Semiclassical Quantum Dynamics and Bohmian Trajectories

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The early days of the twentieth century saw the establishment of quantum mechanics as a novel description of our physical world. Ever since its invention, a basic problem concerns the connection between quantum mechanics and the older, well-understood theory of classical mechanics. It was accepted early on that classical mechanics should be understood as an emergent phenomenon of quantum mechanics, i.e., it should be recovered from the underlying quantum mechanical description when considered over special values of its physical parameters. When trying to follow this basic idea, one immediately faces an obstacle: quantum mechanics and classical mechanics are usually treated within two entirely different mathematical formalisms. While the former is based on the time-evolution of vectors in (infinite-dimensional) Hilbert spaces, the latter is concerned with the dynamics of point particles on a (finite-dimensional) phase space.

Focussing on one of the simplest quantum mechanical systems, we consider the dynamics of a single quantum particle, say, an electron, under the influence of a static external force field mediated by a given real-valued potential $V(x)$, where $x \in \mathbb{R}^3$ denotes the spatial coordinate. The state of the electron at time $t \in \mathbb{R}$ is described by a wave function $\psi(t, \cdot) \in L^2(\mathbb{R}^3; \mathbb{C})$ whose time evolution is governed by Erwin Schrödinger's fundamental equation from 1926:

$$i\varepsilon \frac{\partial}{\partial t}\psi^\varepsilon = -\frac{\varepsilon^2}{2}\Delta_x \psi^\varepsilon + V(x)\psi^\varepsilon, \quad \psi^\varepsilon|_{t=0} = \psi_0^\varepsilon(x).$$

Here we have rescaled the original equation including all physical parameters (mass, charge, the Planck's constant $\hbar$, etc.) into dimensionless units such that only one (small) parameter $\varepsilon > 0$ remains. The latter plays the role of a dimensionless Planck's constant, having the physical unit of an action, i.e. energy $\times$ time. Classical behavior is expected to emerge from quantum dynamics in the limit $\varepsilon \to 0$, incorporating the basic premise that classical mechanics describes systems that vary on energy-time scales much larger than $\hbar$.

However, a moment's reflection reveals that naively passing to the limit $\varepsilon \to 0$ in Schrödinger's equation does not yield anything. Indeed, the classical limit of Schrödinger's equation falls into what is known as "singular limits" for differential equations, a topic with a long history in asymptotic approximation theory. Given the dispersive nature of Schrödinger's equation, we expect solutions ψ^ε to be rapidly oscillating functions in both space and time with frequencies of order $\mathcal{O}(1/\varepsilon)$. In the case where $V \equiv 0$, this is directly seen using the Fourier transform, reaffirming the fact that there is no naive limiting behavior of quantum dynamics as $\varepsilon \to 0$.

In an effort to bypass this problem and give a more direct connection to classical mechanics, Erwin Madelung in 1926 reformulated Schrödinger's equation in terms of a system of equations for the position density $\rho^\varepsilon = |\psi^\varepsilon|^2$ and the current density $J^\varepsilon = \varepsilon \mathrm{Im}(\overline{\psi^\varepsilon}\nabla_x \psi^\varepsilon)$. The hereby obtained system takes the form of a (singular) perturbation of the classical Euler equations of compressible fluid dynamics, and it formally (though not rigorously, in general) converges to the latter in the limit $\varepsilon \to 0$.

Inspired by this reformulation, David Bohm offered in 1952 yet another approach to quantum dynamics: Given any ψ^ε and its associated densities, he postulated that quantum particles will travel along trajectories $t \mapsto X^\varepsilon(t, x) \in \mathbb{R}^3$ obtained from the following dynamical system:

$$\dot{X}^\varepsilon = \frac{J^\varepsilon}{\rho^\varepsilon}, \quad X^\varepsilon(0, x) = x,$$

where the initial data $x \in \mathbb{R}^3$ is in general not known exactly but rather distributed according to the initial probability density $|\psi_0^\varepsilon|^2$. Bohm's interpretation has been controversial within physics, but from a mathematical point of view, one can give a precise and rigorous meaning

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to the dynamical system above and, thus, associate to any given solution ψ^ε of Schrödinger's equation a family of "Bohmian trajectories" X^ε. This point of view offers the advantage that it treats both classical and quantum dynamics on an equal, trajectory-based footing (as Schrödinger's equation remains in the background, used only to define the position and current densities at each space-time point). Ideally, one would like to study the Bohmian trajectories X^ε and recover from them the well-known trajectories of classical point particles in the limit $\varepsilon \to 0$. In the situation at hand, these would simply correspond to Newton's second law written in the form $\dot{X} = P$, $\dot{P} = -\nabla V(X)$, where $(X, P) \in \mathbb{R}^6$ denotes the position and momentum of the particle at time t.

