

WKB ANALYSIS OF BOHMIAN DYNAMICS

ABSTRACT. We consider a semi-classically scaled Schrödinger equation with WKB initial data. We prove that in the classical limit the corresponding Bohmian trajectories converge (locally in measure) to the classical trajectories before the appearance of the first caustic. In a second step we show that after caustic onset this convergence in general no longer holds. In addition, we provide numerical simulations of the Bohmian trajectories in the semiclassical regime which illustrate the above results.

1. INTRODUCTION

1.1. Bohmian trajectories and Bohmian measures. Bohmian mechanics was developed by D. Bohm in 1952, cf. [11, 12], as an alternative to the usual theory of quantum mechanics (for a broader introduction and a historic overview of the subject we refer to [8, 13, 22]). To this end, Bohmian mechanics is based on the dynamics of point particles, in $d \in \mathbb{N}$ spatial dimension, whose motion is guided by Schrödinger's wave function $\psi^\varepsilon(t, \cdot) \in L^2(\mathbb{R}^d; \mathbb{C})$. The dynamics of the latter, is, as usual, governed by the Schrödinger equation, which in the following will be written as

$$i\varepsilon \partial_t \psi^\varepsilon = -\frac{\varepsilon^2}{2} \Delta \psi^\varepsilon + V(x) \psi^\varepsilon, \quad \psi^\varepsilon|_{t=0} = \psi_0^\varepsilon, \quad (1)$$

where $x \in \mathbb{R}^d$, $t \in \mathbb{R}_+$, and $V(x) \in \mathbb{R}$ denotes a given external potential (satisfying some regularity assumptions to be specified below). In (1), we assume that we have already rescaled the equation in dimensionless form such that only one *semi-classical parameter* $0 < \varepsilon \ll 1$ remains. In other words, ε plays the role of a scaled Planck's constant \hbar . It is by now a classical (and well studied) problem of quantum mechanics to understand the emergence of classical physics from (1) in the limit $\varepsilon \simeq \hbar \rightarrow 0$, see, e.g., [45, 48] for a general introduction. In the following we shall be interested in this question from the point of view of Bohmian dynamics.

To this end, we first recall that to any sufficiently regular wave function $\psi^\varepsilon \in H^1(\mathbb{R}^d; \mathbb{C})$ one can associate two basic real-valued densities. Namely, the *position* and the *current-density*, defined by

$$\rho^\varepsilon(t, x) = |\psi^\varepsilon(t, x)|^2, \quad J^\varepsilon(t, x) = \varepsilon \operatorname{Im}(\overline{\psi^\varepsilon(t, x)} \nabla \psi^\varepsilon(t, x)), \quad (2)$$

and which satisfy the conservation law

$$\partial_t \rho^\varepsilon + \operatorname{div}_x J^\varepsilon = 0.$$

These two quantities play an important role in Bohmian mechanics. Namely, given any $\psi^\varepsilon(t, x)$, one defines ε -dependent particle-trajectories $X_t^\varepsilon : y \mapsto X^\varepsilon(t, y) \in \mathbb{R}^d$, via the following differential equation

$$\dot{X}^\varepsilon(t, y) = u^\varepsilon(t, X^\varepsilon(t, y)), \quad X^\varepsilon(0, y) = y \in \mathbb{R}^d,$$

where u^ε denotes the quantum mechanical velocity field, (formally) given by

$$u^\varepsilon(t, x) := \frac{J^\varepsilon(t, x)}{\rho^\varepsilon(t, x)} = \varepsilon \operatorname{Im} \left(\frac{\nabla \psi^\varepsilon(t, x)}{\psi^\varepsilon(t, x)} \right). \quad (3)$$

In addition, one assumes that the initial position $y \in \mathbb{R}^d$ is *distributed* according to the measure $\rho_0^\varepsilon \equiv |\psi_0^\varepsilon|^2 \in L^1_+(\mathbb{R}^d)$. The latter can be seen as a reflection of Born's statistical law of quantum randomness [14].

Although the interpretation of X_t^ε as particle trajectories remains controversial from the physics point of view (see, e.g., [37]), its mathematical foundation is *solid*. Indeed, it was rigorously proved in [9, 51] that, even though u^ε is *not* necessarily continuous, the Bohmian flow $y \mapsto X^\varepsilon(t, y)$ is well-defined $\rho_0^\varepsilon - a.e.$ for all $t \in \mathbb{R}_+$ (provided some mild assumptions on the potential V). In addition, it was shown that, for all times $t \in \mathbb{R}_+$, the position density $\rho^\varepsilon(t, x)$ is given by the *push-forward* of the initial density $\rho_0^\varepsilon(x)$ under the mapping X_t^ε , i.e., for any non-negative Borel function $\sigma : \mathbb{R}^d \rightarrow [0, +\infty]$ it holds:

$$\int_{\mathbb{R}^d} \sigma(x) \rho^\varepsilon(t, x) dx = \int_{\mathbb{R}^d} \sigma(X^\varepsilon(t, y)) \rho_0^\varepsilon(y) dy. \quad (4)$$

More recently, a phase space description of Bohmian mechanics was rigorously introduced in [43] through the definition of the following class of non-negative phase space measures:

Definition 1.1 (Bohmian measures). Let $\varepsilon > 0$ be a given scale and $\psi^\varepsilon \in H^1_\varepsilon(\mathbb{R}^d)$ be a sequence of wave functions with corresponding densities $\rho^\varepsilon, J^\varepsilon$. Then, the associated *Bohmian measure* $\beta^\varepsilon \equiv \beta^\varepsilon[\psi^\varepsilon] \in \mathcal{M}^+(\mathbb{R}_x^d \times \mathbb{R}_p^d)$ is given by

$$\langle \beta^\varepsilon, \varphi \rangle := \int_{\mathbb{R}^d} \rho^\varepsilon(x) \varphi \left(x, \frac{J^\varepsilon(x)}{\rho^\varepsilon(x)} \right) dx, \quad \forall \varphi \in C_0(\mathbb{R}_x^d \times \mathbb{R}_p^d).$$

Here and in the following, \mathcal{M}^+ denotes the set of non-negative Borel measures on phase-space. Moreover, $\langle \cdot, \cdot \rangle$ denotes the corresponding duality bracket between $\mathcal{M}^+(\mathbb{R}_x^d \times \mathbb{R}_p^d)$ and $C_0(\mathbb{R}_x^d \times \mathbb{R}_p^d)$, where C_0 is the closure (with respect to the uniform norm) of the set of continuous functions with compact support. In other words, the Bohmian measure β^ε associated to $\rho^\varepsilon, J^\varepsilon$ is given by

$$\beta^\varepsilon(t, x, p) := \rho^\varepsilon(t, x) \delta(p - u^\varepsilon(t, x)), \quad (5)$$

where u^ε is defined by (3) and $\delta(p - \cdot)$ denotes the d -dimensional delta distribution with respect to the momentum variable $p \in \mathbb{R}^d$. Note that even though u^ε is not well defined at points where $\rho^\varepsilon(t, x) = 0$, the Bohmian measure β^ε is. Moreover, from (5) it immediately follows, that the zeroth and first moment of β^ε with respect to $p \in \mathbb{R}^d$ yield the quantum mechanical particle and current densities, i.e.,

$$\rho^\varepsilon(t, x) = \int_{\mathbb{R}^d} \beta^\varepsilon(t, x, dp), \quad J^\varepsilon(t, x) = \int_{\mathbb{R}^d} p \beta^\varepsilon(t, x, dp),$$

Concerning the dynamics of β^ε it was shown in [43] that the results of [9, 51] can be transferred into phase space. More precisely, [43, Lemma 2.5] states that for all $t \in \mathbb{R}_+$, the measure $\beta^\varepsilon(t, x, p)$ is given by the push-forward of the initial measure

$$\beta_0^\varepsilon(y, p) = \rho_0^\varepsilon(y) \delta(p - u_0^\varepsilon(y)),$$

under the following ε -dependent phase-space flow (defined $\beta_0^\varepsilon - a.e.$):

$$\begin{cases} \dot{X}^\varepsilon(t, y) = P^\varepsilon(t, y), & X^\varepsilon(0, y) = y, \\ \dot{P}^\varepsilon(t, y) = -\nabla V(X^\varepsilon(t, y)) - \nabla V_B^\varepsilon(t, X^\varepsilon(t, y)), & P^\varepsilon(0, y) = u_0^\varepsilon(y), \end{cases} \quad (6)$$

where $V_B^\varepsilon(t, x)$, denotes the *Bohm potential* [22, 53]:

$$V_B^\varepsilon := -\frac{\varepsilon^2}{2\sqrt{\rho^\varepsilon}} \Delta \sqrt{\rho^\varepsilon}. \quad (7)$$

Thus, for any non-negative Borel function $\varphi : \mathbb{R}_x^d \times \mathbb{R}_p^d \rightarrow [0, +\infty]$ it holds

$$\iint_{\mathbb{R}_{x,p}^{2d}} \varphi(x, p) \beta^\varepsilon(t, dx, dp) = \int_{\mathbb{R}^d} \varphi(X^\varepsilon(t, y), P^\varepsilon(t, y)) \rho_0^\varepsilon(y) dy. \quad (8)$$

Note that (6) is the characteristic flow of the following perturbed Burgers' type equation

$$\partial_t u^\varepsilon + (u^\varepsilon \cdot \nabla) u^\varepsilon + \nabla V = \frac{\varepsilon^2}{2\sqrt{\rho^\varepsilon}} \Delta \sqrt{\rho^\varepsilon}, \quad u^\varepsilon|_{t=0} = u_0^\varepsilon,$$

which allows us to identify $\dot{X}^\varepsilon(t, y) = P^\varepsilon(t, y) = u^\varepsilon(t, X^\varepsilon(t, y))$.

The system (6) can be interpreted as a perturbation of the classical Hamiltonian equations of motion for classical point particles, cf. [4], which are formally obtained from (6) by letting $\varepsilon \rightarrow 0_+$. Obviously, this corresponds to a highly singular limiting procedure which is by no means straightforward. In order to gain more insight, we shall in the next subsection recall some, by now classical, material on the asymptotic analysis of ψ^ε .

1.2. WKB asymptotics. A possible way to describe these asymptotics of the semi-classical wave function ψ^ε as $\varepsilon \rightarrow 0_+$ is based on the time-dependent *WKB method*, cf. [15, 45, 48] for a general introduction. One thereby makes the ansatz [40]

$$\psi^\varepsilon(t, x) = a^\varepsilon(t, x) e^{iS(t, x)/\varepsilon} \quad (9)$$

for some ε -independent (real-valued) phase function $S(t, x) \in \mathbb{R}$ and an (in general complex valued) amplitude $a^\varepsilon(t, x) \in \mathbb{C}$ satisfying

$$a^\varepsilon \sim a + \varepsilon a_1 + \varepsilon^2 a_2 + \dots,$$

in the sense of asymptotic expansions. Assuming for the moment that a^ε and S are sufficiently smooth, one can plug (9) into (1) and compare equal powers of ε in the resulting expression. This yields a *Hamilton-Jacobi equation* for the phase, see, e.g., [16, 40, 45]:

$$\partial_t S + \frac{1}{2} |\nabla S|^2 + V(x) = 0, \quad S|_{t=0} = S_0, \quad (10)$$

and a transport equation for the leading order amplitude

$$\partial_t a + \nabla a \cdot \nabla S + \frac{a}{2} \Delta S = 0, \quad a|_{t=0} = a_0. \quad (11)$$

Note that the latter can be rewritten in the form of a conservation law for the leading order particle density $\rho := |a|^2$, i.e.,

$$\partial_t \rho + \operatorname{div}(\rho \nabla S) = 0. \quad (12)$$

The main problem of the WKB approach is that (10) in general does not admit unique smooth solutions for all times. This can be seen, from the method of characteristics (see, e.g., [23]), where one needs to solve the following Hamiltonian system:

$$\begin{cases} \dot{X}(t, y) = P(t, y), & X(0, y) = y, \\ \dot{P}(t, y) = -\nabla V(X(t, y)), & P(0, y) = \nabla S_0(y). \end{cases} \quad (13)$$

By the Cauchy-Lipschitz theorem, this system of ordinary differential equations can be solved at least locally in-time, which yields a flow map $X_t : y \mapsto X(t, y)$. If we denote the corresponding inverse mapping by $Y_t : x \mapsto Y(t, x)$, i.e., $Y_t \circ X_t = \text{id}$, then the phase function S satisfying (10) is found to be [16, 23]

$$S(t, x) = S_0(Y(t, x)) + \int_0^t \left(\frac{1}{2} |P(\tau, y)|^2 - V(X(\tau, y)) \right) d\tau \Big|_{y=Y(t, x)}. \quad (14)$$

Given such a smooth phase function S , one can, in a second step, integrate the amplitude equation (11) along the flow X_t to obtain the amplitude in the following form [16, 45]:

$$a(t, x) = \frac{a_0(Y(t, x))}{\sqrt{J_t(Y(t, x))}}, \quad (15)$$

where $J_t(y) := \det \nabla_y X(t, y)$ is the Jacobian determinant of the map $y \mapsto X(t, y)$. Under the assumptions of our paper (to be stated later on), the flow X_t indeed exists globally in-time. The problem, however, is that in general there is a (possibly, very short) time $T^* > 0$ at which the flow X_t ceases to be one-to-one. Points $x \in \mathbb{R}^d$ at which this happens are *caustic points* and T^* is called the *caustic onset time* [32]. More precisely, let

$$\mathcal{C}_t = \{x \in \mathbb{R}^d : \text{there is } y \in \mathbb{R}^d \text{ such that } x = X(t, y) \text{ and } J_t(y) = 0\},$$

then the *caustic set* is defined by $\mathcal{C} := \{(x, t) : x \in \mathcal{C}_t\}$ and the caustic onset time is

$$T^* := \inf\{t \in \mathbb{R}_+ : \mathcal{C}_t \neq \emptyset\}.$$

For $t > T^*$ the solution of (10), obtained by the method of characteristics, typically becomes multi-valued due to the possibility of crossing trajectories, see Fig. 1. On the other hand, weak solutions to (10), which can be uniquely defined (for

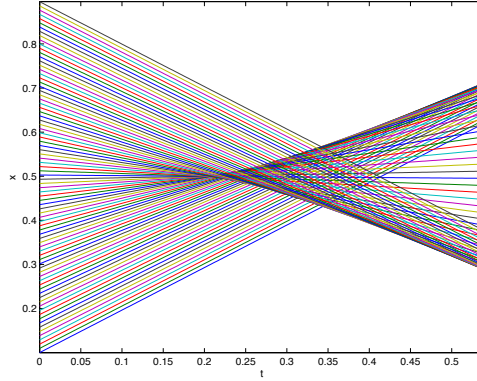


FIGURE 1. Classical trajectories for initial data $\nabla S_0(x) = -\tanh(5x - \frac{5}{2})$

example, by invoking the Lax-Olejnik formula [23]) are not smooth in general and thus plugging (9) into (1) is no longer justified. From the physical point of view T^* marks the generation of new frequencies within ψ^ε not captured by the simple one phase WKB ansatz (9). Indeed, it is well known that for $t > T^*$ one generically

requires a *multi-phase* WKB ansatz to correctly describe the asymptotic behavior of ψ^ε , see [32, 45, 48] and Section 5 for more details.

