On Wigner and Bohmian measures in semi-classical quantum dynamics

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   - Bohmian dynamics

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Basic setting

Consider the time-evolution of $\psi^\varepsilon(t,\cdot) \in L^2(\mathbb{R}^d;\mathbb{C})$ governed by Schrödinger's equation:

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

where $x \in \mathbb{R}^d$, $t \in \mathbb{R}$, and $0 < \varepsilon \leq 1$ a (small) semi-classical parameter.

The potential $V(x) \in \mathbb{R}$ is assumed to be smooth and $V \in L^\infty(\mathbb{R}^d)$. Then, the Hamiltonian

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

is ess. self-adjoint on $L^2(\mathbb{R}^d)$ and thus $\psi^\varepsilon(t) = e^{-itH^\varepsilon/\varepsilon}\psi_0$, $\forall t \in \mathbb{R}$.

Basic conservation laws for mass and energy:

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

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

The initial data initial data ψ_0 is assumed to satisfy:

$$M^\varepsilon(0) = \|\psi_0^\varepsilon\|_{L^2}^2 = 1, \quad \sup_{0<\varepsilon\leq 1} E^\varepsilon(0) \leq C < +\infty.$$

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This implies (since $V(x) \geq 0$ w.r.o.g.) that $\psi^\varepsilon(t)$ is ε-oscillatory:

$$\forall t \in \mathbb{R} : \qquad \sup_{0<\varepsilon\leq 1} \left(\|\psi^\varepsilon(t)\|_{L^2} + \|\varepsilon\nabla\psi^\varepsilon(t)\|_{L^2}\right) < +\infty.$$

The wave function ψ^ε can be used to define observable densities, i.e. (real-valued) quadratic quantities of ψ^ε.

Two important examples are the position and the current density:

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

which satisfy the so-called Quantum hydrodynamic system (QHD):

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

Bohmian dynamics

In Bohmian mechanics [Bohm '52] one defines particle-trajectories

$$X^\varepsilon(t,\cdot):\mathbb{R}^d\to\mathbb{R}^d;\quad y\mapsto x\equiv X^\varepsilon(t,y),$$

via the following ODE:

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

where the initial $y\in\mathbb{R}^d$ are assumed to be distributed according to $\rho_0^\varepsilon\equiv|\psi_0^\varepsilon|^2$ and the velocity field u^ε is (formally) given by

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

Even though u^ε is (highly) singular, it can be proved [Berndl et al. '95] that, for all $t \in \mathbb{R}$: $X^\varepsilon(t,\cdot)$ is well-defined $\rho_0^\varepsilon - a.e.$ and that

$$\rho^\varepsilon(t) = X^\varepsilon(t,\cdot) \# \rho_0^\varepsilon,$$

i.e. $\rho^\varepsilon(t,x)$ is the push-forward of ρ_0^ε under the mapping $X^\varepsilon(t,\cdot)$:

$$\int_{\mathbb{R}^d} \sigma(x)\rho^\varepsilon(t,x)dx = \int_{\mathbb{R}^d} \sigma(X^\varepsilon(t,y))\rho_0^\varepsilon(y)dy, \quad \sigma \in C_0(\mathbb{R}^d).$$

The latter is often called equivariance of the measure $\rho^\varepsilon(t,\cdot)$, see [Teufel and Tumulka '05].

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Then, since $\dot X^\varepsilon = u^\varepsilon(t, X^\varepsilon(t,y))$:

$$\dot P^\varepsilon = \frac{d}{dt} u^\varepsilon(t, X^\varepsilon(t,y)) = \partial_t u^\varepsilon + u^\varepsilon \cdot \nabla u^\varepsilon$$

and using the QHD system (rewritten in terms of $\rho^\varepsilon, u^\varepsilon$) gives:

$$(1) \qquad \begin{cases} \dot X^\varepsilon = P^\varepsilon, & X^\varepsilon(0,y) = y \\ \dot P^\varepsilon = -\nabla V(X^\varepsilon) - \nabla V_B^\varepsilon(t, X^\varepsilon), & P^\varepsilon(0,y) = u_0^\varepsilon(y), \end{cases}$$

with $V_B^\varepsilon := -\frac{\varepsilon^2}{2\sqrt{\rho^\varepsilon}} \Delta \sqrt{\rho^\varepsilon}$, the so-called Bohm potential.

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3. is used for multi-particle computation in quantum chemistry, cf. [Gindensperger et al. '00];
4. allows for a comparison to the well-known theory of Wigner functions and Wigner measures;
5. could provide a possible starting point for an optimal-mass transportation formulation of quantum dynamics.

