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ON THE DYNAMICS OF BOHMIAN MEASURES

PETER MARKOWICH, THIERRY PAUL, AND CHRISTOF SPARBER

ABSTRACT. We revisit the concept of Bohmian measures recently introduced by the authors in [19]. We rigorously prove that for sufficiently smooth wave functions the corresponding Bohmian measure furnishes a distributional solution of a nonlinear Vlasov-type equation. Moreover, we study the associated defect measures appearing in the classical limit. In one space dimension, this yields a new connection between mono-kinetic Wigner and Bohmian measures. In addition, we shall study the dynamics of Bohmian measures associated to so-called semi-classical wave packets. For these type of wave functions, we prove local in-measure convergence of a rescaled sequence of Bohmian trajectories towards the classical Hamiltonian flow on phase space. Finally, we construct an example of wave functions whose limiting Bohmian measure is not mono-kinetic but nevertheless equals the associated Wigner measure.

1. INTRODUCTION AND MAIN RESULTS

1.1. Background on Bohmian measures. We consider the time-evolution of quantum mechanical wave functions $\psi^\varepsilon(t, \cdot) \in L^2(\mathbb{R}^d; \mathbb{C})$ governed by the Schrödinger equation:

$$(1.1) \quad i\varepsilon \partial_t \psi^\varepsilon = -\frac{\varepsilon^2}{2} \Delta \psi^\varepsilon + V(x) \psi^\varepsilon, \quad \psi^\varepsilon(t=0, x) = \psi_0^\varepsilon \in L^2(\mathbb{R}^d),$$

where $x \in \mathbb{R}^d$, $t \in \mathbb{R}$, and $V \in L^\infty(\mathbb{R}^d; \mathbb{R})$ a given bounded potential (satisfying some additional regularity assumptions given below). In addition, we have rescaled all physical parameters such that only one *semi-classical parameter* $0 < \varepsilon \leq 1$ remains. We shall from now on assume that $\|\psi_0^\varepsilon\|_{L^2} = 1$, which is henceforth propagated in time, i.e.

$$(1.2) \quad \|\psi^\varepsilon(t)\|_{L^2} = \|\psi_0^\varepsilon\|_{L^2} = 1.$$

In addition, we also have *conservation of energy*, i.e.

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

Throughout this work, we shall assume that

$$(1.3) \quad \sup_{0 < \varepsilon \leq 1} E^\varepsilon(0) < +\infty.$$

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In other words, we assume ψ_0^ε to have bounded initial energy, uniformly in ε . In view of (1.2), one can define out of $\psi^\varepsilon(t, x) \in \mathbb{C}$ real-valued probability densities from which one computes expectation values of physical observables. Possibly, the two most important such densities are the *position* and the *current-density*, given by

$$(1.4) \quad \rho^\varepsilon(t, x) = |\psi^\varepsilon(t, x)|^2, \quad J^\varepsilon(t, x) = \varepsilon \operatorname{Im}(\overline{\psi^\varepsilon(t, x)} \nabla \psi^\varepsilon(t, x)).$$

Already in 1926, the same year in which Schrödinger exhibited the eponymous equation, it has been realized by Madelung [18] that these densities can be used to rewrite (1.1) in hydrodynamical form. The corresponding *quantum hydrodynamic system* reads

$$(1.5) \quad \begin{cases} \partial_t \rho^\varepsilon + \operatorname{div} J^\varepsilon = 0, \\ \partial_t J^\varepsilon + \operatorname{div} \left(\frac{J^\varepsilon \otimes J^\varepsilon}{\rho^\varepsilon} \right) + \rho^\varepsilon \nabla V = \frac{\varepsilon^2}{2} \rho^\varepsilon \nabla \left(\frac{\Delta \sqrt{\rho^\varepsilon}}{\sqrt{\rho^\varepsilon}} \right). \end{cases}$$

More precisely, it can be proved that under sufficient regularity assumptions on $V(x)$ and $\psi^\varepsilon(t, x)$, each of the nonlinear terms arising in this system is well-defined in the sense of distributions, see [12, Lemma 2.1]. However, the converse direction, i.e. reconstructing ψ^ε from the solution of (1.5), is still open so far (see e.g. [2] and the references given therein).

The quantum-hydrodynamic system (1.5) can also be seen as the starting point of *Bohmian mechanics* [4, 5]. In this theory, one defines an ε -dependent flow-map

$$X_t^\varepsilon : \mathbb{R} \times \mathbb{R}^d \rightarrow \mathbb{R}^d; \quad x \mapsto X^\varepsilon(t, x)$$

via the following differential equation

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

where the vector field u^ε is (formally) given by

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

and the initial data is assumed to be distributed according to $\rho_0^\varepsilon(x) \equiv |\psi_0^\varepsilon(x)|^2$. It has been rigorously proved in [3] (see also [26]) that $X^\varepsilon(t, \cdot)$ is for all $t \in \mathbb{R}$ well-defined ρ_0^ε -*a.e.* and that

$$\rho^\varepsilon(t, x) = X_t^\varepsilon \# \rho_0^\varepsilon(x),$$

i.e. $\rho^\varepsilon(t, x)$ is the *push-forward* of the initial density $\rho_0^\varepsilon(x)$ under the mapping $X_t^\varepsilon : x \mapsto X^\varepsilon(t, x)$, see Definition (3.1) below. This can be seen as the Eulerian viewpoint of Bohmian mechanics.

Bohmian mechanics can be reformulated in its Lagrangian form, by using the concept of *Bohmian measures*, recently introduced by the authors in [19]:

Definition 1.1. For $\psi^\varepsilon \in H^1(\mathbb{R}^d)$, with associated densities $\rho^\varepsilon, J^\varepsilon$ as in (1.4), and a given $\varepsilon > 0$, we define the corresponding *Bohmian measure* $\beta^\varepsilon \equiv \beta^\varepsilon[\psi^\varepsilon] \in \mathcal{M}^+(\mathbb{R}_x^d \times \mathbb{R}_p^d)$ via

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

where $C_0(\mathbb{R}_x^d \times \mathbb{R}_p^d)$ denotes the space of continuous function vanishing at infinity and $\mathcal{M}^+(\mathbb{R}_x^d \times \mathbb{R}_p^d)$ the set of non-negative Radon measures on phase space.

It has been shown in [19] that if $\psi^\varepsilon(t, x)$ solves (1.1), then the corresponding Bohmian $\beta^\varepsilon(t, x, p)$ measure is the push-forward of

$$(1.6) \quad \beta^\varepsilon[\psi_0^\varepsilon] \equiv \beta_0^\varepsilon(x, p) = \rho_0^\varepsilon(x) \delta(p - u_0(x)),$$

under the ε -dependent phase space flow

$$(1.7) \quad \Phi_t^\varepsilon : (x, p) \mapsto (X^\varepsilon(t, x, p), P^\varepsilon(t, x, p))$$

induced by

$$(1.8) \quad \begin{cases} \dot{X}^\varepsilon = P^\varepsilon, \\ \dot{P}^\varepsilon = -\nabla V(X^\varepsilon) - \nabla V_B^\varepsilon(t, X^\varepsilon), \end{cases}$$

where $V_B^\varepsilon(t, x)$, denotes the so-called *Bohm potential* (see [10, 11, 22]).

$$(1.9) \quad V_B^\varepsilon(t, x) := -\frac{\varepsilon^2}{2} \frac{\Delta \sqrt{\rho^\varepsilon(t, x)}}{\sqrt{\rho^\varepsilon(t, x)}}.$$

More precisely, under mild regularity assumptions on V , the flow Φ_t^ε is shown to exist globally in time for almost all $(x, p) \in \mathbb{R}^{2d}$, relative to the measure β_0^ε and is continuous in time on its maximal open domain, cf. [19, Lemma 2.5]. Note that the specific form of the initial data (1.6) implies that Φ_t^ε is projected onto a *Lagrangian sub-manifold* of phase space

$$\mathcal{L}^\varepsilon := \{(x, p) \in \mathbb{R}_x^d \times \mathbb{R}_p^d : p = u_0^\varepsilon(x)\},$$

whose time-evolution is governed by the Bohmian flow (1.8).

The fact that $\beta^\varepsilon(t) = \Phi_t^\varepsilon \# \beta_0^\varepsilon(x)$, is usually called *equivariance* of Bohmian measures [10] and makes $\beta^\varepsilon(t)$ a natural starting point for the investigation of the classical limit as $\varepsilon \rightarrow 0_+$ of Bohmian mechanics. In [19] we gave an extensive study (invoking Young measure theory) of the possible oscillation and concentration phenomena appearing in β^ε as $\varepsilon \rightarrow 0_+$ and compared our findings to the by now classical theory of *Wigner measures*, cf. [13, 17, 25]. One thereby associated to any wave function ψ^ε a phase space function $w^\varepsilon[\psi^\varepsilon] \equiv w^\varepsilon$, defined by

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

This definition yields the so-called *Wigner function* $w^\varepsilon(t)$ associated to $\psi^\varepsilon(t)$ [27]. It is well known that although $w^\varepsilon(t, x, p) \not\geq 0$ in general, it admits as $\varepsilon \rightarrow 0_+$ a weak limit $w(t) \in \mathcal{M}^+(\mathbb{R}_x^d \times \mathbb{R}_p^d)$, usually called *Wigner measure* (or semi-classical measure). The latter is known to give the possibility to describe in a ‘‘classical’’ manner the expectation values of physical observables, for all $t \in \mathbb{R}$, via

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

where $\text{Op}^\varepsilon(a)$ is the Weyl-quantized operator associated to the classical symbol $a \in C_b^\infty(\mathbb{R}_x^d \times \mathbb{R}_p^d)$.