The study of the classical limit of Bohmian trajectories has, in recent years, been a topic of intense research for me and several of my colleagues. Unfortunately, the rather complicated and nonlinear relation between X^ε and ψ^ε makes this a challenging endeavor. Instead of trying to tackle the Bohmian trajectories directly, we first focussed our efforts on a family of phase-space measures β^ε, which we called "Bohmian measures" and which are known to be equivariant with respect to the Bohmian flow. Their classical limit as $\varepsilon \to 0$ (defined in a certain weak sense) can be rigorously studied, and one can show that the resulting limiting measure β^0 not only concentrates on the classical limit of the Bohmian trajectories but also incorporates the classical limits of the densities ρ^ε and J^ε. It remains an open question, however, under which circumstances other physically relevant quantities are correctly described by the Bohmian measure as $\varepsilon \to 0$.

Returning to the study of the classical limit of the Bohmian trajectories themselves, the results available to date require additional assumptions on the potential V and, more importantly, on the considered class of initial wave functions ψ_0^ε. On the positive side, one can show that for initial data given by semiclassical wave packets (these are wave functions known to optimize Heisenberg's uncertainty principle), the Bohmian trajectories stay within a neighborhood of size $\mathcal{O}(\sqrt{\varepsilon})$ of the corresponding classical trajectories for all times $t \in [0, T]$. Surprisingly, though, one can also show that for more general initial data of WKB type, the Bohmian trajectories generically do *not* converge to the corresponding classical ones. More precisely, the limit coincides only with the expected classical one, up to a (small) time $t_* > 0$, depending on the initial data. For $t \geq t_*$ one can prove that the limiting Bohmian dynamics differs from the corresponding classical one by means of a continuity argument (see Figure 1 for an illustration). A more precise description of the limit for $t \geq t_*$ remains a big open question.

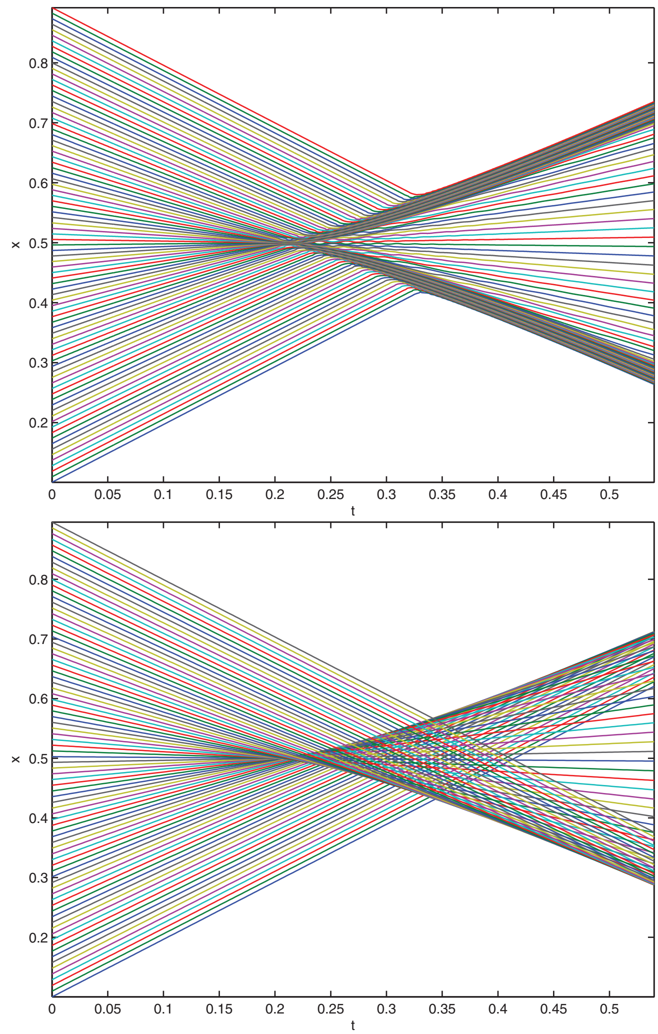

Figure 1. Left: Bohmian trajectories $X^\varepsilon(t, x)$ for WKB initial data and small $\varepsilon = 10^{-2}$. Right: The corresponding classical trajectories, exhibiting interference for $t \geq t_* \approx 0.2$. For more details, see [1].

Reference

1. A. Figalli, C. Klein, P. Markowich, and C. Sparber, WKB analysis of Bohmian dynamics, *Comm. Pure Appl. Math.* **67** (2014), no. 4, 581–620. MR 3168122

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Christof Sparber's research focuses on partial differential equations in mathematical physics and related fields.

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