

On the Global Existence of Bohmian Mechanics

K. Berndl¹, D. Dürr¹, S. Goldstein², G. Peruzzi³, and N. Zanghì⁴

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

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

³ Sezione INFN Firenze, Largo Fermi, 2, 50125 Firenze, Italy

⁴ Dipartimento di Fisica, Università di Genova, Sezione INFN Genova,
Via Dodecaneso 33, 16146 Genova, Italy

August 9, 1994

Abstract. We show that the particle motion in Bohmian mechanics, given by the solution of an ordinary differential equation, exists globally: For a large class of potentials the singularities of the velocity field and infinity will not be reached in finite time for typical initial values. A substantial part of the analysis is based on the probabilistic significance of the quantum flux. We elucidate the connection between the conditions necessary for global existence and the self-adjointness of the Schrödinger Hamiltonian.

1 Introduction

Bohmian mechanics [7, 8, 4, 13, 14, 17] is a Galilean invariant theory for the motion of point particles. Consider a system of N particles with masses m_1, \dots, m_N and potential $V = V(\mathbf{Q}_1, \dots, \mathbf{Q}_N)$, where $\mathbf{Q}_k \in \mathbb{R}^\nu$ denotes the position of the k -th particle. The relevant configuration space is an open subset of $\nu N = d$ -dimensional space \mathbb{R}^d , for example the complement of the set of singularities of V , and shall be denoted by Ω . The state of the N -particle system is given by the configuration $Q = (\mathbf{Q}_1, \dots, \mathbf{Q}_N) \in \Omega$ and the Schrödinger wave function ψ on configuration space Ω . On the subset of Ω where the wave function $\psi \neq 0$ and is

differentiable, it generates a velocity field $v^\psi = (\mathbf{v}_1^\psi, \dots, \mathbf{v}_N^\psi)$

$$\mathbf{v}_k^\psi(q) = \frac{\hbar}{m_k} \operatorname{Im} \frac{\nabla_k \psi(q)}{\psi(q)} \quad (1)$$

the integral curves of which are the trajectories of the particles. Thus the time evolution of the state (Q_t, ψ_t) is given by a first-order ordinary differential equation for the configuration Q_t

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

and Schrödinger's equation for the wave function ψ_t

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

where ∇_k and Δ_k denote the gradient and the Laplace operator in \mathbb{R}^ν and the potential V is a real-valued function on Ω .

Bohmian mechanics may be regarded as a fundamental nonrelativistic quantum theory, from which the quantum formalism—operators as observables, the uncertainty principle, etc.—emerges as “measurement” formalism. It resolves all problems associated with the measurement problem in quantum mechanics [7, 8, 4, 13, 14, 17]. It accounts for the “collapse” of the wave function, for quantum randomness as expressed by Born's law $\rho = |\psi|^2$, and familiar (macroscopic) reality. For a thorough analysis of the physics entailed by Bohmian mechanics see [7, 8, 13, 11], and [14] for a short overview of [13].

Here we are concerned with the mathematical problem of the 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 (2, 3) with $Q_{t_0} = Q_0$ and $\psi_{t_0} = \psi_0$ exist uniquely and globally in time. (Note that Schrödinger's equation (3) is independent of the particle motion, while for solving the Equation (2) for the particle motion we need the wave function ψ_t .) Our first motivation for addressing this problem is the fact that the velocity field (1) exhibits rather obviously possible catastrophic events for the motion: v^ψ is singular at the nodes of ψ , i.e., at points where $\psi = 0$, so that the solution would break down if a node were reached. Furthermore, the solution may cease to exist at singularities of the wave function (if it has singularities), at the boundary of Ω (if it has a boundary), and because of “explosion,” that is the escape to infinity of a particle in a finite amount of time—events which have analogues in the N -body problem (of gravitational interaction) in Newtonian mechanics.

Recall that the problem of the existence of dynamics in Newtonian mechanics is notoriously difficult [26, 12]. In addition to the possibility of routine collision singularities, the N -body problem with $N > 3$ yields marvelous scenarios of so-called pseudocollisions, where some particles, while oscillating wildly, reach infinity in finite time. Examples of such catastrophies have been constructed by Mather and McGehee [24],¹ by Gerver [16], and by Xia [38]. While, for the case of a “solar system” with small “planetary” masses, Arnold [2] established global existence (and much more) “for the majority of initial conditions for which the eccentricities and inclinations of the Kepler ellipses are small,” and while Saari [34] has established global existence for “almost all initial conditions (in the sense of Lebesgue measure and Baire category)” for the 4-body problem, for systems of more than four particles it is not known whether the initial conditions leading to such catastrophies are atypical, i.e., form a set of Lebesgue measure zero—though this is certainly expected by most experts to be the case [12] (though not by all [25]). Indeed, apart from obvious scenarios—such as the particles moving apart sufficiently rapidly—and those covered by some version of the KAM theorem [3], for $N \geq 5$ it cannot, so far as we know, even be precluded on the basis of what has so far been proven that this set has full measure!

It is remarkable that the situation in the corresponding quantum system is very different. 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 \mathcal{H} . U_t is generated by a self-adjoint operator H , which on smooth wave functions in $\mathcal{H} = L^2(\Omega)$ is given by

$$H = -\sum_{k=1}^N \frac{\hbar^2}{2m_k} \Delta_k + V = H_0 + V, \quad (4)$$

i.e., Schrödinger’s equation is regarded as the “generator equation” for U_t . Hence the “problem of the existence of dynamics” for Schrödinger’s equation is reduced to that of 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 large classes of potentials, including singular potentials like the Coulomb potential, which is of primary physical interest [20, 32]. We shall discuss the meaning and the status of the self-adjointness of the Hamiltonian from the perspective of Bohmian mechanics in Section 4. It may be worthwhile to note, however, that the sufficiency of establishing only the

¹However, this example, which is 1-dimensional, involves an infinite number of binary collisions before the system explodes and thus does not describe a true pseudocollision.

self-adjointness of the Hamiltonian for a satisfactory physical interpretation has been questioned by Radin and Simon [29]: “Interestingly enough, while Kato’s result ‘solves’ the dynamical existence question in the quantum case, it says nothing about the question of $\mathbf{x}(t)^2$ remaining finite in time! From its physical interpretation, proof of such regularity property is clearly desirable.”

In Bohmian mechanics we have not only Schrödinger’s equation (3) to consider, but also the differential equation (2), governing the motion of the particles. Thus the question of existence of the dynamics of Bohmian mechanics draws again nearer to the situation in Newtonian mechanics, as it depends now on detailed regularity properties of the velocity field v^ψ (1). *Local* existence and uniqueness of Bohmian trajectories is guaranteed if the velocity field v^ψ is locally Lipschitz continuous. We therefore certainly need greater regularity for the wave function ψ than merely that ψ be in $L^2(\Omega)$.

Global existence is more delicate. In addition to the nodes of ψ , there are singularities comparable to those of Newtonian mechanics. Firstly, even for a globally smooth velocity field the solution of (2) may explode, i.e., it may reach infinity in finite time. Secondly, the boundary points of Ω , typically the singular points of the potential, are reflected in singular behavior of the wave function at such points, giving rise to singularities in the velocity field (1).²

The problem we address is the following: Suppose that at some arbitrary “initial time” ($t_0 = 0$) the N -particle configuration lies in the complement of the set of nodes and singularities of ψ_0 . Does the trajectory develop in a finite amount of time into a singularity of the velocity field v^ψ , or does it reach infinity in finite time? According to Theorem 3.1 and Corollary 3.2, the answer is negative for “typical” initial values, for a large class of potentials including the physically most interesting case of N -particle Coulomb interaction with arbitrary charges and masses. While we consider in this paper only particles without spin, Bohmian mechanics can be naturally defined for spinor-valued wave functions as well [4, 8, 17]. We shall deal with spin, including the motion in a magnetic field, in a subsequent work.

The quantity of central importance for our proof of these results—as well as for the question of the self-adjointness of the Hamiltonian—turns out to be the quantum flux $J^\psi(q, t) = (j^\psi, |\psi|^2)$, a $(d+1)$ -vector, with $j^\psi = v^\psi |\psi|^2$ the quantum

²For example, the ground state wave function of one particle in a Coulomb potential $V(q) = 1/|q|$, $q \in \mathbb{R}^3$ (“hydrogen atom”) has the form $e^{-|q|}$, which is not differentiable at the point $q = 0$ of the potential singularity.

probability current. The absolute value of the flux through any surface in $\Omega \times \mathbb{R}$ controls the probability that a trajectory crosses that surface. Surfaces of interest for us are the boundaries of neighborhoods around all the singular points for Bohmian mechanics. Loosely speaking, the importance of the quantum flux flows from the following insight: “If there is no absolute flux into the singular points, the singular points are not reached.”

We remark that the quantum flux is, in fact, important for most applications of quantum physics, as well as for the mathematics revolving around the self-adjointness of Schrödinger operators. Heuristically, the “right” behavior of the quantum flux at the critical points ensures self-adjointness of the Hamiltonian—i.e., conservation of probability. But suppose we ask, probability of what? The usual answer—the probability of finding a particle in a certain region—is *justified* by Bohmian mechanics: A particle is found in a certain region because, in fact, it’s there. By incorporating the positions of the particles into the theory, and thus interpreting the quantum flux as a flux of particles moving along trajectories, Bohmian mechanics can be regarded as providing the basis for all intuitive reasoning in quantum mechanics. (For more on this point, see also [7, 8, 4, 13, 14, 17, 11].)

The paper is organized as follows: In Section 2, the relevant notion of “typicality” is discussed. Section 3 contains our main results. In Section 3.1 we present the broad structure of the argument and in Section 3.2 we show how to transform the problem to that of controlling flux integrals. The main theorem and corollary are proven in Section 3.3. In Section 4 we discuss various aspects of the self-adjointness of the Hamiltonian from the point of view of Bohmian mechanics. In particular, in Section 4.1 we show that in $d = 1$ dimensions global existence holds under conditions which in certain respects are milder than those of Theorem 3.1.

This is the first work concerned with a rigorous examination of the problem of existence of the motion in Bohmian mechanics. For the related theory of Nelson, stochastic mechanics, this question has been discussed by Nelson [28] and also by Carlen [9]. The behavior of the Bohmian motion at the nodes of ψ has been addressed by Bohm [7] and Holland [17]. Bohm argues that particles are either repelled from the nodes or cross them with infinite speed. (Bohm, however, was not concerned with the question of existence but with consistency with “ $\rho = |\psi|^2$.”) Holland claims to show that a trajectory cannot reach a node

unless it is always at some node. His argument, however, is circular, in that it requires the very regularity whose breakdown at nodes is the source of difficulty.

Here is a simple counterexample to the claims of Bohm and Holland: Consider the one-dimensional harmonic oscillator (with $\hbar = m = \omega = 1$) and take as the wave function of the particle a superposition of the ground state and the second excited state, $\psi_t(q) = e^{-q^2/2} e^{-it/2} [1 + (1 - 2q^2)e^{-2it}]$. This wave function has nodes (among others) at $q = 0$, $t = (n + \frac{1}{2})\pi$ for all integers n . It leads to a velocity field which is an odd function of q , i.e., which defines a motion which is reflection invariant. Therefore $Q_t = 0$, $t \neq (n + \frac{1}{2})\pi$, is a solution of (2) which runs—first—into the node $(0, \pi/2)$ (with velocity 0 and which furthermore may be consistently continued through the nodes).