Similarly to that, we were able to establish in [19] the existence of a limiting non-negative phase space measure $\beta(t) \in \mathcal{M}^+(\mathbb{R}_x^d \times \mathbb{R}_p^d)$, such that, after extracting an appropriate sub-sequence (denoted by the same symbol):

$$\beta^\varepsilon \xrightarrow{\varepsilon \rightarrow 0_+} \beta \quad \text{in } C_b(\mathbb{R}_t; \mathcal{M}^+(\mathbb{R}_x^d \times \mathbb{R}_p^d)) \text{ w} - *.$$

If, in addition, $\psi^\varepsilon(t)$ is ε -oscillatory, i.e.

$$(1.10) \quad \sup_{0 < \varepsilon \leq 1} (\|\psi^\varepsilon(t)\|_{L^2} + \|\varepsilon \nabla \psi^\varepsilon(t)\|_{L^2}) < +\infty.$$

one can prove (cf. [19, Lemma 3.2]) that the limiting phase space measure $\beta(t)$ incorporates the classical limit of the particle and current density in the sense that

$$(1.11) \quad \rho^\varepsilon(t, x) \xrightarrow{\varepsilon \rightarrow 0^+} \int_{\mathbb{R}^d} \beta(t, x, dp),$$

and

$$(1.12) \quad J^\varepsilon(t, x) \xrightarrow{\varepsilon \rightarrow 0^+} \int_{\mathbb{R}^d} p \beta(t, x, dp).$$

Hereby the limits have to be understood in $\mathcal{M}^+(\mathbb{R}_x^d)$ w-*, uniformly on compact time-intervals $I \subset \mathbb{R}_t$. Note that condition (1.10) is satisfied for all $t \in \mathbb{R}$, in view of (1.2), the conservation of energy and our initial assumption (1.3) (since for any $V \in L^\infty(\mathbb{R}^d)$ we can assume w.r.o.g. $V(x) \geq 0$). This is the reason to impose (1.2) and (1.3), throughout this work.

In other words, the limiting Bohmian measure $\beta(t)$ therefore yields the classical limit of the quantum mechanical position and current densities, by taking the zeroth and first moment with respect to $p \in \mathbb{R}^d$, analogous to the case of Wigner measures. Other quantum mechanical observable densities, however, might not be described correctly in the limit $\varepsilon \rightarrow 0_+$. In fact, the limiting $\beta(t)$ is found to be in general different from the Wigner measure $w(t)$, cf. the examples given in Section 5 of [19].

1.2. Main results. The main objective of the current work is to analyze the dynamics of $\beta^\varepsilon(t)$. Note that the equivariance property strongly suggests that $\beta^\varepsilon(t)$ satisfies the following nonlinear *Vlasov-type equation*

$$(1.13) \quad \begin{cases} \partial_t \beta^\varepsilon + p \cdot \nabla_x \beta^\varepsilon - \nabla_x \left(V - \frac{\varepsilon^2}{2} \frac{\Delta_x \sqrt{\rho^\varepsilon}}{\sqrt{\rho^\varepsilon}} \right) \cdot \nabla_p \beta^\varepsilon = 0, \\ \rho^\varepsilon(t, x) = \int_{\mathbb{R}^d} \beta^\varepsilon(t, x, dp), \end{cases}$$

subject to initial data $\beta_0^\varepsilon(x, p)$ given by (1.6). Note that the system (1.13) can be written in one line as

$$(1.14) \quad \partial_t \beta^\varepsilon + p \cdot \nabla_x \beta^\varepsilon - \nabla_x \left(V - \frac{\varepsilon^2}{2} \frac{\Delta_x \sqrt{\int_{\mathbb{R}^d} \beta^\varepsilon dp}}{\sqrt{\int_{\mathbb{R}^d} \beta^\varepsilon dp}} \right) \cdot \nabla_p \beta^\varepsilon = 0,$$

Due to the strong nonlinear nature of this equation and in particular due to possible singularities at points $x \in \mathbb{R}^d$ where $\rho^\varepsilon(t, x) = 0$, it is a non-trivial task to rigorously prove that $\beta^\varepsilon(t)$ furnishes a distributional solution to (1.13). It will be one of the goals of this work to show that this is indeed the case. To this end, we shall derive appropriate bounds for all terms arising in the weak formulation of (1.13) after being evaluated at Bohmian measures. This rigorously establishes the existence of a nonlinear evolution equation for $\beta^\varepsilon(t)$ in a similar spirit as the results of [12] for the quantum hydrodynamic system (1.5). More precisely, the first main result of this work is as follows:

Theorem 1.1. *Let $V \in C_b^1(\mathbb{R}^d; \mathbb{R})$ and $\psi_0^\varepsilon \in H^3(\mathbb{R}^d)$ with corresponding $\rho_0^\varepsilon, J_0^\varepsilon$ defined by (1.4). Then, for all $\varepsilon > 0$, the Bohmian measure*

$$\beta^\varepsilon(t, x, p) = \rho^\varepsilon(t, x) \delta\left(p - \frac{J^\varepsilon(t, x)}{\rho^\varepsilon(t, x)}\right),$$

is a weak solution of (1.13) in $\mathcal{D}'(\mathbb{R}_t \times \mathbb{R}_x^d \times \mathbb{R}_p^d)$ and in $\mathcal{D}'([0, \infty) \times \mathbb{R}_x^d \times \mathbb{R}_p^d)$ with initial data (1.6).

In a second step we shall study the classical limit of equation (1.13). To this end, let us recall, cf. [19, Definition 3.4], that a measure $\mu \in \mathcal{M}^+(\mathbb{R}_x^d \times \mathbb{R}_p^d)$ is said to be *mono-kinetic*, if there exists a $\rho \in \mathcal{M}^+(\mathbb{R}_x^d)$ and a function $u(x)$ defined $\rho - a.e.$, such that

$$\mu(x, p) = \rho(x) \delta(p - u(x)).$$

Obviously, such mono-kinetic phase space measures define Lagrangian sub-manifolds and are thus particularly interesting for our purposes. Clearly $\beta^\varepsilon(t)$ is mono-kinetic by definition, its limit however, will not be in general. To get further insight, we pass to the limit $\varepsilon \rightarrow 0_+$ (after extraction of a subsequence) in the first three linear terms of equation (1.13). This naturally leads to the following definition of a possible *defect* $\mathcal{F}(t, x, p) \in \mathbb{R}^d$: Along a chosen sub-sequence $\{\varepsilon_n\}_{n \in \mathbb{N}}$, let

$$(1.15) \quad \mathcal{F} := \lim_{\varepsilon \rightarrow 0_+} (\operatorname{div}_p(\nabla_x V_B^\varepsilon \beta^\varepsilon)), \quad \text{in } \mathcal{D}'(\mathbb{R}_t \times \mathbb{R}_x^d \times \mathbb{R}_p^d),$$

such that

$$\partial_t \beta + p \cdot \nabla_x \beta - \nabla_x V \cdot \nabla_p \beta = \mathcal{F},$$

A partial characterization of the defect \mathcal{F} , will be given in Section 4. In particular, it yields to the following result:

Theorem 1.2. *Let $d = 1$ and $\beta^\varepsilon(t)$ solve (1.13). In addition assume that at $t = 0$, the limiting measure satisfies*

$$\beta_0(x, p) = w_0(x, p) = \rho_0(x) \delta(p - u_0(x)),$$

where $w_0(x, p)$ is the Wigner measure associated to $\psi_0^\varepsilon(x)$. Then, on any time-interval $I \subseteq \mathbb{R}_t$, on which $w(t)$ is mono-kinetic, i.e.

$$w(t, x, p) = \rho(t, x) \delta(p - u(t, x)),$$

it holds $\beta(t, x, p) = w(t, x, p)$, in the sense of measures.

In contrast to the results of [19], where we established certain criteria for $\psi^\varepsilon(t)$, yielding mono-kinetic Wigner and/or limiting Bohmian measures, this result directly gives $\beta(t) = w(t)$ from the fact that the Wigner measure is mono-kinetic. It is well known, cf. [12, 25] that the Wigner measure is generically mono-kinetic before *caustics*, i.e. before the appearance of the first shock in the (field driven) Burgers equation

$$(1.16) \quad \partial_t u + (u \cdot \nabla)u + \nabla V(x) = 0.$$

Note however, that there are situations in which w is of the form given in Theorem 1.2 (2) even *after* caustics, see e.g. Example 4 given in [12] and Example 1 in [25], both of which furnish so-called *point caustics*, i.e. caustics where all the rays of geometric optics cross at one point. The result given above therefore shows that in some situations the limiting Bohmian measure $\beta(t)$ can indeed give the correct classical limit (for all physical observables) *even after caustics*. In addition, Theorem 1.2 (2) generalizes [19, Proposition 6.1], at least in $d = 1$ spatial dimensions.