Coming back to Bohmian dynamics, we note that for wave functions ψ^ε given in WKB form (9), it holds $J^\varepsilon = |a^\varepsilon|^2 \nabla S$ and thus, the quantum mechanical velocity field is given by

$$u^\varepsilon(t, x) = \frac{J^\varepsilon(t, x)}{\rho^\varepsilon(t, x)} = \nabla S(t, x).$$

Identifying $u_0(y) = \nabla S_0(y)$, one may regard the system (6) as a nonlinear perturbation of the Hamiltonian system (13) and one consequently expects the Bohmian trajectories $(X^\varepsilon, P^\varepsilon)$ to converge to the corresponding classical Hamiltonian flow (X, P) , in the limit $\varepsilon \rightarrow 0_+$. One of the main results of this paper is, that, at least before caustic onset, this convergence indeed holds true (in a sense to be made precise, see Theorem 3.1). After caustic onset, however, the situation in general is much more complicated in view of Fig. 1. Indeed, as a second main result of our work, we shall show that in general one cannot expect the Bohmian trajectories to converge to the (multi-valued) classical flow, see Theorem 5.4. The problem of giving a precise description of the classical limit of the Bohmian trajectories $X^\varepsilon, P^\varepsilon$ after caustic onset therefore remains largely open.

The situation concerning the classical (weak) limit of the Bohmian measure β^ε as $\varepsilon \rightarrow 0_+$ is slightly better, though. In particular, by invoking some well-known results from Fourier integral operators, we will show how to compute the classical limit of β^ε , even after caustic onset. The latter will be compared with the well-known form of the *Wigner measure* associated to ψ^ε . The Wigner measure (also called semi-classical defect measure) is a well established tool in semiclassical analysis, which allows to efficiently describe the classical limit of quantum mechanical observables, cf. [2, 24, 27, 41, 49]. For completeness, the definition of the Wigner measure and its main properties will be recalled in Section 4.2. We will show that, even though the two limiting measures in general do not coincide, their zeroth and first moment (yielding the classical limit of ρ^ε and J^ε) always do¹.

The rest of the paper is organized as follows: In Section 2 we describe some general properties of Bohmian dynamics and of the Young measures associated to the Bohmian trajectories. These properties will be used in Section 3 to prove that the Bohmian trajectories converge to the classical ones before caustic onset. In Section 4 we prove a general result about Bohmian measures associated to multi-phase WKB states. This result is then used in Section 5 to show that, even in the free case (where $V(x) \equiv 0$), the Bohmian measure may differ from the Wigner measure, and that in general the Bohmian trajectories do not converge to the Hamiltonian ones after caustics. Finally, in Section 6 we present numerical simulations of Bohmian trajectories in the regime $0 < \varepsilon \ll 1$.

2. MATHEMATICAL PRELIMINARIES

In the following subsection, we shall impose assumptions on the potential V and the initial data ψ_0^ε which will allow us to retain some basic results of [43], guaranteeing the existence of a weak limit of β^ε , as $\varepsilon \rightarrow 0_+$. An extension of these

¹A more detailed study of the connection between Bohmian measures and Wigner measures can be found in [43]. In the current paper, we use the Wigner measure only as a way of shedding some light onto the classical limit of the Bohmian measure after caustic onset and to prove the aforementioned fact on the particle and current densities.

earlier results will be the proof of a certain a-priori estimate for P^ε . The latter will be used in Subsection 2.2 to infer an important new property of the Young measure associated to the Bohmian flow.

2.1. Basic a-priori estimates and existence of a limiting measure. From now on the potential V will satisfy the following assumptions.

Assumption 2.1. The potential $V \in C^\infty(\mathbb{R}^d; \mathbb{R})$ is assumed to be bounded below and sub-quadratic, i.e.,

$$\partial_x^k V \in L^\infty(\mathbb{R}^d), \quad \forall k \in \mathbb{N}^d \text{ such that } |k| \geq 2.$$

Since V is bounded below, without loss of generality we can assume $V(x) \geq 0$. Assumption 2.1 is (by far) sufficient to guarantee the existence of a unique strong solution $\psi^\varepsilon \in C(\mathbb{R}^d; L^2(\mathbb{R}^d))$ to (1), satisfying two basic conservation laws of quantum mechanics. Namely, conservation of the total *mass*

$$M^\varepsilon(t) := \int_{\mathbb{R}^d} |\psi^\varepsilon(t, x)|^2 dx = M^\varepsilon(0), \quad (16)$$

and the *total energy*

$$E^\varepsilon(t) := \frac{\varepsilon^2}{2} \int_{\mathbb{R}^d} |\nabla \psi^\varepsilon(t, x)|^2 dx + \int_{\mathbb{R}^d} V(x) |\psi^\varepsilon(t, x)|^2 dx = E^\varepsilon(0). \quad (17)$$

Note that the kinetic energy of ψ^ε can be written in terms of ρ^ε and u^ε as

$$\begin{aligned} E_{kin}(t) &:= \frac{\varepsilon^2}{2} \int_{\mathbb{R}^d} |\nabla \psi^\varepsilon(t, x)|^2 dx \\ &= \frac{1}{2} \int_{\mathbb{R}^d} |u^\varepsilon(t, x)|^2 \rho^\varepsilon(t, x) dx + \frac{\varepsilon^2}{2} \int_{\mathbb{R}^d} |\nabla \sqrt{\rho^\varepsilon(t, x)}|^2 dx, \end{aligned} \quad (18)$$

which allows to define $u^\varepsilon \in L^2(\mathbb{R}^d; \rho^\varepsilon dx)$, for any ψ^ε with finite kinetic energy.

A direct consequence of these conservation laws is the following a-priori estimate which we shall use in the proof of Proposition 2.4 below.

Lemma 2.1. *Let V satisfy Assumption 2.1, $\psi_0^\varepsilon \in H^1(\mathbb{R}^d)$, and let P^ε be as in (6). Then, it holds:*

$$\int_0^T \int_{\mathbb{R}^d} |P^\varepsilon(t, y)|^2 \rho_0^\varepsilon(y) dy dt \leq T E^\varepsilon(0), \quad \forall T \in \mathbb{R}_+.$$

Proof. Let us recall that $\rho^\varepsilon(t, x)$ is the push forward of ρ_0^ε under the mapping X_t^ε , i.e., identity (4) holds true for all $t \in \mathbb{R}_+$. Using this identity with $\sigma(\cdot) = |P^\varepsilon(t, \cdot)|^2$ and recalling that $P^\varepsilon(t, y) = \dot{X}^\varepsilon(t, y) = u^\varepsilon(t, X^\varepsilon(t, y))$, we find

$$\begin{aligned} \int_0^T \int_{\mathbb{R}^d} |P^\varepsilon(t, y)|^2 \rho_0^\varepsilon(y) dy dt &= \int_0^T \int_{\mathbb{R}^d} |u^\varepsilon(t, X^\varepsilon(t, y))|^2 \rho_0^\varepsilon(y) dy dt \\ &= \int_0^T \int_{\mathbb{R}^d} |u^\varepsilon(t, y)|^2 \rho^\varepsilon(t, y) dy dt. \end{aligned}$$

In view of energy conservation, the last term on the right hand side is bounded by

$$\int_0^T \int_{\mathbb{R}^d} |u^\varepsilon(t, y)|^2 \rho^\varepsilon(t, y) dy dt \leq \int_0^T E^\varepsilon(t) dt = T E^\varepsilon(0),$$

as desired. \square

In addition to Assumption 2.1, we require the following basic properties for the initial datum ψ_0^ε .

Assumption 2.2. The initial data of (1) satisfy $M^\varepsilon(0) \equiv \|\psi_0^\varepsilon\|_{L^2}^2 = 1$, and there exists $C_0 > 0$ such that

$$\sup_{0 < \varepsilon \leq 1} E^\varepsilon(0) \leq C_0.$$

Remark 2.2. The normalization $\|\psi_0^\varepsilon\|_{L^2}^2 = 1$ is imposed for the sake of mathematical convenience. From a physical point of view, it is required for the usual probabilistic interpretation of quantum mechanics in which $\rho^\varepsilon = |\psi^\varepsilon|^2$ denotes the probability measure of finding the particle within a certain spatial region $\Omega \subseteq \mathbb{R}^d$.

Assumption 2.2, together with conservation of mass and energy and the fact that $V(x) \geq 0$, implies that for all $t \in \mathbb{R}_+$:

$$\sup_{0 < \varepsilon \leq 1} (\|\psi^\varepsilon(t)\|_{L^2} + \|\varepsilon \nabla \psi^\varepsilon(t)\|_{L^2}) < +\infty. \quad (19)$$

In other words, $\psi^\varepsilon(t)$ is ε -oscillatory and we are in the framework of [43]. Indeed, it was shown in [43, Lemma 3.1] that (19) implies the existence of a limiting measure $\beta(t) \in \mathcal{M}^+(\mathbb{R}_x^d \times \mathbb{R}_p^d)$ such that, up to extraction of a subsequence, it holds:

$$\beta^\varepsilon \xrightarrow{\varepsilon \rightarrow 0_+} \beta, \quad \text{in } L^\infty(\mathbb{R}_t; \mathcal{M}^+(\mathbb{R}_x^d \times \mathbb{R}_p^d)) \text{ weak-}^*, \quad (20)$$

and we also have

$$\rho^\varepsilon(t, x) \xrightarrow{\varepsilon \rightarrow 0_+} \int_{\mathbb{R}^d} \beta(t, x, dp), \quad J^\varepsilon(t, x) \xrightarrow{\varepsilon \rightarrow 0_+} \int_{\mathbb{R}^d} p \beta(t, x, dp), \quad (21)$$

where the limits have to be understood in $L^\infty(\mathbb{R}_t; \mathcal{M}^+(\mathbb{R}_x^d))$ weak- $*$.

2.2. Young measures of Bohmian trajectories. The limiting Bohmian measure β is intrinsically connected to the Young measure (or parametrized measure) of the Bohmian dynamics. To this end, we first note that $\Phi^\varepsilon(t, y) \equiv (X^\varepsilon(t, y), P^\varepsilon(t, y))$ is measurable in t, y and thus, there exists an associated Young measure

$$\Upsilon_{t,y} : \mathbb{R}_t \times \mathbb{R}_y^d \rightarrow \mathcal{M}^+(\mathbb{R}_y^d \times \mathbb{R}_p^d) : (t, y) \mapsto \Upsilon_{t,y}(dx, dp),$$

which is defined through the following limit (see [6, 34, 47]): for any test function $\sigma \in L^1(\mathbb{R}_t \times \mathbb{R}_y^d; C_0(\mathbb{R}^{2d}))$,

$$\lim_{\varepsilon \rightarrow 0} \iint_{\mathbb{R} \times \mathbb{R}^d} \sigma(t, y, \Phi_\varepsilon(t, y)) dy dt = \iint_{\mathbb{R} \times \mathbb{R}^d} \iint_{\mathbb{R}^{2d}} \sigma(t, y, x, p) \Upsilon_{t,y}(dx, dp) dy dt.$$

Having in mind (8), if we assume in addition that

$$\rho_0^\varepsilon \xrightarrow{\varepsilon \rightarrow 0_+} \rho_0, \quad \text{strongly in } L^1_+(\mathbb{R}^d),$$

we easily get the following identity:

$$\beta(t, x, p) = \int_{\mathbb{R}_y^d} \Upsilon_{t,y}(x, p) \rho_0(y) dy. \quad (22)$$

Here, β is the limiting Bohmian measure obtained in (20) for a specific subsequence. The relation (22) has already been observed in [43] and can be used to infer the following a-priori estimate on $\Upsilon_{t,y}$.

Lemma 2.3. *Let Assumptions 2.1 and 2.2 hold, and assume in addition that $\rho_0^\varepsilon \xrightarrow{\varepsilon \rightarrow 0_+} \rho_0$ strongly in $L^1_+(\mathbb{R}^d)$. Then, for any $T \in \mathbb{R}_+$, there exists a $C = C(T) > 0$ such that*

$$\int_0^T \iiint_{\mathbb{R}^{2d} \times \mathbb{R}^d} |p|^2 \rho_0(y) \Upsilon_{t,y}(dx, dp) dy dt \leq C(T).$$

Proof. Using (22) we see that

$$\iiint_{\mathbb{R}^{2d} \times \mathbb{R}^d} |p|^2 \rho_0(y) \Upsilon_{t,y}(dx, dp) dy = \iint_{\mathbb{R}^{2d}} |p|^2 \beta(t, dx, dp).$$

Now we recall that, by definition,

$$\beta^\varepsilon(t, x, p) = \rho^\varepsilon(t, x) \delta(p - u^\varepsilon(t, x))$$

and hence

$$\iint_{\mathbb{R}^{2d}} |p|^2 \beta^\varepsilon(t, dx, dp) = \int_{\mathbb{R}^d} |u^\varepsilon(t, x)|^2 \rho^\varepsilon(t, x) dx \leq 2E_{\text{kin}}^\varepsilon(t) \leq C(T),$$

in view of (18) and energy conservation. This uniform (in ε) bound together with Fatou's lemma implies

$$\iint_{\mathbb{R}^{2d}} |p|^2 \beta(t, dx, dp) \leq C(T),$$

and the assertion is proved. \square

Lemma 2.3 together with Lemma 2.1 will be used to prove the following important property for the zeroth moment of $\Upsilon_{t,y}$.

Proposition 2.4. *Let Assumptions 2.1 and 2.2 hold, and assume in addition that $\rho_0^\varepsilon \xrightarrow{\varepsilon \rightarrow 0^+} \rho_0$ strongly in $L^1_+(\mathbb{R}^d)$. Denote*

$$\mathbf{v}_{t,y}(x) := \int_{\mathbb{R}^d} \Upsilon_{t,y}(x, dp).$$

Then $\mathbf{v}_{t,y} \in \mathcal{M}^+(\mathbb{R}^d_x)$ solves, a.e. with respect to the measure $\rho_0(y)$, the following transport equation

$$\partial_t \mathbf{v}_{t,y} + \operatorname{div}_x \left(\int_{\mathbb{R}^d} p \Upsilon_{t,y}(x, dp) \right) = 0, \quad \mathbf{v}_{t=0,y}(x) = \delta(x - y),$$

in the sense of distributions on $\mathcal{D}'(\mathbb{R}_t \times \mathbb{R}^d_x)$.

This transport equation will play a crucial role in the convergence proof of Bohmian trajectories before caustic onset.