2 Equivariance and Typicality

The dynamical system defined by Bohmian mechanics is associated with a natural measure, given by the density $|\psi_0|^2$ on configuration space Ω . If ψ_0 is normalized, i.e., if the L^2 -norm $\|\psi_0\| = (\int_{\Omega} |\psi_0|^2 dq)^{1/2} = 1$, then the density $|\psi_0|^2$ defines a probability measure on configuration space Ω , which we shall denote by \mathbf{P} , that plays the role usually played by the “equilibrium measure.” Thus \mathbf{P} defines our notion of “typicality” [13]. *Given* the existence of the dynamics Q_t for configurations—the result we establish here—the notion of typicality is time independent by equivariance [13]:

$$\rho_0 = |\psi_0|^2 \implies \rho_t = |\psi_t|^2 \quad \text{for all } t \in \mathbb{R}, \quad (5)$$

where ρ_t denotes the probability density on configuration space Ω at time t —the image density of ρ_0 under the motion Q_t . This follows from comparing the continuity equation for an ensemble density $\rho_t(q)$

$$\frac{\partial \rho_t(q)}{\partial t} + \sum_{k=1}^N \nabla_k \cdot [\mathbf{v}_k^{\psi_t}(q) \rho_t(q)] = 0 \quad (6)$$

with the quantum continuity equation

$$\frac{\partial |\psi_t(q)|^2}{\partial t} + \sum_{k=1}^N \nabla_k \cdot \mathbf{j}_k^{\psi_t}(q) = 0 \quad (7)$$

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

$$\mathbf{j}_k^{\psi} = \mathbf{v}_k^{\psi} |\psi|^2 = \frac{\hbar}{2im_k} (\psi^* \nabla_k \psi - \psi \nabla_k \psi^*). \quad (8)$$

We further denote the space-time current, the quantum flux, by $J^\psi = (j^\psi, |\psi|^2)$. In our proof of global existence, this quantity gives the basic estimate for the probability that a trajectory reaches singularities of the velocity field or infinity.

It is at this stage important to bear in mind the conceptual difference between the Equations (6) and (7). The continuity equation (6), even without global existence of differentiable trajectories Q_t , holds “locally” on the set where v^ψ is smooth, with ρ_t suitably interpreted. This understanding is indeed basic to all our proofs.

Equation (7), on the other hand, is an identity for every ψ_t which satisfies Schrödinger’s equation classically. This is seen by calculating

$$\frac{\partial |\psi_t|^2}{\partial t} = \frac{1}{i\hbar}(\psi_t^* H \psi_t - \psi_t H \psi_t^*). \quad (9)$$

But, without having established global existence, 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 is indeed a classical probability current, propagating the ensemble density $|\psi|^2$ along the integral curves of the vector field v^ψ .

3 Global existence and uniqueness

We make the following general assumptions:

A1: *The potential V is a C^∞ -function on Ω .*

A2: *The Hamiltonian H is a self-adjoint extension of $H|_{C_0^\infty(\Omega)}$ with domain $\mathcal{D}(H)$.*

A3: *The initial wave function ψ_0 is a C^∞ -vector of H , $\psi_0 \in C^\infty(H)$, and is normalized, $\|\psi_0\| = 1$.*

The boundary $\partial\Omega$ of the configuration space Ω will be denoted by \mathcal{S} . (Recall that usually \mathcal{S} is the set of singularities of the potential.) $C_0^\infty(\Omega)$, the set of C^∞ -functions with compact support contained in Ω , is dense in $L^2(\Omega)$, and the Hamiltonian is symmetric on this set. Since H is real, i.e., commutes with complex conjugation, there always exist self-adjoint extensions. The set of admissible initial wave functions, $C^\infty(H) = \bigcap_{n=1}^\infty \mathcal{D}(H^n)$, is dense in $L^2(\Omega)$ and invariant under the time evolution $e^{-itH/\hbar}$, and is therefore a core, i.e., a domain of essential self-adjointness for H .³

³Some special C^∞ -vectors are eigenfunctions and “wave packets” $\psi \in \text{Ran}(P_{[a,b]})$, where $P_{[a,b]}$ denotes the spectral projection of H to the finite energy interval $[a, b]$.

In Lemma 6.1 we show that as a consequence of A1–A3 we may regard $\psi_t = e^{-itH/\hbar}\psi_0$ as being in $C^\infty(\Omega \times \mathbb{R})$ (and thus as a classical solution of Schrödinger’s equation). Then the velocity field v^ψ (cf. (1)) is C^∞ on the complement of the set \mathcal{N} of nodes of ψ , $\mathcal{N} := \{(q, t) \in \Omega \times \mathbb{R} : \psi(q, t) = 0\}$, i.e., on the set of “good” points

$$\mathcal{G} := (\Omega \times \mathbb{R}) \setminus \mathcal{N},$$

which is an open subset of $\mathbb{R}^d \times \mathbb{R}$. Let \mathcal{G}_t denote the slice of \mathcal{G} at a fixed time t : $\mathcal{G}_t := \Omega \setminus \mathcal{N}_t$, where $\mathcal{N}_t := \{q \in \Omega : \psi(q, t) = 0\}$. Then by a standard theorem of existence and uniqueness of ordinary differential equations, for all initial values (q_0, t_0) in \mathcal{G} there exist $\tau^-(q_0, t_0) < t_0$, $\tau(q_0, t_0) > t_0$, and a unique maximal (non-extendible) solution Q of (2) on the time interval $(\tau^-(q_0, t_0), \tau(q_0, t_0))$. From continuous dependence on initial values, the domain D of the maximal solution $Q(t; q_0, t_0)$,

$$D := \{(t, q_0, t_0) : (q_0, t_0) \in \mathcal{G}, t \in (\tau^-(q_0, t_0), \tau(q_0, t_0))\}, \quad (10)$$

is an open subset of \mathbb{R}^{d+2} (and Q is locally Lipschitz continuous on D with respect to (t, q_0, t_0)). Thus τ is lower semi-continuous and hence, in particular, measurable. Because of the time translation invariance of the theory, we may fix $t_0 = 0$, writing $\tau(q_0)$ for $\tau(q_0, 0)$, with similar notation for τ^- . Under additional conditions on Ω and H (see Corollary 3.2), we shall show that $\tau(q_0) = \infty$ for typical q_0 , i.e., we show that the solution exists globally in time \mathbf{P} -almost surely:

$$\mathbf{P}(\tau < \infty) = 0. \quad (11)$$

This is equivalent to

$$\forall T < \infty : \mathbf{P}(\tau < T) = 0. \quad (12)$$

(Note that by time translation invariance and equivariance, $\mathbf{P}(\tau < \infty) = 0$ for all $\psi_0 \in C^\infty(H)$ implies that $\mathbf{P}(\tau^- > -\infty) = 0$ for all $\psi_0 \in C^\infty(H)$, so that (11) indeed implies global existence and uniqueness.)

3.1 The program

We view the maximal solution Q_t as a stochastic process on \mathcal{G}_0 equipped with the probability measure \mathbf{P} , i.e., q_0 is distributed according to the probability density $|\psi_0|^2$. The basic criterion for global existence arises from the following properties of the maximal solution. The set of limit points $L(q_0)$ of the trajectory starting

at q_0 ($q^* \in L : \Leftrightarrow$ there is a sequence $t_k, t_k \rightarrow \tau \equiv \tau(q_0)$ with $\lim_{k \rightarrow \infty} Q_{t_k} = q^*$) is either empty—this is equivalent to $\lim_{t \nearrow \tau} |Q_t| = \infty$ —or nonempty, in which case, if $\tau < \infty$, $(q^*, \tau) \in \partial \mathcal{G}$ for all $q^* \in L$. (The solution Q need not be continuous at $t = \tau$, i.e., L might contain more than one point, and there might additionally be sequences $t_k \rightarrow \tau$ along which $|Q_{t_k}| \rightarrow \infty$.) We thus have to see whether trajectories come too close to the boundary of \mathcal{G} or to infinity. We do this by checking whether they reach the boundary of \mathcal{G}^n , an increasing ($\mathcal{G}^{n_1} \subset \mathcal{G}^{n_2}$ for $n_1 < n_2$) sequence of open sets $\mathcal{G}^n \subset \mathcal{G}$, $\overline{\mathcal{G}^n} \subset \mathcal{G}$, which are bounded in configuration space, i.e., for all $T \in \mathbb{R}$, the set $\mathcal{G}_{[0,T]}^n := \mathcal{G}^n \cap (\mathbb{R}^d \times [0, T])$ is bounded.

For $q_0 \in \mathcal{G}_0^n$, we introduce the stopping time $\tau^n(q_0)$, at which the process Q_t first hits the boundary of \mathcal{G}^n :

$$\tau^n(q_0) := \sup\{s > 0 : (Q_t(q_0), t) \in \mathcal{G}^n \text{ for all } t \leq s\}.$$

Now, from the elementary theory of ordinary differential equations, for all $q_0 \in \mathcal{G}_0^n$,

$$\text{if } \tau(q_0) < \infty, \text{ then } \tau^n(q_0) < \tau(q_0) \text{ and } (Q_{\tau^n(q_0)}(q_0), \tau^n(q_0)) \in \partial \mathcal{G}^n. \quad (13)$$

Furthermore, the sequence τ^n is increasing in n . For all n and all $T \leq \infty$, we have

$$\{q_0 \in \mathcal{G}_0 : \tau < T\} \subset (\mathcal{G}_0 \setminus \mathcal{G}_0^n) \cup \{q_0 \in \mathcal{G}_0^n : \tau^n < T\}$$

and therefore

$$\mathbf{P}(\{q_0 \in \mathcal{G}_0 : \tau < T\}) \leq \mathbf{P}(\mathcal{G}_0 \setminus \mathcal{G}_0^n) + \mathbf{P}(\{q_0 \in \mathcal{G}_0^n : \tau^n < T\}) \quad (14)$$

Thus to obtain the global existence and uniqueness of Bohmian mechanics for typical initial configurations, it is sufficient to establish the vanishing of the right hand side of (14) as $n \rightarrow \infty$ for some sequence of sets \mathcal{G}^n . (Note as a matter of fact that the right hand side of (14) decreases as n increases.)

To proceed, we need to separate different parts of the boundary of \mathcal{G}^n which we shall treat in different ways: those close to infinity, those close to $\mathcal{S} = \partial \Omega$, and those close to the set \mathcal{N} of nodes of the wave function. We introduce \mathcal{K}^n , a sequence of bounded open sets exhausting \mathbb{R}^d , $\mathcal{K}^n \nearrow \mathbb{R}^d$; \mathcal{S}^δ , a sequence of closed neighborhoods of \mathcal{S} of “thickness δ ”; and \mathcal{N}^ϵ , a sequence of closed neighborhoods of \mathcal{N} of “thickness ϵ .” (For the following general remarks, we do not need to specify these sets more concretely; this will be done in Section 3.3.) Thus the

index n accordingly gets replaced by $\epsilon\delta n$. $\mathcal{G}^{\epsilon\delta n}$ then denotes the set of “ ϵ - δ - n -good” points in configuration-space-time:

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

and $\mathcal{G}_t^{\epsilon\delta n}$ denotes the slice at a fixed time $t \in \mathbb{R}$:

$$\mathcal{G}_t^{\epsilon\delta n} := (\mathcal{K}^n \cap \Omega) \setminus (\mathcal{S}^\delta \cup \mathcal{N}_t^\epsilon).$$

Furthermore, we define

$$\mathcal{G}_{(0,T)}^{\delta n} := ((\mathcal{K}^n \cap \Omega) \setminus \mathcal{S}^\delta) \times (0, T). \quad (15)$$

From (13), we may write, with $x := (Q_{\min(\tau^{\epsilon\delta n}, T)}, \min(\tau^{\epsilon\delta n}, T))$,

$$\begin{aligned} \{q_0 \in \mathcal{G}_0^{\epsilon\delta n} : \tau^{\epsilon\delta n} < T\} &= \{q_0 \in \mathcal{G}_0^{\epsilon\delta n} : x \in \partial\mathcal{G}^{\epsilon\delta n} \cap (\mathbb{R}^d \times (0, T))\} \\ &= \{q_0 \in \mathcal{G}_0^{\epsilon\delta n} : x \in \partial\mathcal{N}^\epsilon \cap \mathcal{G}_{(0,T)}^{\delta n}\} \\ &\cup \{q_0 \in \mathcal{G}_0^{\epsilon\delta n} : x \in (\partial\mathcal{S}^\delta \cap \Omega) \times (0, T)\} \\ &\cup \{q_0 \in \mathcal{G}_0^{\epsilon\delta n} : x \in (\partial\mathcal{K}^n \cap \Omega) \times (0, T)\}. \end{aligned} \quad (16)$$

and therefore we arrive at

$$\begin{aligned} \mathbf{P}(\{q_0 \in \mathcal{G}_0^{\epsilon\delta n} : \tau^{\epsilon\delta n} < T\}) &\leq \mathbf{P}(\{q_0 \in \mathcal{G}_0^{\epsilon\delta n} : x \in \partial\mathcal{N}^\epsilon \cap \mathcal{G}_{(0,T)}^{\delta n}\}) \\ &\quad + \mathbf{P}(\{q_0 \in \mathcal{G}_0^{\epsilon\delta n} : x \in (\partial\mathcal{S}^\delta \cap \Omega) \times (0, T)\}) \\ &\quad + \mathbf{P}(\{q_0 \in \mathcal{G}_0^{\epsilon\delta n} : x \in (\partial\mathcal{K}^n \cap \Omega) \times (0, T)\}). \end{aligned} \quad (17)$$

By virtue of (14) (almost sure) global existence follows if for *some suitable* choice of sets \mathcal{N}^ϵ , \mathcal{S}^δ , and \mathcal{K}^n , $\mathbf{P}(\mathcal{G}_0 \setminus \mathcal{G}_0^{\epsilon\delta n})$ and the right hand side of (17) can be made arbitrarily small by appropriately choosing ϵ , δ and n .