Bohmian measures

Definition

Fix $\varepsilon > 0$ and let $\psi^\varepsilon \in H^1(\mathbb{R}^d)$, with associated densities $\rho^\varepsilon, J^\varepsilon$. Then, $\beta^\varepsilon \in \mathcal{M}^+(\mathbb{R}^d_x \times \mathbb{R}^d_p)$ is given by

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

In other words

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

i.e. a mono-kinetic phase space distribution. It, formally, defines a Lagrangian sub-manifold of phase space

$$\mathcal{L}^\varepsilon := \{(x,p) \in \mathbb{R}^d_x \times \mathbb{R}^d_p : p = u^\varepsilon(x)\},$$

Analogous to classical kinetic theory, we have

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

However, for the second moment, we find

$$\iint_{\mathbb{R}^{2d}} \frac{|p|^2}{2}\, \beta^\varepsilon(x, dp) = \frac{1}{2} \int_{\mathbb{R}^d} \frac{|J^\varepsilon(x)|^2}{\rho^\varepsilon(x)} dx$$

which is not equal to the quantum mechanical kinetic energy:

$$E_{\rm kin} := \frac{\varepsilon^2}{2} \int_{\mathbb{R}^d} |\nabla \psi^\varepsilon(x)|^2 dx = \frac{1}{2} \int_{\mathbb{R}^d} \frac{|J^\varepsilon(x)|^2}{\rho^\varepsilon(x)} + \frac{\varepsilon^2}{2} \int_{\mathbb{R}^d} |\nabla \sqrt{\rho^\varepsilon}|^2 dx,$$

i.e. we are missing the term of order $\mathcal{O}(\varepsilon^2)$.

Dynamics of Bohmian measures

Denote by $\Phi_t^\varepsilon := (X^\varepsilon(t,y), P^\varepsilon(t,y))$ the (ε-dependent) phase space flow induced by (1).

Lemma (Equivariance of β)

The mapping Φ_t^ε exists globally in-time for almost all $(x,p) \in \mathbb{R}^{2d}$, relative to the measure

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

Moreover Φ_t^ε is continuous in time on its maximal open domain and

$$\beta^\varepsilon(t) = \Phi_t^\varepsilon \# \beta_0^\varepsilon,$$

i.e. $\beta^\varepsilon(t)$ is the push-forward of β^ε under the flow Φ_t^ε.

Classical limit of Bohmian measures

Lemma (Existence of a limiting measure)

Let $\psi^\varepsilon(t)$ be ε-oscillatory, i.e

$$\sup_{0<\varepsilon\leqslant 1}\left(\|\psi^\varepsilon(t)\|_{L^2}+\|\varepsilon\nabla\psi^\varepsilon(t)\|_{L^2}\right)<+\infty.$$

Then, up to extraction of sub-sequences, it holds:

$$\beta^\varepsilon \overset{\varepsilon\to 0_+}{\longrightarrow} \beta \quad \textit{in } L^\infty(\mathbb{R}_t;\mathcal{M}^+(\mathbb{R}^d_x\times\mathbb{R}^d_p))\,\mathrm{w}-*.$$

for some classical limit $\beta(t)\in\mathcal{M}^+(\mathbb{R}^d_x\times\mathbb{R}^d_p)$. Moreover,

$$\rho^\varepsilon(t,x) \overset{\varepsilon\to 0_+}{\longrightarrow} \int_{\mathbb{R}^d}\beta(t,x,dp),\quad J^\varepsilon(t,x) \overset{\varepsilon\to 0_+}{\longrightarrow} \int_{\mathbb{R}^d} p\,\beta(t,x,dp).$$

Thus, the limiting measure $\beta(t)$ incorporates (for all times $t \in \mathbb{R}$), the classical limit of the quantum mechanical position and current densities $\rho^\varepsilon(t), J^\varepsilon(t)$.

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Remark (Tightness)

If in addition $\rho^\varepsilon(t) = |\psi^\varepsilon(t)|^2$ is tight, we also have

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

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Q: Can we say more about $\beta(t)$, e.g., when is $\beta(t)$ mono-kinetic ?

