



HAL
open science

STRONG AND WEAK SEMICLASSICAL LIMIT FOR SOME ROUGH HAMILTONIANS

Agissilaos Athanassoulis, Thierry Paul

► **To cite this version:**

Agissilaos Athanassoulis, Thierry Paul. STRONG AND WEAK SEMICLASSICAL LIMIT FOR SOME ROUGH HAMILTONIANS. 2011. inria-00533558v7

HAL Id: inria-00533558

<https://inria.hal.science/inria-00533558v7>

Preprint submitted on 2 Feb 2011 (v7), last revised 6 Aug 2011 (v8)

HAL is a multi-disciplinary open access archive for the deposit and dissemination of scientific research documents, whether they are published or not. The documents may come from teaching and research institutions in France or abroad, or from public or private research centers.

L'archive ouverte pluridisciplinaire **HAL**, est destinée au dépôt et à la diffusion de documents scientifiques de niveau recherche, publiés ou non, émanant des établissements d'enseignement et de recherche français ou étrangers, des laboratoires publics ou privés.

STRONG AND WEAK SEMICLASSICAL LIMIT FOR SOME ROUGH HAMILTONIANS

AGISSILAOS ATHANASSOULIS AND THIERRY PAUL

ABSTRACT. We present several results concerning the semiclassical limit of the time dependent Schrödinger equation with potentials whose regularity doesn't guarantee the uniqueness of the underlying classical flow. Different topologies for the limit are considered and the situation where two bicharacteristics can be obtained out of the same initial point is emphasized.

CONTENTS

1.	Introduction	1
2.	Main results	4
3.	Definitions and Notations	7
4.	Proofs	8
4.1.	Proof of Theorem 2.1	8
4.2.	Proof of Theorem 2.2	10
4.3.	Proof of Theorem 2.3	13
5.	Examples	15
5.1.	Examples for Theorem 2.2	16
5.2.	Examples for Theorem 2.3	19
6.	Auxiliary results	22
	References	27

1. INTRODUCTION

Consider a wavefunction $u^\varepsilon(x, t) : \mathbb{R}^n \times \mathbb{R} \rightarrow \mathbb{C}$ satisfying the Schrödinger equation,

$$(1.1) \quad \begin{aligned} i\varepsilon \frac{\partial}{\partial t} u_t^\varepsilon(x) &= \left(-\frac{\varepsilon^2}{2} \Delta + V(x) \right) u_t^\varepsilon(x), \\ u_{t=0}^\varepsilon &= u_0^\varepsilon(x), \end{aligned}$$

or a mixed state D_t^ε satisfying the Heisenberg-von Neumann equation:

$$(1.2) \quad \begin{aligned} i\varepsilon \frac{\partial}{\partial t} D_t^\varepsilon &= \left[-\frac{\varepsilon^2}{2} \Delta + V, D_t^\varepsilon \right], \\ D_{t=0}^\varepsilon &= D_0^\varepsilon. \end{aligned}$$

Typically one considers trace-class operators, and the trace is preserved in time $tr(D^\varepsilon(t)) = tr(D_0^\varepsilon)$.

The small parameter ε is called Planck's constant in the context of quantum mechanics, and its physical meaning is that of the lengthscale of oscillation of the wavefunction in space.

Several techniques have been developed for the study of the semiclassical limit $\varepsilon \rightarrow 0$ of (1.1). One is based on the Wigner transform (WT) [9, 10, 13]. The WT $W_t^\varepsilon(x, k)$ of the wavefunction u_t^ε is, defined in the standard semiclassical scaling,

$$(1.3) \quad W_t^\varepsilon(x, k) = W^\varepsilon[u_t^\varepsilon](x, k) = \int_{y \in \mathbb{R}^n} e^{-2\pi i y k} u_t^\varepsilon(x + \varepsilon \frac{y}{2}) \bar{u}_t^\varepsilon(x - \varepsilon \frac{y}{2}) dy.$$

In that case W_t^ε corresponds to a *pure state*. A Wigner function W^ε need not be the Wigner transform of a wavefunction u ; when working with *mixed states*, i.e. with equation (1.2), the Wigner function can be

$$(1.4) \quad W_t^\varepsilon(x, k) = W^\varepsilon[D_t](x, k) = \int_{y \in \mathbb{R}^n} e^{-2\pi i y k} K_t^\varepsilon(x + \varepsilon \frac{y}{2}, x - \varepsilon \frac{y}{2}) dy$$

where $K_t^\varepsilon(x, y)$ is the integral kernel of the mixed-state D_t^ε . It evolves in time under the well-known Wigner equation,

$$(1.5) \quad \begin{aligned} & \partial_t W_t^\varepsilon(x, k) + 2\pi k \cdot \partial_x W_t^\varepsilon(x, k) + \\ & + \frac{2}{\varepsilon} Re \left[i \int e^{2\pi i S x} \widehat{V}(S) W_t^\varepsilon(x, k - \frac{\varepsilon S}{2}) dS \right] = 0, \end{aligned}$$

$$W_{t=0}^\varepsilon = W_0^\varepsilon.$$

An important feature of the Wigner transform is that (under appropriate conditions) it allows for a very natural and compact description of the semiclassical limit: the WT has a physically meaningful limit as ε tends to zero, while in general the wavefunction u^ε itself does not. The limit (in the weak-* topology of an appropriate algebra of test functions), called the Wigner measure,

$$W_t^\varepsilon \rightharpoonup W_t^0,$$

satisfies the Liouville equation of classical mechanics

$$(1.6) \quad \partial_t W^0 + 2\pi k \partial_x W^0 - \frac{1}{2\pi} \partial_x V \partial_k W^0 = 0,$$

$$W_0^0 = \lim_{\varepsilon \rightarrow 0} W_0^\varepsilon.$$

In general the Wigner measure W^0 is a non-negative measure on phase-space, associated with the family of initial data $\{W_0^\varepsilon\}$. For the precise formulation of the result, see e.g. [13]. The limit problem (1.6) is well-posed in general for $V(x) \in C^{1,1}$.