Proof. As a first, preparatory step we shall prove that, for all test functions $\zeta \in C_0(\mathbb{R}_t \times \mathbb{R}^d_y)$, $\sigma \in C_0(\mathbb{R}^d_x)$:

$$\begin{aligned} \lim_{\varepsilon \rightarrow 0^+} \int_0^T \int_{\mathbb{R}^d} P^\varepsilon(t, y) \zeta(t, y) \sigma(X^\varepsilon(t, y)) \rho_0^\varepsilon(y) dy dt = \\ \int_0^T \zeta(t, y) \iint_{\mathbb{R}^{2d}} p \sigma(x) \Upsilon_{t,y}(dx, p) \rho_0(y) dy dt, \end{aligned} \quad (23)$$

To this end, let $K > 0$ and $\chi_K \in C_c^\infty(\mathbb{R}^d)$ be such that $\chi_K(p) = 1$ for $|p| \leq K$, and $\chi_K(p) = 0$ for $|p| > K + 1$. Then, by writing $P^\varepsilon = \chi_K(P^\varepsilon) + (1 - \chi_K(P^\varepsilon))$ we can decompose

$$\int_0^T \int_{\mathbb{R}^d} \zeta(t, y) \sigma(X^\varepsilon(t, y)) P^\varepsilon(t, y) \rho_0^\varepsilon(y) dy dt = I_1^{\varepsilon, K} + I_2^{\varepsilon, K}.$$

Because of the strong convergence of ρ_0^ε , the first term on the right hand side has the following limit:

$$I_1^{\varepsilon, K} \xrightarrow{\varepsilon \rightarrow 0^+} \int_0^T \zeta(t, y) \iint_{\mathbb{R}^{2d}} \sigma(x) \chi_K(p) \Upsilon_{t,y}(dx, dp) \rho_0(y) dy dt,$$

On the other hand, by having in mind the result of Lemma 2.1, the second term on the right hand side can be estimated by

$$\begin{aligned} |I_2^{\varepsilon,K}| &\leq C \int_0^T \int_{|P^\varepsilon| \geq K} |P^\varepsilon(t,y)| \rho_0^\varepsilon(y) dy, dt \\ &\leq \frac{C}{K} \int_0^T \int_{\mathbb{R}^d} |P^\varepsilon(t,y)|^2 \rho_0^\varepsilon(y) dy, dt \leq \frac{CT}{K} E^\varepsilon(0). \end{aligned}$$

In view of Lemma 2.3 we can let $K \rightarrow +\infty$, which yields $|I_2^{\varepsilon,K}| \xrightarrow{K \rightarrow +\infty} 0$ and the validity of (23).

With (23) in hand, we shall now show that $v_{t,y}$ indeed obeys the transport equation given above. Let $\zeta, \varphi \in C_c^\infty(\mathbb{R}^d)$, $\sigma \in C_c^\infty[0, \infty)$, be smooth compactly supported test functions. Then by (23) we get

$$\begin{aligned} &\int_0^\infty \iint_{\mathbb{R}^{2d}} \left(\partial_t \sigma(t) \varphi(x) + \sigma(t) p \cdot \nabla_x \varphi(x) \zeta(y) \right) \Upsilon_{y,t}(x, dp) \rho_0(y) dy dt \\ &= \lim_{\varepsilon \rightarrow 0^+} \int_0^\infty \int_{\mathbb{R}^d} \left(\partial_t \sigma(t) \varphi(X^\varepsilon(t,y)) + \sigma(t) P^\varepsilon(t,y) \cdot \nabla_x \varphi(X^\varepsilon(t,y)) \zeta(y) \right) \rho_0(dy) dt. \end{aligned}$$

Recalling that $P^\varepsilon(t,y) = \dot{X}^\varepsilon(t,y)$, which implies that

$$P^\varepsilon(t,y) \cdot \nabla_x \varphi(X^\varepsilon(t,y)) = \frac{d}{dt} \varphi(X^\varepsilon(t,y)),$$

we obtain

$$\begin{aligned} &\int_0^\infty \int_{\mathbb{R}^d} \left(\partial_t \sigma(t) \varphi(X^\varepsilon(t,y)) + \sigma(t) P^\varepsilon(t,y) \cdot \nabla_x \varphi(X^\varepsilon(t,y)) \zeta(y) \right) \rho_0(dy) dt \\ &= \int_0^\infty \int_{\mathbb{R}^d} \left(\partial_t \sigma(t) \varphi(X^\varepsilon(t,y)) + \sigma(t) \frac{d}{dt} \varphi(X^\varepsilon(t,y)) \zeta(y) \right) \rho_0(y) dy dt \\ &= \int_{\mathbb{R}^d} \sigma(0) \varphi(X^\varepsilon(0,y)) \zeta(y) \rho_0(y) dy \\ &= \int_{\mathbb{R}^d} \sigma(0) \varphi(y) \zeta(y) \rho_0(y) dy. \end{aligned}$$

where in going from the second to the third we have integrated by parts with respect to time, and from the third to the fourth line we have used that $X^\varepsilon(0,y) = y$ by definition. The obtained expression in the last line is nothing but the initial condition, since

$$\iint_{\mathbb{R}^d} \varphi(y) \zeta(y) \rho_0(y) dy = \iint_{\mathbb{R}^{2d}} \varphi(x) \Upsilon_{0,y}(x, dp) \zeta(y) \rho_0(y) dy,$$

is equivalent to saying that

$$v_{0,y}(x) \equiv \int_{\mathbb{R}^d} \Upsilon_{0,y}(x, dp) = \delta(x-y), \quad \rho_0(dy) - a.e.$$

□

Having collected all necessary properties of $\Upsilon_{t,y}$ we shall prove the convergence of Bohmian trajectories (before caustic onset) in the next section.

Remark 2.5. For completeness, we want to mention that $\Upsilon_{t,y}$ is indeed a probability measure on $\mathbb{R}_x^d \times \mathbb{R}_p^d$ for a.e. y, t , provided the sequence $\{\psi^\varepsilon\}_{0 < \varepsilon \leq 1}$ is compact at infinity (tight), i.e.,

$$\lim_{R \rightarrow \infty} \limsup_{\varepsilon \rightarrow 0^+} \int_{|x| \geq R} |\psi^\varepsilon(t,x)|^2 dx = 0.$$

Indeed if the latter holds true, it was shown in [43, Lemma 3.2] that

$$\lim_{\varepsilon \rightarrow 0_+} M^\varepsilon(t) \equiv \lim_{\varepsilon \rightarrow 0_+} \iint_{\mathbb{R}^{2d}} \beta^\varepsilon(t, dx, dp) = \iint_{\mathbb{R}^{2d}} \beta(t, dx, dp),$$

and having in mind our normalization $M^\varepsilon(t) = 1$, we conclude

$$1 = \iint_{\mathbb{R}^{2d}} \beta(t, dx, dp) = \iiint_{\mathbb{R}^{2d} \times \mathbb{R}^d} \rho_0(y) \Upsilon_{t,y}(dx, dp) dy,$$

in view of (22). Define

$$\alpha_{t,y} := \iint_{\mathbb{R}^{2d}} \Upsilon_{t,y}(dx, dp) \leq 1.$$

Then, since $\int_{\mathbb{R}^d} \rho_0(dy) = 1$, we conclude $\alpha_{y,t} = 1$ a.e.. However, we shall not use this property in the following.

3. CONVERGENCE OF BOHMIAN TRAJECTORIES BEFORE CAUSTIC ONSET

So far we have not specified the initial data ψ_0^ε to be of WKB form. By doing so, we can state the first main result of our work (recall the definition of sub-quadratic, given in Assumption 2.1).

Theorem 3.1. *Let Assumptions 2.1 hold, and let ψ_0^ε be given in WKB form*

$$\psi_0^\varepsilon(x) = a_0(x) e^{iS_0(x)/\varepsilon}, \quad (24)$$

with amplitude $a_0 \in \mathcal{S}(\mathbb{R}^d; \mathbb{C})$ and sub-quadratic phase $S_0 \in C^\infty(\mathbb{R}^d; \mathbb{R})$. Then, there exists a caustic onset time $0 < T^* \leq \infty$ such that:

(i) *For all compact time-intervals $I_t \subset [0, T^*)$, the Bohmian measure β^ε associated to $\rho^\varepsilon, J^\varepsilon$ satisfies*

$$\beta^\varepsilon \xrightarrow{\varepsilon \rightarrow 0_+} \rho(t, x) \delta(p - \nabla S(t, x)), \text{ in } L^\infty(I_t; \mathcal{M}^+(\mathbb{R}_x^d \times \mathbb{R}_p^d)) \text{ weak-}^*,$$

where $\rho \in C^\infty(I_t; \mathcal{S}(\mathbb{R}^d))$ and $S \in C^\infty(I_t \times \mathbb{R}^d)$ solve the WKB system (12), (10).

(ii) *The corresponding Bohmian trajectories satisfy*

$$X^\varepsilon \xrightarrow{\varepsilon \rightarrow 0_+} X, \quad P^\varepsilon \xrightarrow{\varepsilon \rightarrow 0_+} P$$

locally in measure on $\{I_t \times \text{supp } \rho_0\} \subseteq \mathbb{R}_t \times \mathbb{R}_x^d$, where $\rho_0 = |a_0|^2$, and (X, P) are as in (13). More precisely, for every $\delta > 0$ and every Borel set $\Omega \subseteq \{I_t \times \text{supp } \rho_0\}$ with finite Lebesgue measure \mathcal{L}^{d+1} , it holds

$$\lim_{\varepsilon \rightarrow 0} \mathcal{L}^{d+1}(\{(t, y) \in \Omega : |(X^\varepsilon(t, y), P^\varepsilon(t, y)) - (X(t, y), P(t, y))| \geq \delta\}) = 0.$$

Assertion (i) is classical in term of Wigner measures, cf. [26, 49]. For Bohmian measures, the same result has been proved more recently in [43]. Of course, both results are themselves a consequence of the validity of the WKB expansion before caustic onset, cf. [16, 40]. Since the obtained (mono-kinetic) form of the limiting measure will be used to show Assertion (ii), we shall recall the proof of (i) for the sake of completeness.

Assertion (ii) shows, that before caustic onset, the Bohmian trajectories converge locally in measure to the corresponding classical flow. Clearly, if $a_0(x) > 0$ for all $x \in \mathbb{R}^d$, and thus $\text{supp } \rho_0 = \mathbb{R}^d$, we obtain local in measure convergence of the Bohmian trajectories on all of $I_t \times \mathbb{R}_x^d$. After selecting an appropriate subsequence $\{\varepsilon_n\}_{n \in \mathbb{N}}$ this also implies (see, e.g., [10]) *almost everywhere convergence*

on any finite subset of $I_t \times \mathbb{R}_x^d$. Moreover, since, by definition, $\dot{X}^\varepsilon = P^\varepsilon$, the convergence in measure of P^ε to P combined with the L^2 bound from Lemma 2.1 implies that, for \mathcal{L}^d -a.e. y , the curves $X^\varepsilon(\cdot, y)$ converge *uniformly* to $X(\cdot, y)$ on the time interval I_t .

Proof of Theorem 3.1. We first note that (24) implies

$$E^\varepsilon(0) = \frac{1}{2} \int_{\mathbb{R}^d} |a_0|^2 |\nabla S|^2 dx + \frac{\varepsilon^2}{2} \int_{\mathbb{R}^d} |\nabla a_0|^2 dx + \int_{\mathbb{R}^d} V(x) |a_0|^2 dx.$$

Since $a_0 \in \mathcal{S}(\mathbb{R}^d)$, we see that Assumption 2.2 is satisfied and thus all the results established in Section 2 apply. In particular, we have the existence of a limiting Bohmian measure $\beta \in L^\infty(\mathbb{R}_t; \mathcal{M}^+(\mathbb{R}_x^d \times \mathbb{R}_p^d))$ weak-*. In order to prove Assertion (i) we need to show that before caustic onset, this limiting measure is given by a *mono-kinetic* phase space distribution, i.e.,

$$\beta(t, x, p) = \rho(t, x) \delta(p - \nabla S(t, x)). \quad (25)$$

In [43] sufficient conditions for β being mono-kinetic have been derived. In particular, it is proved in there that (25) holds as soon as one has strong L^1 convergence of ρ^ε and J^ε in the limit $\varepsilon \rightarrow 0_+$. To show that this is indeed the case, we shall rely on the so-called modified WKB approximation introduced in [31] and further developed in [15]: Define a complex-valued amplitude a^ε by setting

$$a^\varepsilon(t, x) = \psi^\varepsilon(t, x) e^{-iS(t, x)/\varepsilon}, \quad (26)$$

where ψ^ε solves (1) and S is a smooth solution of the Hamilton-Jacobi equation (10). Next, we recall that the results of [15] (see also [16]) ensure that under our assumptions there is a time $T^* > 0$, independent of $x \in \mathbb{R}^d$, such that, for all compact subsets $I_t \subset [0, T^*)$, the Hamiltonian flow (13) is well-defined, and there exists a unique (sub-quadratic) phase function $S \in C^\infty(I_t \times \mathbb{R}^d)$, given by (14). Consequently, this also ensures the existence of a smooth amplitude $a \in C^\infty(I_t; \mathcal{S}(\mathbb{R}^d))$ given by (15).

With this result in hand, a straightforward computation shows that a^ε , defined in (26), solves

$$\partial_t a^\varepsilon + \nabla a^\varepsilon \cdot \nabla S + \frac{a^\varepsilon}{2} \Delta S = i \frac{\varepsilon}{2} \Delta a^\varepsilon, \quad a^\varepsilon(0, x) = a_0(x). \quad (27)$$

This equation can be considered as a perturbation of (11). Indeed, if we denote the difference by $w^\varepsilon := a^\varepsilon - a$, then w^ε satisfies

$$\partial_t w^\varepsilon + \nabla w^\varepsilon \cdot \nabla S + \frac{w^\varepsilon}{2} \Delta S = i \frac{\varepsilon}{2} \Delta a^\varepsilon, \quad w^\varepsilon(0, x) = 0,$$

where the source term on the right hand side is formally of order $O(\varepsilon)$. Invoking energy estimates, one can prove (see [15, Proposition 3.1]) that for any time-interval $I_t \subset [0, T^*)$, there exists a unique solution $a^\varepsilon \in C(I_t; H^s(\mathbb{R}^d))$ of (27), and that

$$\|w^\varepsilon\|_{L^\infty(I_t; H^s(\mathbb{R}^d))} \equiv \|a^\varepsilon - a\|_{L^\infty(I_t; H^s(\mathbb{R}^d))} = O(\varepsilon), \quad \forall s \geq 0.$$

Writing the mass and current densities as

$$\rho^\varepsilon = |\psi^\varepsilon|^2 = |a^\varepsilon|^2, \quad J^\varepsilon = \varepsilon \operatorname{Im}(\overline{\psi^\varepsilon} \nabla \psi^\varepsilon) = |a^\varepsilon|^2 \nabla S + \varepsilon \operatorname{Im}(\overline{a^\varepsilon} \nabla a^\varepsilon),$$

and using the fact that $H^s(\mathbb{R}^d) \hookrightarrow L^\infty(\mathbb{R}^d)$ for $s > d/2$, this consequently implies

$$\rho^\varepsilon \xrightarrow{\varepsilon \rightarrow 0_+} \rho, \quad \text{in } L^\infty(I_t; L^1(\mathbb{R}^d)) \text{ strongly,}$$

and

$$J^\varepsilon \xrightarrow{\varepsilon \rightarrow 0^+} \rho u, \quad \text{in } L^\infty(I_t; L^1_{\text{loc}}(\mathbb{R}^d)^d) \text{ strongly,}$$

where $\rho = |a|^2$ and $u = \nabla S$ are smooth solutions of the WKB system:

$$\begin{aligned} \partial_t \rho + \operatorname{div}_x(\rho u) &= 0, & \rho(0, x) &= |a_0(x)|^2, \\ \partial_t u + u \cdot \nabla u + \nabla V(x) &= 0, & u(0, x) &= \nabla S_0(x). \end{aligned}$$

In particular, we infer that $P(t, y) = \nabla S(t, X(t, y)) = u(t, X(t, y))$ and, in view of (15), we also have that the density $\rho = |a|^2$ is given by

$$\rho(t, x) = \frac{\rho_0(Y(t, x))}{J_t(Y(t, x))}, \quad t \in [0, T^*]. \quad (28)$$

The strong convergence of $\rho^\varepsilon, J^\varepsilon$ together with [43, Theorem 3.6] then directly imply that the limiting measure β is given by (25) and thus Assertion (i) is proved.

