the origin of absolute uncertainty, *J. Stat. Phys.* **67**, 843 (1992).

3. M. Daumer, D. Dürr, S. Goldstein, and N. Zanghì, On the role of operators in quantum theory, in preparation.

4. K. Berndl, D. Dürr, S. Goldstein, G. Peruzzi, and N. Zanghì, On the global existence of Bohmian mechanics, in preparation.

5. M. Reed, B. Simon, "Methods of Modern Mathematical Physics II," Academic Press, San Diego (1975).