It was already observed in [13] that there are certain cases where semiclassical convergence to the Liouville equation could be shown, but the Liouville equation itself is not well posed – namely for $V(x) \in C^1 \setminus C^{1,1}$. The result then becomes as follows: the Wigner measure is a weak solution of the Liouville equation – but there is not enough information to select the correct weak solution. Families of initial data whose evolution oscillate between the several solutions of the Liouville equation were constructed in [13].

The one-dimensional case study considered in [13] was essentially equivalent to the following:

One considers the potential

$$(1.7) \quad V(x) = -|x|^{1+\theta} \cdot \beta(x)$$

with $\theta \in (0, 1)$, $C^\infty \ni \beta = 1$ on $[-1, +1]$, and $\beta(x) = 0$ for $|x| \geq 2$. Then one can easily check that there exist, for t small enough, two families of bicharacteristics starting near the origin at $t = 0$, namely

$$(1.8) \quad (X^\pm(t), P^\pm(t)) = (\pm c_0 t^\nu, \pm \frac{c_0 \nu}{2\pi} t^{\nu-1}),$$

with $\nu = \frac{2}{1-\theta}$ and $c_0 = \left(\frac{(1-\theta)^2}{2}\right)^{1-\theta}$.

In this case it is possible to find semiclassical limits where one wavepacket (a δ -function in classical phase-space) splits in two wavepackets. (In this particular example it happens immediately, i.e. $\forall t > 0$; different examples can be constructed where it happens after an ε -independent time t_*). The mass of each wavepacket depends on information which can be easily extracted from the quantum problem, but lost if we take the limit as usual in a straightforward way.

Weak semiclassical limits with rough potentials were also considered recently in [2] where the hypothesis on the potential is essentially, among other properties, that its gradient is in BV_{loc} (allowing for a Coulomb part to be added). It was proved there, roughly speaking, that the Wigner measure of the solutions of (1.1) at time t , after averaging over initial data, tends weakly to the push-forward of its initial value by the flow associated to the underlying classical Hamiltonian system of ODEs by the Ambrosio-DiPerna-Lions theory [1, 7] (see also [8] for the same construction with density matrices). In particular this averaging condition forbids concentrating initial data, a fact consistent with the weak limit strategy and the fact that the flow is not defined everywhere.

Our results concern less general potentials than those treated in [2, 8] (still giving rise to ill-posed classical dynamics of course), but can deal with initial data concentrating to singular measures.

Other problems where the Wigner measure does not satisfy one well-posed Liouville equation have attracted attention recently. The difficulties can originate from lack of smoothness of the potential [11], or working on a torus instead of Euclidean space [14].

The first of our results deals with the case study from [13] mentioned earlier. Our second Theorem gives a general result concerning the approximation, in strong topology, of the Wigner function of the solution of (1.4) with the solution of a “smoothed” Liouville equation. Our third results goes back to the weak approximation, but with explicit remainder estimates.

2. MAIN RESULTS

We will use a space of test-functions introduced in [13]: let

$$(2.1) \quad \mathcal{A} = \{ \phi \in C_0(\mathbb{R}^{2n}) \mid \int \sup_x |\mathcal{F}_{k \rightarrow K}[\phi(x, k)]| dK < \infty \},$$

equipped with the norm

$$(2.2) \quad \|\phi\|_{\mathcal{A}} = \int \sup_x |\mathcal{F}_{k \rightarrow K}[\phi(x, k)]| dK.$$

Our first result will focus on the case study presented in the introduction; a family of initial data which concentrates at the origin at time $t = 0$ and splits into two separated wave packets at time $t > 0$. This is only an example among several others presented in section 5 and the more general results of the paper are given by the Theorems 2.2 and 2.3 below.

Theorem 2.1. *Let V given by (1.7) and*

$$(2.3) \quad W_0^\varepsilon(x, k) = \lambda^{\frac{7+3\theta}{30}} w(\lambda^{\frac{1+\theta}{6}} x, \lambda^{\frac{1-\theta}{15}} k) * \left(\frac{2}{\varepsilon}\right)^n e^{-2\pi \frac{x^2+k^2}{\varepsilon}}$$

with $\lambda = \log(\frac{1}{\varepsilon})$, $w \in H^2 \cap L^\infty \cap L^1$, $w(x, k) \geq 0$, $\text{supp } w \subseteq \{|x|^2 + |k|^2 < 1\}$, $\int w(x, k) dx dk = 1$.

Then $\exists T > 0$ such that for all $t \in [0, T]$, the solution W_t^ε of (1.5) converges in weak-* sense in \mathcal{A}' to

$$(2.4) \quad W_t^0 = c_+ \delta_{(X^+(t), P^+(t))} + c_- \delta_{(X^-(t), P^-(t))},$$

with $(X^\pm(t), P^\pm(t))$ given by (1.8) and

$$c_\pm = \int_{\pm x > 0} w(x, k) dx dk.$$

Remark: The fact that the initial data contain a smoothing by $(\frac{2}{\varepsilon})^n e^{-2\pi \frac{x^2+k^2}{\varepsilon}}$ ensures that W_0^ε corresponds to a density matrix, i.e. a positive trace-class operator (see e.g. Exemple III.7 of [13], or lemma 6.7).

In Remarque IV.3 of [13], one can find a construction of a family of normalized wave functions u_ε^+ concentrating at the origin, and whose Wigner functions, after extraction of a subsequence, converge to a Dirac mass centered on $(X^+(t), P^+(t))$. The same construction is obviously possible in order to get a family u_ε^- whose Wigner functions, after extraction of a subsequence, converge to a Dirac mass centered on $(X^-(t), P^-(t))$. Defining $D_0^\varepsilon = \frac{1}{\sqrt{2}}(|u_\varepsilon^+\rangle\langle u_\varepsilon^+| + |u_\varepsilon^-\rangle\langle u_\varepsilon^-|)$ one can check that the Wigner function of D_0^ε

will follow the conclusion of Theorem 2.1. However the present construction is different, more precise and is not obtained through compactness arguments: there is no need of extraction of subsequence, the scaling property is explicit (it is given by an implicit diagonal argument in a two scale sequence in [13]) and the choice of the initial datum is somewhat more general. The construction of [13] is based on the more-or-less explicit understanding of the flow around the singular point, while our approximation (i.e. Theorems 2.2 and 2.3 below) is built around a graceful degradation property (in a sense analogous to the use of the term, e.g., in [12]) of the flow (properties 1 and 2 in section 5), and applies automatically, whenever that property holds, to more general and less explicit potentials. Let us also remark the similarity with the long-time behaviour around a regular separatrix, studied extensively in [15].