3.2 The flux argument

Consider the random trajectory $(\mathcal{G}_0, \mathbf{P}, \tilde{Q}_t)$ obtained by stopping the original process Q_t at time τ and placing it in the cemetery \dagger : The process $\tilde{Q}_t : \mathcal{G}_0 \longrightarrow \Omega \cup \{\dagger\}$ is defined, for all $t \geq 0$, by

$$\tilde{Q}_t(q_0) := \begin{cases} Q_t(q_0) & \text{for } t < \tau(q_0) \\ \dagger & \text{for } t \geq \tau(q_0). \end{cases} \quad (18)$$

Let ρ_t be the image density of \tilde{Q}_t restricted to Ω .

Denote by \mathcal{I} the set

$$\mathcal{I} := \{(Q_t(q_0), t) : t \in (\tau^-(q_0), \tau(q_0)) \text{ and } q_0 \in \mathcal{G}_0\},$$

and by $\mathcal{I}_t := \text{Ran}\tilde{Q}_t \setminus \{\dagger\}$ ($\mathcal{I}_t \subset \mathcal{G}_t$) its time- t slice. \mathcal{I} is an open subset of \mathcal{G} . (\mathcal{I} can be identified with $D \cap (\{0\} \times \mathbb{R}^{d+1})$, cf. (10).) Clearly $\rho_t = 0$ on $\mathcal{G}_t \setminus \mathcal{I}_t$ for $t > 0$. Note that on \mathcal{I} both $|\psi_t|^2$ and ρ_t are solutions of the continuity equation (6) restricted to \mathcal{I} with the same initial data. Uniqueness of solutions of quasilinear first order partial differential equations on the set where the characteristics exist implies that for all $t \geq 0$

$$\rho_t(q) = |\psi_t(q)|^2 \text{ for all } q \in \mathcal{I}_t. \quad (19)$$

Consider now a smooth surface Σ in \mathcal{G} . Recalling the probabilistic meaning 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 (including tangential “crossings” in which the trajectory remains on the same side of Σ) is given by

$$\int_{\Sigma} |J_t(q) \cdot U| d\sigma \quad (20)$$

where U denotes the local unit normal vector at (q, t) . ($\int_{\Sigma} (J \cdot U) d\sigma$ is the expected number of *signed* crossings.) (Consider first a small surface element which the trajectory can cross at most once. The probability density for this crossing is readily calculated to be $|J \cdot U|$. Invoking the linearity of the expectation value yields then the general statement.)⁴

The probability of crossing Σ (at least once) is hence bounded by (20). From (19) we obtain that

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

and thus we arrive at the bound

$$\mathbf{P}(\tilde{Q}_t \text{ crosses } \Sigma) \leq \int_{\Sigma} |J^{\psi_t}(q) \cdot U| d\sigma. \quad (21)$$

If now the sets \mathcal{N}^ϵ , \mathcal{S}^δ , and \mathcal{K}^n are chosen in such a way that their boundaries are piecewise integrable surfaces, the events on the r.h.s. of (17) are crossings by

⁴In stochastic mechanics [28], which involves the same quantum flux, the particle trajectories are realizations of a diffusion process and are hence not differentiable, i.e., velocities do not exist. Thus in stochastic mechanics the flux does not have the same probabilistic significance and hence the subsequent arguments are not valid for stochastic mechanics.

\tilde{Q}_t through the respective surfaces, and hence (21) implies the following bounds for the terms in (17):

$$\begin{aligned} \mathbf{P}(x \in (\partial\mathcal{N}^\epsilon \cap \mathcal{G}_{(0,T)}^{\delta n})) &\leq \int_{\partial\mathcal{N}^\epsilon \cap \mathcal{G}_{(0,T)}^{\delta n}} |J^{\psi_t}(q) \cdot U| d\sigma := \mathbf{N}(\epsilon, \delta, n), \\ \mathbf{P}(x \in ((\partial\mathcal{S}^\delta \cap \Omega) \times (0, T))) &\leq \int_{(\partial\mathcal{S}^\delta \cap \Omega) \times (0, T)} |J^{\psi_t}(q) \cdot U| d\sigma := \mathbf{S}(\delta), \quad (22) \\ \mathbf{P}(x \in ((\partial\mathcal{K}^n \cap \Omega) \times (0, T))) &\leq \int_{(\partial\mathcal{K}^n \cap \Omega) \times (0, T)} |J^{\psi_t}(q) \cdot U| d\sigma =: \mathbf{I}(n). \end{aligned}$$

(If a boundary happens to be the empty set, the corresponding integral of course vanishes.)

It seems intuitively rather clear⁵ that all the flux integrals should vanish in the limit $\epsilon \rightarrow 0, \delta \rightarrow 0$, and $n \rightarrow \infty$: It seems fairly obvious that the “nodal integral” $\mathbf{N}(\epsilon, \delta, n)$ should vanish as $\epsilon \rightarrow 0$ since J^{ψ_t} is zero at the nodes.⁶ The “singularity integral” $\mathbf{S}(\delta)$ should vanish in the limit $\delta \rightarrow 0$ if the set \mathcal{S} has codimension greater than 1, which is usually the case. Furthermore, $j^\psi = 0$ at \mathcal{S} is a natural boundary condition defining a domain of self-adjointness of the Hamiltonian. Finally, the “infinity integral” $\mathbf{I}(n)$ should tend to zero as $n \rightarrow \infty$ since $\psi_t(q)$ (which is sufficiently smooth) and hence $J^{\psi_t}(q)$ should rapidly go to zero as $|q| \rightarrow \infty$.

3.3 Global existence of Bohmian mechanics

Our main result is the following theorem:

Theorem 3.1 *Assume A2, A3, and further*

A1': *A1 and $\mathcal{S} \subset \bigcup_{l=1}^m \mathcal{S}_l$, where $m < \infty$ and the \mathcal{S}_l are $(d-3)$ -dimensional hyperplanes;*

A4: *$\int_0^T \|\nabla\psi_t\|^2 dt < \infty$ for all $0 < T < \infty$.*

Then $\mathbf{P}(\tau < \infty) = 0$.

Since \mathcal{S}_l is a $(d-3)$ -dimensional hyperplane, it may be written as $\mathcal{S}_l = \{\mathbf{y}_l = \mathbf{a}_l\}$ with \mathbf{y}_l denoting the map $\mathbb{R}^d \rightarrow \mathbb{R}^3, q \mapsto (q \cdot y_l^1, q \cdot y_l^2, q \cdot y_l^3)$ where y_l^1, y_l^2, y_l^3 are 3 orthogonal unit vectors normal to the hyperplane \mathcal{S}_l and $\mathbf{a}_l \in \mathbb{R}^3$ a constant.

⁵By mentioning these heuristics we do not wish to suggest the structure of the rigorous proof given in the next section, nor need this proof sustain these heuristics.

⁶One might worry about the “size of $\partial\mathcal{N}$ ” being uncontrollably large. However, since ψ is a complex smooth function, \mathcal{N} might be expected to have codimension 2 “generically,” so $\partial\mathcal{N}^\epsilon$ should have small area.

The Condition A1' on the shape of \mathcal{S} fits well with the 3-dimensionality of physical space. If V is a central potential, \mathcal{S}_l is of the form $\{\mathbf{q}_i = 0\}$, and for a pair potential, \mathcal{S}_l is of the form $\{\mathbf{q}_i - \mathbf{q}_j = 0\}$ for some $1 \leq i < j \leq N$. (Note that if $d = \nu N < 3$, Assumption A1' demands that $\mathcal{S} = \emptyset$.)

Under the Assumption A1', the configuration space $\Omega = \mathbb{R}^d \setminus \mathcal{S}$; in particular, $L^2(\Omega) = L^2(\mathbb{R}^d)$.⁷ Recall that H_0 denotes the self-adjoint operator

$$H_0 = - \sum_{k=1}^N \frac{\hbar^2}{2m_k} \Delta_k$$

on the Hilbert space $\mathcal{H} = L^2(\Omega) = L^2(\mathbb{R}^d)$.

The Condition A4 of “finite integrated kinetic energy” may be ensured by bounding the quadratic form $(\nabla\psi_t, \nabla\psi_t) \leq M(\psi_t, H_0\psi_t)$ with $M = (2/\hbar^2) \max(m_1, \dots, m_N)$ by the form $(\psi_t, H\psi_t)$, which is finite and independent of t for ψ_0 (and hence ψ_t) in the form domain [31] $\mathcal{Q}(H) (\supset \mathcal{D}(H))$ of the Hamiltonian H .⁸ The following corollary shows that Theorem 3.1 indeed implies the global existence and uniqueness of Bohmian mechanics for all $\psi_0 \in C^\infty(H)$ for a large class of Hamiltonians.

Corollary 3.2 *Assume*

A1'': *A1' and $V = V_1 + V_2$, where V_1 is bounded below, and V_2 is H_0 -form bounded with relative bound $a < 1$,*

A2': *H is the form sum $H_0 + V$ [15],*

and A3. Then $\mathbf{P}(\tau < \infty) = 0$ and Bohmian mechanics exists uniquely and globally in time \mathbf{P} -almost surely.

Proof. We show that A4 holds: That V_2 is H_0 -form bounded means that $\mathcal{Q}(H_0) \subset \mathcal{Q}(V_2)$ and that for $\psi \in \mathcal{Q}(H_0)$ there exist constants $a, b > 0$ such that

$$|(\psi, V_2\psi)| \leq a(\psi, H_0\psi) + b(\psi, \psi).$$

⁷Thus Theorem 3.1 does not cover the case of a bounded configuration space Ω , for which boundary conditions of Dirichlet or Neumann (or mixed) type are normally imposed. See, however, our Theorem 4.1.

⁸Note that the notation $(\psi, A\psi)$ for the quadratic form associated with the self-adjoint operator A is symbolic: Only for $\psi \in \mathcal{D}(A)$ does it coincide with the indicated scalar product in $\mathcal{H} = L^2(\mathbb{R}^d)$; more generally it can be defined via the spectral representation for A .

Since $V_1(q) \geq -c$, $c > 0$, for all $q \in \Omega$, we obtain for $\psi \in \mathcal{Q}(H) = \mathcal{Q}(H_0) \cap \mathcal{Q}(V_1)$ that

$$\begin{aligned} (1-a)(\psi, H_0\psi) &\leq (\psi, (H_0 + V_2)\psi) + b(\psi, \psi) \\ &\leq (\psi, (H_0 + V_1 + V_2)\psi) + c(\psi, \psi) + b(\psi, \psi) \\ &= (\psi, H\psi) + (b+c)(\psi, \psi). \end{aligned}$$

Hence with $a < 1$ we have that for $\psi_0 \in \mathcal{Q}(H) \subset \mathcal{Q}(H_0)$ and all t

$$\begin{aligned} \frac{1}{M}(\nabla\psi_t, \nabla\psi_t) &\leq (\psi_t, H_0\psi_t) \leq \frac{1}{1-a}(\psi_t, H\psi_t) + \frac{b+c}{1-a}(\psi_t, \psi_t) \\ &= \frac{1}{1-a}(\psi_0, H\psi_0) + \frac{b+c}{1-a}\|\psi_0\|^2 \end{aligned}$$

and A4 follows. \square

The class of H_0 -form bounded potentials, with arbitrary small relative bound a , includes for example $R+L^\infty$ or $L^{3/2}+L^\infty$ on \mathbb{R}^3 , where R is the Rollnik class. (For details, see for example [21, 36, 32].) Therefore such H_0 -form bounded potentials include power law interactions $1/r^\alpha$ 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 [20].) Furthermore, harmonic and anharmonic (positive) potentials are included, and arbitrarily strong positive repulsive potentials.