Remark 1.2. Equation (1.16) can be seen as the formal limit obtained from (1.1) by means of WKB analysis. One thereby seeks solution to (1.1) in the following form

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

with (real-valued) ε -independent phase S and (possibly complex-valued) amplitude $a^\varepsilon \sim a_0 + \varepsilon a_1 + \varepsilon^2 \dots$, in the sense of formal asymptotics. Plugging this ansatz into (1.1) and neglecting terms of order $\mathcal{O}(\varepsilon^2)$ yields (1.16) upon identifying $u = \nabla S$, cf. [25] for more details (see also Section 6 of [19] where the connection between WKB analysis and Bohmian measures is discussed).

Finally, we shall consider the particular case where $\psi^\varepsilon(t)$ is a so-called *semi-classical wave packet* (or coherent state). The classical limit of Bohmian trajectories in this particular situation has been recently studied in [9]. There it has been shown that the Bohmian trajectories $X^\varepsilon(t, x)$ converge (in some suitable topology) to $X(t)$, the classical particle trajectory induced by the Hamiltonian system

$$(1.17) \quad \begin{cases} \dot{X} = P, & X(0) = x_0, \\ \dot{P} = -\nabla V(X), & P(0) = p_0. \end{cases}$$

One should note that the mathematical methods used in [9] are rather different from ours and that no convergence result for $P^\varepsilon(t)$ is given, except for $p_0 = 0$ (and, as a variant, for a class of time-averaged Bohmian momenta). In comparison to that, the use of $\beta^\varepsilon(t)$, together with the Young measure theory developed in [19], allows us to conclude the following result:

Theorem 1.3. *Let $V \in C_b^3(\mathbb{R}^d)$. In addition, assume that ψ_0^ε is of the following form*

$$\psi_0^\varepsilon(x) = \varepsilon^{-d/2} a \left(\frac{x - x_0}{\sqrt{\varepsilon}} \right) e^{ip_0 \cdot x / \varepsilon}, \quad x_0, p_0 \in \mathbb{R},$$

with given ε -independent amplitude $a \in \mathcal{S}(\mathbb{R})$.

(1) *Then, the limiting Bohmian measure satisfies*

$$\beta(t, x, p) = w(t, x, p) = \|a\|_{L^2}^2 \delta(x - X(t)) \delta(p - P(t)),$$

where $X(t), P(t)$ are the classical trajectories defined by (1.17).

(2) *Consider the following re-scaled Bohmian trajectories*

$$Y^\varepsilon(t, y) = X^\varepsilon(t, x_0 + \sqrt{\varepsilon}y), \quad Z^\varepsilon(t, y) = P^\varepsilon(t, x_0 + \sqrt{\varepsilon}y),$$

where $X^\varepsilon(t, x), P^\varepsilon(t, x)$ solve (1.8) subject to initial data $(x, p_0) \in \mathcal{L}^\varepsilon$, i.e. with constant initial velocity $u_0^\varepsilon(x) = p_0 \in \mathbb{R}^d$ induced by ψ_0^ε . Then

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

locally in measure on $\mathbb{R}_t \times \mathbb{R}_x^d$. More precisely, for every $\delta > 0$ and every Borel set $\Omega \subseteq \mathbb{R}_t \times \mathbb{R}_x^d$ with finite Lebesgue measure,

$$(1.18) \quad \lim_{\varepsilon \rightarrow 0} \mathbb{L}(\{(t, y) \in \Omega : |(Y^\varepsilon(t, y), Z^\varepsilon(t, y)) - (X(t), P(t))| \geq \delta\}) = 0,$$

where \mathbb{L} denotes the Lebesgue measure.

Let us compare now our results with the corresponding ones in [9]: Besides the fact that we are able to infer convergence of the Bohmian momentum $P^\varepsilon(t)$, the topology we use is different from the one used there. Rephrased in our notation [9]

proves that, for all $T > 0$ and $\gamma > 0$ there exists some $R < \infty$ such that, for all ε small enough,

$$(1.19) \quad \mathbb{P}_{\rho_0^\varepsilon}(\{x_0 \in \mathbb{R}^3 \mid \max_{t \in [0, T]} |X^\varepsilon(t, x_0) - X(t)| \leq R\sqrt{\varepsilon}\}) > 1 - \gamma,$$

where $\mathbb{P}_{\rho_0^\varepsilon}$ is the probability measure with density $\rho_0^\varepsilon = |\psi_0^\varepsilon(x)|^2$. We see clearly that the comparison between the two results is not straightforward, as (1.19) measures the “good” points and (1.18) the “bad” ones. Moreover, (1.19) is more precise for finite times, whereas (1.18) doesn’t require a-priori bounds on the time dependence and additionally implies almost everywhere convergence of sub-sequences, see Remark 5.3. It would certainly be interesting to study the link between the two approaches more precisely.

Remark 1.3. In view of Theorem 1.2 and Theorem 1.3 one might guess that $w = \beta$ only if both are mono-kinetic phase space distributions. This is consistent with the examples given in [19] but still wrong in general. Indeed, in the appendix of the present work, we shall construct a family of wave functions ψ^ε for which $w = \beta$ is absolutely continuous with respect to the Lebesgue measure on \mathbb{R}_p^d . This henceforth closes a gap in the case studies given in [19].

The paper is now organized as follows: In the upcoming section we collect some basic mathematical estimates needed throughout this work. In Section 3 we establish the fact that $\beta^\varepsilon(t)$ indeed furnishes a distributional solution of (1.13). In Section 4 the defect \mathcal{F} will be partially characterized, yielding the proof of Theorem 1.2. In Section 5, the particular case of semi-classical wave packets will be studied including the proof of Theorem 1.3. Finally, in Appendix A we shall present an example in which $w = \beta$ but not mono-kinetic.

2. STATIC ESTIMATES

In order to establish the weak formulation of (1.13), we shall heavily rely on the following static, i.e. time-independent, estimate.

Proposition 2.1. *Let $\psi \in C^2(\mathbb{R}^d)$, then it holds:*

$$|\operatorname{div}(\nabla|\psi| \otimes \nabla|\psi|)| \leq d \left(\sup_{\ell j k} |\partial_\ell \partial_j \psi \partial_k \psi| + \frac{1}{2} \left| \operatorname{Im} \left(\frac{\nabla \psi}{\psi} \right) \right| \sup_{\ell j} |\partial_\ell \psi \partial_j \psi| \right),$$

with $j, \ell, k = 1, \dots, d$.

Proof. We denote $\partial_j := \partial_{x_j}$ and first compute

$$\partial_j |\psi| = \frac{\bar{\psi} \partial_j \psi + \psi \overline{\partial_j \psi}}{2(\psi \bar{\psi})^{1/2}},$$

which yields

$$\partial_\ell |\psi| \partial_j |\psi| = \operatorname{Re} \left(\partial_\ell \psi \overline{\partial_j \psi} + \frac{\bar{\psi}}{\psi} \partial_\ell \psi \partial_j \psi \right),$$

Using this we can write

$$(2.1) \quad \operatorname{div}(\nabla|\psi| \otimes \nabla|\psi|) = \sum_{k=1}^d \operatorname{Re} \partial_k \left(\partial_\ell \psi \overline{\partial_j \psi} + \frac{\bar{\psi}}{\psi} \partial_\ell \psi \partial_j \psi \right),$$

where each term in this series will be estimated separately (and in the same way). In order to handle terms in which the partial derivative ∂_k acts on $\bar{\psi}/\psi$ we note that

$$\partial_k \left(\frac{\bar{\psi}}{\psi} \right) = \frac{\partial_k \bar{\psi}}{\psi} - \frac{\partial_k \psi \bar{\psi}}{\psi^2} = \left(\frac{\partial_k \bar{\psi}}{\bar{\psi}} - \frac{\partial_k \psi}{\psi} \right) \frac{\bar{\psi}}{\psi},$$

and we henceforth obtain

$$\partial_\ell \psi \partial_j \psi \partial_k \left(\frac{\bar{\psi}}{\psi} \right) = \frac{1}{2} \operatorname{Im} \left(\frac{\partial_k \psi}{\psi} \right) \partial_\ell \psi \partial_j \psi \frac{\bar{\psi}}{\psi}.$$

Using this on the r.h.s. of (2.1) and summing up all terms yields the assertion of the lemma. \square

In the upcoming analysis, we shall use the established estimate in the following form, where we denote by $\|f\|_{\dot{H}^1} := \|\nabla f\|_{L^2}$ the usual $\dot{H}^1(\mathbb{R}^d)$ semi-norm:

Corollary 2.2. *Fix $\varepsilon > 0$. Then for any $\psi^\varepsilon \in H_{\text{loc}}^2(\mathbb{R}^d)$ and for any test function $\varphi \in \mathcal{D}(\mathbb{R}_x^d \times \mathbb{R}_p^d)$, we have*

$$(2.2) \quad \left| \int_{\mathbb{R}^d} \operatorname{div} (\nabla \sqrt{\rho^\varepsilon} \otimes \nabla \sqrt{\rho^\varepsilon}) \varphi \left(x, \frac{J^\varepsilon}{\rho^\varepsilon} \right) dx \right| \leq M^\varepsilon < +\infty,$$

where $\rho^\varepsilon, J^\varepsilon$ are defined in (1.4). Explicitly, we find

$$\begin{aligned} M^\varepsilon &\leq \frac{d}{\varepsilon} \|\psi^\varepsilon\|_{\dot{H}^1(\Omega)}^2 \sup_{\xi \in \mathbb{R}^d} \int_{\mathbb{R}^d} |\xi \varphi(x, \xi)| dx \\ &\quad + \varepsilon d \|\psi^\varepsilon\|_{\dot{H}^1(\Omega)} \|\nabla \psi^\varepsilon\|_{\dot{H}^1(\Omega)} \sup_{\xi \in \mathbb{R}^d} \int_{\mathbb{R}^d} |\varphi(x, \xi)| dx, \end{aligned}$$

where $\Omega \subset \mathbb{R}^d$ denotes any compact set containing the support of $\varphi(\cdot, p)$ for all $p \in \mathbb{R}^d$.

Proof. The proof follows directly from the estimate given in Proposition 2.1 and a density argument in $H_{\text{loc}}^2(\mathbb{R}^d)$. \square

In order to understand how M^ε behaves with respect to ε we first note that due to the semi-classical scaling of the equation (1.1) $\|\psi^\varepsilon(t)\|_{\dot{H}^1}$ is not uniformly bounded as $\varepsilon \rightarrow 0_+$. In fact $\psi^\varepsilon(t)$ is ε -oscillatory for all $t \in \mathbb{R}$ and thus each derivative scales like $1/\varepsilon$. Invoking the conservation laws of mass and energy, we have to use the re-scaled semi-norms $\|f\|_{\dot{H}_\varepsilon^1} := \|\varepsilon \nabla f\|_{L^2}$ in order to write M^ε in terms of uniformly bounded (w.r.t. ε) expressions. Doing so, we find that $M^\varepsilon = \mathcal{O}(1/\varepsilon^3)$ as $\varepsilon \rightarrow 0_+$.

Remark 2.3. Note, however, that if ψ^ε is of WKB type, i.e. $\psi^\varepsilon(x) = a(x)e^{iS(x)/\varepsilon}$ with real-valued phase $S(x) \in \mathbb{R}$ and ε -independent amplitude a , then the left hand side in (2.2) obviously is bounded as $\varepsilon \rightarrow 0$, although the right hand side blows up. In addition, it is easy to check that if one takes a superposition of two WKB states (such that $\nabla S_1 \neq \nabla S_2$), the bound (2.2) is easily saturated.

3. BOHMIAN MEASURES AS DISTRIBUTIONAL SOLUTIONS OF (1.13)

3.1. Mathematical preliminaries. Let us first note that the assumption $V \in C_b^1(\mathbb{R}^d; \mathbb{R})$ is sufficient to ensure that, for each $\varepsilon > 0$, the Hamiltonian operator

$$H^\varepsilon = -\frac{\varepsilon^2}{2}\Delta + V(x),$$

is essentially self-adjoint on $D(H^\varepsilon) = H^2(\mathbb{R}^d) \subset L^2(\mathbb{R}^d)$. It therefore generates a unitary (strongly continuous) group $U^\varepsilon(t) = e^{-itH^\varepsilon/\varepsilon}$ on $L^2(\mathbb{R}^d)$, which ensures the global existence of a unique solution $\psi^\varepsilon(t) = U^\varepsilon(t)\psi_0$ of the Schrödinger equation (1.1), such that

$$\|\psi^\varepsilon(t, \cdot)\|_{L^2} = \|\psi_0^\varepsilon\|_{L^2}.$$

Moreover, since $\psi_0^\varepsilon \in H^3 \subset D(H^\varepsilon)$, standard semi-group theory [23] imply $\psi^\varepsilon(t) \in D(H^\varepsilon) = H^2(\mathbb{R}^d)$, for all $t \in \mathbb{R}$. Clearly, this also yields that $\rho^\varepsilon(t) \in L^1(\mathbb{R}^d; \mathbb{R})$ as well as $J^\varepsilon(t) \in L^1(\mathbb{R}^d; \mathbb{R}^d)$, for all $t \in \mathbb{R}$ and that

$$E^\varepsilon(t) = E^\varepsilon(0) < +\infty,$$

providing a rigorous basis for the conservation of mass and energy. In addition, since H^ε and $U^\varepsilon(t)$ commute, and we obtain that

$$\|(H^\varepsilon)^{n/2}\psi^\varepsilon(t)\|_{L^2(\mathbb{R}^d)} = \|(H^\varepsilon)^{n/2}\psi_0^\varepsilon\|_{L^2(\mathbb{R}^d)}.$$

Since $V \in L^\infty(\mathbb{R}^d)$ the latter is equivalent to the n -th Sobolev norm

$$\|f\|_{H^n} := \|(1 + |\xi|^{n/2})\widehat{f}\|_{L^2},$$

and we immediately infer the following result:

Lemma 3.1. *Under the assumptions of Theorem 1.1, $\psi^\varepsilon(t) \in H^3(\mathbb{R}^d)$ for all $t \in \mathbb{R}$.*

With this result in hand, we are sure to be able to apply the estimates established in Section 2.

3.2. Weak formulation of (1.13). In order to make sense of $\beta^\varepsilon(t)$ as a weak solution of (1.13), the main problem is to understand the weak formulation of $\nabla_x V_B^\varepsilon \cdot \nabla_p \beta^\varepsilon = \text{div}_p(V_B^\varepsilon \nabla_x \beta^\varepsilon)$. To this end, consider a class of test-functions $\varphi(t, x, p) = \chi(t, x)\sigma(p)$ with $\chi \in C_0^\infty(\mathbb{R}_t \times \mathbb{R}_x^d)$, $\sigma \in C_0^\infty(\mathbb{R}_p^d)$ and compute

$$\begin{aligned} & \int_0^\infty \iint_{\mathbb{R}^{2d}} \nabla_x V_B^\varepsilon \cdot \nabla_p \varphi(t, x, p) d\beta^\varepsilon(t, dx, dp) dt = \\ & = \int_0^\infty \int_{\mathbb{R}^d} \chi(t, x) \nabla_x V_B^\varepsilon(t, x) \cdot \nabla \sigma(u^\varepsilon(t, x)) \rho^\varepsilon(t, dx) dt. \end{aligned}$$

since, by definition, $\beta^\varepsilon(t, x, p) = \rho^\varepsilon(t, x)\delta(p - u^\varepsilon(t, x))$ where denote $u^\varepsilon := \frac{J^\varepsilon}{\rho^\varepsilon}$, i.e. the quantum mechanical velocity field. The following lemma then shows that this weak formulation indeed makes sense.

Lemma 3.2. *Let $\varepsilon > 0$. For $\sigma \in C_0^\infty(\mathbb{R}_p^d)$ and $\chi \in C_0^\infty(\mathbb{R}_t \times \mathbb{R}_x^d)$ we have*

$$\int_0^\infty \int_{\mathbb{R}^d} |\chi(x, t)| |\nabla \sigma(u^\varepsilon(x, t))| |\nabla_x V_B^\varepsilon(x, t)| \rho^\varepsilon(t, x) dx dt < +\infty.$$

This result is key in proving that Bohmian measures furnishes a distributional solution of (1.13).