We turn now to the more general results of this paper.

In the sequel we will consider potentials V satisfies the following assumption:

Assumption 1.

$$(2.5) \quad \int_{\mathbb{R}^n} |\widehat{V}(S)| \frac{S^2}{1+S^2} dS < \infty,$$

and moreover there are constants $C > 0, \theta \in (0, 1)$ such that for $m \in \{0, 1, 2\}$

$$\forall 1 \leq a \leq b \leq +\infty : \int_{|S| \in (a, b)} |\widehat{V}(S)| |S|^m dS \leq \frac{C}{m-1-\theta} (b^{m-1-\theta} - a^{m-1-\theta})$$

This is closely modeled after $V(x) = C|x|^{1+\theta}$; indeed it is easy to check that the aforementioned potential satisfies this condition. In section 5, we will also see some other relevant types of singularities (also generated from $|x|^{1+\theta}$ in some sense).

Denote

$$(2.6) \quad \widetilde{V}^\gamma(x) = \left(\frac{2}{\varepsilon^\gamma}\right)^{\frac{n}{2}} \int e^{-\frac{2\pi}{\varepsilon^\gamma}|x-x'|^2} V(x') dx'.$$

Theorem 2.2. *Let us suppose that Assumption 1 holds, and there exist $T > 0, \delta \in (0, \frac{\theta}{2+\theta}), \gamma > \frac{2}{1+\theta}$ and $[W_0^\varepsilon] \in H^2(\mathbb{R}^{2n})$ such that*

$$(2.7) \quad \|[W_0^\varepsilon] - W_0^\varepsilon\|_{L^2} = o(1)\|W_0^\varepsilon\|_{L^2}$$

and the solution of

$$(2.8) \quad \partial_t \rho + 2\pi k \partial_x \rho - \frac{1}{2\pi} \partial_x \widetilde{V}^\gamma \cdot \partial_x \rho = 0,$$

with initial condition $\rho(t=0) = [W_0^\varepsilon]$ satisfies

$$(2.9) \quad \|\rho(t)\|_{H^2} = O(\varepsilon^{-\delta} \|W_0^\varepsilon\|_{L^2})$$

uniformly on $[0, T]$.

Then the Wigner function W_t^ε of the solution of (1.4) satisfies, uniformly on $[0, T]$,

$$(2.10) \quad \|W_t^\varepsilon - \rho_1^\varepsilon(t)\|_{L^2} = O(\varepsilon^\kappa \|W_0^\varepsilon\|_{L^2} + \|W_0^\varepsilon - [W_0^\varepsilon]\|_{L^2}) = o(\|W_0^\varepsilon\|_{L^2}).$$

where ρ_1^ε is the solution of (2.8) with initial datum $\rho_1^\varepsilon(t=0) = W_0^\varepsilon$ and $\kappa = \min\{\gamma^{\frac{1+\theta}{2}} - 1, \frac{\theta}{2+\theta} - \delta\}$.

Our next result deals with the weak-* limit in ε (which in general is not in L^2).

Theorem 2.3. *Assume that the hypotheses of Theorem 2.2 hold and $\rho_1^\varepsilon(t)$ is as in Theorem 2.2. Moreover, in addition to the condition (2.7) we assume that*

$$(2.11) \quad \|[W_0^\varepsilon] - W_0^\varepsilon\|_{L^2} = o(1),$$

$\|W_0^\varepsilon\|_{L^2} = o(\varepsilon^{-\kappa})$, and the initial data W_0^ε corresponds to a density matrix, i.e. it is the Wigner function of a positive trace-class operator D_0^ε , $\text{tr}(D_0^\varepsilon) = 1 \forall \varepsilon > 0$.

For $\phi \in \mathcal{A}$ denote

$$E^\varepsilon(\phi) = \langle W_t^\varepsilon - \rho_1^\varepsilon(t), \phi \rangle.$$

and, for brevity, by $F(\varepsilon)$ the bound of equation (2.10), namely

$$F(\varepsilon) = C(\varepsilon^\kappa \|W_0^\varepsilon\|_{L^2} + \|[W_0^\varepsilon] - W_0^\varepsilon\|_{L^2}) = o(1),$$

for some large enough constant $C > 0$.

Then, $\forall \phi \in \mathcal{A}$, $t \geq 0$, the following estimate holds:

$$(2.12) \quad |E^\varepsilon(\phi)| \leq F(\varepsilon) \|\phi\|_{\mathcal{A}} + \frac{2^n \pi^{\frac{n}{2}}}{\sqrt{\Gamma(n+1)}} \sqrt{F(\varepsilon)} + \\ + (1 + \|[W_0^\varepsilon]\|_{L^1}) \|(1 - \chi_{F(\varepsilon)^{\frac{1}{2n}}}) \phi\|_{\mathcal{A}}$$

where $\chi \in C^\infty(\mathbb{R}^{2n}, [0, 1])$ is any cutoff function, $\chi(z) = 1 \forall |z| < 1$, $\chi(z) = 0 \forall |z| > 2$, and $\chi_M(z) := \chi(Mz)$.

Remark: The last term in rhs of equation (2.12) can be further estimated if there is more information on ϕ , and in particular its decay in the k variable.