In order to prove (ii) we first note that for every fixed $t \in [0, T^*]$, the limiting measure $\beta(t)$ is carried by the set

$$\mathcal{G}_t = \{(x, p) \in \mathbb{R}^{2d} : p = u(t, x)\}.$$

The identity (22) then implies that a.e. in y the measure $\Upsilon_{t,y}$ is also carried by the same set and we consequently infer

$$\Upsilon_{t,y}(x, p) = \mu_{t,y}(x) \delta(p - u(t, x)),$$

where $\mu_{t,y}$ is the Young measure associated to $X^\varepsilon(t, y)$.

By taking the zeroth moment of $\Upsilon_{t,y}$ with respect to $p \in \mathbb{R}^d$ we realize that indeed $\mu_{t,y} = \nu_{t,y}$, with $\nu_{t,y}$ defined in Proposition 2.4. We thus find that $\mu_{t,y}$ solves, in the sense of distributions:

$$\partial_t \mu_{t,y} + \operatorname{div}_x(u \mu_{t,y}) = 0, \quad \mu_{t=0,y}(x) = \delta(x - y),$$

a.e. with respect to the measure $\rho_0(y)$. In other words, $\mu_{t,y}(x)$ solves the same transport equation as the limiting density $\rho(t, x)$ does. In view of (28), we therefore conclude that, before caustic onset, $\mu_{t,y}$ is given by

$$\mu_{t,y}(x) = \frac{1}{J_t(Y(t, x))} \delta(Y(t, x) - y), \quad \rho_0 - a.e..$$

Multiplying by a test function $\varphi \in C_0(\mathbb{R}_x^d \times \mathbb{R}_y^d)$ and performing the change of variable $x = Y(t, x)$, we consequently find

$$\langle \mu_{t,y}, \varphi \rangle = \iint_{\mathbb{R}^{2d}} \frac{1}{J_t(Y(t, x))} \delta(Y(t, x) - y) \varphi(x, y) dx dy = \int_{\mathbb{R}^d} \varphi(X(t, y), y) dy,$$

and thus we can also express $\mu_{t,y} = \delta(x - X(t, y))$. In summary we obtain that

$$\Upsilon_{t,y}(x, p) = \delta(x - X(t, y)) \delta(p - u(t, X(t, y))).$$

a.e. on $\operatorname{supp} \rho_0 \subseteq \mathbb{R}^d$. In other words, the Young measure $\Upsilon_{t,y}$ is supported in a single point (on phase space). By a well known result in measure theory, cf. [34, Proposition 1], this is equivalent to the local in-measure convergence of the associated family of trajectories $X^\varepsilon, P^\varepsilon$ and we are done. \square

The proof in particular shows, that, at least before caustic onset, the Young measure $\Upsilon_{t,y}$ is independent of the choice of ρ_0^ε , even though the Bohmian flow X^ε is not.

Remark 3.2. It is certainly possible to obtain Theorem 3.1 under weaker regularity assumption on V, a_0^ε , and S_0 , which are imposed here only for the sake of simplicity. The assumption of V and S_0 being sub-quadratic, however, cannot be relaxed, if one wants to guarantee the existence of a non-zero caustic onset time $T^* > 0$ uniformly in $x \in \mathbb{R}^d$, see, e.g., [15] for a counter-example. Explicit examples of initial phases S_0 , for which $T^* = +\infty$ (i.e., no caustic) are easily found in the case $V(x) \equiv 0$. Namely, either plane waves: $S_0(x) = k \cdot x$, where $k \in \mathbb{R}^d$ is a given wave vector, or $S_0(x) = -|x|^2$, yielding a rarefaction wave for $t \in \mathbb{R}_+$, see [26]. In these situations, we obtain in-measure convergence of the Bohmian trajectories $(X^\varepsilon, P^\varepsilon)$, and consequently also uniform convergence of X^ε , locally on every Borel set $\Omega \subseteq \{\mathbb{R}_t \times \text{supp } \rho_0\}$ with finite Lebesgue measure.

4. SUPERPOSITION OF WKB STATES AND BOHMIAN MEASURES

4.1. Bohmian measure for multi-phase WKB states. In view of Fig. 1, we expect that for $|t| > T^*$, i.e., after caustic onset, the correct asymptotic description of ψ^ε is given by a superposition of WKB states, also known as *multi-phase ansatz*. In order to gain more insight into situations where this is indeed the case we shall, as a first step, study the classical limit of the corresponding Bohmian measure. To this end, let $\Omega \subset \mathbb{R}_t \times \mathbb{R}_x^d$ be some open set and consider ψ^ε to be given in the following form:

$$\psi^\varepsilon(t, x) = \sum_{j=1}^N b_j(t, x) e^{iS_j(t, x)/\varepsilon} + r_\varepsilon(t, x), \quad (29)$$

where $b_j \in C^\infty(\Omega; \mathbb{C})$ are some smooth amplitudes and the real-valued phases $S_j \in C^\infty(\Omega; \mathbb{R})$ locally solve

$$\partial_t S_j + \frac{1}{2} |\nabla S_j|^2 + V(x) = 0 \quad \text{for all } j = 1, \dots, N, \quad (30)$$

In addition, r_ε denotes a possible remainder term (the assumptions on which will be made precise in the theorem below).

Remark 4.1. As we shall see in Section 5, the multi-phase WKB form (29) can be rigorously established, locally on every connected component of $(\mathbb{R}_t \times \mathbb{R}_x^d) \setminus \mathcal{C}$, i.e., locally away from caustics.

The second main result of this work establishes an explicit formula for the limiting Bohmian measure β associated to a wave function of the form (29). More precisely we prove the following:

Theorem 4.2. *Let ψ^ε be as in (29), with $b_j \in C^\infty(\Omega; \mathbb{C})$, $S_j \in C^\infty(\Omega; \mathbb{R})$, for all $j = 1, \dots, N$, where $\Omega \subset [0, T] \times \mathbb{R}^d$ denotes some open set. Assume, in addition,*

$$\nabla S_j \neq \nabla S_k \quad \text{for all } j \neq k \in \{1, \dots, N\}, \quad (31)$$

and that the remainder $r_\varepsilon(t, x)$ satisfies

$$\|r_\varepsilon\|_{L_{\text{loc}}^2(\Omega)} = o(1), \quad \|\varepsilon \nabla r_\varepsilon\|_{L_{\text{loc}}^2(\Omega)} = o(1) \quad \text{as } \varepsilon \rightarrow 0_+. \quad (32)$$

Then

$$\beta^\varepsilon \xrightarrow{\varepsilon \rightarrow 0_+} \beta(t, x, p), \text{ in } L^\infty([0, T]; \mathcal{M}^+(\mathbb{R}_x^d \times \mathbb{R}_p^d)) \text{ weak-}^*,$$

where β is given by

$$\beta(t, x, p) = \int_{\mathbb{T}^N} \Gamma(t, x, \theta) \delta\left(p - \frac{\sum_{j,k=1}^N \nabla S_j(t, x) \Gamma_{j,k}(t, x, \theta)}{\Gamma(t, x, \theta)}\right) d\theta.$$

with $\theta = (\theta_1, \dots, \theta_N) \in \mathbb{T}^N$, and

$$\Gamma(t, x, \theta) := \left| \sum_{j=1}^N b_j(t, x) e^{i\theta_j} \right|^2, \quad \Gamma_{j,k}(t, x, \theta) := \operatorname{Re} \left(b_j \bar{b}_k e^{i(\theta_j - \theta_k)} \right). \quad (33)$$

The above formula for β generalizes equation (6.6) given in [43] and states that β in general is a *diffuse measure* in the momentum variable $p \in \mathbb{R}^d$, unless all but one $b_j = 0$. Note that, in the case where $N = 1$, β simplifies to a mono-kinetic phase space measure, i.e.,

$$\beta(t, x, p) = |b(t, x)|^2 \delta(p - \nabla S(t, x)).$$

We already know from Assertion (i) of Theorem 3.1 that this holds for $|t| < T^*$, i.e., before caustic onset.

Proof. By our assumptions, it is easy to check that $\rho^\varepsilon = |\psi^\varepsilon|^2 = \tilde{\rho}^\varepsilon + r_{1,\varepsilon}$ and $J^\varepsilon = \varepsilon \operatorname{Im}(\overline{\psi^\varepsilon}(t, x) \nabla \psi^\varepsilon(t, x)) = \tilde{J}^\varepsilon + r_{2,\varepsilon}$, where

$$\tilde{\rho}^\varepsilon := \sum_{j,k=1}^N b_j \bar{b}_k e^{i(S_j - S_k)/\varepsilon}, \quad \tilde{J}^\varepsilon := \sum_{j,k=1}^N \nabla S_j \operatorname{Re} \left(b_j \bar{b}_k e^{i(S_j - S_k)/\varepsilon} \right).$$

and

$$\|r_{1,\varepsilon}\|_{L^1_{\text{loc}}(\Omega)} = o(1), \quad \|r_{2,\varepsilon}\|_{L^1_{\text{loc}}(\Omega)} = o(1).$$

In order to derive the classical limit as $\varepsilon \rightarrow 0_+$ of the Bohmian measure β^ε , we need to compute the limit of expressions of the following form

$$\iint_{\Omega} \sigma(t, x) \rho^\varepsilon(t, x) \varphi \left(t, \frac{J^\varepsilon(t, x)}{\rho^\varepsilon(t, x)} \right) dx dt, \quad (34)$$

where $\varphi, \sigma \in C_c^\infty([0, T] \times \mathbb{R}^d; \mathbb{R})$ are smooth and compactly supported. To this end, we first note that, because φ is smooth and compactly supported, the map

$$\mathbb{R}^+ \times \mathbb{R}^d \ni (s, v) \mapsto s \varphi \left(t, \frac{v}{s} \right)$$

is Lipschitz (uniformly with respect to t), which implies

$$\left\| \rho^\varepsilon \varphi \left(t, \frac{J^\varepsilon}{\rho^\varepsilon} \right) - \tilde{\rho}^\varepsilon \varphi \left(t, \frac{\tilde{J}^\varepsilon}{\tilde{\rho}^\varepsilon} \right) \right\|_{L^1_{\text{loc}}(\Omega)} \leq C \left(\|r_{1,\varepsilon}\|_{L^1_{\text{loc}}(\Omega)} + \|r_{2,\varepsilon}\|_{L^1_{\text{loc}}(\Omega)} \right) = o(1).$$

In particular, to compute the limit as $\varepsilon \rightarrow 0_+$ of the expression in (34) it suffices to consider

$$\iint_{\Omega} \sigma(t, x) \tilde{\rho}^\varepsilon(t, x) \varphi \left(t, \frac{\tilde{J}^\varepsilon(t, x)}{\tilde{\rho}^\varepsilon(t, x)} \right) dx dt. \quad (35)$$

We now use the following result, whose proof is postponed to the end.

Lemma 4.3. *There exists a set $\Sigma \subset \Omega$ of \mathcal{L}^{d+1} -measure zero such that, for all $j, k, \ell \in \{1, \dots, N\}$ with $k \neq \ell$,*

$$\frac{S_j(t, x) - S_k(t, x)}{S_j(t, x) - S_\ell(t, x)} \notin \mathbb{Q} \quad \text{for all } (t, x) \in \Omega \setminus \Sigma.$$

Using this lemma, we deduce that for \mathcal{L}^{d+1} -a.e. (t, x) , the frequencies

$$\frac{S_1(t, x) - S_k(t, x)}{\varepsilon}, \quad k = 2, \dots, N,$$

are all rationally independent, which implies that the “trajectories”

$$\varepsilon \mapsto \left(\cos\left(\frac{S_2 - S_1}{\varepsilon}\right), \dots, \cos\left(\frac{S_N - S_1}{\varepsilon}\right) \right)$$

and

$$\varepsilon \mapsto \left(\sin\left(\frac{S_2 - S_1}{\varepsilon}\right), \dots, \sin\left(\frac{S_N - S_1}{\varepsilon}\right) \right)$$

are both dense on the $(N - 1)$ -dimensional torus \mathbb{T}^{N-1} . By standard results on two-scale convergence (see for instance [1]), we consequently obtain that for any continuous and compactly supported test function $\vartheta : \Omega \times \mathbb{C}^{N-1} \rightarrow \mathbb{R}$,

$$\begin{aligned} \int_{\Omega} \vartheta \left(t, x, e^{i(S_2 - S_1)/\varepsilon}, \dots, e^{i(S_N - S_1)/\varepsilon} \right) dx dt \\ \xrightarrow{\varepsilon \rightarrow 0^+} \int_{\Omega} \int_{\mathbb{T}^{N-1}} \vartheta \left(t, x, e^{i\theta_1}, \dots, e^{i\theta_{N-1}} \right) d\theta_1 \dots d\theta_{N-1} dx dt. \end{aligned}$$

Moreover, we observe that for any j, k we can write

$$\frac{S_j - S_k}{\varepsilon} = \frac{S_j - S_1}{\varepsilon} + \frac{S_1 - S_k}{\varepsilon}.$$

Hence the expression in (35) converges to

$$\begin{aligned} \iint_{\Omega} \sigma(t, x) \int_{\mathbb{T}^{N-1}} \sum_{j,k=1}^N b_j \bar{b}_k e^{i(\theta_{j-1} - \theta_{k-1})} \\ \varphi \left(t, \frac{\sum_{j,k=1}^N \nabla S_j \operatorname{Re}(b_j \bar{b}_k e^{i(\theta_{j-1} - \theta_{k-1})})}{\sum_{j,k=1}^N b_j \bar{b}_k e^{i(\theta_{j-1} - \theta_{k-1})}} \right) d\theta_1 \dots d\theta_{N-1} dx dt, \end{aligned}$$

where by convention $\theta_0 \equiv 0$. Finally, let us observe that one can also rewrite the obtained expression in a more symmetric form by performing the change of variables $\theta_{j-1} \leftrightarrow \theta_j - \theta_1$, and it is immediate to check that under this transformation the above expression is equal to

$$\iint_{\Omega} \sigma(t, x) \int_{\mathbb{T}^N} \Gamma(t, x, \theta) \varphi \left(t, \frac{\sum_{j,k=1}^N \nabla S_j \Gamma_{j,k}(t, x, \theta)}{\Gamma(t, x, \theta)} \right) d\theta dx dt,$$

where $\theta = (\theta_1, \dots, \theta_N)$, and Γ and $\Gamma_{j,k}$ are defined in (33). By the arbitrariness of φ and σ , this proves the desired result. \square

We are now left with the proof of Lemma 4.3.