Proof. A simple computation shows that

$$\begin{aligned}\rho^\varepsilon \nabla_x V_B^\varepsilon &= \frac{\varepsilon^2}{2} \nabla \Delta \rho^\varepsilon - \frac{\varepsilon^2}{4} \operatorname{div} \left(\frac{\nabla \rho^\varepsilon \otimes \nabla \rho^\varepsilon}{\rho^\varepsilon} \right) \\ &= \frac{\varepsilon^2}{2} \nabla \Delta \rho^\varepsilon - \varepsilon^2 \operatorname{div} (\nabla \sqrt{\rho^\varepsilon} \otimes \nabla \sqrt{\rho^\varepsilon}).\end{aligned}$$

Inserting this into the weak formulation of $\nabla_x V_B^\varepsilon \cdot \nabla_p \beta^\varepsilon$, we can estimate

$$\begin{aligned}& \int_0^\infty \int_{\mathbb{R}^d} |\chi(x, t)| |\nabla \sigma(u^\varepsilon(x, t))| |\nabla_x V_B^\varepsilon(x, t)| \rho^\varepsilon(x) dx dt \\ & \leq \frac{\varepsilon^2}{2} \int_0^\infty \int_{\mathbb{R}^d} |\chi(x, t)| |\nabla \sigma(u^\varepsilon(x, t))| |\nabla \Delta \rho^\varepsilon| dx dt + \\ & \quad + \varepsilon^2 \int_0^\infty \int_{\mathbb{R}^d} |\chi(x, t)| |\nabla \sigma(u^\varepsilon(x, t))| |\operatorname{div} (\nabla \sqrt{\rho^\varepsilon} \otimes \nabla \sqrt{\rho^\varepsilon})| dx dt\end{aligned}$$

The two terms on the right hand side can be treated as follows: By Lemma 3.1 we have $\psi^\varepsilon \in H^3(\mathbb{R}^d)$ and thus $\nabla \Delta \rho^\varepsilon$ is in $L^1(\mathbb{R})$, for all $t \in \mathbb{R}$. Therefore

$$\int_0^\infty \int_{\mathbb{R}^d} |\chi(t, x)| |\nabla \sigma(u^\varepsilon(x, t))| |\nabla \Delta \rho^\varepsilon| dx dt < +\infty.$$

On the other hand, inequality (2.2) directly yields (for any fixed $\varepsilon > 0$)

$$\int_0^\infty \int_{\mathbb{R}^d} |\chi(t, x)| |\nabla \sigma(u^\varepsilon(x, t))| |\operatorname{div} (\nabla \sqrt{\rho^\varepsilon} \otimes \nabla \sqrt{\rho^\varepsilon})| dx dt < +\infty,$$

and the assertion is proved. \square

As a final preliminary step, let us recall the classical notion of the *push-forward for measures*: Let $\mu_0 \in \mathcal{M}(\mathbb{R}^d)$ and $f : \mathbb{R}^d \rightarrow \mathbb{R}^d$ a measurable map. Then $\mu_1 = X \# \mu_0$ is called the *push-forward of μ_0 under f* , if for every $\sigma \in C_0(\mathbb{R}^d)$, it holds:

$$(3.1) \quad \int_{\mathbb{R}^d} \sigma(x) \mu_1(x) dx = \int_{\mathbb{R}^d} \sigma(f(x)) \mu_0(x) dx,$$

By a straightforward approximation argument this condition can be relaxed in order to take into account test-functions σ which are (only) integrable with respect to μ_1 , but not necessarily C_0 . In the following we shall use this slightly more general definition of push-forwards (the reason will become clear in the proof given below). In particular, we have

$$\int_0^\infty \iint_{\mathbb{R}^{2d}} \varphi(t, x, p) d\beta^\varepsilon(t, dx, dp) dt = \int_0^\infty \int_{\mathbb{R}^d} \varphi(t, X^\varepsilon(t, x), u^\varepsilon(t, x)) \rho_0^\varepsilon(dx) dt,$$

by using the fact that $\beta^\varepsilon(t, x, p)$ is the push-forward of the measure $\rho_0^\varepsilon(x) \delta(p - u_0(x))$ under the Bohmian phase space flow Φ_t^ε defined in (1.7).

Proof of Theorem 1.1. Let $\varphi \in C_0^\infty([0, +\infty) \times \mathbb{R}_x^d \times \mathbb{R}_p^d)$ be a test-function such that $\varphi(t, x, p) = \chi(t, x) \sigma(p)$. Then, the weak formulation of (1.13) reads

$$\int_0^\infty \iint_{\mathbb{R}^{2d}} ((\partial_t \chi(t, x) + p \cdot \nabla_x \chi(t, x)) \sigma(p) - \chi(t, x) \nabla_x (V + V_B^\varepsilon) \cdot \nabla_p \sigma) \beta^\varepsilon(t, dx, dp) dt$$

First, consider the term involving $\nabla_x V_B^\varepsilon$: Having in mind the result of Lemma 3.2, we are allowed to consider $\chi(t, x) \nabla_x V_B^\varepsilon(t, x) \cdot \nabla \sigma(u^\varepsilon(t, x))$ as a test-function which

is integrable with respect to $\rho^\varepsilon(t, x)$. Thus, we can apply the push-forward formula 3.1 and infer

$$\begin{aligned} & \int_0^\infty \iint_{\mathbb{R}^{2d}} \chi(t, x) \nabla_x V_B^\varepsilon(t, x) \cdot \nabla \sigma(p) \beta^\varepsilon(t, dx, dp) dt = \\ & = \int_0^\infty \int_{\mathbb{R}^d} \chi(t, X^\varepsilon(t, x)) \nabla_x V_B^\varepsilon(t, X^\varepsilon(t, x)) \cdot \nabla \sigma(u^\varepsilon(t, X^\varepsilon(t, x))) \rho_0^\varepsilon(dx) dt. \end{aligned}$$

In addition, the fact that $J^\varepsilon = \rho^\varepsilon u^\varepsilon \in L^1(\mathbb{R}^d)$ implies that the “test-function” $\sigma(u^\varepsilon(t, x)) u^\varepsilon(t, x) \cdot \nabla \chi(t, x)$ is integrable with respect to ρ^ε (note however, that $u^\varepsilon(t, x)$ in general is not continuous). Thus we can again apply the (generalized) push-forward formula 3.1 to obtain

$$\begin{aligned} & \int_0^\infty \iint_{\mathbb{R}^{2d}} \sigma(p) p \cdot \nabla_x \chi(t, x) \beta^\varepsilon(t, dx, dp) dt = \\ & = \int_0^\infty \int_{\mathbb{R}^d} \sigma(u^\varepsilon(t, x)) u^\varepsilon(t, x) \cdot \nabla \chi(t, x) \rho_0^\varepsilon(dx) dt. \end{aligned}$$

All the other terms appearing in the weak formulation of (1.13) can then be treated analogously. Having in mind the ODE system (1.8), we consequently arrive at

$$\begin{aligned} & \int_0^\infty \iint_{\mathbb{R}^{2d}} ((\partial_t \chi + p \cdot \nabla_x \chi) \sigma(p) - \chi \nabla_x (V + V_B^\varepsilon) \cdot \nabla_p \sigma) \beta^\varepsilon(t, dx, dp) dt \\ & = \int_0^\infty \int_{\mathbb{R}^d} \frac{d}{dt} (\chi(t, X^\varepsilon(t, x)) \sigma(u^\varepsilon(t, x))) \rho_0^\varepsilon(dx) dt \\ & = - \int_{\mathbb{R}^d} \chi(t, x) \sigma(u_0^\varepsilon(x)) \rho_0^\varepsilon(dx). \end{aligned}$$

This proves that the Bohmian measure $\beta^\varepsilon(t)$ furnishes a weak solution of (1.13) in $\mathcal{D}'([0, \infty) \times \mathbb{R}_x^d \times \mathbb{R}_p^d)$ with initial data (1.6). The proof for $\mathcal{D}'(\mathbb{R}_t \times \mathbb{R}_x^d \times \mathbb{R}_p^d)$ is analogous. \square

4. STUDY OF POSSIBLE DEFECTS

Having established the fact that β^ε is indeed a weak solution of (1.13), we first rewrite the equation in the following form

$$(4.1) \quad \partial_t \beta^\varepsilon + p \cdot \nabla_x \beta^\varepsilon - \nabla_x V \cdot \nabla_p \beta^\varepsilon = \operatorname{div}_p (\nabla_x V_B^\varepsilon \beta^\varepsilon),$$

where V_B is the Bohm potential defined in (1.9). Using the weak convergence results given in [19] we can pass to the limit on the left hand side of this equation (up to extraction of sub-sequences) in order to obtain

$$(4.2) \quad \partial_t \beta + p \cdot \nabla_x \beta - \nabla_x V \cdot \nabla_p \beta = \mathcal{F}$$

where the defect \mathcal{F} is defined in (1.15). In order to gain some information on \mathcal{F} (and prove Theorem 1.2), we first derive from (4.2) the following equation for the first moment of $\beta(t)$ with respect to $p \in \mathbb{R}^d$:

$$(4.3) \quad \partial_t J + \operatorname{div}_x \int_{\mathbb{R}_p^d} p \otimes p \beta(t, x, dp) - \rho \nabla_x V = - \int_{\mathbb{R}_p^d} p \mathcal{F}(t, x, p) dp,$$

where ρ, J denote the classical limits of $\rho^\varepsilon, J^\varepsilon$ given by (1.11) and (1.12). To proceed further we need the following result.

Lemma 4.1. *Let $\mu \in \mathcal{M}^+(\mathbb{R}_x^d \times \mathbb{R}_p^d)$ be such that*

$$\int_{\mathbb{R}_p^d} \mu(x, dp) = \rho \in \mathcal{M}^+(\mathbb{R}^d), \quad \int_{\mathbb{R}_p^d} p\mu(x, dp) = \rho(x)u(x),$$

for some function $u(x) \in \mathbb{R}^d$ defined ρ -a.e.. Then it holds

$$\int_{\mathbb{R}_p^d} p \otimes p \mu(x, dp) \geq \rho u \otimes u,$$

with equality if and only if $\mu(x, p) = \rho(x)\delta(p - u(x))$.