Corollary 2.4. *If the assumptions of Theorem 2.3 are satisfied and $\|[W_0^\varepsilon]\|_{L^1}$ is uniformly bounded in ε , then*

$$\lim_{\varepsilon \rightarrow 0} E^\varepsilon(\phi) = 0 \quad \forall \phi \in \mathcal{A}, t \geq 0,$$

and therefore the Wigner function W^ε has a weak-* limit in \mathcal{A}' if and only if ρ_1^ε has a weak-* limit, and the two are equal, i.e.

$$(2.13) \quad \exists W_t^0 : \lim_{\varepsilon \rightarrow 0} \langle W_t^\varepsilon, \phi \rangle = \langle W_t^0, \phi \rangle \quad \forall \phi \in \mathcal{A}, t \in [0, T],$$

if and only if

$$(2.14) \quad \lim_{\varepsilon \rightarrow 0} \langle \rho_1^\varepsilon(t), \phi \rangle = \langle W_t^0, \phi \rangle \quad \forall \phi \in \mathcal{A}, \quad t \in [0, T].$$

In other words, under the assumptions of theorem 2.3, one has to solve equation (2.8) in order to compute the propagation in time, $\rho_1^\varepsilon(t)$, and then take the limit $\varepsilon \rightarrow 0$. This no longer makes sense if the semiclassical limit is taken *before* time propagation. That is, unlike what happens with regular potentials, the semiclassical limit and the propagation in time by (a regularization of) the Liouville flow no longer commute.

$$\begin{array}{ccc} \rho_1^\varepsilon(0) & \xrightarrow{\circ\phi_\varepsilon^t} & \rho_1^\varepsilon(t) \\ \varepsilon \rightarrow 0 \downarrow & & \downarrow \varepsilon \rightarrow 0 \\ W^0(0) & & W^0(t) \end{array}$$

FIGURE 1. In some cases, there is not enough information in $W^0(0)$ to determine $W^0(t)$.

Organization of the paper: Proofs of the main Theorems are in section 4. Checking the assumptions of the Theorems for various concrete problems is done in section 5. Certain auxiliary results we use are collected in section 6.

3. DEFINITIONS AND NOTATIONS

The Fourier transform is defined as

$$(3.1) \quad \widehat{f}(k) = \mathcal{F}_{x \rightarrow k} [f(x)] = \int_{x \in \mathbb{R}^n} e^{-2\pi i k x} f(x) dx.$$

For compactness, we will use the following notations:

$$\begin{aligned} T_\varepsilon^V W &= \frac{2}{\varepsilon} \operatorname{Re} \left[i \int e^{2\pi i S x} \widehat{V}(S) W(x, k - \frac{\varepsilon S}{2}) dS \right] = \\ &= 2\mathcal{F}_{X, K \rightarrow x, k}^{-1} \left[\int \widehat{V}(S) \widehat{W}(X - S, K) \frac{\sin(\pi \varepsilon S K)}{\varepsilon} dS \right], \\ T_0^V W &= -\frac{1}{2\pi} \partial_x \widetilde{V} \cdot \partial_x W = \\ &= 2\pi \mathcal{F}_{X, K \rightarrow x, k}^{-1} \left[\int \widehat{V}(S) \widehat{W}(X - S, K) S \cdot K dS \right]. \end{aligned}$$

The Sobolev norms of order m on phase-space will be defined as follows:

$$\|f\|_{W^{m,p}(\mathbb{R}^{2n})} = \sum_{|a|+|b| \leq m} \|\partial_x^a \partial_k^b f\|_{L^p(\mathbb{R}^{2n})},$$

where of course a and b are multi-indices of length n each. Moreover, $H^m(\mathbb{R}^{2n}) = W^{m,2}(\mathbb{R}^{2n})$.

4. PROOFS

4.1. Proof of Theorem 2.1. Observe that λ as used in the statement of theorem 2.1 is an effective upper bound; if we replace λ by $\lambda' \leq \lambda$, $\frac{1}{\lambda'} = o(1)$, the theorem still holds.

In this section we will show that Theorem 2.1 follows from Theorems 2.2, 2.3.

Remarks on notation:

- In this section we use the notation $R = \lambda^{-\frac{1}{3}}$.
- Denote

$$(4.1) \quad f_0^\varepsilon(x, k) = \lambda^{\frac{7+3\theta}{30}} w(\lambda^{\frac{1+\theta}{6}} x, \lambda^{\frac{1-\theta}{15}} k),$$

where of course $\lambda = \log(\frac{1}{\varepsilon})$, i.e. $W_0^\varepsilon = f_0^\varepsilon * (\frac{2}{\varepsilon})^n e^{-2\pi \frac{x^2+k^2}{\varepsilon}}$. One should note that

$$(4.2) \quad \|W_\varepsilon^0 - f_0^\varepsilon\|_{L^2} \leq \sqrt{\varepsilon} \|f_0^\varepsilon\|_{H^1} = O(\varepsilon^{\frac{1}{2}-\eta}) \quad \forall \eta \in (0, \frac{1}{2})$$

(The approximation follows from a standard observation on smoothing operators, see e.g. [4] for a proof).

(Moreover, since by construction the constant κ of Theorem 2.2 is $\kappa < \frac{1}{3}$, the error $\|W_\varepsilon^0 - f_0^\varepsilon\|_{L^2}$ can indeed be dropped without loss of generality, when invoking Theorem 2.3 – and Theorem 2.2 through it).

In lemma 5.3 it is shown essentially that Theorem 2.3 applies if $n = 1$, $V(x) = -|x|^{1+\theta}$ in $\{|x| < 1\}$ (with a smooth cutoff outside of that, the specifics of which are irrelevant) and $W_0^\varepsilon = \delta_x^{-1} \delta_k^{-1} w(\frac{x}{\delta_x}, \frac{k}{\delta_k})$, where $\delta_k = R^{\frac{1+\theta}{2}}$, $\delta_x = R^{\frac{1-\theta}{5}}$. (We avoid duplicating parts of the proof of lemma 5.3 here. Moreover, it is completely straightforward to see that the assumptions not checked explicitly there also hold). Therefore corollary 2.4 applies, i.e. it suffices to find the limit in ε of ρ_1^ε .