Proof of Lemma 4.3. The set Σ can be described as

$$\bigcup_{j,k,\ell, k \neq \ell} \bigcup_{m \neq n \in \mathbb{Z}} S_{j,k,\ell}^{m,n},$$

where

$$S_{j,k,\ell}^{m,n} := \{(t, x) \in \Omega : m[S_j(t, x) - S_k(t, x)] + n[S_j(t, x) - S_\ell(t, x)] = 0\}.$$

We now claim that each $S_{j,k,\ell}^{m,n}$ is a smooth hypersurface in Ω , which implies in particular that $S_{j,k,\ell}^{m,n}$ (and so also Σ) has measure zero. To prove that this is indeed the case, it suffices to check, in view of the implicit function theorem, that the gradient of the function

$$(t, x) \mapsto m[S_j(t, x) - S_k(t, x)] + n[S_j(t, x) - S_\ell(t, x)]$$

is nowhere zero. Assume by contradiction that this is not the case, i.e., there exists a point $(t, x) \in \Omega$ where

$$\begin{aligned}(m+n)\partial_t S_j(t, x) &= m\partial_t S_k(t, x) + n\partial_t S_\ell(t, x), \\ (m+n)\nabla S_j(t, x) &= m\nabla S_k(t, x) + n\nabla S_\ell(t, x).\end{aligned}$$

By (30), the first equation above becomes

$$(m+n)|\nabla S_j(t, x)|^2 = m|\nabla S_k(t, x)|^2 + n|\nabla S_\ell(t, x)|^2,$$

which combined with the second equation gives

$$(m+n) \left| \frac{m}{m+n} \nabla S_k(t, x) + \frac{n}{m+n} \nabla S_\ell(t, x) \right|^2 = m|\nabla S_k(t, x)|^2 + n|\nabla S_\ell(t, x)|^2.$$

By strict convexity of $|\cdot|^2$, the above relation is possible if and only if $\nabla S_k(t, x) = \nabla S_\ell(t, x)$, which contradicts (31) and concludes the proof. \square

4.2. Comparison to Wigner measures. An important consequence of Theorem 4.2 concerns the connection between the limiting Bohmian measure β and the Wigner measure $w \in \mathcal{M}^+(\mathbb{R}_x^d \times \mathbb{R}_p^d)$ associated to ψ^ε . To this end, let us first recall the definition of the ε -scaled Wigner transform w^ε given in [3, 27, 41]:

$$w^\varepsilon(t, x, p) := \frac{1}{(2\pi)^d} \int_{\mathbb{R}^d} \psi^\varepsilon\left(t, x - \frac{\varepsilon}{2}\eta\right) \overline{\psi^\varepsilon}\left(t, x + \frac{\varepsilon}{2}\eta\right) e^{i\eta \cdot p} d\eta.$$

Provided $\psi^\varepsilon(t)$ is uniformly bounded in L^2 with respect to ε , it is well known that, cf. [27, 41] there exists a limit $w(t, x, p)$ such that

$$w^\varepsilon \xrightarrow{\varepsilon \rightarrow 0^+} w, \text{ in } L^\infty(\mathbb{R}_t; \mathcal{M}^+(\mathbb{R}_x^d \times \mathbb{R}_p^d)) \text{ weak-}^*.$$

In addition, one finds $w(t) \in \mathcal{M}^+(\mathbb{R}_x^d \times \mathbb{R}_p^d)$, usually called *Wigner measure* (or semi-classical defect measure). The latter is known to give the possibility to compute the classical limit of all expectation values of physical observables via

$$\lim_{\varepsilon \rightarrow 0} \langle \psi^\varepsilon(t), \text{Op}^\varepsilon(a) \psi^\varepsilon(t) \rangle_{L^2(\mathbb{R}^d)} = \iint_{\mathbb{R}_{x,p}^{2d}} a(x, p) w(t, x, p) dx dp,$$

where the $\text{Op}^\varepsilon(a)$ is a self-adjoint operator obtained by Weyl-quantization of the corresponding classical symbol $a \in \mathcal{S}(\mathbb{R}_x^d \times \mathbb{R}_p^d)$, see [27, 49] for a precise definition. In addition, if $\psi^\varepsilon(t)$ is ε -oscillatory, i.e., satisfies (19), we also have that the zeroth and first p -moment of w yield the classical limit of ρ^ε and J^ε , i.e.,

$$\rho^\varepsilon(t, x) \xrightarrow{\varepsilon \rightarrow 0^+} \int_{\mathbb{R}^d} w(t, x, dp), \quad J^\varepsilon(t, x) \xrightarrow{\varepsilon \rightarrow 0^+} \int_{\mathbb{R}^d} p w(t, x, dp),$$

where the limits have to be understood in $L^\infty(\mathbb{R}_t; \mathcal{M}^+(\mathbb{R}_x^d))$ weak- * . Note that this is indeed *analogous* to (21).

For a given superposition of WKB states such as (29), the associated Wigner measure has been computed in [41] (see also [49]): under the same assumption on the phases, i.e., $\nabla S_j \neq \nabla S_k$ for all $j \neq k$, one explicitly finds

$$w(t, x, p) = \sum_{j=1}^N |b_j(t, x)|^2 \delta(p - \nabla S_j(t, x)). \quad (36)$$

From this explicit formula we immediately conclude the following important corollary.

Corollary 4.4. *Let $b_j \neq 0$. Then, under the same assumptions as in Theorem 4.2 we have that, in the sense of measures, $\beta = w$ if and only if $N = 1$.*

Proof. For $b_j \neq 0$ and $N > 1$ we see from Theorem 4.2 that β is a diffuse measure in the momentum variable $p \in \mathbb{R}^d$, and thus $\beta \neq w$ in view of (36). On the other hand, if $N = 1$ then, both w and β simplify to the same mono-kinetic phase space distribution. \square

In view of Assertion (i) of Theorem 3.1 we conclude that before caustic onset, the classical limit of all physical observables can be computed by taking moments of the limiting Bohmian measure, since in fact $\beta = w$ for $|t| < T^*$. After caustic onset, however, this is in general *no longer* the case (see Section 5).

Still, we do know (by weak compactness arguments) that the *zeroth* and *first moments* w.r.t. $p \in \mathbb{R}^d$ of β and w are *the same* for all times $t \in \mathbb{R}$. For completeness, we check this explicitly in the case of multi-phase WKB states: using the fact that

$$\int_{\mathbb{T}} \cos(\theta) d\theta = \int_{\mathbb{T}} \sin(\theta) d\theta = 0,$$

we compute

$$\begin{aligned} \int_{\mathbb{R}^d} \beta(t, x, dp) &= \sum_{j,k=1}^N b_j(t, x) \bar{b}_k(t, x) \int_{\mathbb{T}^N} e^{i(\theta_j - \theta_k)} d\theta_1 \dots d\theta_N \\ &= \sum_{j=1}^N |b_j(t, x)|^2 = \int_{\mathbb{R}^d} w(t, x, dp). \end{aligned}$$

Moreover

$$\begin{aligned} \int_{\mathbb{R}^d} p \beta(t, x, dp) &= \sum_{j,k=1}^N \nabla S_j(t, x) \int_{\mathbb{T}^N} \operatorname{Re} \left(b_j(t, x) \bar{b}_k(t, x) e^{i(\theta_j - \theta_k)} \right) d\theta_1 \dots d\theta_N \\ &= \sum_{j=1}^N \nabla S_j(t, x) |b_j(t, x)|^2 = \int_{\mathbb{R}^d} p w(t, x, dp). \end{aligned}$$

In other words, in the case of multi-phase WKB states, the difference between w and β can only manifest itself in p -moments of order two or higher.

5. A COMPLETE DESCRIPTION IN THE FREE CASE AND POSSIBLE EXTENSIONS

In this section we shall give a (fairly) complete description of the classical limit of Bohmian dynamics in the case of the *free Schrödinger equation* corresponding to $V = 0$. The proof will rely on classical stationary phase techniques. For the case $V \neq 0$ decisively more complicated methods based on Fourier integral operators have to be employed, as will be discussed in Section 5.3.

5.1. Multi-phase WKB for vanishing potential. Consider the free Schrödinger equation with WKB initial data:

$$i\varepsilon \partial_t \psi^\varepsilon + \frac{\varepsilon^2}{2} \Delta \psi^\varepsilon = 0, \quad \psi^\varepsilon|_{t=0} = a_0(x) e^{iS_0(x)/\varepsilon}, \quad (37)$$

In this case, we find the free Hamilton-Jacobi equation, which is obviously given by

$$\partial_t S + \frac{1}{2} |\nabla S|^2 = 0, \quad S|_{t=0} = S_0, \quad (38)$$

and the corresponding classical Hamiltonian equations (13) simplify to

$$\begin{cases} \dot{X}(t, y) = P(t, y), & X(0, y) = y, \\ \dot{P}(t, y) = 0, & P(0, y) = \nabla S_0(y). \end{cases} \quad (39)$$

This implies that, for all $t \in \mathbb{R}_+$, $P(t, y) = \nabla S_0(y)$ and

$$X(t, y) = y + t\nabla S_0(y). \quad (40)$$

Consequently, the caustic set is given by $\mathcal{C}_{\text{free}} = \{(x, t) : x \in \mathcal{C}_t^{\text{free}}\}$ where for $x \equiv X(t, y)$ we set:

$$\mathcal{C}_t^{\text{free}} = \{x \in \mathbb{R}^d : \exists y \in \mathbb{R}^d \text{ satisfying (40) and } \det(\text{Id} + t\nabla^2 S_0(y)) = 0\}.$$

In particular, we see that in the free case, the caustic onset time $T^* > 0$ is solely determined by the (sub-quadratic) initial phase $S_0(y)$. In order to proceed we need to slightly strengthen our assumption on the initial phase S_0 .

Assumption 5.1. The initial phase $S_0 \in C^\infty(\mathbb{R}^d; \mathbb{R})$ is assumed to be sub-quadratic and

$$\lim_{|y| \rightarrow \infty} \frac{|\nabla S_0(y)|}{|y|} = 0.$$

In other words we need that S_0 grows strictly less than quadratically at infinity. This is the same assumption as in [7], guaranteeing that the map $y \mapsto X(t, y)$ is proper and onto.

In the following we shall denote by $x \mapsto y \equiv Y(t, x)$ the inverse mapping of (40). Clearly, for $|t| > T^*$ this inverse will not be unique in general, i.e., for each fixed $(t, x) \in \mathbb{R}_t \times \mathbb{R}_x^d$ there is $N(t, x) \in \mathbb{N}$ and corresponding $Y_j(t, x)$, with $j = 1, \dots, N(t, x)$, satisfying the implicit relation

$$Y_j(t, x) + t\nabla S_0(Y_j(t, x)) = x. \quad (41)$$

Assumption 5.1 guarantees that in each connected component of $(\mathbb{R}_t \times \mathbb{R}^d) \setminus \mathcal{C}_{\text{free}}$ there are only finitely many $\{Y_j(t, x)\}$. (This follows by properness of the characteristic map and the implicit function theorem, see [7, Lemma 1.1].) In addition, in each such connected component $N(t, x) = \text{const}$. Moreover, under the same assumptions on S_0 , we already know that the caustic onset time T^* is positive, and thus there is exactly one connected component Ω_0 of $(\mathbb{R}_t \times \mathbb{R}^d) \setminus \mathcal{C}_{\text{free}}$ containing $\{t = 0\}$.

In order to proceed further, we also recall that the solution of (37) admits an explicit representation in the form of an ε -oscillatory integral

$$\psi^\varepsilon(t, x) = \left(\frac{1}{\sqrt{2\pi i \varepsilon t}} \right)^d \int_{\mathbb{R}^d} a_0(y) e^{i\Phi(t, x, y)/\varepsilon} dy, \quad (42)$$

where the phase is given by

$$\Phi(t, x, y) := S_0(y) + \frac{|x - y|^2}{2t}. \quad (43)$$

It is well known that, for $\varepsilon \rightarrow 0_+$, the representation formula (42) can be treated by the stationary phase techniques (see, e.g., Theorem 7.7.6. of [32]) and we consequently obtain the following lemma.

Lemma 5.1. *Let $a_0 \in \mathcal{S}(\mathbb{R}^d; \mathbb{C})$ and S_0 satisfy Assumption 5.1. Then, for all $(t, x) \in (\mathbb{R}_t \times \mathbb{R}^d) \setminus \mathcal{C}_{\text{free}}$ the solution of (37) satisfies*

$$\psi^\varepsilon(t, x) \stackrel{\varepsilon \rightarrow 0_+}{=} \sum_{j=1}^{N(t, x)} a_j(t, x) e^{i\pi\kappa_j(t, x)/4} e^{i\Phi(t, x, Y_j(t, x))/\varepsilon} + r_\varepsilon(t, x), \quad (44)$$

where $\Phi(t, x, y)$ is given by (43), $\kappa_j(t, x) \in \mathbb{N}$ denotes the Maslov factor, and

$$a_j(t, x) = \frac{a_0(Y_j(t, x))}{|\det(\text{Id} + t\nabla^2 S_0(Y_j(t, x)))|^{1/2}}. \quad (45)$$

In addition, the remainder r^ε satisfies

$$\|r_\varepsilon\|_{C^0(\Omega)} = O(\varepsilon), \quad \|r_\varepsilon\|_{C^1(\Omega)} = O(1) \quad \text{as } \varepsilon \rightarrow 0_+, \quad (46)$$

uniformly on compact subsets $\Omega \subset (\mathbb{R}_t \times \mathbb{R}^d) \setminus \mathcal{C}_{\text{free}}$.

Remark 5.2. The first remainder estimate $\|r_\varepsilon\|_{C^0(\Omega)} = O(\varepsilon)$ is classical, whereas the second one can be obtained by noticing that the operator ∇ commutes with the free Schrödinger equation (37). Thus, we find that $\nabla\psi^\varepsilon$ satisfies an integral representation analogous to (42), i.e.,

$$\nabla\psi^\varepsilon(t, x) = \left(\frac{1}{\sqrt{2\pi i \varepsilon t}} \right)^d \int_{\mathbb{R}^d} e^{i|x-y|^2/(2t\varepsilon)} \nabla\psi_0^\varepsilon(y) dy.$$

By applying the stationary phase lemma to this oscillatory integral one readily infers the estimate $\|r_\varepsilon\|_{C^1(\Omega)} = O(1)$.

Next, we note that, in view of (43) and (41), we explicitly have

$$\begin{aligned} \Phi(t, x, Y_j(t, x)) &\equiv S_0(Y_j(t, x)) + \frac{1}{2t}|x - Y_j(t, x)|^2 \\ &= S_0(Y_j(t, x)) + \frac{t}{2}|\nabla S_0(Y_j(t, x))|^2. \end{aligned} \quad (47)$$

On the other hand, since for $V(x) = 0$ it holds that $P(t, y) = \nabla S_0(y)$ (i.e., P is constant along the characteristics), the solution formula (14) yields, for all $j = 1, \dots, N$:

$$\begin{aligned} S_j(t, x) &= S_0(Y_j(t, x)) + \int_0^t \frac{1}{2}|P(\tau, y)|^2 d\tau \Big|_{y=Y_j(t, x)} \\ &= S_0(Y_j(t, x)) + \frac{t}{2}|\nabla S_0(Y_j(t, x))|^2. \end{aligned} \quad (48)$$

We consequently infer that $\Phi(t, x, Y_j(t, x)) \equiv S_j(t, x)$ is a smooth solution of the free Hamilton-Jacobi equation (38) for all $j = 1, \dots, N(t, x)$. Obviously, we also have that a_j given by (45) solves the corresponding transport equation (15) with $S \equiv S_j$.

Remark 5.3. An alternative way of showing that $\Phi(t, x, Y_j(t, x))$ solves the free Hamilton-Jacobi equation is to plug (47) into (38) and use (41) to implicitly differentiate with respect to t and x . A lengthy but straightforward computation then yields the desired result.