Proof. The proof follows directly from the Cauchy-Schwartz inequality (see also Lemma 3.5 in [12]) applied to

$$\sum_{\ell, j=1}^d \int_{\mathbb{R}^d} \rho(x) \varphi_\ell(x) \varphi_j(x) u_\ell(x) u_j(x) dx,$$

where $\varphi \in C_0^\infty(\mathbb{R}^d)$. Equality then holds if and only if there exists a constant $C \in \mathbb{R}$, such that

$$\forall \varphi \in C_0^\infty : \sum_{\ell, j=1}^d p_\ell \varphi_j(x) = C \sum_{\ell, j=1}^d u_\ell(x) \varphi_j(x), \quad \mu - a.e.$$

which clearly implies that $p_\ell = Cu_\ell(x)$ and thus for any $x \in \mathbb{R}^d$, $\mu(x, \cdot)$ must concentrate on the set of points $\{Cu_\ell(x)\}_{\ell=1}^d$. \square

Using the result of this lemma we can rewrite (4.3) as

$$(4.4) \quad \partial_t J + \operatorname{div}_x(\rho u \otimes u) - \rho \nabla_x V = - \int_{\mathbb{R}_p^d} p \mathcal{F}(t, x, p) dp - \operatorname{div}_x(\rho \mathcal{B}),$$

with a defect $\mathcal{B}(t, x) \geq 0$. In addition we know that

$$\mathcal{B}(t, x) = 0, \text{ if and only if, } \beta(t, x, p) = \rho(t, x)\delta(p - u(t, x)).$$

On the other hand, we can consider the equation for $\beta^\varepsilon(t)$, take first the moment w.r.t. p and then pass to the limit $\varepsilon \rightarrow 0_+$: Multiplying (4.1) by $p \in \mathbb{R}^d$ and integrating yields the equation for the current density in the quantum hydrodynamical system (1.5), i.e.

$$(4.5) \quad \partial_t J^\varepsilon + \operatorname{div} \left(\frac{J^\varepsilon \otimes J^\varepsilon}{\rho^\varepsilon} \right) + \rho^\varepsilon \nabla V = \rho^\varepsilon \nabla V_B^\varepsilon,$$

where we have used the fact that

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

since β^ε is mono-kinetic by definition. Using this, we can define a defect $\mathcal{C}(t, x) \geq 0$ via

$$(4.6) \quad \lim_{\varepsilon \rightarrow 0_+} \left(\frac{J^\varepsilon \otimes J^\varepsilon}{\rho^\varepsilon} \right) = \int_{\mathbb{R}^d} p \otimes p \beta(t, x, dp) + \mathcal{C}(t, x),$$

where the limit has to be understood in $\mathcal{D}'(\mathbb{R}_t \times \mathbb{R}_x^d)$. In addition, we know that

$$\rho^\varepsilon \nabla V_B^\varepsilon = \frac{\varepsilon^2}{2} \nabla \Delta \rho^\varepsilon - \varepsilon^2 \operatorname{div} (\nabla \sqrt{\rho^\varepsilon} \otimes \nabla \sqrt{\rho^\varepsilon}),$$

where the first term tends to zero as $\varepsilon \rightarrow 0_+$ by linearity. This consequently yields

$$(4.7) \quad \partial_t J + \operatorname{div}(\rho u \otimes u) + \rho \nabla V = -\operatorname{div}(\mathcal{A} + \rho \mathcal{B} + \mathcal{C}),$$

where $\mathcal{A}(t, x)$ is defined by

$$(4.8) \quad \varepsilon^2 \operatorname{div}(\nabla \sqrt{\rho^\varepsilon} \otimes \nabla \sqrt{\rho^\varepsilon}) \xrightarrow{\varepsilon \rightarrow 0_+} \mathcal{A} \quad \text{in } \mathcal{D}'(\mathbb{R}_t \times \mathbb{R}_x^d).$$

In summary, we have the following partial characterization of \mathcal{F} .

Lemma 4.2. *The defect \mathcal{F} defined in (1.15) satisfies*

$$(4.9) \quad \int_{\mathbb{R}^d} p \mathcal{F}(t, x, p) dp = -\operatorname{div}(\mathcal{A}(t, x) + \mathcal{C}(t, x)),$$

where \mathcal{A}, \mathcal{C} are given by (4.8), (4.6), respectively.

In a last step, this can now be compared with the classical limit of the quantum hydrodynamic system (1.5) via Wigner measures. In [12] it has been shown that

$$J^\varepsilon(t, x) \xrightarrow{\varepsilon \rightarrow 0_+} J(t, x) := \int_{\mathbb{R}^d} w(t, x, dp)$$

satisfies

$$(4.10) \quad \partial_t J + \operatorname{div}(\rho u \otimes u) + \rho \nabla V = -\operatorname{div} \rho \mathcal{T},$$

with a temperature tensor $\mathcal{T}(t, x) \geq 0$. The latter is found to be equal to zero, if and only if $w(t, x, p) = \rho(t, x) \delta(p - u(t, x))$. This can now be used as follows:

Proof of Theorem 1.2. Let $d = 1$. Having in mind that, by assumption, the initial limiting Bohmian and Wigner measures are equal $\beta_0(x, p) = w_0(x, p)$, the uniqueness of solutions, together with (4.10) and (4.7), implies

$$(4.11) \quad \rho \mathcal{T} = \mathcal{A} + \rho \mathcal{B} + \mathcal{C}, \quad \text{in } \mathcal{D}'(\mathbb{R}_t \times \mathbb{R}_x^d),$$

Since all terms on the right hand side are greater or equal to zero, we infer that

$$w(t, x, p) = \rho(t, x) \delta(p - u(t, x)), \quad \text{if and only if, } \mathcal{A} = \mathcal{B} = \mathcal{C} = 0.$$

By definition, this implies that

$$\rho^\varepsilon \nabla V_B^\varepsilon \xrightarrow{\varepsilon \rightarrow 0_+} 0,$$

as well as

$$\lim_{\varepsilon \rightarrow 0_+} \int_{\mathbb{R}^d} p \otimes p \beta^\varepsilon(t, x, dp) = \int_{\mathbb{R}^d} p \otimes p \beta(t, x, dp) = \rho u \otimes u.$$

By Lemma 4.1, we conclude $\beta(t, x, p) = \rho(t, x) \delta(p - u(t, x))$ and the assertion is proved. \square

Remark 4.3. In dimensions $d > 1$ we can not conclude as before, since identity (4.11) has to be replaced by

$$\rho \mathcal{T} = \mathcal{A} + \rho \mathcal{B} + \mathcal{C} + \mathcal{D},$$

for some \mathcal{D} satisfying $\operatorname{div} \mathcal{D}(t, x) = 0$.

5. BOHMIAN MEASURES FOR SEMI-CLASSICAL WAVE PACKETS

The theory of semi-classical wave packets is very well developed, see e.g. [14, 15, 20, 21] and the references given therein (see also [1, 6] for a recent application in the context of nonlinear Schrödinger equations). It allows to approximate the solution to (1.1) via

$$(5.1) \quad \psi^\varepsilon(t, x) \stackrel{\varepsilon \rightarrow 0^+}{\sim} u^\varepsilon(t, x) = \varepsilon^{-d/2} v \left(t, \frac{x - X(t)}{\sqrt{\varepsilon}} \right) e^{i(P(t) \cdot (x - X(t)) + S(t))/\varepsilon},$$

where $P(t), X(t)$ solve the Hamiltonian system (1.17) and $S(t)$ is the associated classical action, i.e.

$$S(t) = \int_0^t \frac{1}{2} |P(s)|^2 - V(X(s)) ds.$$

The envelope function $v(t, y)$ is thereby found to be a solution of the following ε -independent Schrödinger equation (see also the proof of Theorem 1.3 below):

$$(5.2) \quad i\partial_t v = -\frac{1}{2} \Delta_y v + \frac{1}{2} (Q(t)y, y)v, \quad v(t=0, y) = a(y),$$

where $Q(t) := \text{Hess } V(X(t))$ denotes the Hessian of the potential $V(x)$ evaluated at the classical trajectory $X(t)$ and $a \in \mathcal{S}$ is induced by the initial data ψ_0^ε given in Theorem 1.3. In other words, $v(t, x)$ solves a linear Schrödinger equation with time-dependent quadratic potential.

Under suitable assumptions on V (satisfied by the hypothesis of Theorem 1.3), one can show, see e.g. [1, 14, 15, 6, 20, 21], that the coherent state $u^\varepsilon(t, x)$ approximates the exact solution $\psi^\varepsilon(t, x)$ of (1.1) in the following sense

$$(5.3) \quad \|\psi^\varepsilon(t, \cdot) - u^\varepsilon(t, \cdot)\|_{L^2(\mathbb{R}^d)} \leq C\sqrt{\varepsilon}e^{Ct},$$

provided the initial data $\psi^\varepsilon(0, x)$ is of the form given in Theorem 1.3.

Remark 5.1. Note that in contrast to the WKB approximation, the coherent state ansatz does not suffer from the appearance of caustics (although it is sensitive to them through equation (5.2) where the caustics are somehow hidden). In addition, it assumes that the amplitude concentrates on the scale $\sqrt{\varepsilon}$. The latter has been shown to be a critical scaling in the theory of Bohmian measures, cf. [19].