Claim: With $[W_0^\varepsilon]$ defined as in equation (5.15), we have

$$(4.3) \quad \|W_0^\varepsilon - [W_0^\varepsilon]\|_{L^1} = o(1).$$

Proof of the claim: We will work separately for the two terms

$$\|W_0^\varepsilon - [W_0^\varepsilon]\|_{L^1} \leq \|W_0^\varepsilon - f_0^\varepsilon\|_{L^1} + \|f_0^\varepsilon - [W_0^\varepsilon]\|_{L^1}.$$

First of all, it is obvious that

$$\int_{|(x,k)|>2} |f_0^\varepsilon - W_0^\varepsilon| dx dk = \int_{|(x,k)|>2} |W_0^\varepsilon| dx dk = O(\varepsilon^\infty).$$

Moreover, using the Jensen inequality, one sees that

$$\begin{aligned} \int_{|(x,k)|<2} |f_0^\varepsilon - W_0^\varepsilon| dx dk &\leq \sqrt{\int_{|(x,k)|<2} dx dk} \sqrt{\int_{|(x,k)|<2} |f_0^\varepsilon - W_0^\varepsilon|^2 dx dk} \leq \\ &\leq C \|f_0^\varepsilon - W_0^\varepsilon\|_{L^2}, \end{aligned}$$

and therefore

$$\|W_0^\varepsilon - f_0^\varepsilon\|_{L^1} \leq O(\varepsilon^\infty) + C \|f_0^\varepsilon - W_0^\varepsilon\|_{L^2} = o(1).$$

Moreover,

$$\begin{aligned} \|f_0^\varepsilon - [W_0^\varepsilon]\|_{L^1} &\leq C \delta_x^{-1} \delta_k^{-1} \int_{|x|<CR} |w(\frac{x}{\delta_x}, \frac{k}{\delta_k})| dx dk = \\ (4.4) \quad &= \int_{|x|<C\frac{R}{\delta_x}} |w(x, k)| dx dk \leq C \delta_x^{-1} R = o(1). \end{aligned}$$

The proof of the claim is complete.

This means that ρ_2^ε and ρ_1^ε (the evolution under equation (2.8) of $[W_0^\varepsilon]$, W_0^ε respectively) are interchangeable for our purposes, since

$$\langle \rho_1^\varepsilon, \phi \rangle = \langle \rho_2^\varepsilon, \phi \rangle + \langle \rho_1^\varepsilon - \rho_2^\varepsilon, \phi \rangle$$

and

$$|\langle \rho_1^\varepsilon - \rho_2^\varepsilon, \phi \rangle| \leq \|\rho_1^\varepsilon - \rho_2^\varepsilon\|_{L^1} \|\phi\|_{L^\infty} \leq \|W_0^\varepsilon - [W_0^\varepsilon]\|_{L^1} \|\phi\|_{\mathcal{A}}.$$

(We used the obvious bound $\|\phi\|_{L^\infty} \leq \|\phi\|_{\mathcal{A}} = \int \sup_x |\mathcal{F}_{k \rightarrow K}[\phi(x, k)]| dK$).

In particular, this means we can always work with $|x| > CR$, since ρ_2^ε stays outside of $\{|x| < CR\}$ by construction. This allows certain ODEs we will use to be well-posed. Without loss of generality we will work for $x > 0, k > 0$ (working with $k < 0$ makes no difference other than the opposite sign in the explicit expression for $K(0)$ in equation (4.5), the case $x < 0$ follows by symmetry). Denote by $X(t), K(t)$ the unique solution of

$$(4.5) \quad \begin{aligned} \dot{X}(t) &= 2\pi K(t), & \dot{K}(t) &= \frac{1+\theta}{2\pi} (X(t))^\theta, \end{aligned}$$

$$X(0) = CR, \quad K(0) = |X(0)|^{\frac{1+\theta}{2}},$$

i.e. the only branch of the level set of $\{2\pi^2 k^2 + V(x)\} = 0$ in $\{x > R \wedge k > 0\}$.

The interesting property of this trajectory is that, unlike what happens with regular potentials, it leaves zero in finite time (more generally, i.e. without restricting to $\{x > R \wedge k > 0\}$, it reaches *and* leaves zero in finite time).

Claim: *We will show that any characteristic of the Liouville equation (2.8) starting in $\{x > R \wedge k > 0\} \cap \text{supp}[W_0^\varepsilon]$ converges to $X(t), K(t)$ defined in equation (4.5).*

Then it follows that

$$\chi_{x>0}(x, k)[W_0^\varepsilon] \rightharpoonup \int \chi_{x>0}(x, k)[W_0^\varepsilon] dx dk \delta(x - X(t), k - K(t)).$$

Repeating the argument for $x < 0$ gives a limit of two delta functions leaving zero along different trajectories.

Proof of the claim: Denote by $X_1(t), K_1(t)$ the solution of

$$(4.6) \quad \begin{aligned} \dot{X}_1(t) &= 2\pi K_1(t), & \dot{K}_1(t) &= -\frac{1}{2\pi} \partial_x \tilde{V}^\gamma(X_1(t)), \\ X_1(0) &= x_0, & K_1(0) &= k_0, \end{aligned}$$

where of course $(x_0, k_0) \in \{x > R \wedge k > 0\} \cap \text{supp}[W_0^\varepsilon]$ are as in the statement of the claim). Then equation (4.6) can be recast as

$$(4.7) \quad \begin{aligned} \dot{X}_1(t) &= 2\pi K_1(t), & \dot{K}_1(t) &= -\frac{1}{2\pi} V_x(X_1(t)) - \frac{1}{2\pi} (\partial_x \tilde{V}^\gamma(X_1(t)) - V_x(X_1(t))), \\ X_1(0) &= x_0, & K_1(0) &= k_0. \end{aligned}$$

Here we use the estimate $|\partial_x \tilde{V}^\gamma(X_1(t)) - V_x(X_1(t))| \leq CR^{\theta-1} \varepsilon^{\frac{\gamma}{2}} = o(1)$ (see lemma 6.2 with $V'(x)$ in the place of f). It is clear now that any such characteristic converges to

$$(4.8) \quad \begin{aligned} \dot{X}_2(t) &= 2\pi K_2(t), & \dot{K}_2(t) &= -\frac{1}{2\pi} V_x(X_2(t)), \\ X_2(0) &= x_0, & K_2(0) &= k_0. \end{aligned}$$

To conclude observe that trajectory $X_2(t), K_2(t)$ is squeezed between two level sets of $2\pi^2 k^2 + V(x)$ converging to each other (namely between $\{2\pi^2 k^2 + V(x)\} = V(CR)$ and $\{2\pi^2 k^2 + V(x)\} = V(R^{\frac{1-\theta}{5}})$).