Proof of Theorem 3.1. We establish (12)—for all $0 < T < \infty$, $\mathbf{P}(\tau < T) = 0$ —following the program described in Section 3.1 and the flux argument of Section 3.2.

We first choose suitable sets \mathcal{N}^ϵ , \mathcal{S}^δ , and \mathcal{K}^n . Let $\epsilon > 0$. Set

$$\mathcal{N}^\epsilon := \bigcup_{k: C^\epsilon(k) \cap \mathcal{N} \neq \emptyset} C^\epsilon(k), \quad (23)$$

where $(C^\epsilon(k))_{k \in \mathbb{N}}$ is a “partition” of configuration-space-time into closed cubes with side length ϵ whose edges are parallel to the canonical basis vectors of \mathbb{R}^{d+1} . Let $\delta = (\delta_1, \dots, \delta_m)$, $\delta_l > 0$ for all l . Recalling that $\mathcal{S} \subset \bigcup_{l=1}^m \mathcal{S}_l$ with $\mathcal{S}_l = \{\mathbf{y}_l = \mathbf{a}_l\}$, set

$$\mathcal{S}^\delta := \bigcup_{l=1}^m \mathcal{S}_l^{\delta_l}, \quad \mathcal{S}_l^{\delta_l} := \{q \in \mathbb{R}^d : \text{dist}(q, \mathcal{S}_l) \leq \delta_l\} = \{|\mathbf{y}_l - \mathbf{a}_l| \leq \delta_l\}.$$

For the cutoff at infinity we choose open balls with radii $n \in \mathbb{R}^+$:

$$\mathcal{K}^n := \{q \in \mathbb{R}^d : |q| < n\}.$$

By virtue of (14), (17), and (22), we obtain that for all $0 < T < \infty$

$$\begin{aligned} \mathbf{P}(\tau < T) &\leq \mathbf{P}(\mathcal{G}_0 \setminus \mathcal{G}_0^{\epsilon\delta n}) + \mathbf{P}(\tau^{\epsilon\delta n} < T) \\ &\leq \mathbf{P}(\mathcal{G}_0 \setminus \mathcal{G}_0^{\epsilon\delta n}) + \mathbf{P}(x \in (\partial\mathcal{N}^\epsilon \cap \mathcal{G}_{(0,T)}^{\delta n})) \\ &\quad + \mathbf{P}(x \in (\partial\mathcal{S}^\delta \times (0, T))) + \mathbf{P}(x \in ((\partial\mathcal{K}^n \cap \Omega) \times (0, T))) \\ &\leq \mathbf{P}(\mathcal{G}_0 \setminus \mathcal{G}_0^{\epsilon\delta n}) + \mathbf{N}(\epsilon, \delta, n) + \mathbf{S}(\delta) + \mathbf{I}(n) \end{aligned} \quad (24)$$

For the first term on the right hand side of (24) recall that $\mathcal{G}_0^{\epsilon\delta n} = (\mathcal{K}^n \cap \Omega) \setminus (\mathcal{N}_0^\epsilon \cup \mathcal{S}^\delta)$; therefore

$$\mathcal{G}_0 \setminus \mathcal{G}_0^{\epsilon\delta n} = (\mathcal{G}_0 \setminus \mathcal{K}^n) \cup (\mathcal{G}_0 \cap \mathcal{S}^\delta) \cup (\mathcal{G}_0 \cap \mathcal{N}_0^\epsilon),$$

and thus

$$\mathbf{P}(\mathcal{G}_0 \setminus \mathcal{G}_0^{\epsilon\delta n}) \leq \mathbf{P}(\mathcal{G}_0 \setminus \mathcal{K}^n) + \mathbf{P}(\mathcal{G}_0 \cap \mathcal{S}^\delta) + \mathbf{P}(\mathcal{G}_0 \cap \mathcal{N}_0^\epsilon).$$

The vanishing of the three terms on the right hand side in the limit $n \rightarrow \infty$, $\delta \rightarrow 0$, resp. $\epsilon \rightarrow 0$, follows easily from the facts that \mathbf{P} is a probability measure with density $|\psi_0|^2$, and that the respective sets tend to \mathbf{P} -measure 0 sets.

The vanishing of the remaining terms in (24) is the content of the following lemmas:

Lemma 3.3 *Assume A1–A4. For all $0 < T < \infty$ there exists a sequence n_k , $n_k \rightarrow \infty$ as $k \rightarrow \infty$, with*

$$\lim_{k \rightarrow \infty} \mathbf{I}(n_k) = 0.$$

Lemma 3.4 *Assume A1', and A2–A4. Then there exists a sequence of m -vectors $\delta^{(k)}$, $|\delta^{(k)}| \rightarrow 0$ as $k \rightarrow \infty$ (with $\delta_l^{(k)} > 0$ for all l, k), with*

$$\lim_{k \rightarrow \infty} \mathbf{S}(\delta^{(k)}) = 0.$$

Lemma 3.5 *Assume A1–A3. For all $0 < T < \infty$, $n < \infty$ and $\delta > 0$,*

$$\lim_{\epsilon \rightarrow 0} \mathbf{N}(\epsilon, \delta, n) = 0.$$

These lemmas will be proven below. Lemmas 3.3, 3.4, and 3.5 imply that the r.h.s. of (24) can be made arbitrarily small. (Note that if $d < 3$, Assumption A1' demands that $\mathcal{S} = \emptyset$, and hence that $\mathbf{S} \equiv 0$, so that Lemma 3.4 is trivial in this case.) \square

Proof of Lemma 3.3.

$$\begin{aligned} \mathbf{I}(n) &= \int_{(\partial\mathcal{K}^n \cap \Omega) \times (0, T)} |J^{\psi_t}(q) \cdot U| \, d\sigma = \int_0^T \int_{\partial\mathcal{K}^n \cap \Omega} |j^{\psi_t}(q) \cdot u| \, ds \, dt \\ &\leq \mu \int_0^T \int_{\partial\mathcal{K}^n \cap \Omega} |\psi_t| |\nabla \psi_t| \, ds \, dt =: \mu \tilde{\mathbf{I}}(n) \end{aligned}$$

with $\mu = \hbar / \min(m_1, \dots, m_N)$, ds the $(d-1)$ -dimensional surface element of $\partial\mathcal{K}^n$, and u the local unit normal vector of this surface. To show that $\tilde{\mathbf{I}}(n)$ goes to 0 along some sequence n_k , we prove a stronger statement, namely that $\tilde{\mathbf{I}}(n)$ is integrable over n . This is immediate since $\int_0^\infty \tilde{\mathbf{I}}(n) \, dn$ yields the *volume* integral of $|\psi_t| |\nabla \psi_t|$, which is easily estimated:

$$\begin{aligned} \int_0^\infty \tilde{\mathbf{I}}(n) \, dn &= \int_0^T \int_{\Omega} |\psi_t| |\nabla \psi_t| \, dq \, dt \\ &\leq \int_0^T \|\psi_t\| \|\nabla \psi_t\| \, dt = \int_0^T \|\nabla \psi_t\| \, dt < \infty, \end{aligned}$$

where we have used A4 for the last inequality. We may thus conclude that there exists a sequence $(n_k)_k$ with $n_k \rightarrow \infty$ as $k \rightarrow \infty$, along which $\tilde{\mathbf{I}}(n_k) \rightarrow 0$. This proves Lemma 3.3. \square

Proof of Lemma 3.4. We may assume that $d \geq 3$. We shall use the following Inequality: For $\psi \in \mathcal{Q}(H_0)$

$$\int_{\mathbb{R}^d} \frac{|\psi|^2}{4|\mathbf{y}_l - \mathbf{a}_l|^2} \, dq \leq \int_{\mathbb{R}^d} |\nabla \psi|^2 \, dq. \quad (25)$$

This is a straightforward extension of the inequality known as Hardy's inequality or the "uncertainty principle lemma" (see, for example, [32]) usually given for $\psi \in C_0^\infty(\mathbb{R}^3)$:

$$\int_{\mathbb{R}^3} \frac{|\psi|^2}{4r^2} \, d\mathbf{r} \leq \int_{\mathbb{R}^3} |\nabla \psi|^2 \, d\mathbf{r}.$$

(One immediately obtains (25) for $d = 3$ and $\psi \in C_0^\infty(\mathbb{R}^3)$. Then, viewing $\psi \in C_0^\infty(\mathbb{R}^d)$ as $\psi \in C_0^\infty(\mathbb{R}^3)$ by keeping all coordinates fixed except \mathbf{y}_l , one extends this inequality easily to $C_0^\infty(\mathbb{R}^d)$. It is then further extendible to $\psi \in \mathcal{Q}(H_0)$ because $C_0^\infty(\mathbb{R}^d)$ is dense in $\mathcal{Q}(H_0)$ with respect to the H_0 -form norm.)

First we estimate

$$\begin{aligned} \mathbf{S}(\delta) &= \int_{\partial \mathcal{S}^\delta \times (0, T)} |J^{\psi_t}(q) \cdot U| \, d\sigma = \int_0^T \int_{\partial \mathcal{S}^\delta} |j^{\psi_t}(q) \cdot u| \, ds \, dt \\ &\leq \mu \sum_{l=1}^m \int_0^T \int_{\partial \mathcal{S}_l^{\delta_l} \cap \Omega} |\psi_t| |\nabla \psi_t| \, ds \, dt =: \mu \sum_{l=1}^m \tilde{\mathbf{S}}_l(\delta_l). \end{aligned}$$

We now integrate $(1/|\mathbf{y}_l - \mathbf{a}_l|) \tilde{\mathbf{S}}_l(\delta_l)$ over $\delta_l = |\mathbf{y}_l - \mathbf{a}_l|$: By the definition of $\mathcal{S}_l^{\delta_l} = \{|\mathbf{y}_l - \mathbf{a}_l| \leq \delta_l\}$, this yields the *volume* integral of $(|\psi|/|\mathbf{y}_l - \mathbf{a}_l|) |\nabla \psi|$, which may be bounded as follows:

$$\begin{aligned} \int_0^\infty \frac{1}{\delta_l} \tilde{\mathbf{S}}_l(\delta_l) \, d\delta_l &= \int_0^T \int_{\Omega} \frac{|\psi_t|}{|\mathbf{y}_l - \mathbf{a}_l|} |\nabla \psi_t| \, dq \, dt \\ &= \int_0^T \int_{\mathbb{R}^d} \frac{|\psi_t|}{|\mathbf{y}_l - \mathbf{a}_l|} |\nabla \psi_t| \, dq \, dt \leq \int_0^T \left\| \frac{\psi_t}{|\mathbf{y}_l - \mathbf{a}_l|} \right\| \|\nabla \psi_t\| \, dt \\ &\leq 2 \int_0^T \|\nabla \psi_t\|^2 \, dt < \infty \end{aligned}$$

using Schwarz's inequality and the Inequality (25). Since $1/\delta_l$ is not integrable at $\delta_l = 0$, for each l there exists a sequence $\delta_l^{(k)}$ with $\delta_l^{(k)} \rightarrow 0$ as $k \rightarrow \infty$, along which $\tilde{\mathbf{S}}_l(\delta_l^{(k)}) \rightarrow 0$. This proves Lemma 3.4. \square

Proof of Lemma 3.5. This proof is more involved than the previous ones, since the nodal set is unknown. The basic idea is the following: Where the $(d+1)$ -gradient $\psi' = \left(\nabla \psi, \frac{\partial \psi}{\partial t}\right)$ is small the current is very small, and where ψ' is not small the surface area can be controlled.