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Young measures

We briefly recall the definitiion of Young measures:

Let $f_\varepsilon : \mathbb{R}^d \to \mathbb{R}^m$ be a sequence of measurable functions. Then, there exists a mapping

$$\Upsilon_\zeta : \mathbb{R}^d \to \mathcal{M}^+(\mathbb{R}^m),$$

called the Young measure associated to f_ε, such that (after selection of an appropriate subsequence):

1. $\zeta \mapsto \langle \Upsilon_\zeta, g \rangle$ is measurable for all $g \in C_0(\mathbb{R}^m)$;
2. For any test function $\sigma \in L^1(\Omega; C_0(\mathbb{R}^m))$:

$$\lim_{\varepsilon \to 0} \int_{\mathbb{R}^d} \sigma(\zeta, f_\varepsilon(\zeta))\, d\zeta = \int_{\mathbb{R}^d} \int_{\mathbb{R}^m} \sigma(\zeta, \lambda) d\Upsilon_\zeta(\lambda)\, d\zeta.$$

Using the push-forward formula $\beta^\varepsilon(t) = \Phi_t^\varepsilon \,\#\, \beta_0^\varepsilon$ and passing to the limit $\varepsilon \to 0_+$ implies:

Lemma (Connection to Young measures)

Denote by

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

the Young measure associated to the Bohmian flow $X^\varepsilon(t,y), P^\varepsilon(t,y)$.

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Then, if $\rho_0^\varepsilon \stackrel{\varepsilon \to 0_+}{\longrightarrow} \rho_0,$ *strongly in* $L_+^1(\mathbb{R}^d)$*, the following identity holds*

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

Wigner transforms and Wigner measures

For any $\varepsilon > 0$, one defines Wigner function $w^\varepsilon(t) \in L^2(\mathbb{R}^d_x \times \mathbb{R}^d_p)$:

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

The function $w^\varepsilon \in L^2(\mathbb{R}^d_x \times \mathbb{R}^d_p)$ solves a nonlocal dispersive equation. In general, $w^\varepsilon(t,x,p) \not\geq 0$ and thus not a probability measure.

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It is well known [Lions and Paul '93] that if $\psi^\varepsilon(t)$ is ε-oscillatory, then, up to extraction of sub-sequences,

$$w^\varepsilon \stackrel{\varepsilon \to 0_+}{\longrightarrow} w \quad \text{in } C_{\rm b}(\mathbb{R}_t; \mathcal{D}'(\mathbb{R}^d_x \times \mathbb{R}^d_p))\, \mathrm{w}-*.$$

where $w(t) \in \mathcal{M}^+(\mathbb{R}^d_x \times \mathbb{R}^d_p)$ is the Wigner measure, satisfying the classical Liouville equation:

$$\partial_t w + p\cdot\nabla_x w - \nabla_x V \cdot \nabla_p w = 0, \quad \text{in } \mathcal{D}'(\mathbb{R}^x_p \times \mathbb{R}^d_p).$$

Moreover, if $\psi^\varepsilon(t)$ is ε-oscillatory, then we also have

$$\rho^\varepsilon(t,x) \stackrel{\varepsilon\to 0_+}{\longrightarrow} \int_{\mathbb{R}^d} w(t,x,dp), \quad J^\varepsilon(t,x) \stackrel{\varepsilon\to 0_+}{\longrightarrow} \int_{\mathbb{R}^d} p\, w(t,x,dp).$$

More generally, for any (smooth) quantum mechanical observable

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

where $\mathrm{Op}^\varepsilon(a)$ is the Weyl-quantized operator associated to the classical symbol $a \in C_{\mathrm{b}}^\infty(\mathbb{R}^d_x \times \mathbb{R}^d_p)$.

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Q: Under which circumstances do we know that $w = \beta$?

Results on the connection of w and β

For simplicity we shall suppress any t-dependence in the following.

Theorem (Sub-critical case)

Assume that ψ^ε is uniformly bounded in $L^2(\mathbb{R}^d)$ and that in addition

$$\varepsilon \nabla \psi^\varepsilon \stackrel{\varepsilon \to 0_+}{\longrightarrow} 0, \quad \text{in } L^2_{\text{loc}}(\mathbb{R}^d).$$

Then, up to extraction of subsequences, it holds

$$w(x,p) = \beta(x,p) \equiv \rho(x)\, \delta(p).$$

Wave functions ψ^ε which neither oscillate nor concentrate on the scale ε (but maybe on some larger scale), yield in the classical limit the same mono-kinetic Bohmian or Wigner measure with $p = 0$.

For the next result we use the representation

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

with $S^\varepsilon(x) \in \mathbb{R}$ defined $\rho^\varepsilon \equiv |a^\varepsilon|^2 - a.e.$ (up to additives of $2\pi n, n \in \mathbb{N}$).