Essentially the same analysis applies to the example of lemma 5.4 as well.

4.2. Proof of Theorem 2.2. It will be helpful to recall the main objects we are going to use here. The WT for this problem, $W = W^\varepsilon(x, k, t)$, satisfies the well-known Wigner equation (1.5) with initial data W_0^ε . Moreover, W_1^ε and ρ_2^ε are defined as follows

$$(4.9) \quad \begin{cases} \partial_t W_1^\varepsilon + 2\pi k \cdot \partial_x W_1^\varepsilon + T_\varepsilon^{\tilde{V}^\gamma} W_1^\varepsilon = 0, \\ W_1^\varepsilon(t=0) = W_0^\varepsilon, \end{cases}$$

and ρ_2^ε ,

$$(4.10) \quad \begin{cases} \partial_t \rho_2^\varepsilon + 2\pi k \partial_x \rho_2^\varepsilon + T_0^{\tilde{V}^\gamma} \rho_2^\varepsilon = 0, \\ \rho_2^\varepsilon(t=0) = [W_0^\varepsilon], \end{cases}$$

Of course recall that ρ_1^ε was defined as the solution of equation (2.8) with initial data $\rho_1\varepsilon(t=0) = W_0^\varepsilon$.

We partition the proof as follows:

$$(4.11) \quad \begin{aligned} \|W^\varepsilon - \rho_1^\varepsilon\|_{L^2} &\leq \|W^\varepsilon - W_1^\varepsilon\|_{L^2} + \\ &+ \|W_1^\varepsilon - \rho_2^\varepsilon\|_{L^2} + \|\rho_1^\varepsilon - \rho_2^\varepsilon\|_{L^2} = o(1)\|W_0^\varepsilon\|_{L^2}. \end{aligned}$$

We will use without further comments the elementary observation

$$(4.12) \quad \left\| \int f(x-s, k)g(s)ds \right\|_{L^2(\mathbb{R}^{2n})} \leq \|g\|_{L^1(\mathbb{R}^n)} \|f\|_{L^2(\mathbb{R}^{2n})}$$

Lemma 4.1 ($W \approx W_1$). $\forall t \in [0, T]$

$$\|W_1^\varepsilon(t) - W^\varepsilon(t)\|_{L^2} = O(\varepsilon^{\gamma\frac{1+\theta}{2}-1}\|W_0^\varepsilon\|_{L^2}).$$

Proof: Denote

$$(4.13) \quad h^\varepsilon = W^\varepsilon - W_1^\varepsilon.$$

Obviously,

$$(4.14) \quad \begin{aligned} \partial_t h + 2\pi k \partial_x h + T \tilde{V}^\gamma h &= -T^{V-\tilde{V}^\gamma} W_1^\varepsilon, \\ h(x, k, 0) &= 0. \end{aligned}$$

Since the Wigner equation has a bounded L^2 propagator, it suffices to bound in L^2 the rhs. Indeed, we have

$$(4.15) \quad \begin{aligned} \|T^{V-\tilde{V}^\gamma} W_1^\varepsilon\|_{L^2} &= C \left\| \int \widehat{V}(S)(1 - e^{-\frac{\pi}{2}\varepsilon^\gamma S^2}) \widehat{W}_1^\varepsilon(X-S, K) \frac{\sin(\pi\varepsilon SK)}{\varepsilon} dS \right\|_{L^2} \leq \\ &\leq O(\varepsilon^{-1}) \|\widehat{V}(S)(1 - e^{-\frac{\pi}{2}\varepsilon^\gamma S^2})\|_{L^1} \|W_1^\varepsilon\|_{L^2} \leq \\ &\leq O(\varepsilon^{-1}) \|W_1^\varepsilon\|_{L^2} \left[\varepsilon^\gamma \int_{|S| \leq \varepsilon^{-\frac{\gamma}{2}}} |\widehat{V}(S)| |S|^2 dS + \int_{|S| \geq \varepsilon^{-\frac{\gamma}{2}}} |\widehat{V}(S)| dS \right] = \\ &= O(\varepsilon^{-1}) \|W_1^\varepsilon\|_{L^2} \left[\varepsilon^\gamma + \varepsilon^\gamma \int_{\rho \in (1, \varepsilon^{-\frac{\gamma}{2}})} \rho^{-\theta} d\rho + \int_{\rho \geq \varepsilon^{-\frac{\gamma}{2}}} \rho^{-2-\theta} d\rho \right] = \\ &= O(\varepsilon^{-1}) \|W_0^\varepsilon\|_{L^2} \left[\varepsilon^\gamma + \varepsilon^{\gamma[-\frac{1}{2}(1-\theta)+1]} + \varepsilon^{\gamma\frac{1+\theta}{2}} \right]. \end{aligned}$$

Asking that the remainder is small gives

$$\gamma > 1,$$

$$(4.16) \quad \gamma[-\frac{1-\theta}{2} + 1] > 1 \Leftrightarrow \gamma > \frac{2}{1+\theta},$$

$$\gamma \frac{1+\theta}{2} > 1 \Leftrightarrow \gamma > \frac{2}{1+\theta}.$$

So finally with the calibration $\gamma > \frac{2}{1+\theta}$ the proof of lemma 4.1 is complete.