Let $\eta > 0$. We split the part of \mathcal{N}^ϵ contributing to the surface $\partial \mathcal{N}^\epsilon \cap \mathcal{G}_{(0, T)}^{\delta_n}$ into two (not necessarily disjoint) sets:

$$\mathcal{N}_>^\epsilon := \bigcup_{k \in I_>} C^\epsilon(k), \quad \text{and} \quad \mathcal{N}_<^\epsilon := \bigcup_{k \in I_<} C^\epsilon(k) \quad \text{with}$$

$$I_> := \{k : C^\epsilon(k) \cap \{(q, t) : \psi(q, t) = 0, |\psi'(q, t)| > \eta\} \cap \mathcal{G}_{(0, T)}^{\delta_n} \neq \emptyset\}$$

$$I_< := \{k : C^\epsilon(k) \cap \{(q, t) : \psi(q, t) = 0, |\psi'(q, t)| \leq \eta\} \cap \mathcal{G}_{(0, T)}^{\delta_n} \neq \emptyset\}$$

Then

$$\mathbf{N}(\epsilon, \delta, n) = \int_{\partial \mathcal{N}^\epsilon \cap \mathcal{G}_{(0, T)}^{\delta_n}} |J^{\psi_t}(q) \cdot U| \, d\sigma \leq \int_{\partial \mathcal{N}_>^\epsilon} |J^{\psi_t}(q)| \, d\sigma + \int_{\partial \mathcal{N}_<^\epsilon} |J^{\psi_t}(q)| \, d\sigma \quad (26)$$

On the compact set $\overline{\mathcal{G}_{(-1, T+1)}^{(\delta/2)(n+1)}}$ (cf. (15)) there exist a global Lipschitz constant L for ψ' , and a global bound K for $|\psi'|$. Observe that for $\epsilon < \min(\delta/(2\sqrt{d}), 1/\sqrt{d})$, $\mathcal{N}_>^\epsilon \subset \mathcal{G}_{(-1, T+1)}^{(\delta/2)(n+1)}$. Let therefore $\epsilon < \min(\delta/(2\sqrt{d}), 1/\sqrt{d})$.

Consider first $\mathcal{N}_<^\epsilon$. In this set the flux $|J^\psi|$ is very small. We may estimate the integral by simply taking an appropriate bound of $|J^\psi|$ times the total area of the surfaces of *all* the cubes. In every ϵ -cube C^ϵ of $\mathcal{N}_<^\epsilon$ there is a point $(q^*, t^*) \in \mathcal{N}$ with $|\psi'(q^*, t^*)| \leq \eta$. Thus (in every ϵ -cube of $\mathcal{N}_<^\epsilon$ and hence) for all $(q, t) \in \mathcal{N}_<^\epsilon$

$$|\psi'(q, t)| \leq \eta + L\sqrt{d+1}\epsilon.$$

$|\psi|$ is thus bounded on (every ϵ -cube of $\mathcal{N}_<^\epsilon$ and hence on) $\mathcal{N}_<^\epsilon$ by $(\eta + L\sqrt{d+1}\epsilon)\sqrt{d+1}\epsilon =: c_1\eta\epsilon + c_2\epsilon^2$. The flux is then bounded by

$$\begin{aligned} |J^\psi| &= \sqrt{(|\psi|^2)^2 + |j^\psi|^2} \leq |\psi|^2 + |j^\psi| \leq |\psi|^2 + \mu|\psi||\nabla\psi| \\ &\leq (c_1\eta\epsilon + c_2\epsilon^2)^2 + \mu(c_1\eta\epsilon + c_2\epsilon^2)(\eta + L\sqrt{d+1}\epsilon) \end{aligned} \quad (27)$$

To bound the surface area of $\mathcal{N}_<^\epsilon$, we simply add the areas of the surfaces of all ϵ -cubes in $\mathcal{G}_{(-1, T+1)}^{(\delta/2)(n+1)}$. The number of ϵ -cubes in $\mathcal{G}_{(-1, T+1)}^{(\delta/2)(n+1)}$ is bounded by c_3/ϵ^{d+1} with

$$c_3(n, T, d) = (T+2)(2n+2)^d,$$

and the surface area of a single cube is equal to $2(d+1)\epsilon^d$. Thus for the surface area of $\partial\mathcal{N}_<^\epsilon$ we have the bound

$$|\partial\mathcal{N}_<^\epsilon| \leq \frac{2(d+1)c_3}{\epsilon} \quad (28)$$

and combining (27) and (28) we obtain that

$$\begin{aligned} \int_{\partial\mathcal{N}_<^\epsilon} |J^\psi| d\sigma &\leq \left(\sup_{\mathcal{N}_<^\epsilon} |J^\psi| \right) (|\partial\mathcal{N}_<^\epsilon|) \\ &\leq \frac{2(d+1)c_3}{\epsilon} ((c_1\eta\epsilon + c_2\epsilon^2)^2 + \mu(c_1\eta\epsilon + c_2\epsilon^2)(\eta + L\sqrt{d+1}\epsilon)) \\ &= O(\eta^2), \quad \epsilon \rightarrow 0. \end{aligned} \quad (29)$$

Consider next the set $\mathcal{N}_>^\epsilon$. On this set we can control the size of the nodal surface. To do this we use a further partition of configuration-space-time into cubes $(C^\gamma(k))_{k \in \mathbb{N}}$ of side length γ (with sides parallel to the sides of the C^ϵ -cubes). We choose γ so small that any C^γ -cube which contains or overlaps the interior of a C^ϵ -cube of $\mathcal{N}_>^\epsilon$ lies completely in $\mathcal{G}_{(-1, T+1)}^{(\delta/2)(n+1)}$, i.e., $\gamma < \min(\delta/(2\sqrt{d}) - \epsilon, (1/\sqrt{d}) - \epsilon)$. (γ will later be chosen to be proportional to η , and we shall take the limit $\epsilon \rightarrow 0$ for fixed η , so that $\gamma \gg \epsilon$ eventually.)

We show now that in each γ -cube the number of ϵ -cubes in $\mathcal{N}_>^\epsilon$ is small, at least compared with $(\frac{2}{\epsilon})^{d+1}$. Consider a γ -cube $C^\gamma(k)$ containing or overlapping the interior of a C^ϵ -cube of $\mathcal{N}_>^\epsilon$. Then there is a point $(q^*, t^*) \in \mathcal{N} \cap C_\epsilon^\gamma(k)$ with $|\psi'(q^*, t^*)| > \eta$, where $C_\epsilon^\gamma(k)$ is the “ ϵ -fattened” γ -cube, i.e., the cube of side $\gamma + 2\epsilon$ with the same center as $C^\gamma(k)$. That $|\psi'(q^*, t^*)| > \eta$ implies that

$$|\psi'_i(q^*, t^*)| > \frac{\eta}{\sqrt{2}}$$

for either $i = 1$ or $i = 2$ (or both), with $\psi_1 := \operatorname{Re} \psi$ and $\psi_2 := \operatorname{Im} \psi$.

Let e_k be that basis vector which is closest to the direction of $\psi'_i(q^*, t^*)$, i.e., for which $|e_k \cdot \psi'_i(q^*, t^*)|$ is maximal. Thus

$$|e_k \cdot \psi'_i(q^*, t^*)| > \frac{\eta}{\sqrt{2(d+1)}}$$

and hence we have that for all $(q, t) \in C_\epsilon^\gamma(k)$

$$|e_k \cdot \psi'_i(q, t)| > \frac{\eta}{\sqrt{2(d+1)}} - L\sqrt{d+1}(\gamma + 2\epsilon).$$

Now choose γ such that $L\sqrt{d+1}(\gamma + 2\epsilon) = \eta / (2\sqrt{2(d+1)})$, i.e., introduce $c_4 := 1 / (2L\sqrt{2(d+1)})$ and set $\gamma = c_4\eta - 2\epsilon$. Then for all $(q, t) \in C_\epsilon^\gamma(k)$

$$|e_k \cdot \psi'_i(q, t)| > \frac{\eta}{2\sqrt{2(d+1)}}. \quad (30)$$

Let x and y be two space-time points in $C_\epsilon^\gamma(k) \cap \mathcal{N}^\epsilon$ with $\psi(y) = 0$ and $x - y = le_k, l > 0$. Then, on the one hand, by the global bound K on $|\psi'|$ we have that

$$|\psi_i(x)| \leq K\sqrt{d+1}\epsilon.$$

On the other hand, it follows from (30) that $|\psi_i(x)| \geq l\eta / (2\sqrt{2(d+1)})$. Thus $l \leq 2K\sqrt{2(d+1)}\epsilon / \eta =: c_5\epsilon / \eta$. Therefore the number of ϵ -cubes in $\mathcal{N}_>^\epsilon$ contained in $C_\epsilon^\gamma(k)$ and lying in an e_k -column—the set of e_k -translates of an ϵ -cube—is bounded by $(c_5/\eta) + 1$. (This is a rather crude estimate. The number of such cubes is in fact bounded by $2d + \sqrt{d} + 2$, independent of η , as can easily be seen by controlling also the projection of ψ'_i orthogonal to e_k .)

Now the number of e_k -columns in $C_\epsilon^\gamma(k)$ is no greater than $[(\gamma/\epsilon) + 2]^d$, while the number of γ -cubes in $\mathcal{G}_{(-1, T+1)}^{(\delta/2)(n+1)}$ is bounded by c_3/γ^{d+1} . Thus we obtain a bound for the surface area of $\mathcal{N}_>^\epsilon$:

$$|\partial\mathcal{N}_>^\epsilon| \leq \left(\frac{c_5}{\eta} + 1\right) \left(\frac{c_4\eta}{\epsilon}\right)^d \frac{c_3}{(c_4\eta - 2\epsilon)^{d+1}} 2(d+1)\epsilon^d.$$

$|J^\psi|$ may be estimated (as in (27)) by invoking now the global bound K for $|\psi'|$ to yield

$$|J^\psi| \leq K^2(d+1)\epsilon^2 + \mu K^2\sqrt{d+1}\epsilon$$

on $\mathcal{N}_>^\epsilon$. Thus we arrive at the estimate

$$\begin{aligned} & \int_{\partial\mathcal{N}_>^\epsilon} |J| d\sigma & (31) \\ & \leq \left(\frac{c_5}{\eta} + 1\right) \left(\frac{c_4\eta}{\epsilon}\right)^d \frac{c_3}{(c_4\eta - 2\epsilon)^{d+1}} 2(d+1)\epsilon^d \left(K^2(d+1)\epsilon^2 + \mu K^2\sqrt{d+1}\epsilon\right) \end{aligned}$$

Using (29) and (31), by letting first $\epsilon \rightarrow 0$ and then $\eta \rightarrow 0$, it follows from (26) that $\lim_{\epsilon \rightarrow 0} \mathbf{N}(\epsilon, \delta, n) = 0$. \square

3.4 Remarks

3.4.1. It is an immediate consequence of continuous dependence on initial conditions for solutions of ODE's that the probabilistic negligibility of the set of "bad" initial values $\mathcal{B} := \{q_0 \in \mathcal{G}_0 : \tau(q_0) < \infty\}$, $\mathbf{P}(\mathcal{B}) = 0$, implies the negligibility of \mathcal{B} in the topological sense: \mathcal{B} is of first category in \mathcal{G}_0 , i.e., it is contained in a countable union of nowhere dense (in \mathcal{G}_0) sets. (Take $\mathcal{B}_t = \{q \in \mathcal{G}_0 : \tau(q) \leq t\}$; cf. also [34].) In other words: Global existence of Bohmian mechanics is typical and generic.

3.4.2. Since \mathbf{P} is equivalent to the Lebesgue measure \mathbf{L} on \mathcal{G}_0 , we have also that $\mathbf{L}(\mathcal{B}) = 0$ and we thus have the global existence and uniqueness of Bohmian mechanics \mathbf{L} -a.s. on \mathcal{G}_0 .

3.4.3. The flux argument shows that any given hypersurface in $\Omega \times \mathbb{R}$ (where ψ is C^∞) of codimension greater than 1 will (almost surely) not be reached.

3.4.4. We have shown that under certain conditions on the initial wave function and the Hamiltonian, particle trajectories exist as solutions of (2) globally in time for \mathbf{P} -almost all initial conditions. In the introduction we have already given an example showing that in general (i.e., assuming merely the conditions of Theorem 3.1 or Corollary 3.2) this result does not hold for *all* initial configurations. However, in that example the dynamics is uniquely extendible to a global dynamics $Q : \mathbb{R}^2 \rightarrow \mathbb{R}$, $(q, t) \mapsto Q_t(q)$. There are 3 continuous trajectories which

periodically run into nodes of the wave function, while the other trajectories are global solutions of (2). This extended dynamics $Q_t(q)$ is continuous.