Proof of Theorem 1.3. We first note that the solution to (5.2) satisfies $\|v(t, \cdot)\|_{L^2} = \|a\|_{L^2}$ for all $t \in \mathbb{R}$. Thus, the Wigner transformation of $u^\varepsilon(t, x)$ satisfies

$$w^\varepsilon[u^\varepsilon] \stackrel{\varepsilon \rightarrow 0^+}{\rightarrow} w \quad \text{in } C_b(\mathbb{R}_t; \mathcal{M}^+(\mathbb{R}_x^d \times \mathbb{R}_p^d)) \text{ w-}^*$$

The corresponding Wigner measure is well known, cf. [17, 19]:

$$w(t, x, p) = \|a\|_{L^2}^2 \delta(x - X(t)) \delta(p - P(t)).$$

From the estimate (5.3) and the classical results given in [17] we conclude that the Wigner transformation of the exact solution $w^\varepsilon[\psi^\varepsilon]$ converges to the same limiting measure w , uniformly on compact time-intervals $I \subset \mathbb{R}_t$.

In order to prove that $w(t) = \beta(t)$, we perform the following unitary transformation

$$(5.4) \quad \psi^\varepsilon(t, x) = \varepsilon^{-d/2} v^\varepsilon \left(t, \frac{x - X(t)}{\sqrt{\varepsilon}} \right) e^{i(P(t) \cdot (x - X(t)) + S(t))/\varepsilon}.$$

Using this transformation, equation (1.1) is easily found to be equivalent to

$$(5.5) \quad i\partial_t v^\varepsilon = -\frac{1}{2}\Delta_y v^\varepsilon + V^\varepsilon(t, y)v^\varepsilon, \quad v^\varepsilon(t=0, x) = a(x),$$

where $V^\varepsilon(t, y)$ is given by

$$V^\varepsilon(t, y) = \frac{1}{\varepsilon} (V(X(t) + \sqrt{\varepsilon}y) - V(X(t)) - \sqrt{\varepsilon}\nabla V(X(t)) \cdot y).$$

Obviously, for C^2 potentials V equation (5.5) converges to (5.2) as $\varepsilon \rightarrow 0_+$. This together with sufficient a-priori bounds on $v^\varepsilon(t)$ yields the estimate (5.3), cf. [6] for more details. On the other hand, using (5.4), the Bohmian measure $\beta^\varepsilon(t)$ of the exact solution $\psi^\varepsilon(t)$ can be seen to act on Lipschitz test-function $\varphi \in C_0(\mathbb{R}_x^d \times \mathbb{R}_p^d)$ via

$$\langle \beta^\varepsilon(t), \varphi \rangle = \int_{\mathbb{R}^d} |v^\varepsilon(t, y)|^2 \varphi \left(X(t) + \sqrt{\varepsilon}y, \sqrt{\varepsilon}\text{Im} \left(\frac{\nabla v^\varepsilon(t, y)}{v^\varepsilon(t, y)} \right) + P(t) \right) dy.$$

Using the Lipschitz continuity of φ we can estimate

$$\begin{aligned} & \left| \varphi \left(X(t) + \sqrt{\varepsilon}y, \sqrt{\varepsilon}\text{Im} \left(\frac{\nabla v^\varepsilon(t, y)}{v^\varepsilon(t, y)} \right) + P(t) \right) - \varphi(X(t), P(t)) \right| \\ & \leq C_\varphi \sqrt{\varepsilon} \left(|y| + \left| \text{Im} \left(\frac{\nabla v^\varepsilon(t, y)}{v^\varepsilon(t, y)} \right) \right| \right), \end{aligned}$$

for some positive constant $C_\varphi > 0$. In view of this, we obtain

$$\begin{aligned} & \left| \langle \beta^\varepsilon(t), \varphi \rangle - \int_{\mathbb{R}^d} |v^\varepsilon(y, t)|^2 \varphi(X(t), P(t)) dy \right| \\ & \leq C_\varphi \sqrt{\varepsilon} \int_{\mathbb{R}^d} |y| |v^\varepsilon(t, y)|^2 dy + \sqrt{\varepsilon} \int_{\mathbb{R}^d} |v^\varepsilon(t, y)| |\nabla v^\varepsilon(t, y)| dy \\ & \leq C_\varphi \sqrt{\varepsilon} \|v^\varepsilon(t)\|_{L^2} (\|x|v^\varepsilon(t)\|_{L^2} + \|\nabla v^\varepsilon(t)\|_{L^2}), \end{aligned}$$

where the last inequality follows from Cauchy-Schwartz. In order to proceed further we need the following lemma.

Lemma 5.2. *Let $V \in C_b^3(\mathbb{R}^d)$. Then the solution of (5.5) satisfies*

$$\|x|v^\varepsilon(t)\|_{L^2} \leq C_1, \quad \|\nabla v^\varepsilon(t)\|_{L^2} \leq C_2, \quad \forall t \in \mathbb{R},$$

where C_1, C_2 are some positive constants, independent of ε .

Proof of Lemma 5.2. In [6] it is shown in there that, if V is sub-quadratic, i.e. $\partial^\gamma V(x) \in L^\infty$, for all $|\gamma| \geq 2$, it holds:

$$(5.6) \quad \|x|v^\varepsilon(t, \cdot)\|_{L^2} \leq C_1, \quad \|x|^3 v^\varepsilon(t)\|_{L^2} \leq C_3, \quad \forall t \in \mathbb{R}.$$

It therefore only remains to show the estimate for $\nabla v^\varepsilon(t)$. This follows by considering the energy corresponding to (5.5), i.e.

$$E^\varepsilon(t) = \frac{\varepsilon^2}{2} \int_{\mathbb{R}^d} |\nabla v^\varepsilon(t, x)|^2 dx + \int_{\mathbb{R}^d} V^\varepsilon(t, x) |v^\varepsilon(t, x)|^2 dx,$$

which satisfies

$$\frac{d}{dt} E^\varepsilon(t) = \int_{\mathbb{R}^d} \partial_t V^\varepsilon(t, x) |v^\varepsilon(t, x)|^2 dx.$$

Since

$$|\partial_t V^\varepsilon(t, x)| \leq |\dot{X}(t)| |y|^3 \sqrt{\varepsilon} \sup |\partial^3 V(X(t) + s\sqrt{\varepsilon}y)|,$$

the assumption $V \in C_b^3$, together with (5.6), yields the desired bound on $\nabla v^\varepsilon(t)$. \square

Using the a-priori estimates established in Lemma 5.2 we obtain

$$\left| \langle \beta^\varepsilon(t), \varphi \rangle - \int_{\mathbb{R}^d} |v^\varepsilon(y, t)|^2 \varphi(X(t), P(t)) dy \right| \xrightarrow{\varepsilon \rightarrow 0^+} 0.$$

In other words, we have that

$$(5.7) \quad \beta(t) = \|v(t, \cdot)\|_{L^2}^2 \delta(x - X(t)) \delta(p - P(t)),$$

Having in mind that $\|v(t, \cdot)\|_{L^2} = \|a\|_{L^2}$ this proves assertion (1) of Theorem 1.3.

In order to conclude assertion (2) we recall the following formula, stated in [19, Remark 3.8]. For all $t \in \mathbb{R}$ and for all test-functions $\varphi \in C_0(\mathbb{R}_x^d \times \mathbb{R}_p^d)$, $\chi \in C_0(\mathbb{R}_t)$ it holds

$$\begin{aligned} \int_{\mathbb{R}} \chi(t) \iint_{\mathbb{R}^{2d}} \varphi(x, p) \beta^\varepsilon(t, dx, dp) dt &= \int_{\mathbb{R}} \chi(t) \int_{\mathbb{R}^d} \varphi(X^\varepsilon(t, x), P^\varepsilon(t, x)) \rho_0^\varepsilon(x) dx dt \\ &= \int_{\mathbb{R}} \chi(t) \int_{\mathbb{R}^d} \varphi(X^\varepsilon(t, x_0 + \sqrt{\varepsilon}y), P^\varepsilon(t, x_0 + \sqrt{\varepsilon}y)) |a(y)|^2 dy dt \end{aligned}$$

where in the second equality we set $y = (x - x_0)/\sqrt{\varepsilon}$ and recall that the initial density is given by

$$\rho_0^\varepsilon(x) = \varepsilon^{-d/2} \left| a \left(\frac{x - x_0}{\sqrt{\varepsilon}} \right) \right|^2.$$