Moreover:

Lemma 4.2 ($W_1 \approx \rho_2^\varepsilon$). $\forall t \in [0, T]$

$$(4.17) \quad \|W_1^\varepsilon(t) - \rho_2^\varepsilon(t)\|_{L^2} = O(\varepsilon^{\frac{\theta}{2+\theta}-\delta} \|W_0^\varepsilon\|_{L^2}).$$

Proof: It is straightforward to check that

$$(4.18) \quad \begin{aligned} \partial_t \widehat{W}_1^\varepsilon - 2\pi X \cdot \partial_K \widehat{W}_1^\varepsilon + 2 \int \widehat{V}^\gamma(S) \widehat{W}_1^\varepsilon(X - S, K) \frac{\sin(\pi \varepsilon S \cdot K)}{\varepsilon} dS &= 0, \\ \partial_t \widehat{\rho}_2^\varepsilon - 2\pi X \cdot \partial_K \widehat{\rho}_2^\varepsilon + 2\pi \int \widehat{V}^\gamma(S) \widehat{\rho}_2^\varepsilon(X - S, K) S \cdot K dS &= 0, \end{aligned}$$

and therefore, if $f = \widehat{W}_1^\varepsilon - \widehat{\rho}_2^\varepsilon$,

$$(4.19) \quad \begin{aligned} \partial_t f - 2\pi X \cdot \partial_K f + 2 \int \widehat{V}^\gamma(S) f(X - S, K) \frac{\sin(\pi \varepsilon S \cdot K)}{\varepsilon} dS &= \\ = 2 \int \widehat{V}^\gamma(S) \widehat{\rho}_2^\varepsilon(X - S, K) \left(1 - \frac{\sin(\pi \varepsilon S \cdot K)}{\pi \varepsilon S \cdot K}\right) \pi S \cdot K dS, \\ f(x, k, 0) &= W_0^\varepsilon - [W_0^\varepsilon]. \end{aligned}$$

Using the Duhamel formula,

$$(4.20) \quad \begin{aligned} \|f(t)\|_{L^2} &\leq \|W_0^\varepsilon - [W_0^\varepsilon]\|_{L^2} + \\ &+ 2T \sup_{t \in [0, T]} \left\| \int \widehat{V}^\gamma(S) \widehat{\rho}_2^\varepsilon(X - S, K, t) \left(1 - \frac{\sin(\pi \varepsilon S \cdot K)}{\pi \varepsilon S \cdot K}\right) \pi S \cdot K dS \right\|_{L^2}. \end{aligned}$$

Recall that the first term above is (relatively) small by assumption; we will work out the other term:

To bound that, first of all observe that

$$(4.21) \quad \left| \frac{\sin(\pi \varepsilon S \cdot K)}{\pi \varepsilon S \cdot K} - 1 \right| \leq C \min\{1, |\pi \varepsilon S \cdot K|\}$$

and therefore for any $b < 0$

(4.22)

$$\begin{aligned}
& \left\| \int \widehat{V}^\gamma(S) \widehat{\rho}_2^\varepsilon(X - S, K) \left(1 - \frac{\sin(\pi \varepsilon S \cdot K)}{\pi \varepsilon S \cdot K} \right) \pi S \cdot K dS \right\|_{L^2} \leq \\
& \leq C \varepsilon \left\| \int_{0 \leq |S| \leq 1} |\widehat{V}^\gamma(S)| \cdot |S|^2 |\widehat{\rho}_2^\varepsilon(X - S, K)| \cdot |K|^2 dS \right\|_{L^2} + \\
& \quad + \varepsilon^{1+2b} \left\| \int_{1 < |S| < \varepsilon^b} \widehat{V}^\gamma(S) \widehat{\rho}_2^\varepsilon(X - S, K) |K|^2 dS \right\|_{L^2} + \\
& \quad + \left\| \int_{|S| > \varepsilon^b} \widehat{V}^\gamma(S) \widehat{\rho}_2^\varepsilon(X - S, K) |SK| dS \right\|_{L^2} \leq \\
& \leq C \left(\varepsilon^{1+2b} \|\widehat{V}(S) \min\{|S|^2, 1\}\|_{L^1} \|\rho_2^\varepsilon\|_{H^2} + \int_{|S| > \varepsilon^b} |\widehat{V}^\gamma(S)| |S| dS \|\rho_2^\varepsilon\|_{H^1} \right) \leq \\
& \leq C \left(\varepsilon^{1+2b} \|\widehat{V} \frac{S^2}{1+S^2}\|_{L^1} \|\rho_2^\varepsilon\|_{H^2} + \int_{\rho=\varepsilon^b}^\infty \rho^{-1-\theta} d\rho \|\rho_2^\varepsilon\|_{H^1} \right) = \\
& = C \left(\varepsilon^{1+2b} \|\rho_2^\varepsilon\|_{H^2} + \varepsilon^{-\theta b} \|\rho_2^\varepsilon\|_{H^1} \leq C(\varepsilon^{1+2b-\delta} + \varepsilon^{-\theta b - \delta}) \|W_0^\varepsilon\|_{L^2} \right)
\end{aligned}$$

Calibrating the parameters is easy; we are given $\theta \in (0, 1)$, δ as in the statement of the theorem and we need to find $b \in (-\frac{1}{2}, 0)$ so that

$$\begin{aligned}
(4.23) \quad & 1 + 2b - \delta > 0, \quad -\theta b - \delta > 0 \Leftrightarrow \\
& \Leftrightarrow \frac{\delta-1}{2} < b < -\frac{\delta}{\theta}.
\end{aligned}$$

It should now be clear that the constraint on δ in statement of the theorem comes from the self-consistency check $-\frac{1}{2} < \frac{\delta-1}{2} < -\frac{\delta}{\theta} < 0$. The proof of lemma 4.2 is complete.

Now the last step is to show that $\rho_2^\varepsilon \approx \rho_1^\varepsilon$; but this follows by construction, since they satisfy the same equation (which has an L^2 -continuous propagator): $\|\rho_2^\varepsilon(t) - \rho_1^\varepsilon(t)\|_{L^2} = \|W_0^\varepsilon - [W_0^\varepsilon]\|_{L^2}$.

The proof of Theorem 2.2 is complete.

4.3. Proof of Theorem 2.3. One observes of course that, by construction,

$$|E^\varepsilon(\phi)| \leq \|\rho_1^\varepsilon(t) - W^\varepsilon(t)\|_{L^2} \|\phi\|_{L^2}.$$

This will be useful in situations when we use a test-function from $\mathcal{A} \cap L^2$.