However, if the trajectory running through the node at $t = 0$, $q = 1$ is analyzed, one finds that locally $Q_t(1) \sim \sqrt[3]{\frac{3}{4}t^2} + 1$, i.e., the map $Q_t(q)$ is not differentiable with respect to t at $t = 0$ for fixed $q = 1$. This may, for example, be seen by considering the flux through $q = 1$ for t near 0, or, what amounts to the same thing, by employing the Formula (41) (see Section 4) expressing the trajectories as curves of constant value of the function $F(q, t) = \int_{-\infty}^q |\psi_t|^2 dx$. (This behavior of trajectories hitting nodes is in fact typical—though it does not occur in the example for the trajectory at the origin; in fact, if $\psi(q, t^*)$ has a node of order k at q^* , $\psi(q, t^*) \sim \alpha x^k$ with $x = q - q^*$, then $F(q, t^*) \sim F(q^*, t^*) + ax^{2k+1}$, $a = \frac{|\alpha|^2}{2k+1}$, and $\frac{\partial F}{\partial t}(q, t^*) = -j^{\psi_{t^*}}(q) \sim bx^{2k}$, so that $F(q, t) \sim F(q^*, t^*) + ax^{2k+1} + bx^{2k}s + cs^2$, $s = t - t^*$, in the vicinity of the node. Thus for $c \neq 0$, the equation $F(q, t) = F(q^*, t^*)$ implies that $x \sim \sqrt[2k+1]{-\frac{c}{a}s^2}$.)

Concerning the regularity of $Q_t(q)$ in q at fixed t , one sees in the example that for suitable choices of initial time the solution map will fail to be differentiable at $q = 0$ (where there will be a fifth root singularity) or at $q = \pm 1$ (where there will be a cube root singularity) as a function of q for fixed t .

For an even stronger breakdown of regularity in q for fixed t , consider the harmonic oscillator in 3 dimensions, and take the $(n = 1, l = 1)$ -state $\psi(q, t) = r e^{-(r^2+z^2)/2} e^{i\phi} e^{-5it/2}$ in cylindrical coordinates. This wave function vanishes only at $r = 0$, i.e., on the z -axis. Particles circle around the z -axis with angular velocity $1/r^2$. The map Q is uniquely extendable to a global dynamics given by a continuous map, which is however not differentiable with respect to q , by defining $Q_t(q_0) = q_0$ for all t and $q_0 \in \mathcal{N}_0$.

It is possible also to give an example in which the extended map must fail even to be continuous with respect to q for fixed t : Consider free motion in 1 dimension, and let the wave function ψ be even, (real and positive), C^∞ , and supported on $[-b, -a] \cup [a, b]$ with $0 < a < b < \infty$. Then $\psi \in C^\infty(H_0)$. Moreover, there is a $t_1 > 0$ such that $(e^{iH_0 t_1/\hbar} \psi)(0) \neq 0$. Let $\psi_0 = e^{iH_0 t_1/\hbar} \psi$. ψ_t is then even for all t , so that the velocity field is odd, i.e., symmetric under reflection. Any extension Q which respects this symmetry must have $Q_t(0) = 0$ for all t . Then the map Q is discontinuous in q for $t = t_1$, and, in fact, any extension must have this discontinuity.

3.4.5. It is well known—at least if V is real analytic in Ω (see for example [30], page 98)—that if ψ vanishes on a nonempty (bounded) open set in configuration-space-time, it vanishes everywhere (in the components of $\Omega \times \mathbb{R}$ that intersect this set). We remark that under the hypotheses of Corollary 3.2, the same conclusion would in fact obtain merely if ψ were to vanish everywhere on the boundary of such a set (and even with the possible exception of a single piece of the boundary contained in a constant-time hyperplane), since it would then follow from global existence and the inaccessibility of the nodes that ψ must vanish everywhere in this set.

3.4.6. The probability of reaching the nodes $\mathbf{P}(x \in (\partial\mathcal{N}^\epsilon \cap \mathcal{G}_{(0,T)}^{\delta n}))$ may also be estimated without using flux integrals. We include this argument, which involves a choice for \mathcal{N}^ϵ different from the one used earlier. We remark that for the new \mathcal{N}^ϵ we can see no reason why $\partial\mathcal{N}^\epsilon$ must be smooth, even piece-wise. Notice also that Lemma 3.6 involves both stronger premises and, since the convergence in it is uniform, a stronger conclusion than the corresponding Lemma 3.5.

Lemma 3.6 *Assume A1–A4 and, for $\epsilon > 0$, let*

$$\mathcal{N}^\epsilon := \{(q, t) \in \Omega \times \mathbb{R} : |\psi_t(q)| \leq \epsilon\}. \quad (32)$$

Then, uniformly in δ and n , with $x := (Q_{\min(\tau^{\epsilon\delta n}, T)}, \min(\tau^{\epsilon\delta n}, T))$,

$$\lim_{\epsilon \rightarrow 0} \mathbf{P}(\{q_0 \in \mathcal{G}_0^{\epsilon\delta n} : x \in (\partial\mathcal{N}^\epsilon \cap \mathcal{G}_{(0,T)}^{\delta n})\}) = 0.$$

The proof involves a fairly standard “existence of dynamics” argument and is analogous to that of Nelson [28] for the similar problem in stochastic mechanics: One looks for an “energy” function on the state space of the motion which becomes infinite on the catastrophic event. With good a priori bounds on the expectation value of that function, one can control the probability of catastrophic events.

Proof. The function which recommends itself here is $\log |\psi|$, i.e., what we control is the “entropy.”

We first present a formal estimate, disregarding the problem that the solution curve $Q_t(q)$ starting at q may not exist for all times—which is taken care of below.

Let \mathbf{E} denote the expectation with respect to \mathbf{P} . We compute for arbitrary T :

$$\begin{aligned} & \mathbf{E} (|\log |\psi_T(Q_T)| - \log |\psi_0| |) = \mathbf{E} \left(\left| \int_0^T \frac{d}{dt} \log |\psi_t(Q_t)| dt \right| \right) \\ &= \mathbf{E} \left(\left| \int_0^T \left(\frac{1}{2} \frac{1}{|\psi_t(Q_t)|^2} \frac{\partial |\psi_t(Q_t)|^2}{\partial t} + \frac{(\nabla |\psi_t|)(Q_t)}{|\psi_t(Q_t)|} \cdot v^{\psi_t}(Q_t) \right) dt \right| \right) \leq \\ & \int_0^T \mathbf{E} \left(\frac{1}{2} \frac{1}{|\psi_t(Q_t)|^2} \left| \frac{\partial |\psi_t(Q_t)|^2}{\partial t} \right| \right) dt + \int_0^T \mathbf{E} \left(\mu \frac{|\nabla \psi_t(Q_t)|^2}{|\psi_t(Q_t)|^2} \right) dt, \end{aligned} \quad (33)$$

where we used for the inequality the bounds

$$\nabla |\psi| \leq |\nabla \psi| \quad \text{and} \quad |v^\psi| \leq \mu \left| \frac{\nabla \psi}{\psi} \right| \quad (34)$$

Now use the equivariance of $|\psi|^2$ (cf. (5)) to compute the expectation $\mathbf{E}(f_t(Q_t)) = \int_\Omega |\psi_t(q)|^2 (f_t(q)) dq$ and obtain that the right hand side of (33) is equal to

$$\int_0^T \int_\Omega \frac{1}{2} \left| \frac{\partial |\psi_t(q)|^2}{\partial t} \right| dq dt + \mu \int_0^T \int_\Omega |\nabla \psi_t(q)|^2 dq dt. \quad (35)$$

By virtue of (9) we replace $|\partial |\psi_t(q)|^2 / \partial t|$ by $|\psi_t^*(q) H \psi_t(q) - \psi_t(q) H \psi_t^*(q)| / \hbar$. By Schwarz's inequality, the first term of (35) is then bounded by

$$\frac{1}{\hbar} \int_0^T \|\psi_t\| \|H \psi_t\| dt = \frac{T}{\hbar} \|H \psi_0\| < \infty,$$

and the second term is bounded for each $T < \infty$ by Assumption A4.

To construct from this a rigorous proof we need only define a suitable killed process. For $t \geq 0$ we define $Q_t^{\epsilon \delta n} : \mathcal{G}_0^{\epsilon \delta n} \cup \{\dagger\} \longrightarrow \mathcal{G}_t^{\epsilon \delta n} \cup \{\dagger\}$ by

$$Q_t^{\epsilon \delta n}(q) := \begin{cases} Q_t(q) & \text{for } t \leq \tau^{\epsilon \delta n}(q) \\ \dagger & \text{for } t > \tau^{\epsilon \delta n}(q) \end{cases} \quad (36)$$

For completeness, we set $Q_t^{\epsilon \delta n}(\dagger) = \dagger$ for all $t \geq 0$. Consider the probability measure $P_0^{\epsilon \delta n}$ on $\mathcal{G}_0^{\epsilon \delta n} \cup \{\dagger\}$ which has the density

$$\rho_0^{\epsilon \delta n}(q) := |\psi_0(q)|^2 \text{ for } q \in \mathcal{G}_0^{\epsilon \delta n}$$

(and, of course, $P_0^{\epsilon \delta n}(\dagger) = 1 - \int_{\mathcal{G}_0^{\epsilon \delta n}} \rho_0^{\epsilon \delta n}(q) dq$). The image measure of the process $Q_t^{\epsilon \delta n}$ is denoted by $P_t^{\epsilon \delta n} := P_0^{\epsilon \delta n} \circ (Q_t^{\epsilon \delta n})^{-1}$ and has the density $\rho_t^{\epsilon \delta n}$ on $\mathcal{G}_t^{\epsilon \delta n}$. From the definition of \mathcal{N}^ϵ (32),

$$\{q_0 \in \mathcal{G}_0^{\epsilon \delta n} : x \in (\partial \mathcal{N}^\epsilon \cap \mathcal{G}_{(0,T)}^{\delta n})\} \subset \{q_0 \in \mathcal{G}_0^{\epsilon \delta n} : |\psi(x)| = \epsilon\}. \quad (37)$$

Since we keep δ and n fixed, and since the estimates are independent of δ and n , we will omit the indices δ and n on $Q^{\epsilon\delta n}, \mathcal{G}^{\epsilon\delta n}, \rho^{\epsilon\delta n}$.

Define for $q \in \mathcal{G}_0^\epsilon$ and $t \geq 0$

$$D_t^\epsilon(q) := \log |\psi_{\min(\tau^\epsilon(q), t)}(Q_{\min(\tau^\epsilon(q), t)}(q))| - \log |\psi_0(q)|.$$

One has that

$$D_T^\epsilon(q) = \int_0^T \frac{\partial}{\partial t} D_t^\epsilon(q) dt = \int_0^T f_t \circ Q_t^\epsilon(q) dt,$$

where

$$f_t(y) := \begin{cases} 0 & \text{for } y = \dagger \\ \frac{1}{2} \frac{1}{|\psi_t(y)|^2} \frac{\partial |\psi_t(y)|^2}{\partial t} + \frac{|\nabla |\psi_t(y)||}{|\psi_t(y)|} \cdot v^{\psi_t}(y) & \text{for } y \in \mathcal{G}_t^\epsilon \end{cases}$$

We shall show that uniformly in ϵ

$$\mathbf{P}(\{q \in \mathcal{G}_0^\epsilon : |D_T^\epsilon(q)| > K\}) \rightarrow 0 \text{ as } K \rightarrow \infty. \quad (38)$$

Then, since for q_0 as in (37) $D_T^\epsilon(q_0) = \log \epsilon - \log |\psi_0(q_0)|$, the lemma follows from (38) by observing that

$$\mathbf{P}(\{q \in \mathcal{G}_0^\epsilon : |\log |\psi_0(q)|| > K\}) \rightarrow 0 \text{ as } K \rightarrow \infty$$

holds uniformly in ϵ , which is immediate since the density of \mathbf{P} is $|\psi_0|^2$.

By Markov's inequality we obtain that

$$\mathbf{P}(\{q \in \mathcal{G}_0^\epsilon : |D_T^\epsilon(q)| > K\}) \leq \frac{1}{K} \mathbf{E} \left(\mathbb{1}_{\mathcal{G}_0^\epsilon} \left| \int_0^T f_t \circ Q_t^\epsilon dt \right| \right). \quad (39)$$

Recall now that $\mathbf{P} = P_0^\epsilon$ on \mathcal{G}_0^ϵ , and that $f_t = 0$ at \dagger . Then by the definition of ρ_t^ϵ as the density of the image measure of Q_t^ϵ one obtains that the right hand side of (39) is bounded by

$$\frac{1}{K} \int_0^T \int_{\mathcal{G}_t^\epsilon} \rho_t^\epsilon(q) |f_t(q)| dq dt$$

Using the bounds (19) (with ρ_t replaced by ρ_t^ϵ) and (34) (which holds on \mathcal{G}_t^ϵ) we finally obtain that

$$\mathbf{P}(\{q \in \mathcal{G}_0^\epsilon : |D_T^\epsilon(q)| > K\}) \leq \frac{1}{K} \left(\int_0^T \int_\Omega \frac{1}{2} \left| \frac{\partial |\psi_t(q)|^2}{\partial t} \right| dq dt + \mu \int_0^T \int_\Omega |\nabla \psi_t(q)|^2 dq dt \right). \quad (40)$$

The bracket on the r.h.s. is (35). By the Assumptions A3 and A4, (35) is finite and hence the r.h.s. of (40) goes to zero uniformly in ϵ as $K \rightarrow \infty$. Thus we have established Lemma 3.6. \square

4 Bohmian mechanics and self-adjointness

4.1. In this subsection we shall discuss the necessity of certain assumptions under which we have established global existence of the Bohmian particle motion (cf. Theorem 3.1 and Corollary 3.2). We shall investigate in particular the assumptions concerning self-adjointness of the Hamiltonian.