For completeness we also recall that the Maslov factor is explicitly given by [32]

$$\mathbb{N} \ni \kappa_j(t, x) = m_j^+(t, x) - m_j^-(t, x),$$

where $m^\pm(t, x) \in \mathbb{N}$ denotes, respectively, the number of positive or negative eigenvalues of the matrix $\text{Id} + t\nabla^2 S_0(Y_j(t, x))$. Note that κ_j can also be written in the form

$$\kappa_j(t, x) = d - 2m_j^-(t, x).$$

By the implicit function theorem, $\kappa(t, x) = \text{const.}$ in every connected component of $(\mathbb{R}_t \times \mathbb{R}_x^d) \setminus \mathcal{C}_{\text{free}}$, see, e.g., [7].

5.2. WKB analysis of Bohmian dynamics in the free case. From what is said above, we infer that in each connected component Ω of $(\mathbb{R}_t \times \mathbb{R}_x^d) \setminus \mathcal{C}_{\text{free}}$, the solution ψ^ε admits the approximation (44), so Theorem 4.2 can be applied after identifying

$$b_j(t, x) = a_j(t, x)e^{i\pi\kappa_j(t, x)/4} \equiv a_j(t, x)e^{i\pi\kappa_\Omega/4}, \quad j = 1, \dots, N(t, x) \equiv N_\Omega,$$

where $\kappa_\Omega \in \mathbb{R}$ and $N_\Omega \in \mathbb{N}$ are constants depending only on Ω . Consequently, we obtain the following result.

Theorem 5.4. *Let $a_0 \in \mathcal{S}(\mathbb{R}^d; \mathbb{C})$ and S_0 satisfy Assumption 5.1. Denote by Ω_0 the connected component of $(\mathbb{R}_t \times \mathbb{R}_x^d) \setminus \mathcal{C}_{\text{free}}$ containing $\{t = 0\}$. Then it holds:*

(i) *The limiting Bohmian measure satisfies*

$$\beta(t, x, p) = w(t, x, p) = \rho(t, x)\delta(p - u(t, x)), \quad \forall (t, x) \in \Omega_0,$$

and the Bohmian trajectories converge

$$X^\varepsilon(t, y) \xrightarrow{\varepsilon \rightarrow 0^+} y + t\nabla S_0(y), \quad P^\varepsilon(t, y) \xrightarrow{\varepsilon \rightarrow 0^+} \nabla S_0(y),$$

locally in measure on $\Omega_0 \cap \{\mathbb{R}_t \times \text{supp}\rho_0\}$.

(ii) *Outside of Ω_0 there are regions $\Omega \subseteq (\mathbb{R}_t \times \mathbb{R}_x^d) \setminus \mathcal{C}_{\text{free}}$ where $\beta \neq w$ and where the Bohmian momentum P^ε does not converge locally in-measure to the classical momentum P .*

(iii) *There exist initial data a_0 such that, outside of Ω_0 , there are regions $\tilde{\Omega} \subseteq (\mathbb{R}_t \times \mathbb{R}_x^d) \setminus \mathcal{C}_{\text{free}}$ in which both X^ε and $P^\varepsilon = \dot{X}^\varepsilon$ do not converge to the classical flow.*

Note that Assertion (i) is slightly stronger than Theorem 3.1 (i) in the sense that Ω_0 is strictly larger than $[0, T^*) \times \mathbb{R}_x^d$. The proof shows that if $|a_0| > 0$ on all of \mathbb{R}^d , Assertion (ii) holds for any connected component $\Omega \neq \Omega_0$ whose boundary intersects the boundary of Ω_0 .

Proof. We first note that for all $(t, x) \in \Omega_0$ it holds $N(t, x) = 1$ and $\kappa_j(t, x) = 0$. In view of the remainder estimates stated in Lemma 5.1 we thus can apply Theorem 4.2 with $N = 1$ to obtain

$$\beta(t, x, p) = \rho(t, x)\delta(p - \nabla S(t, x)),$$

where $\rho = |a|^2$. With this in mind, the result on the convergence of the Bohmian trajectories follows verbatim from the proof of Theorem 3.1 (ii). This proves the first assertion.

In order to prove Assertion (ii), we first note that outside of Ω_0 we have (in general) more than one branch, i.e., $N(t, x) > 1$. For instance, assume that $|a_0| > 0$ on \mathbb{R}^d , and let $\Omega \neq \Omega_0$ be a connected component whose boundary intersects the boundary of Ω_0 . Then it is not difficult to see that $N_\Omega \neq 1$, as otherwise one could show that no caustics can occur on $\partial\Omega_0 \cap \partial\Omega$. Next, we recall that in each connected component Ω of $(\mathbb{R}_t \times \mathbb{R}_x^d) \setminus \mathcal{C}_{\text{free}}$ the phase $\Phi(t, x, Y_j(t, x)) \equiv S_j(t, x)$ is a

smooth solution of the Hamilton-Jacobi equation (10). By the method of characteristics we have that

$$\nabla\Phi(t, x, Y_j(t, x)) \equiv \nabla S_j(t, x) = P(t, Y_j(t, x)) = \nabla S_0(Y_j(t, x)),$$

since $P(t, y)$ is constant along characteristics (recall that $V(x) = 0$). Hence, assuming by contradiction that $\nabla S_j = \nabla S_k$ for some $j \neq k$, the above identity together with (40) yields $Y_j(t, x) = Y_k(t, x)$, which is impossible by construction. This implies that in each connected component Ω we can apply Theorem 4.2 to conclude that β in general is a diffuse measure in $p \in \mathbb{R}^d$, unless all but one of the $a_j = 0$ in Ω . In view of (45), the latter cannot be the case if $|a_0| > 0$ on \mathbb{R}^d . Corollary 4.4 then immediately implies $\beta \neq w$. On the other hand, since for WKB initial data we have that ρ_0^ε is indeed ε -independent, we can apply (22) in Ω to infer that the Young measure $\Upsilon_{t,y}$ is diffusive in p (since β is). This, however, prohibits the convergence of P^ε locally in measure, since the latter is equivalent to $\Upsilon_{t,y}$ being concentrated in a single point.

The result in (ii) may still give some hopes for the convergence of X^ε to X , since the fact that $\dot{X}^\varepsilon = P^\varepsilon$ gives more compactness for the curves in the x -variables. However, we shall see that this is not the case.

Consider indeed the example described in Fig. 1 and Fig. 7 (so $d = 1$). These figures suggest that for ψ_0^ε as in (56) convergence should not hold. To show this rigorously, we begin by observing that $\rho(t, x) > 0$ on $\mathbb{R}_t \times \mathbb{R}_x$ (this follows from the explicit formula for $\rho = |a|^2$, but it can also be seen from Fig. 1 observing there only the trajectories starting inside $[0, 1]$ are plotted). Since ρ is smooth, this implies that for $R, T > 0$ there exists a positive constant $c_{R,T}$ such that

$$\rho(t, x) \geq c_{R,T} \quad \text{for } (t, x) \in [0, T] \times [-R, R].$$

In particular, since ψ^ε is given by (44) with r_ε small in C^0 , see (46), it follows that

$$\rho^\varepsilon(t, x) \geq \frac{c_{R,T}}{2} \quad \text{for } (t, x) \in [0, T] \times [-R, R] \quad (49)$$

for all $\varepsilon > 0$ sufficiently small (the smallness depending on T and R). Recalling that

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

and that J^ε and ρ^ε are both smooth, it follows from (49) that u^ε is smooth as well inside $[0, T] \times [-R, R]$. In particular, by the Cauchy-Lipschitz theorem, the Bohmian trajectories X^ε can never cross inside $[0, T] \times [-R, R]$. Since by symmetry $X^\varepsilon(t, 1/2) = 1/2$ for all $t \geq 0$ (see Fig. 1 and Fig. 7), this implies in particular that, for all $t \in [0, T]$:

$$X^\varepsilon(t, x) \geq 1/2 \quad \forall x \geq 1/2, \quad X^\varepsilon(t, x) \leq 1/2 \quad \forall x \leq 1/2.$$

Letting $\varepsilon \rightarrow 0$ we deduce that X^ε does not converge to X (locally) in measure on $\tilde{\Omega} \equiv [0, T] \times [-R, R]$, since otherwise the above property would give

$$X(t, x) \geq 1/2 \quad \forall x \geq 1/2, \quad X(t, x) \leq 1/2 \quad \forall x \leq 1/2$$

for all $t \geq 0$, which is not the case (see Fig. 1). This proves Assertion (iii). \square

Remark 5.5. Note that for $|t| > T^*$, i.e., after caustic onset, the Wigner measure is given by (36) for all $(t, x) \in (\mathbb{R}_t \times \mathbb{R}_x^d) \setminus \mathcal{C}_{\text{free}}$. In particular, this shows that w is *insensitive* to the Maslov phase shifts, since $|a_j|^2 = |b_j|^2$ for all $j = 1, \dots, N(t, x)$. The limiting Bohmian measure β , however, *incorporates* these phase shifts in view

of the formula given in Theorem 4.2. However, as we have seen in Section 4.2 these phase shift do not enter in the classical limit of ρ^ε and J^ε .

5.3. Extension to the non-zero potential case. In the case where $V(x) \neq 0$ the situation becomes considerably more complicated, due to a lack of an explicit integral representation for the exact solution ψ^ε of (1). The only exception therefrom is the case of a polynomial $V(x)$ of degree (at most) two, in which case one has *Mehler's formula* replacing (42), see, e.g., [33]. In order to proceed further in situations where V is a more general (sub-quadratic) potential, one needs to approximate the full Schrödinger propagator

$$U^\varepsilon(t) = e^{-iH^\varepsilon t}, \quad \text{with } H^\varepsilon = -\frac{\varepsilon^2}{2}\Delta + V(x),$$

for $0 < \varepsilon \ll 1$ by a semi-classical *Fourier integral operator* [20, 48]. Early results on this can be found in [18, 25], where the occurrence of caustics makes the approximation valid only locally in-time. This problem can be overcome, by considering a class of Fourier integral operators whose Schwartz kernel furnishes an ε -oscillatory integral with *complex* phase and quadratic imaginary part, see [39, Theorem 2.1] for a precise definition. Using this, the authors of [39] construct a global in-time approximation of $U^\varepsilon(t)$ for potentials satisfying $V \in C_b^\infty(\mathbb{R}^d)$, i.e., smooth and bounded together with all derivatives (see also [29, 35] for closely related results with slightly different assumptions). By applying the stationary phase lemma to this type of (global) Fourier integral operator, one infers the following result, as a slight generalization of [39, Theorem 5.1]:

Fix a point $(t_0, x_0) \in (\mathbb{R}_t \times \mathbb{R}_x^d) \setminus \mathcal{C}$, i.e., away from caustics, and as before denote by $Y_j(t, x)$ and $j = 1, \dots, N = N(t, x) \in \mathbb{N}$, the solutions of the equation $x = X(t, y)$, where $t \mapsto X(t, y)$ is the classical flow map induced by (13). Let $\{y \in \mathbb{R}^d : |a_0(y)| > 0\}$, be a sufficiently small neighborhood of

$$\{Y_1(t_0, x_0), \dots, Y_N(t_0, x_0)\} \subset \mathbb{R}^d, \quad (50)$$

i.e., the points obtained by tracing back the classical trajectories intersecting in $(t_0, x_0) \in (\mathbb{R}_t \times \mathbb{R}_x^d) \setminus \mathcal{C}$. Then the solution of (1) at $t = t_0$ admits the following approximative behavior:

$$\psi^\varepsilon(t_0, x) \stackrel{\varepsilon \rightarrow 0^+}{\approx} \sum_{j=1}^{N(t, x)} a_j(t_0, x) e^{i\pi(m_j^+(t_0, x) - m_j^-(t_0, x))/4} e^{iS_j(t_0, x)/\varepsilon} + r_\varepsilon(t_0, x), \quad (51)$$

where the amplitudes a_j and the (real-valued) phases S_j are, respectively, given by (15) and (14) with Y replaced by $Y_j(t_0, x)$, and $m_j^+(t_0, x)$ (resp. $m_j^-(t_0, x)$) is the number of positive (resp. negative) eigenvalues of the matrix $\nabla_y X_t(Y_j(t_0, x))$. In addition, the remainder r_ε satisfies

$$\|r_\varepsilon(t_0, \cdot)\|_{L^2(\Lambda)} = O(\varepsilon),$$

where $x \in \Lambda \subset \mathbb{R}^d$ is a *sufficiently small* neighborhood of $x_0 \in \mathbb{R}^d$. The above result (the proof of which can be found in [7]) replaces Lemma 5.1, valid in the free case. Note however, that one only infers a local result in some sufficiently small neighborhood of $x_0 \in \mathbb{R}^d$, provided the initial amplitude a_0 is sufficiently concentrated on (50). In order to obtain an estimate for $\varepsilon \nabla r_\varepsilon$, we note that by applying the Hamiltonian H^ε to (1), and having in mind that $V \in L^\infty(\mathbb{R}^d)$, we infer

$$\sup_{0 < \varepsilon \leq 1} \|\varepsilon^2 \Delta \psi^\varepsilon(t, \cdot)\|_{L^2} \leq C, \quad \forall t \in \mathbb{R}_+,$$

where $C > 0$ is independent of ε . In view of (51), we consequently obtain that $\|\varepsilon^2 \Delta r_\varepsilon\|_{L^2}$ is uniformly bounded w.r.t. ε and hence we can interpolate

$$\|\varepsilon \nabla r_\varepsilon\|_{L^2}^2 \leq C \|r_\varepsilon\|_{L^2} \|\varepsilon^2 \Delta r_\varepsilon\|_{L^2} = O(\varepsilon),$$

to obtain $\|\varepsilon \nabla r_\varepsilon\|_{L^2} = O(\sqrt{\varepsilon}) = o(1)$, as required in Theorem 4.2. In order to apply the latter we also require $\nabla S_j \neq \nabla S_k$ for $j \neq k \in \{1, \dots, N\}$. This follows, from similar arguments as has been done in the free case. Indeed, if the gradients were the same, by following backward the Hamiltonian flow we would get that the curves were starting from the same point, which is a contradiction.

Thus, after using appropriate localization arguments, the multi-phase form (51) combined with Theorem 4.2 allows to infer the *same* qualitative picture for the classical limit of Bohmian dynamics in the case $V \neq 0$, as we showed above for the free case. Using the same notation as above, we can summarize our discussion as follows.

Proposition 5.6. *Let $V \in C_b^\infty(\mathbb{R}^d)$ and S_0 satisfy Assumption 5.1. Let $(t_0, x_0) \in (\mathbb{R}_t \times \mathbb{R}_x^d) \setminus \mathcal{C}$, and assume that $\{y \in \mathbb{R}^d : |a_0(y)| > 0\}$ is a sufficiently small neighborhood of $\{Y_1(t_0, x_0), \dots, Y_N(t_0, x_0)\}$. Then there exists a small neighborhood $\mathcal{U} \subset \mathbb{R}_t \times \mathbb{R}_x^d$ of (t_0, x_0) such that $\beta \neq w$ inside $\mathcal{U} \times \mathbb{R}_p^d$. In particular, the Bohmian trajectories $(X^\varepsilon, P^\varepsilon)$ do not converge locally in measure to the classical Hamiltonian flow.*

6. NUMERICAL SIMULATION OF BOHMIAN TRAJECTORIES

In this section we shall numerically study the behavior of Bohmian trajectories, mainly in the semiclassical regime $0 < \varepsilon \ll 1$ and in particular in situations where caustics appear in the corresponding classical limit. Let us remark that the numerical implementation of Bohmian trajectories is used in applications of quantum chemistry, cf. [19, 28, 46], in particular in molecular dynamics, where the use of Bohmian trajectories allows for a unified approach in the computation of multi-particle systems. Indeed, it is an important challenge in quantum chemistry to model and to numerically solve processes in which some particles are rather heavy and thus behave essentially classically (e.g., the atomic nuclei of molecules), whereas others are very light and thus require a quantum mechanical treatment (e.g. the electrons). From the numerical point of view, the main problem is to compute the Bohm potential V_B^ε in an efficient and accurate manner, in particular in higher dimensions. In order to do so, Lagrangian schemes are often used, for which the authors of [46] propose the implementation of a Delaunay tessellation in order to be able to accurately compute Bohmian trajectories in two and three spatial dimensions. For a broader introduction to this subject we refer to [53].