Theorem (WKB wave functions)

Let ψ^ε be as above. If $\varepsilon \nabla \sqrt{\rho^\varepsilon} \stackrel{\varepsilon \to 0_+}{\longrightarrow} 0$, in $L^2_{\mathrm{loc}}(\mathbb{R}^d)$, and if

$$\varepsilon \sup_{x \in \Omega^\varepsilon} \left| \frac{\partial^2 S^\varepsilon}{\partial x_\ell \partial x_j} \right| \stackrel{\varepsilon \to 0_+}{\longrightarrow} 0, \quad \forall\, \ell, j \in 1, \dots, d,$$

where Ω^ε is an open set containing supp ρ^ε, then it holds

$$\lim_{\varepsilon \to 0_+} |\langle w^\varepsilon, \varphi \rangle - \langle \beta^\varepsilon, \varphi \rangle| = 0, \quad \forall\, \varphi \in C_0(\mathbb{R}^d_x \times \mathbb{R}^d_p).$$

This result can be shown to be almost sharp.

Case studies

Example (Oscillatory function)

Let $f \in \mathcal{S}(\mathbb{R}^d;\mathbb{C})$, $g \in C^\infty(\mathbb{R}^d,\mathbb{C})$ s.t. $g(y+\gamma) = g(y)$, $\gamma \in \Gamma \simeq \mathbb{Z}^d$ and

$$\psi^\varepsilon(x) = f(x) g\left(\frac{x}{\varepsilon}\right).$$

Then, $\beta = w$ if, and only if, $g(y) = \alpha e^{ik\cdot y}$, $\alpha \in \mathbb{R}$, $k \in \Gamma^*$.

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Example (Concentrating function)

$$\psi^\varepsilon(x) = \varepsilon^{-d/2} f\left(\frac{x-x_0}{\varepsilon}\right),$$

with $f \in \mathcal{S}(\mathbb{R}^d;\mathbb{C})$. Thus $|\psi^\varepsilon|^2 \rightharpoonup \delta(x-x_0)$. Then, $\beta = w$ iff $f \equiv 0$.

Example (Semi-classical wave packet)

$$\psi^\varepsilon(x) = \varepsilon^{-d/4} f\left(\frac{x - x_0}{\sqrt{\varepsilon}}\right) e^{ip_0\cdot x/\varepsilon}, \quad x_0, p_0 \in \mathbb{R}^d,$$

with $f \in \mathcal{S}^\infty(\mathbb{R}^d; \mathbb{C})$, concentrating “only” on the scale $\sqrt{\varepsilon}$ (such ψ^ε are often called “coherent states”).

Then, one easily computes

$$w = \beta = \|f\|^2_{L^2}\, \delta(p - p_0)\delta(x - x_0).$$

This phase-space distribution describes classical (point) particles with position x_0 and momentum p_0.

Semi-classical wave packtes

Denote by $X(t), P(t)$ the solution of the classical Hamiltonian system

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

and assume the initial data to be a coherent state, i.e.

$$\psi_0^\varepsilon(x) = \varepsilon^{-d/4} f\left(\frac{x - x_0}{\sqrt{\varepsilon}}\right) e^{ip_0 \cdot x/\varepsilon}, \quad x_0, p_0 \in \mathbb{R}^d,$$

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In addition, we recall that a sequence $\{f_\varepsilon\}_{0<\varepsilon\leqslant 1} : \mathbb{R}^d \to \mathbb{R}$ is said to converge locally in measure to f, if for every $\delta > 0$ and every Borel set Ω with finite Lebesgue measure:

$$\lim_{\varepsilon\to 0} \text{meas}\big\{(x \in \Omega \mid f_\varepsilon(x) - f(x)| \geqslant \delta)\big\} = 0.$$

Theorem (Convergence of Bohmian trajectories)

Let $V \in C^3_{\mathrm{b}}(\mathbb{R}^d)$ *and* ψ_0^ε *a coherent state at* x_0, p_0.

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Let $V \in C_{\mathrm{b}}^3(\mathbb{R}^d)$ *and* ψ_0^ε *a coherent state at* x_0, p_0.

1. *Then, the limiting Bohmian measure satisfies*

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

where $X(t), P(t)$ *are the classical Hamiltonian trajectories.*

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where $X(t), P(t)$ are the classical Hamiltonian trajectories.