By Corollary 3.2 we obtain global existence if the Hamiltonian is the *form sum* $H_0 + V$, and if the potential V satisfies certain conditions leading in particular to the Hamiltonian's being bounded from below. These conditions on the Hamiltonian guarantee in particular that Assumption A4 of Theorem 3.1 is satisfied. In the case of one particle moving on the half line $\Omega = (0, \infty)$, we shall prove, without invoking A4, global existence for a certain class of potentials for arbitrary self-adjoint extensions, which furthermore may be unbounded below.

Theorem 4.1 *Let $\Omega = (0, \infty)$, $\mathcal{H} = L^2(\Omega)$, and suppose $V \in C^\infty(\Omega)$ is such that $H_0 + V$ is in the limit point case at infinity (see for example [37]). Let H be an arbitrary self-adjoint extension of $(H_0 + V)|_{C_0^\infty(\Omega)}$, and let $\psi_0 \in C^\infty(H)$ with $\|\psi_0\| = 1$. Then $\mathbf{P}(\tau < \infty) = 0$.*

It follows for example from Theorem X.8 in [32] that if $V(r) \geq -kr^2$ for $r > c$ with $c, k \geq 0$, then $H_0 + V$ is in the limit point case at infinity.

Consider as an example the potential $V(q) = -c/q^2$ with $c > 0$ large enough: The Hamiltonian $H = H_0 + V$ is in the limit circle case at 0, in the limit point case at infinity, and unbounded above and below (cf. for example [32]). Thus by Weyl's limit point-limit circle criterion there is a one-parameter family of (similarly unbounded) self-adjoint extensions of $H|_{C_0^\infty(\Omega)}$ for all of which, by Theorem 4.1, Bohmian mechanics exists uniquely and globally for \mathbf{P} -almost all initial values.

The proof employs a new definition of the particle dynamics in one dimension which extends the solution to (2) and is interesting in its own right. (In fact, this definition extends the Bohm motion, defined by (1) and (2), to an equivariant motion for all $\psi \in L^2$!) Let $Q_t(q_0)$ be defined implicitly by

$$\int_{-\infty}^{Q_t(q_0)} |\psi_t(q)|^2 dq = \int_{-\infty}^{q_0} |\psi_0(q)|^2 dq.$$

$Q_t(q_0)$ is well-defined if

$$F(q, t) := \int_{-\infty}^q |\psi_t|^2 dx$$

is strictly monotonic in q . This is the case except at extended intervals with $\psi_t = 0$, where $F(\cdot, t)$ has a plateau. To define $Q_t(q_0)$ globally for $q_0 \in \mathbb{R}$, set for example

$$Q_t(q_0) := \min\{q : F(q, t) = F(q_0, 0)\} \quad (41)$$

(and $Q_t(q_0) = -\infty$ if $F(q_0, 0) = 0$, $Q_t(q_0) = \infty$ if $F(q_0, 0) = 1$).

Proof. From Lemma 6.1 we obtain that $\psi \in C^\infty(\Omega \times \mathbb{R})$. Therefore, using the continuity of the scalar product and the L^2 -differentiability of $t \mapsto \psi_t$,

$$F(q, t) = \int_0^q |\psi_t|^2 dx = (\mathbb{1}_{[0, q]} \psi_t, \psi_t)$$

(where (\cdot, \cdot) denotes the scalar product in $\mathcal{H} = L^2(\Omega)$) is jointly continuous and differentiable. Clearly $F(0, t) = 0$, $\lim_{q \rightarrow \infty} F(q, t) = 1$, and $\partial F / \partial q = |\psi_t(q)|^2$. Moreover,

$$\frac{\partial F(q, t)}{\partial t} = \int_0^q \frac{\partial |\psi_t|^2}{\partial t} dx = -j_t(q) + \lim_{c \rightarrow 0} j_t(c) = -j_t(q).$$

Here the existence of $\lim_{c \rightarrow 0} j_t(c)$ follows for $\psi \in C^\infty(H)$ from partial integration of $\int_c^d (\psi^*(H\psi) - (H\psi^*)\psi) dx$ and Schwarz's inequality; the value 0 for $\lim_{c \rightarrow 0} j_t(c) = 0$ follows from the symmetry of H together with the fact that $\lim_{d \rightarrow \infty} j_t(d) = 0$, which holds because H is in the limit point case at infinity. (See for example [37].)

For all t and all $q_0 \in \mathcal{G}_0 = \Omega \setminus \mathcal{N}_0$, let $Q_t(q_0)$ be defined by (41). It follows from the implicit function theorem that $t \mapsto Q_t(q_0)$ is continuous and differentiable for (q_0, t) such that $\psi_t(Q_t(q_0)) \neq 0$, with $dQ_t/dt = j(Q_t)/|\psi_t(Q_t)|^2 = v^{\psi_t}(Q_t)$, i.e., Q_t solves the differential equation (2) on $\mathcal{G} = (\Omega \times \mathbb{R}) \setminus \mathcal{N}$. It remains to show that for \mathbf{P} -almost all initial q_0 , $\tau(q_0) = \sup\{s > 0 : Q_t(q_0) \in \mathcal{G} \text{ for all } t \leq s\}$ is infinite, i.e., (2) has global solutions for almost all initial values.

Now it is obvious from this definition that $Q_t(q_0) \in \Omega$ for all t and all $q_0 \in \mathcal{G}_0$. ($Q_t(q_0) = 0$ corresponds to $F(q_0, 0) = 0$, $Q_t(q_0) = \infty$ to $F(q_0, 0) = 1$, and for $q_0 \in \mathcal{G}_0$, $F(q_0, 0) \in (0, 1)$.) Moreover, by the L^2 -continuity of $t \rightarrow \psi_t$, we have that for $0 < T < \infty$ and $q_0 \in \mathcal{G}_0$, $\inf_{0 \leq t \leq T} Q_t(q_0) > 0$ and $\sup_{0 \leq t \leq T} Q_t(q_0) < \infty$, i.e., the trajectories cannot run into the (only) possible singularity of the potential $\mathcal{S} = \{0\}$ or to infinity in finite time. Thus it remains only to control the probability of hitting \mathcal{N} , for which Lemma 3.5 does the job. We omit the details. \square

4.2. One might now wonder whether we have global existence of Bohmian mechanics for any self-adjoint Schrödinger Hamiltonian (without assuming A4). This is quite trivially wrong, as is easily seen by considering free motion on the interval $\Omega = (0, 1)$. There are self-adjoint extensions of $H_0|_{C_0^\infty(\Omega)}$ with $j(0) = j(1) \neq 0$. (Similarly one might consider potentials on $\Omega = (0, \infty)$ such that $H_0 + V$ is in the limit circle case at infinity.) This corresponds to an incoming flow at 0, balanced by an outgoing flow at 1 (or the other way round) so that the total probability is conserved (a situation which can of course be identified with a motion on a circle). Typically, the particle will reach the boundary of Ω , so that almost sure global existence in the sense of solutions of the differential equation (2) fails. However, the motion is quite trivially extendible in such a way that the trajectories are piecewise solutions of the differential equation: when the boundary of Ω is reached they jump to the other end of Ω . $|\psi|^2$ then remains an equivariant measure. This motion can be described by replacing (41) by

$$Q_t(q_0) := \min\{q : \tilde{F}(q, t) = \tilde{F}(q_0, 0)\}$$

with

$$\tilde{F}(q, t) = \left(F(q, t) - \int_0^t j_s(0) ds \right) \pmod{1}$$

[Another possibility to define a global motion in this case is to use the unmodified (41). This provides then an example of a deterministic dynamics completely different from (and not an extension of) the Bohmian dynamics, ((2) is replaced by the nonlocal form $dQ/dt = (j^\psi - j_t(0))/|\psi|^2$) for which, however, $|\psi|^2$ remains equivariant. With this motion, particles do not jump from 1 to 0 or the other way round. (However, they might all run through nodes!)]

In fact, we expect generally that self-adjointness guarantees (possibly discontinuous) extendibility of the Bohmian motion in such a way that $|\psi|^2$ is an equivariant measure. This is suggested by the fact that the symmetry of the Hamiltonian leads to

$$\lim_{\delta \rightarrow 0, n \rightarrow \infty} \left(\int_{\partial S^\delta \cap \mathcal{K}^n} (j^{\psi_t}(q) \cdot u) ds + \int_{\partial \mathcal{K}^n \setminus S^\delta} (j^{\psi_t}(q) \cdot u) ds \right) = 0,$$

using integration by parts (Green's identity)

$$\int_M \psi^*(H\psi) dq - \int_M (H\psi^*)\psi dq = -i\hbar \int_{\partial M} (j^\psi \cdot u) ds,$$

for $M = \mathcal{K}^n \setminus \mathcal{S}^\delta$. The vanishing of the integrals over the *absolute* flux yields global existence of Bohmian mechanics: In finite time the singularities and infinity are not reached. The flux balance from self-adjointness alone suggests extendibility of the motion: Some parts of the singularities (or infinity) may act as sources, others as sinks.

4.3. For a wider perspective on this matter let us consider a Schrödinger Hamiltonian H on a domain where it is not (essentially) self-adjoint, i.e., where the boundary conditions are too few or too weak. Then, first of all, the time evolution of wave functions is not unique: There are infinitely many different unitary evolutions (corresponding to the different self-adjoint extensions), and there are also semi-groups for which $\|\psi_t\|$ is not conserved. The (essential) self-adjointness of H is equivalent to $\text{Ker}(H^* \pm i) = \{0\}$, so that if H is considered on a domain where it is symmetric but not self-adjoint, then H^* has imaginary eigenvalues. Together with the (space) regularity for eigenstates of the elliptic operator H^* (assuming sufficient regularity for the potential V) we thus obtain classical solutions of Schrödinger’s equation with exponentially decreasing or increasing norm. Since $\rho = |\psi|^2$ still holds on \mathcal{I} (cf. the paragraph around Equation (19)), those solutions lead with positive probability to catastrophic events.

This possibility is not that far-fetched: The Hamiltonian for one particle in a Coulomb field $V(r) = -1/r$ considered on the “natural” domain $C_0^\infty(\mathbb{R}^3 \setminus \{0\})$ is not essentially self-adjoint and hence the time evolution of the wave function is not uniquely defined [22, 19]. There are many properties that mathematically distinguish the self-adjoint extension usually regarded as “the Coulomb Hamiltonian” from other possible extensions. However, we do not know of any convincing (a priori) physical argument for “the Coulomb Hamiltonian” unless one accepts, for example, that the Coulomb potential is a “small perturbation” of the free Hamiltonian [20], or that “in reality the singularity is smeared out.” Of course, if we require that Bohmian mechanics be globally existing, then, as we have argued above, only self-adjoint extensions are possible. But among all self-adjoint extensions Bohmian mechanics seems not to discriminate: While our Corollary 3.2 applies only to the form sum (which is “the Coulomb Hamiltonian”), it is heuristically rather clear (or at least plausible) that Bohmian mechanics should exist globally and uniquely for all the other self-adjoint extensions of $H|_{C_0^\infty(\mathbb{R}^3 \setminus \{0\})}$

as well.⁹

Nonetheless, discussions about the “right” (unitary or contractive) evolution, i.e., about the “right” boundary conditions, as for example in the case of strongly singular potentials like the $1/r^2$ potential (see [10, 23, 27]), do gain now firm ground by taking into account the actual behavior of the particles: Whether or not we should consider the Bohmian particle to be caught at the origin is a matter of the physics we wish to describe: whether or not particles disappear in the nucleus. An axiom, or dogma, of self-adjointness of the Hamiltonian (or equivalently of unitarity of the wave function evolution) appears quite inappropriate from a Bohmian perspective—even though the importance of self-adjointness is profoundly illuminated by this perspective!