Now, let

$$\omega_{t,y} : \mathbb{R}_t \times \mathbb{R}_y^d \rightarrow \mathcal{M}^+(\mathbb{R}_x^d \times \mathbb{R}_p^d); \quad (t, y) \mapsto \omega_{t,y}(x, p),$$

be the Young measure associated to the family of re-scaled Bohmian trajectories

$$Y^\varepsilon(t, y) = X^\varepsilon(t, x_0 + \sqrt{\varepsilon}y), \quad Z^\varepsilon(t, y) = P^\varepsilon(t, x_0 + \sqrt{\varepsilon}y),$$

where we refer to [24] for the definition of Young measures and to [19, 16] for their application in the context of Bohmian measures. Then, by passing to the limit $\varepsilon \rightarrow 0_+$ (after the choice of an appropriate sub-sequence) we find that

$$\int_{\mathbb{R}} \chi(t) \iint_{\mathbb{R}^{2d}} \varphi(x, p) \beta(t, dx, dp) dt = \int_{\mathbb{R}} \chi(t) \int_{\mathbb{R}^d} \varphi(x, p) \omega_{t,y}(dx, dp) |a(y)|^2 dy dt.$$

In other words

$$\beta(t, x, p) = \int_{\mathbb{R}^d} |a(y)|^2 \omega_{t,y}(x, p) dy$$

Upon inserting (5.7) with $\|v(t, \cdot)\|_{L^2} = \|a\|_{L^2}$, this implies

$$\omega_{t,y}(x, p) = \nu(t, y) \delta(p - P(t)) \delta(x - X(t)).$$

Since $0 \leq \nu(y, t) \leq 1$ and

$$\int_{\mathbb{R}^d} |a(y)|^2 dy = \int_{\mathbb{R}^d} |a(y)|^2 \nu(t, y) dy,$$

for all $t \in \mathbb{R}$, we conclude $\nu(t, y) \equiv 1$ a.e. and hence

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

By a well known result of Young measure theory (see e.g. [16, Proposition 1]), we know that the fact that $\omega_{t,x}$ is concentrated in a point is equivalent to the convergence of the re-scaled trajectories, i.e.

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

locally in measure on $\mathbb{R}_t \times \mathbb{R}_y^d$. □

Remark 5.3. In $d = 1$, assertion (1) of Theorem 1.3 directly follows from Theorem 1.2, since $w(t)$ is obviously mono-kinetic. In addition, one should note that the established local in measure convergence implies (see e.g. [8, Section 13]) that there exists a sub-sequence $\{\varepsilon_n\}_{n \in \mathbb{N}}$, going to zero as $n \rightarrow \infty$, such that

$$Y^{\varepsilon_n} \xrightarrow{n \rightarrow \infty} X, \quad Z^{\varepsilon_n} \xrightarrow{n \rightarrow \infty} P, \quad \text{a.e. in } \Omega \subseteq \mathbb{R}_t \times \mathbb{R}_y^d.$$

APPENDIX A. AN EXAMPLE WITH NON MONO-KINETIC LIMITING BOHMIAN MEASURE

In [19] we considered several different examples of ψ^ε and computed the corresponding limiting Bohmian measure β and the corresponding Wigner measure w . We found that in general $w \neq \beta$ except in rather special situations. In fact, in all the examples given in [19] we find $w = \beta$ only in the mono-kinetic case. Together with the results stated in Theorem 1.2 and Theorem 1.3 this might yield the wrong impression that w and β can only coincide if they are both mono-kinetic phase space distributions. The following example will illustrate that this is in general not the case:

Consider an ε -dependent family of wave functions $\{u^\varepsilon\}_{0 < \varepsilon \leq 1}$ given by

$$u^\varepsilon(x) = a^\varepsilon(x) e^{iS^\varepsilon(x)/\varepsilon},$$

where the amplitude a^ε reads

$$a^\varepsilon(x) = \varepsilon^{-\frac{d}{4}} \rho^{1/2} \left(\frac{|x|}{\varepsilon^{1/2}} \right),$$

with some ε -independent profile $\rho \in \mathcal{S}(\mathbb{R}; \mathbb{R})$, satisfying

$$(A.1) \quad \int_0^\infty \frac{(\rho'(r))^2}{\rho(r)} r^{d-1} dr < +\infty.$$

In addition, we assume that $S^\varepsilon \in C_b(\mathbb{R}^d) \cap C_b^2(\mathbb{R}^d / \{0\})$, such that for $|x| > \varepsilon^{3/4}$: $S^\varepsilon(x) = S(x)$, with S even and

$$\lim_{\delta \rightarrow 0} \nabla S(\delta\omega) = \chi(\omega), \quad \forall \omega \in \mathbb{S}^{d-1},$$

with $\chi \in C^\infty(\mathbb{S}^{d-1})$. On the other hand, for $|x| \leq \varepsilon^{3/4}$ we assume that the phase function $S^\varepsilon(x) = S(x)$ is such that

$$\nabla S^\varepsilon(\varepsilon^{3/4}t\omega) = \nabla S(\varepsilon^{3/4}\omega) \frac{1+t}{2} + \nabla S(-\varepsilon^{3/4}\omega) \frac{1-t}{2}, \quad -1 \leq t \leq 1.$$

Lemma A.1. *Let u^ε be as given above, then*

$$\beta(x, p) = w(x, p) = \int_{\mathbb{R}} \rho(|y|) dy \frac{1}{|\mathbb{S}^{d-1}|} \int_{\mathbb{S}^{d-1}} \delta(p - \chi(\omega)) d\omega \otimes \delta(x).$$

Remark A.2. To our knowledge this is the first example in which $\beta = w$ is absolutely continuous with respect to the Lebesgue measure on \mathbb{R}_p^d .

Proof. We first note that, by assumption,

$$|u^\varepsilon(x)|^2 = \varepsilon^{-d/2} \rho \left(\frac{|x|}{\varepsilon^{1/2}} \right) \xrightarrow{\varepsilon \rightarrow 0^+} \delta(x) \int_{\mathbb{R}^d} \rho(|x|) dx.$$

In addition, we also have that $\nabla S^\varepsilon \in W^{1,\infty}(\mathbb{R}^d)$ and $|\partial_\ell \partial_j S^\varepsilon| \leq C\varepsilon^{-3/4}$, for all $\ell, j = 1, \dots, d$. Thus

$$\varepsilon \|\partial_{x_\ell} \partial_{x_j} S^\varepsilon\|_{L^\infty(\mathbb{R}^d)} \xrightarrow{\varepsilon \rightarrow 0^+} 0, \quad \forall \ell, j = 1, \dots, d.$$

Next, we consider $\varepsilon^2|\nabla u^\varepsilon|^2 = \varepsilon^2|\nabla a^\varepsilon|^2 + \rho^\varepsilon|\nabla S^\varepsilon|^2$, where we denote, as usual $\rho^\varepsilon := |u^\varepsilon|^2$. Since $|\nabla S^\varepsilon(x)| \leq C$, by assumption, we infer

$$\int_{\mathbb{R}^d} \rho^\varepsilon(x) |\nabla S^\varepsilon(x)|^2 dx \leq C, \text{ uniformly in } \varepsilon.$$

On the other hand one easily computes

$$\varepsilon^2 \int_{\mathbb{R}^d} |\nabla a^\varepsilon(x)|^2 = \frac{\varepsilon}{4} \int_{\mathbb{R}} \frac{\rho'(|y|)^2}{\rho(|y|)} dy \xrightarrow{\varepsilon \rightarrow 0^+} 0,$$

in view of (A.1). Theorem 4.7 of [19] consequently implies $\beta(x, p) = w(x, p)$ in the sense of measures.

It remains to explicitly compute the limiting measure. To this end, we consider the action of β^ε onto any testfunction $\varphi \in C_0(\mathbb{R}^{2d})$, i.e.

$$\begin{aligned} \langle \beta^\varepsilon, \varphi \rangle &= \varepsilon^{-d/2} \int_{\mathbb{R}^d} \rho \left(\frac{|x|}{\varepsilon^{1/2}} \right) \varphi(x, \nabla S^\varepsilon(x)) dx \\ &= \int_{\mathbb{S}^{d-1}} \int_0^\infty \rho(r) \varphi(\varepsilon^{1/2} r \omega, \nabla S^\varepsilon(\varepsilon^{1/2} r \omega)) r^{d-1} dr d\omega, \end{aligned}$$

by setting $y = r\omega$. It easily follows that as $\varepsilon \rightarrow 0_+$:

$$\langle \beta^\varepsilon, \varphi \rangle \sim \int_{\mathbb{S}^{d-1}} \int_0^\infty \rho(r) r^{d-1} \varphi(0, \nabla S^\varepsilon(\varepsilon^{1/2} r \omega)) dr d\omega.$$

Keeping $r > 0$, $\omega \in \mathbb{S}^{d-1}$ fixed, we see that for ε sufficiently small,

$$\nabla S^\varepsilon(\varepsilon^{1/2} r \omega) = \nabla S(\varepsilon^{1/2} r \omega) \xrightarrow{\varepsilon \rightarrow 0^+} \chi(\omega),$$

since $\varepsilon^{1/2} \gg \varepsilon^{3/4}$. By dominated convergence, we therefore conclude

$$\langle \beta^\varepsilon, \varphi \rangle \xrightarrow{\varepsilon \rightarrow 0^+} \frac{1}{|\mathbb{S}^{d-1}|} \int_{\mathbb{R}} \rho(|y|) dy \int_{\mathbb{S}^{d-1}} \varphi(0, \chi(\omega)) d\omega,$$

and the assertion is proved. \square

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