2. *Consider the following re-scaled Bohmian trajectories*

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

Then

$$Y^\varepsilon \stackrel{\varepsilon \to 0_+}{\longrightarrow} X, \quad Z^\varepsilon \stackrel{\varepsilon \to 0_+}{\longrightarrow} P,$$

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

Remark

This result should be compared with a recent result by [Dürr and Römer '10], which proved

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in-probability induced by the measure $\|\psi_0^\varepsilon\|^2$*, locally on compact time-intervals.*

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1. *we can also prove convergence of the re-scaled Bohmian momentum* Z^{ε}*;*
2. *we do not need a-priori estimates on the time-dependence;*
3. *we immediately obtain existence of a sub-sequence* $\{\varepsilon_n\}$, *such that*
$$Y^{\varepsilon_n} \xrightarrow{n \to \infty} X, \quad Z^{\varepsilon_n} \xrightarrow{n \to \infty} P, \quad \text{a.e. in } \Omega \subseteq \mathbb{R}_t \times \mathbb{R}^d_y.$$

Sketch of proof.

The proof relies on the use of Young measure theory. Let

$$\omega_{t,y} : \mathbb{R}_t \times \mathbb{R}^d_y \to \mathcal{M}^+(\mathbb{R}^d_x \times \mathbb{R}^d_p)\,;\ (t,y) \mapsto \omega_{t,y}(x,p),$$

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Having in mind the particular form of the limiting measure $\beta(t)$, implies

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

This is equivalent to (local) in measure convergence of Y^ε, Z^ε.

WKB analysis of Bohmian trajectories

The, by now, classical, WKB ansatz is

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

with $S(t,x) \in \mathbb{R}$ and $a^\varepsilon \sim a + \varepsilon a_1 + \varepsilon^2 a_2 + \dots$.

Plugging this into Schrödinger's equation and comparing equal powers of ε yields a Hamilton-Jacobi equation for the phase

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

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or, equivalently for $\rho = |a|^2$:

$$\partial \rho + \mathrm{div}(\rho \nabla S) = 0.$$

In order to obtain S one needs to solve the Hamiltonian system:

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

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In general, there is a time $T^* > 0$, at which the flow $X(t,\cdot)$ ceases to be one-to-one. Points $x \in \mathbb{R}^d$ at which this happens are caustic points:

$$\mathscr{C}_t = \{x \in \mathbb{R}^d \, : \, \exists \, y \in \mathbb{R}^d \text{ s.t. } x = X(t,y) \text{ and } \det \nabla_y X(t,y) = 0\}.$$

The caustic set is thus defined by $\mathscr{C} := \{(x,t) : x \in \mathscr{C}_t\}$ and the caustic onset time is

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

For $t > T^*$ the solution of the Hamilton-Jacobi equation (obtained by the method of characteristics), typically becomes multi-valued.

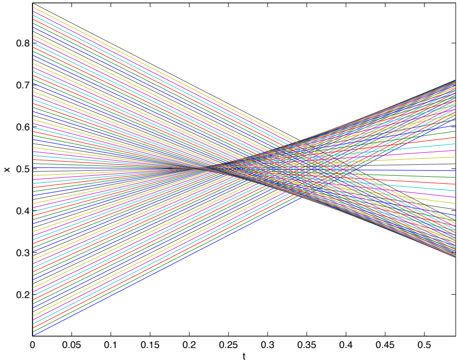

Figure : Classical trajectories for $V(x) = 0$ and $\nabla S_0(x) = -\tanh(5x - \frac{5}{2})$

Theorem (Convergence before caustic onset)

Let $\psi_0^\varepsilon(x) = a_0(x)e^{iS_0(x)/\varepsilon}$ *with* $a_0 \in \mathcal{S}(\mathbb{R}^d;\mathbb{C})$, $S_0 \in C^\infty(\mathbb{R}^d;\mathbb{R})$ *and sub-quadratic.*

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Then, there exists a $T^* > 0$, independent of $x \in \mathbb{R}^d$, such that:

1. *For all compact time-intervals $I_t \subset [0, T^*)$*

$$\beta^\varepsilon \stackrel{\varepsilon\to 0_+}{\longrightarrow} \beta \equiv w(t,x,p) = \rho(t,x)\delta(p - \nabla S(t,x)),$$

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   where $\rho(t,x)$ *and* $S(t,x)$ *solve the WKB system.*

2. *The corresponding Bohmian trajectories satisfy*

$$X^\varepsilon \stackrel{\varepsilon\to 0_+}{\longrightarrow} X, \quad P^\varepsilon \stackrel{\varepsilon\to 0_+}{\longrightarrow} P,$$

   locally in measure on $\{I_t \times \mathrm{supp}\ \rho_0\} \subseteq \mathbb{R}_t \times \mathbb{R}_x^d$, *where* $\rho_0 = |a_0|^2$.