Moreover, the particle picture of Bohmian mechanics naturally yields an interpretation of the current j as a current of particles moving in accordance with the density $|\psi|^2$. In this way, boundary conditions for self-adjointness of the form $j = 0$ at the singularities or $j(in) = j(out)$ may be viewed as “arising from Bohmian mechanics.” For example, the outcome of a detailed analysis of self-adjoint extensions of H_0 on the half line $(0, \infty)$ —there is a one parameter family of self-adjoint extensions H_0^a , the respective domains being defined by $\psi'(0)/\psi(0) = a$, a real, or $\psi(0) = 0$ ($a = \infty$)—is easily guessed from the point of view of Bohmian mechanics by demanding that either $v^\psi(0) = 0$, i.e., $\text{Im}(\psi'(0)/\psi(0)) = 0$, or that $|\psi(0)|^2 = 0$.

4.4. We wish to conclude with some remarks on the general Hilbert space description of orthodox quantum theory viewed from the perspective of Bohmian mechanics. We have discussed the fact that Bohmian mechanics is well defined, i.e., trajectories exist globally and uniquely, for typical initial values and for wave functions which are C^∞ -vectors of the self-adjoint Hamiltonian H . The set

⁹The singularity of the radial current at 0 may be estimated for $\psi = \sum_{l,m} f_{lm}(r)Y_{lm}(\theta, \phi) \in \bigoplus_{l=0}^{\infty} \mathcal{D}(H_{r,l}) \otimes K_l$, where, for angular momentum l , $H_{r,l}$ is the radial part of H and K_l is the corresponding eigenspace of the angular part of $-\frac{\hbar^2}{2m}\Delta$, as follows: $H_{r,l}f_{lm} \in L^2(\mathbb{R}^+, r^2 dr)$ implies for the worst behavior of f_{lm} as $r \rightarrow 0$ that $f_{lm} \sim r^\alpha$ with $\alpha > 1/2$ for $l \geq 1$ resp. $\alpha = -1$ for $l = 0$. Therefore the worst behavior of the radial current $j_r^\psi = \frac{\hbar}{m} \text{Im}\left(\psi^* \frac{\partial \psi}{\partial r}\right)$ as $r \rightarrow 0$ is $j_r^\psi \sim r^{-(3/2)+\epsilon}$ (using the fact that the radial current at 0 vanishes on $\mathcal{D}(H_{r,0})$ for all self-adjoint extensions, cf. the proof of Theorem 4.1). Thus we should have that $\int_{\mathcal{K}^r} |j^\psi \cdot u| ds = \int_{S^2} |j_r^\psi| r^2 d\omega \sim r^{(1/2)+\epsilon} \rightarrow 0$ as $r \rightarrow 0$. For a proof of global existence along the lines of Theorem 3.1, it is necessary also to control the time change of the radial current. However, the global existence for the one-dimensional problem (Theorem 4.1) suggests that this should be possible.

$C^\infty(H)$ is dense and invariant; however, it is most likely not a residual in the norm topology of the Hilbert space $L^2(\Omega)$, i.e., it is presumably not a “generic” set, and it furthermore depends on the Hamiltonian. One might now wonder how Bohmian mechanics can be taken as the basis for the quantum formalism (as has been claimed—see [11]) if the former cannot even be defined for a really “fat” set of wave functions. And since, as we have seen, Bohmian mechanics yields a natural understanding of the (spirit of the) meaning of the self-adjointness of a Schrödinger Hamiltonian, the question should be even more puzzling. The answer is, of course, that the embedding of Bohmian mechanics into a Hilbert space structure is a natural but purely mathematical device. Indeed this answer is (of course, in disguise) commonly accepted—though maybe not as loudly stated: No physicist believes that a generic L^2 -wave function (in the residual sense) results as the “collapsed” wave function from a preparation procedure. The state space of physical wave functions ψ is not the Hilbert space $\mathcal{H} = L^2(\Omega)$ but more or less the space of classical, smooth solutions of Schrödinger’s equation, for the analysis of which the L^2 -norm and hence the Hilbert space structure is of critical importance.

Other aspects of this embedding are commonly taken more seriously: for example, that observables are self-adjoint operators on \mathcal{H} . While we do not wish here to enter into a general discussion of this question (see [11]), we would like once again to comment on the self-adjointness of the Hamiltonian H . The importance of this property is certainly not that “measured energy values must be real” but lies rather in Stone’s theorem: H acts as the generator of a one-parameter unitary group U_t , which gives the time evolution of states $\psi_t = U_t\psi_0$ (or of observables $A_t = U_t^{-1}AU_t$), and hence must be self-adjoint by Stone’s theorem. Why should the time evolution be unitary? Simply because the norm $\|\psi_t\|$ must be invariant, so that the total probability is conserved.

We conclude with some remarks about effective descriptions. We first note that restrictions of configuration space such as described in the last paragraph of Section 4.3 (with a freedom in the boundary condition) are perhaps best understood physically as arising as a limit of a sequence of (moderately realistic) potentials V_n^a tending to “ $V = 0$ for $q > 0$, $V = \infty$ for $q < 0$ ” in a suitable way—such that $H_0 + V_n^a \rightarrow H_0^a$ in an appropriate sense. This problem is analyzed in [35, 1, 5], and in [5] the convergence of the Bohmian trajectories in this limit is derived.

In other physically interesting but complex situations we may have an effective description involving a Hamiltonian which is self-adjoint but not of Schrödinger-

type,¹⁰ so that the probability current j may fail to be of the usual form [cf. Eq. (8)], or where there may in fact be no local conservation law at all for the probability density $|\psi|^2$.

For an example with nonstandard current j , consider the self-adjoint shift operator $H_c = -i\hbar c\nabla$, where c is a constant with the dimension of a velocity. $\psi_t(q) = e^{-itH_c/\hbar}\psi_0(q) = \psi_0(q - ct)$ describes translation without “spreading.” This Hamiltonian may perhaps arise in a limit in which the spreading of the wave function, induced by the Laplacian, can be neglected. In any case, the corresponding current is $j_c = c|\psi|^2$, and the obvious candidate for the “Bohm motion” in this case is $v = j_c/\rho = c$, not (1).

It is conceivable that an approximation procedure leading to an effective Hamiltonian like H_c , when applied to Bohmian mechanics, also converges to a deterministic limit. If so, then $v^\psi = c$ would be the natural guess for the motion in this limit.

For a Hamiltonian with no local conservation law for probability there is of course no “Bohm motion” generalizing (1).

5 Acknowledgements

During this work, we profited from discussions with many colleagues. In particular, we wish to acknowledge helpful discussions with Lara Beraha, Martin Daumer, Joseph Gerver, John Mather, Markus Schneider, Eugene Speer, Avy Soffer, Herbert Spohn, Francois Treves, and Jürgen Weckler. This work was supported by the DFG, by NSF Grant No. DMS-9305930, and by the INFN.

6 Appendix: On the regularity of ψ

Lemma 6.1 *Assume A1–A3, and let $\psi_t(q) = e^{-itH/\hbar}\psi_0(q)$. Then there exists a function $\tilde{\psi} \in C^\infty(\Omega \times \mathbb{R})$ such that for all $t \in \mathbb{R}$ $\tilde{\psi}(q, t) = \psi_t(q)$ for almost all q . ($\tilde{\psi}$ is a classical solution of Schrödinger’s equation.)*

This fact is presumably folklore knowledge to experts in PDE’s, but since we could find no suitable reference—and since it does not appear to be well

¹⁰The modeling of physical situations leads often to idealizations which are very singular. In Newtonian mechanics one considers for example singular evolutions induced by “hard walls” confining a particle or by elastic collision between hard spheres.

known among mathematical physicists—we shall supply a proof. (Hunziker [18] has established space-time regularity of ψ for potentials which are bounded, have bounded derivatives, and are C^∞ on \mathbb{R}^d for ψ_0 in Schwartz space. Also, regularity (in space) of eigenfunctions (for sufficiently regular potentials) is well known [32].)

Proof. We apply standard methods of elliptic regularity (see, for example, [33]) to the elliptic operator L on $\Omega \times \mathbb{R}$

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

From A3, $\psi_t \in C^\infty(H)$, and therefore the functions $\phi_{n,t} := H^n \psi_t (= e^{-itH/\hbar} \phi_{n,0})$ are in $L^2(\Omega)$ for all n and t . With this definition, formally

$$L\psi = \phi_2 + \phi_1, \quad \text{and} \quad L\phi_n = \phi_{n+2} + \phi_{n+1} \quad (42)$$

To apply the theorem of elliptic regularity, we need to show a) that ψ and ϕ_n are locally L^2 in $\Omega \times \mathbb{R}$, therefore locally in the Sobolev space W^0 (we refer to the definitions and theorems of [33], where however W^n is written H^n) in $\Omega \times \mathbb{R}$, and b) that (42) is satisfied in the distributional sense on $\Omega \times \mathbb{R}$. Then, by repeated use of Theorem 8.12 in [33] we obtain that ψ (and ϕ_n) are locally in W^n for all even (positive) integers n . Then by Sobolev's lemma ψ is indeed (almost everywhere equal to) a C^∞ -function on $\Omega \times \mathbb{R}$. (The space-time set of measure 0 on which ψ has to be corrected indeed splits into t -slices that are of measure 0 for all t . This is a consequence of L^2 -continuity of $t \mapsto \psi_t$.)

a) This is an easy consequence of Fubini's theorem if ψ and ϕ_n are jointly measurable in q, t . ψ_t is measurable in q ($\psi_t \in L^2(\Omega)$) and the map $t \mapsto \psi_t$ resp. $t \mapsto \phi_{n,t}$ is weakly measurable (indeed much more is true, namely strong differentiability). Then by a theorem of Bochner and von Neumann [6] joint measurability of $\psi_t(q)$ and $\phi_{n,t}(q)$ in (q, t) follows in the following sense: There exist functions $\tilde{\psi}$ and $\tilde{\phi}_n$ which are jointly measurable in q, t , and for all t $\tilde{\psi}(q, t) = \psi_t(q)$ and $\tilde{\phi}_n(q, t) = \phi_{n,t}(q)$ for almost all $q \in \Omega$. In the following, we shall denote $\tilde{\psi}(q, t)$ and $\tilde{\phi}_n(q, t)$ by $\psi(q, t)$ and $\phi_n(q, t)$ or again by $\psi_t(q)$ and $\phi_{n,t}$, as convenient.

b) First one convinces oneself that ψ and ϕ_n satisfy Schrödinger's equation in the distributional sense, i.e., for all test functions $f \in C_0^\infty(\Omega \times \mathbb{R})$,

$$-i\hbar \int \left(\frac{\partial}{\partial t} f \right) \psi \, dq \, dt = \int (Hf) \psi \, dq \, dt.$$

This follows by looking at the function $G : \mathbb{R} \rightarrow \mathbb{R}, t \mapsto \int f(q, t)\psi(q, t)dq = (f_t^*, \psi_t)$, where (\cdot, \cdot) denotes the scalar product in $L^2(\Omega)$. G has compact support, and its derivative is seen to be

$$\frac{dG(t)}{dt} = \frac{1}{i\hbar}(f_t^*, H\psi_t) + \left(\frac{\partial f_t^*}{\partial t}, \psi_t\right)$$

by the continuity of the scalar product (\cdot, \cdot) and the weak (in $L^2(\Omega)$) differentiability of ψ_t . The same holds with ψ replaced by ϕ_n for all n . Since furthermore $f_t \in \mathcal{D}(H)$ for all t , and therefore $(f_t^*, H\psi_t) = (Hf_t^*, \psi_t)$, ψ and ϕ_n are indeed weak solutions of Schrödinger's equation (and the self-adjoint operator H on $\mathcal{D}(H)$ agrees with the operator on distributions defined by H), i.e., we've arrived at

$$i\hbar \frac{\partial \psi}{\partial t} = H\psi = \phi_1 \quad \text{and} \quad i\hbar \frac{\partial \phi_n}{\partial t} = H\phi_n = \phi_{n+1}$$

weakly, and therefore (42) indeed holds in the distributional sense (on $\Omega \times \mathbb{R}$). \square

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