6.1. Description of the numerical method. For the numerical tracking of Bohmian trajectories $(X^\varepsilon, P^\varepsilon)$ it is necessary to solve the system (6) for a given solution $\psi^\varepsilon(t, x)$ of the Schrödinger equation (1). To this end, we will always consider initial data $\psi_0^\varepsilon \in \mathcal{S}(\mathbb{R}^d)$, i.e., rapidly decreasing functions. This allows to numerically approximate the solution ψ^ε through a truncated Fourier series in the spatial coordinates by choosing the computational domain Ω_{com} sufficiently large, i.e., such that $|\psi^\varepsilon|$ is smaller than machine precision at the $\partial\Omega_{\text{com}}$ (we use double precision which is roughly equivalent to 10^{-16}). Thus the function can be periodically continued as a smooth function with maximal numerical precision. In our

numerical examples, we shall concentrate on the case of $d = 1$ spatial dimension. The x -dependence of ψ^ε is consequently treated with a discrete Fourier transformation realized via a Fast Fourier Transform (FFT) in Matlab. We thereby always choose the resolution large enough so that the modulus of the Fourier coefficients decreases to machine precision which is achieved in the studied examples for 2^{10} to 2^{14} Fourier modes. This resolution enables high precision interpolation from x to X^ε (see below).

For the time-integration of the Schrödinger equation we shall rely on a *time-splitting method*. The basic idea underlying these splitting methods is the Trotter-Kato formula [52], i.e.,

$$\lim_{n \rightarrow \infty} \left(e^{-tA/n} e^{-tB/n} \right)^n = e^{-t(A+B)} \quad (52)$$

where A and B are certain unbounded linear operators, for details see [36]. In particular this includes the cases studied by Bagrinovskii and Godunov in [5] and by Strang [50]. The formula (52) allows to solve an evolutionary equation

$$\partial_t u = (A + B)u, \quad u|_{t=0} = u_0,$$

in the following form

$$u(t) = e^{c_1 \Delta t A} e^{d_1 \Delta t B} e^{c_2 \Delta t A} e^{d_2 \Delta t B} \dots e^{c_k \Delta t A} e^{d_k \Delta t B} u_0,$$

where (c_1, \dots, c_k) and (d_1, \dots, d_k) are sets of real numbers that represent fractional time steps. In the numerical treatment of (1) we shall use a second order Strang splitting, i.e., $c_i = d_i = 1$ for all i except for $c_1 = d_k = 1/2$. The Schrödinger equation is consequently split into the following system:

$$i\varepsilon \partial_t u + \frac{\varepsilon^2}{2} \partial_{xx} u = 0, \quad i\varepsilon \partial_t u = V(x)u.$$

The first equation can then be explicitly integrated in Fourier space, using two FFT's. The second equation can explicitly be solved (in physical space) in the form

$$u(t, x) = e^{-itV(x)/\varepsilon} u_0.$$

Next, in order to solve the Bohmian equations of motion (6) for a given $\psi^\varepsilon(t, x)$, we need to interpolate between the coordinate x , in which ψ^ε is given, and the coordinate X^ε . For this we use that the x -dependence of ψ^ε is treated by Fourier spectral methods. Thus we can apply the representation of ψ^ε in terms of truncated Fourier series not only at the collocation points for which the formulae for the discrete Fourier transform hold, but at *general intermediate* points. The main drawback is that for such points there is no FFT algorithm known and the transformation is thus computationally more expensive. But since we only need to track a limited number of trajectories X^ε and since this interpolation method is of high accuracy, our approach is more efficient than, say, a low order polynomial (*spline*) interpolation (as used, e.g., in [19]). In order to obtain the Bohmian momentum P^ε we interpolate $x \leftrightarrow X^\varepsilon$ within $\psi^\varepsilon(t, x)$ and $\partial_x \psi^\varepsilon(t, x)$, for fixed time $t \in \mathbb{R}$. To this end, we note that the latter is of course determined in Fourier space. We consequently compute P^ε through

$$P^\varepsilon(t, X^\varepsilon) = \varepsilon \operatorname{Im} \left(\frac{\partial_x \psi^\varepsilon(t, X^\varepsilon)}{\psi^\varepsilon(t, X^\varepsilon)} \right).$$

We test the accuracy of the interpolation by comparing different numbers of Fourier modes for the solution of the Schrödinger equation for a given set of computed trajectories. Once machine precision is assured for ψ^ε (i.e., the modulus of the Fourier coefficients decreases below 10^{-12} , in our case), the difference between different interpolates can be shown to be of the same order. Thus we can conclude that the spatial resolution of the trajectories is of the order of 10^{-12} , much better than plotting accuracy.

The time integration of the first equation of the system (6) is performed with an explicit scheme (here, we shall use a standard fourth order Runge-Kutta method). This allows to compute the right-hand side of this equation with the already known values for X^ε at the previous time step. Note that we compute the solution to the Schrödinger equation either exactly in time (if $V(x) = 0$) or with second order time splitting for each stage of the Runge-Kutta scheme (whenever $V(x) \neq 0$). We shall test the accuracy of the time integration scheme by assuring that the difference of the numerical solution for N_t time steps to the solution for $2N_t$ time steps is smaller than 10^{-4} and thus much smaller than plotting accuracy. Typically we use $N_t = 10^4$. In addition the accuracy of the splitting scheme is tested as in [38] by tracing the numerically computed energy $E_{\text{num}}^\varepsilon(t)$ which due to unavoidable numerical errors is indeed a function of time. In our examples, the relative conservation of $E_{\text{num}}^\varepsilon(t)$ is ensured to better than 10^{-7} implying again an accuracy of more than 10^{-5} .

Remark 6.1. For efficiency reasons, the computation of the trajectories X^ε is done at the same time for all X^ε . Thus, in principle, it could happen that the identification of the trajectories in the examples below do not reflect the actual dynamics. By tracing also individual trajectories, i.e., by computing just one X^ε per run, we nevertheless are able to ensure that this is not the case and that the shown trajectories are indeed the correct ones. In particular our numerical code captures the physically important property that Bohmian trajectories *do not cross*, see, e.g., [19] (see also the proof of Theorem 5.4 (iii)). This is indeed a delicate issue in other numerical approaches where the system (13) is numerically integrated with (10) and (11) instead of (1), and where different interpolation techniques are used. The latter have to be chosen in a way to avoid the crossing of the trajectories (see Section 6.2.1 below).

6.2. Case studies. In the following we shall illustrate our analytical results by numerical examples. We shall first consider some test cases which will show that our algorithm is indeed trustworthy even for small $0 < \varepsilon \ll 1$, before we eventually study the case for WKB initial data leading to caustics.

6.2.1. Vortices. Before studying the semiclassical regime we shall show that our numerics displays the important non-crossing property of Bohmian trajectories, which we have seen to be the main obstacle for convergence (as $\varepsilon \rightarrow 0_+$) towards the multi-valued classical flow after caustic onset. For $\varepsilon > 0$, the only possibility for the crossing of Bohmian trajectories stems from nodes of the wave function, i.e., points at which ψ^ε vanishes. Due to the superfluid property of ψ^ε such nodes are physically interpreted as quantum mechanical *vortices*. In the following, we shall numerically study the example given in [9]. More precisely, ψ^ε is given by the superposition of the ground state and the second excited state of the harmonic oscillator (we also put $\varepsilon = 1$ in this example), i.e.,

$$\psi(t, x) = (1 + (1 - 2x^2)e^{-2it}) e^{-x^2 - it/2}.$$

This wave function vanishes for $x = 0$ and for all times $t = (2k + 1)\pi/2$, with $k \in \mathbb{Z}$. To treat the limit ‘0/0’ numerically, we add some quantity of the order of the rounding error to the wave function which will consequently provide the limit with an error of the order of the unavoidable numerical error. The resulting trajectories can be seen in Fig. 2. Note that, indeed, all trajectories avoid the vortices at $t = \pi/2$ and $t = 3\pi/2$, only the trajectory for $x = 0$ passes through these nodes.

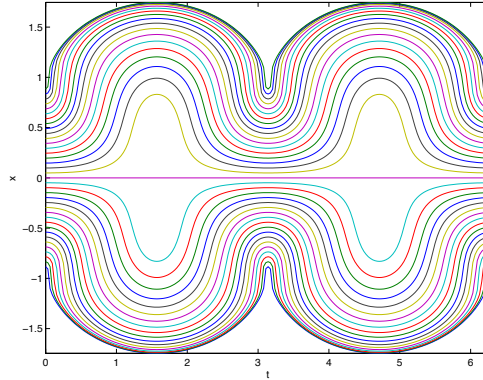


FIGURE 2. Bohmian trajectories for $\varepsilon = 1$ in a harmonic oscillator potential $V(x) = \frac{1}{2}x^2$ with ψ given as a superposition of the ground state and the second excited state.

6.2.2. *Semiclassical wave packets.* Before numerically studying the semiclassical limit of X_t^ε for WKB initial data, we shall test our algorithm in a slightly different situation, which is known to be better behaved as $\varepsilon \rightarrow 0_+$. Indeed, it has been proved in [44] that for the case of *semiclassical wave-packets*, convergence of the Bohmian flow to its corresponding classical counterpart holds in some appropriate topology (see also [21] for a closely related study). At $t = 0$ a semiclassical wave packet is of the form

$$\psi_0^\varepsilon(x) = \varepsilon^{-d/4} a_0 \left(\frac{x - x_0}{\sqrt{\varepsilon}} \right) e^{ik \cdot (x - x_0)/\varepsilon}, \quad a_0 \in \mathcal{S}(\mathbb{R}^d; \mathbb{C}). \quad (53)$$

The main differences between WKB states and semiclassical wave packets are that for the latter, the particle density concentrates in a point, i.e.,

$$\rho_0^\varepsilon(x) \xrightarrow{\varepsilon \rightarrow 0_+} \delta(x - x_0), \quad \text{in } \mathcal{D}'(\mathbb{R}^d),$$

and that the corresponding classical phase space flow does *not exhibit caustics*, cf. [17] for more details. This in particular implies that for semiclassical wave packets one can prove convergence of the Bohmian trajectories on *any* finite time-interval [44]. An example for such a situation (with $k_0 = 0$) can be seen in Fig. 3. The corresponding classical trajectories would be just lines parallel to the t -axis. Since these data do not lead to a caustic, there is just a slight defocusing effect to be seen with respect to the classical trajectories.

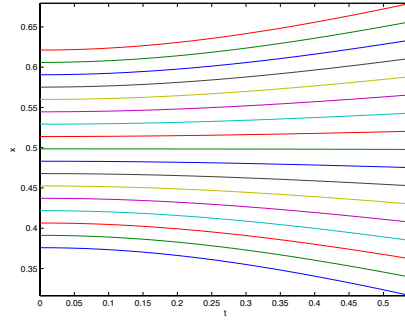


FIGURE 3. Bohmian trajectories for wave packet initial data of the form (53) with $k_0 = 0$, $x_0 = 1/2$, $a_0(z) = e^{-z^2}$ and $\varepsilon = 10^{-3}$.

6.2.3. *Caustics.* In this last subsection we shall, finally, present examples for WKB initial data exhibiting caustics in the classical limit. To this end, we shall first study the case where the caustic is just one single point, i.e., a situation in which all classical trajectories $X(t, y)$ cross at $(x^*, T^*) \in \mathbb{R}_t \times \mathbb{R}_x$. As a particular example, we shall consider the harmonic oscillator with potential

$$V(x) = \frac{1}{2} \left(x - \frac{1}{2} \right)^2, \quad (54)$$

and an initial data in the form

$$\psi_0^\varepsilon(x) = e^{-25(x-1/2)^2}, \quad (55)$$

i.e., a WKB state with Gaussian amplitude and $S_0(x) = 0$. Then, the classical trajectories $X(t, y)$ all intersect in one point as can be seen in Fig. 4.

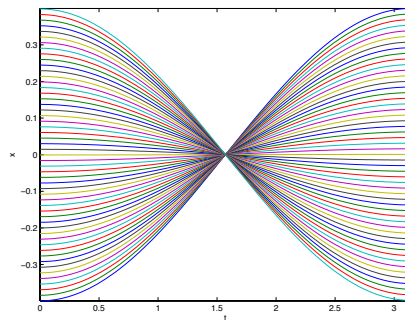


FIGURE 4. Classical trajectories $X(t, y)$ for the harmonic oscillator potential (54) and ψ_0^ε given by (55).

The same situation for the Bohmian trajectories $X^\varepsilon(t, y)$ and $\varepsilon = 10^{-3}$ can be seen in Fig. 5. The closeup of the region of intersection when $\varepsilon = 0$ clearly shows that the trajectories come close to x^* , but keep a finite distance from it except for the one trajectory which is parallel to the t -axis and goes straight through x^* . The

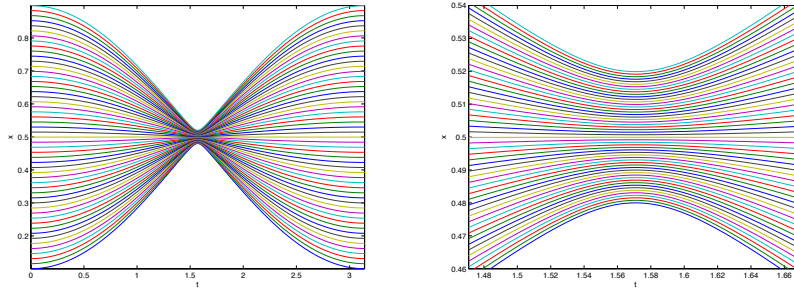


FIGURE 5. Left: Bohmian trajectories $X^\varepsilon(t, y)$ for the harmonic oscillator potential (54) and ψ_0^ε given by (55). Right: A closeup of the central region near x^* .

solution ψ^ε is periodic in time and shows a breather-type behavior with a large $|\psi^\varepsilon|$ at the caustic. We show only a half-period of this periodic motion.