What happens after caustic onset?

Theorem (Non-convergence after caustics)

Denote by Ω_0 *the connected component of* $(\mathbb{R}_t \times \mathbb{R}^d_x) \setminus \mathscr{C}$ *containing* $\{t = 0\}$.

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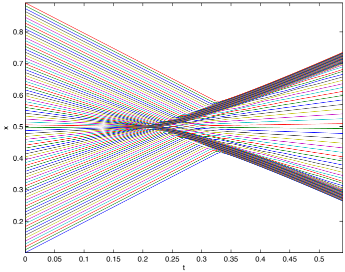
Then there exist initial data $a_0(y)$ *and* $S_0(y)$ *such that, outside of* Ω_0*, there are regions* $\Omega \subseteq (\mathbb{R}_t \times \mathbb{R}^d_x) \setminus \mathscr{C}$ *in which both* X^ε *and* $P^\varepsilon = \dot{X}^\varepsilon$ *do not converge to the classical, multivalued flow.*

Remark

In the free case $V(x) \equiv 0$ *and if* $|a_0| > 0$ *on all of* $\mathbb{R}^d$*, one can show that on any connected component* $\Omega \neq \Omega_0$*, whose boundary intersects* $\partial\Omega_0$ P^ε *does not converge to* P.

The obstruction to convergence stems from the fact that Bohmian trajectories do not cross, even as $\varepsilon \to 0_+$.



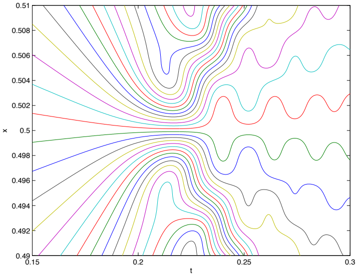


Figure : Left: Bohmian trajectories $X^\varepsilon(t, y)$ with $\varepsilon = 10^{-3}$ in the case $V(x) = 0$ and $\nabla S_0(x) = -\tanh(5x - \frac{5}{2})$. Right: A closeup of the central region.

Oscillations not only appear in the trajectories X^ε, but also in the momentum $P^\varepsilon(t,y) = u^\varepsilon(t, X^\varepsilon(t,y))$. They are reminiscent of so-called dispersive shocks, observed in, e.g. Korteweg-de Vries.

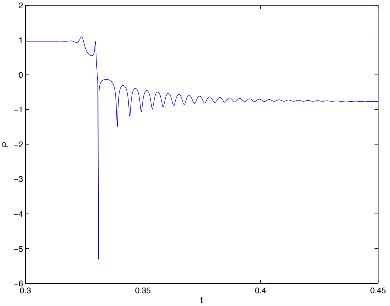


Figure : The quantity $P^\varepsilon(t,y) = u^\varepsilon(t, X^\varepsilon(t,y))$ for $\varepsilon = 10^{-2}$.

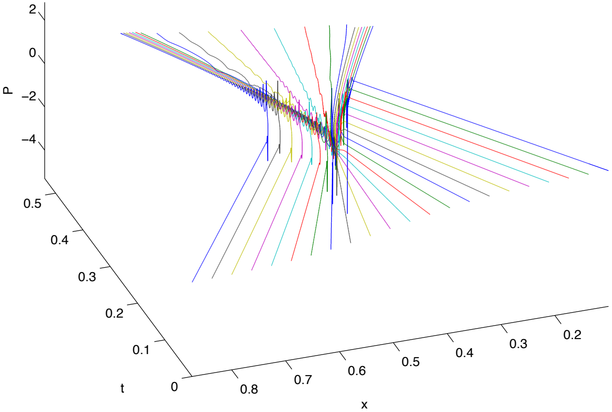


Figure : The quantity $P^\varepsilon(t, y)$ along the Bohmian trajectories $X^\varepsilon(t, y)$.

Open questions

1. What is the limit of $X^\varepsilon(t,y), P^\varepsilon(t,y)$ after caustic onset?

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2. We can compute $\beta(t)$ for $t > T^*$ (using FIO's and stationary phase techniques for the solution of Schrödinger's equation) but what about $\Upsilon_{t,y}$?
3. Which system of equations do the classical limit densities ρ and J satisfy for $t > T^*$?