Next, we consider the case $V(x) = 0$ with WKB initial data

$$\psi_0(x) = e^{-25(x-1/2)^2} e^{iS_0(x)/\varepsilon}, \quad S_0(x) = -\frac{1}{5} \ln \cosh\left(5x - \frac{5}{2}\right) \quad (56)$$

as in [42], i.e., the same amplitude as before but with nonzero initial phase. The time dependence of the density ρ shows a strong maximum followed by a zone of oscillation inside a break-up zone as can be seen in Fig. 6. In this case, the

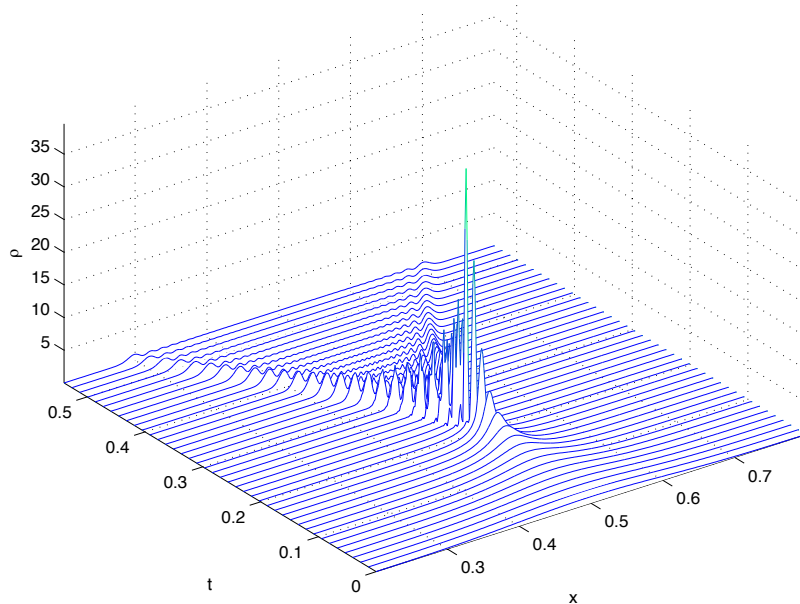


FIGURE 6. Density $\rho = |\psi^\varepsilon|^2$ for $V(x) = 0$ and ψ_0^ε given by (56).

classical trajectories $X(t, y)$ will lead to a diffuse caustic as depicted in Fig. 1. For finite ε , the Bohmian trajectories $X^\varepsilon(t, y)$ obviously do not cross, but there are rapid oscillations within the caustic region as can be seen in Fig. 7.

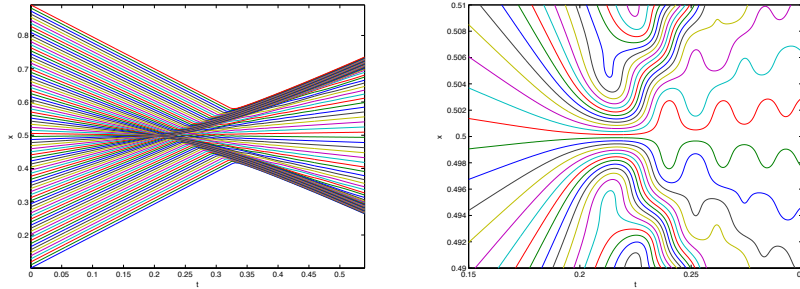


FIGURE 7. Left: Bohmian trajectories $X^\varepsilon(t, y)$ for $V(x) = 0$ and ψ_0^ε given by (56). Right: A closeup of the central region.

However, oscillations do not only appear in the trajectories, but also in the momentum $P^\varepsilon(t, y) = u^\varepsilon(t, X^\varepsilon(t, y))$ along any trajectory X^ε which is “deflected” at the caustic region. This can be clearly seen in Fig. 8 where several P^ε are plotted along the corresponding trajectories X^ε . The oscillations within P^ε are reminiscent of so-called *dispersive shocks*, as observed, e.g., in the Korteweg-de Vries equation with small dispersion, see for instance [30] and references therein. This is even

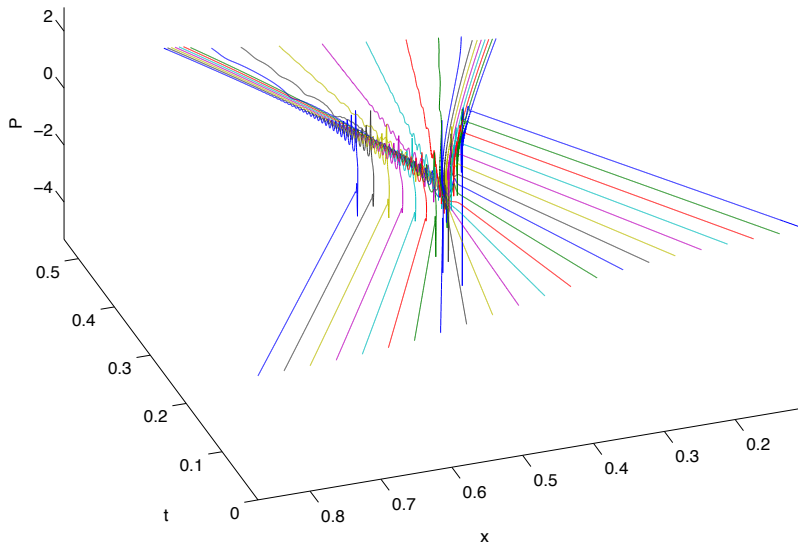


FIGURE 8. The quantity $P^\varepsilon(t, y)$ along the Bohmian trajectories $X^\varepsilon(t, y)$ given Fig. 7.

more visible in Fig. 9 where the oscillations on the left most trajectory in Fig. 8 are shown in dependence of t , thus in a projection onto the t -axis.

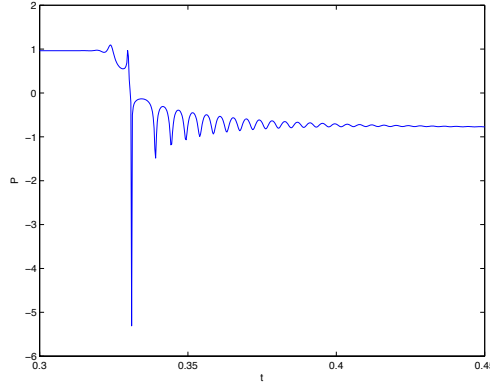


FIGURE 9. The quantity $P^\varepsilon(t, y)$ along the left most trajectory in Fig. 8 in dependence of t .

Figures 5 and 7 suggest the existence of a well defined limiting flow, which can be seen as the dispersive limit (for $\varepsilon \rightarrow 0_+$) of the Bohmian flow X_t^ε . Presumably, the classical limit of Bohmian measures (which can be computed even after caustics, see Theorem 4.2) is then given as the push forward under this limiting flow. Unfortunately, at this point we do not have the tools necessary to describe the limiting flow after caustic onset.

REFERENCES

- [1] Allaire, G. Homogenization and two-scale convergence. *SIAM J. Math. Anal.* **23** (1992), 1482–1518.
- [2] Ambrosio, L.; Figalli, A.; Friesecke, G.; Giannoulis, J.; Paul, T. Semiclassical limit of quantum dynamics with rough potentials and well-posedness of transport equations with measure initial data. *Comm. Pure Appl. Math.* **64** (2011), no. 9, 1199–1242.
- [3] Arnold, A.; López, J. L.; Markowich, P.; Soler, J. An analysis of quantum Fokker-Planck models: a Wigner function approach. *Rev. Mat. Iberoamericana* **20** (2004), no. 3, 771–814.
- [4] Arnold, V. I. *Mathematical Methods of Classical Mechanics*, Springer Verlag, 1989.
- [5] Bagrinovskii, K. A.; Godunov, S. K. Difference Schemes for multi-dimensional Problems, *Dokl. Acad. Nauk.* **115** (1957), 431–433.
- [6] Ball, J. M. A version of the fundamental theorem for Young measures. *PDEs and Continuum Models of Phase Transitions* Lecture Notes in Physics, **344**, Rasche, M., Serre, D., Slemrod, M. (eds.), Springer Verlag, 1989.
- [7] Bardos, C.; Golse, F.; Markowich, P.; Paul, T. Regularity issues in the semiclassical limit of the Schrödinger equation. *Preprint* (2012).
- [8] Berndl, K.; M. Daumer, M.; Dürr, D.; Goldstein, S.; Zanghi, N. A Survey of Bohmian Mechanics *Nuovo Cimento* **110B** (1995), 737–750.
- [9] Berndl, K.; Dürr, D.; Goldstein, S.; Peruzzi, G.; Zanghi, N. On the global existence of Bohmian mechanics. *Comm. Math. Phys.* **173** (1995), 647–673.
- [10] Bogachev, V. I. *Measure Theory*, Springer, Berlin 2006.
- [11] Bohm, D. A Suggested Interpretation of the Quantum Theory in Terms of “Hidden Variables” I. *Phys. Rev.* **85** (1952), 166–179.
- [12] Bohm, D. A Suggested Interpretation of the Quantum Theory in Terms of “Hidden Variables” II. *Phys. Rev.* **85** (1952), 180–193.

- [13] Bohm, D.; Hiley, B.J. *The Undivided Universe*. Routledge, London, 1995.
- [14] Born, M. Zur Quantenmechanik der Stoßvorgänge. *Z. Phys.* **37** (1926), 863.
- [15] Carles, R. WKB analysis for nonlinear Schrödinger equations with potential. *Comm. Math. Phys.* **269** (2007), no. 1, 195–221.
- [16] Carles, R. *Semi-classical analysis for nonlinear Schrödinger equations*. World Scientific, Co. Pte. Ltd., Hackensack, NJ 2008.
- [17] Carles, R.; Fermanian-Kammerer, C. Nonlinear coherent states and Ehrenfest time for Schrödinger equations. *Comm. Math. Phys.* **301** (2011), no. 2, 443–472.
- [18] Chazarain, J. Spectre d'un hamiltonien quantique et mécanique classique. *Comm. Partial Differential Equations* **5** (1980), no. 6, 595–644.
- [19] Deckert, D. A.; Dürr, D.; Pickl, P. Quantum Dynamics with Bohmian Trajectories, *J. Phys. Chem. A* **111** (2007), no. 41, 10325–10330.
- [20] Duistermaat, J. J. *Fourier integral operators*. Progress in Mathematics, 130. Birkhäuser Boston, Inc., Boston, MA, 1996.
- [21] Dürr, D.; Römer, S. On the classical limit of Bohmian mechanics for Hagedorn wave packets. *J. Funct. Anal.* **259** (2010), 2404–2423.
- [22] Dürr, D.; Teufel, S. *Bohmian Mechanics*. Springer Verlag, 2009.
- [23] Evans, L. C. *Partial Differential Equations*, Graduate Studies in Mathematics vol. 19, American Mathematical Society, 2010.
- [24] Figalli, A.; Ligabò, M.; Paul, T. Semiclassical limit for mixed states with singular and rough potentials. *Indiana Univ. Math.*, to appear.
- [25] Fujiwara, D. On a nature of convergence of some Feynman path integrals. I-II. *Proc. Japan Acad. Ser. A Math. Sci.* **55** (1979), no. 8, 273–277.
- [26] Gasser, I.; Markowich, P. A.; Quantum hydrodynamics, Wigner transforms and the classical limit. *Asympt. Anal.* **14** (1997), 97–116.
- [27] Gérard, P.; Markowich, P. A.; Mauser, N. J.; Poupaud, F. Homogenisation Limits and Wigner transforms. *Comm. Pure Appl. Math.* **50** (1997), 323–379.
- [28] Gindensperger E.; Meier C.; Beswick J. A. Mixing quantum and classical dynamics using Bohmian trajectories. *J. Chem. Phys.* **113** (2000), issue 21, 936–9372.
- [29] Graffi S.; Zanelli, L. Global parametrices for the Schrödinger propagator and geometric approach to the Hamilton-Jacobi equation. *Atti Accad. Naz. Lincei Cl. Sci. Fis. Mat. Natur. Rend. Lincei (9) Mat. Appl.* **22** (2011), no. 1, 17–28.
- [30] Grava T.; Klein C. Numerical solution of the small dispersion limit of Korteweg de Vries and Whitham equations. *Comm. Pure Appl. Math.* **60** (2007), no. 11, 1623–1664.
- [31] Grenier, E. Semiclassical limit of the nonlinear Schrödinger equation in small time. *Proc. Amer. Math. Soc.* **126** (1998), no. 2, 523–530.
- [32] Hörmander, L. *The analysis of linear partial differential operators I*, Springer-Verlag, Berlin, 1990.
- [33] Hörmander, L. Symplectic classification of quadratic forms, and general Mehler formulas, *Math. Z.* **219** (1995), no. 3, 413–449.
- [34] Hungerbühler, N. A. Refinement of Ball's Theorem on Young Measures. *New York J. Math.* **3** (1997), 48–53.
- [35] Kapitansky, L; Safarov, Y. A. Parametrix for the nonstationary Schrödinger equation. *Differential operators and spectral theory*, 139–148, Amer. Math. Soc. Transl. Ser. 2, 189, Amer. Math. Soc., Providence 1999.
- [36] Kato, T. Trotter's product formula for an arbitrary pair of self-adjoint contraction semigroups. *Topics in Functional Analysis (Essays dedicated to M. G. Krein on the Occasion of his 70th Birthday)* **3**, 185–195, Academic Press, Boston, 1978.
- [37] Kiessling, M. Misleading signposts along the de Broglie-Bohm road to quantum mechanics, *Found. Physics* **40** (2010), no. 4, 418–429.
- [38] Klein, C. Fourth order time-stepping for low dispersion Korteweg-de Vries and nonlinear Schrödinger equation, *Electronic Trans. Num. Anal.* **29** (2008), 116–135.
- [39] Laptev, A.; Sigal, I. M. Global Fourier integral operators and semiclassical asymptotics, *Rev. Math. Phys.* **12** (2000), no. 5, 749–766.
- [40] Lax, P. D. Asymptotic solutions of oscillatory initial value problems, *Duke Math. J.* **24** (1957), 627–646.

- [41] P. L. Lions and T. Paul, *Sur les mesures de Wigner*. *Rev. Math. Iberoamericana* **9** (1993), 553–618.
- [42] Markowich, P.; Pietra, P.; Pohl, C. Numerical approximation of quadratic observables of Schrödinger-type equations in the semi-classical limit, *Numer. Math.* **81** (1998), 595–630.
- [43] Markowich, P.; Paul, T.; Sparber, C. Bohmian measures and their classical limit, *J. Funct. Anal.* **259** (2010), 1542–1576.
- [44] Markowich, P.; Paul, T.; Sparber, C. On the dynamics of Bohmian measures, *Arch. Ration. Mech. Anal.* **205** (2012), no. 3, 1031–1054.
- [45] Maslov, V.P.; Fedoryuk, M.V. *Semi-classical approximation in quantum mechanics*, Reidel, 1981.
- [46] Nerukh D.; Frederick, J. H. Multidimensional quantum dynamics with trajectories: a novel numerical implementation of Bohmian mechanics. *Chem. Phys. Lett.* **332** (2000), issue 1-2, 145–153.
- [47] Pedregal, P. Optimization, relaxation and Young measures, *Bull. Amer. Math. Soc.* **36** (1999), no. 1, 27–58.
- [48] Robert, D. *Autour de l'Approximation Semi-Classique*, Birkhäuser, Boston, 1987.
- [49] Sparber, C.; Markowich, P.; Mauser, N. Wigner functions vs. WKB methods in multivalued geometrical optics. *Asymptot. Anal.* **33** (2003), no. 2, 153–187.
- [50] Strang, G. On the Construction and Comparison of Difference Schemes. *SIAM J. Numer. Anal.* **5** (1968), 506–517.
- [51] Teufel, S.; Tumulka, R. Simple proof of global existence of Bohmian trajectories. *Comm. Math. Phys.* **258** (2005), 349–365.
- [52] Trotter, H. F. On the Product of Semi-Groups of Operators. *Proceedings of the American Mathematical Society* **10** (1959), 545–551.
- [53] Wyatt, R. E.; Trahan, C. E. *Quantum dynamics with trajectories: introduction to quantum hydrodynamics*, Springer, Berlin 2005.