Since in general there are $\phi \in \mathcal{A} \setminus L^2$, we will also use a variation of the space of test-functions \mathcal{A} introduced earlier: let

$$(4.24) \quad \mathcal{B} = \left\{ \phi \in C_0(\mathbb{R}^{2n}) \mid \int \sup_x |\mathcal{F}_{k \rightarrow K}[\phi(x, k)]| dK + \|\phi\|_{L^2} < \infty \right\}$$

equipped with the norm

$$(4.25) \quad \|\phi\|_{\mathcal{B}} = \|\phi\|_{\mathcal{A}} + \|\phi\|_{L^2}.$$

In particular, it is clear by construction that $\mathcal{B} \subseteq \mathcal{A}$, $\mathcal{A}' \subseteq \mathcal{B}'$, and $\|f\|_{L^2} \leq \|f\|_{\mathcal{B}}$, $\|f\|_{\mathcal{B}'} \leq \|f\|_{L^2}$. Moreover, one easily sees the following

Claim: There is $R > 0$ such that $\|W^\varepsilon - \rho_1^\varepsilon\|_{\mathcal{A}'} < R$.

Proof of the claim: Observe that

$$\begin{aligned} |\langle f, \phi \rangle_{\mathcal{A}', \mathcal{A}}| &= \left| \int_{x, K} \mathcal{F}_{k \rightarrow K}[f(x, k)] \overline{\mathcal{F}_{k \rightarrow K}[\phi(x, k)]} dx dK \right| \leq \\ &\leq \int_K \sup_x |\mathcal{F}_{k \rightarrow K}[\phi(x, k)]| \int_x |\mathcal{F}_{k \rightarrow K}[f(x, k)]| dx dK \leq \\ &\leq \int_K \sup_x |\mathcal{F}_{k \rightarrow K}[\phi(x, k)]| dK \sup_x \int_x |\mathcal{F}_{k \rightarrow K}[f(x, k)]| dx, \end{aligned}$$

i.e.

$$\|f\|_{\mathcal{A}'} \leq \sup_K \int_x \mathcal{F}_{k \rightarrow K}[f(x, k)] dx = \sup_K \int_x \left| \int_k e^{-2\pi i k K} f(x, k) dk \right| dx \leq \|f\|_{L^1}.$$

To conclude we use the singular value decomposition of the initial data: if $D_0^\varepsilon = \sum_m \lambda_m |u_m\rangle \langle u_m|$, then

$$W_0^\varepsilon = \sum_m \lambda_m \int e^{-2\pi i k y} u_m^\varepsilon(x + \frac{\varepsilon y}{2}) \overline{u_m^\varepsilon(x - \frac{\varepsilon y}{2})} dy,$$

and

$$W^\varepsilon(t) = \sum_m \lambda_m \int e^{-2\pi i k y} u_m^\varepsilon(x + \frac{\varepsilon y}{2}, t) \overline{u_m^\varepsilon(x - \frac{\varepsilon y}{2}, t)} dy,$$

where of course each of $u_m(t)$, $\|u_m\|_{L^2} = 1$, satisfies the Schrödinger equation (1.1). The point is that the singular values are time-independent and, especially for positive operators, are controlled by the trace:

$$D_0^\varepsilon > 0 \Rightarrow \lambda_m > 0 \quad \forall m \quad \Rightarrow \quad \text{tr}(D_0^\varepsilon) = \sum_m \lambda_m = \|\lambda_m\|_{l^1}.$$

We readily observe that

$$\sup_K \int_x |\mathcal{F}_{k \rightarrow K}[W^\varepsilon(x, k)]| dx = \sup_K \int_x \sum_m |\lambda_m u_m^\varepsilon(x + \frac{\varepsilon K}{2}) \overline{u_m^\varepsilon(x - \frac{\varepsilon K}{2})}| dx \leq \text{tr}(D_0^\varepsilon),$$

and of course

$$\|\rho_1^\varepsilon(t)\|_{L^1} = \|[W_0^\varepsilon]\|_{L^1}.$$

The proof of the claim is complete; it is obvious that $R \leq \text{tr}(D_0^\varepsilon) + \|[W_0^\varepsilon]\|_{L^1}$.

We will also use the following:

Claim: Let $\chi \in C^\infty(\mathbb{R}^{2n}, [0, 1])$ be a cutoff function, $\chi(z) = 1 \quad \forall |z| < 1$, $\chi(z) = 0 \quad \forall |z| > 2$, and denote $\phi_M(x, k) = \chi(\frac{(x, k)}{M})$. Then,

$$\|\phi_M\|_{L^2} \leq \frac{2^n \pi^{\frac{n}{2}}}{\Gamma(\frac{n}{2} + 1)} M^n \|\phi\|_{\mathcal{A}},$$

and

$$\lim_{M \rightarrow \infty} \|\phi_M - \phi\|_{\mathcal{A}} = 0.$$

Proof of the claim: First of all, $\chi(x, k) \in \mathcal{S}(\mathbb{R}^{2n}) \subseteq \mathcal{A}(\mathbb{R}^{2n})$. Moreover, keeping in mind that $\|\phi\|_{L^\infty} \leq \|\phi\|_{\mathcal{A}}$,

$$\|\phi_M\|_{L^2} \leq \|\phi\|_{L^\infty} \sqrt{\int_{|(x,k)| < 2M} dx dk} \leq \frac{2^n \pi^{\frac{n}{2}}}{\sqrt{\Gamma(n+1)}} M^n \|\phi\|_{\mathcal{A}}.$$

The second part, i.e.

$$\lim_{M \rightarrow \infty} \|\phi_M - \phi\|_{\mathcal{A}} = 0$$

follows e.g. from the density of $\mathcal{S}(\mathbb{R}^{2n})$ in \mathcal{A} [13]. Additional information on the decay of ϕ is needed in order to estimate more precisely the rate of convergence.

The proof of the claim is complete.

It is clear now how, given a $\phi \in \mathcal{A}$, we can select a family $\{\phi_M\} \subseteq \mathcal{B}$ such that $\|\phi_M - \phi\|_{\mathcal{A}} \rightarrow 0$ as $M \rightarrow \infty$. Moreover set for brevity

$$F(\varepsilon) = C(\varepsilon^\kappa \|W_0^\varepsilon\|_{L^2} + \|[W_0^\varepsilon] - W_0^\varepsilon\|_{L^2})$$

for some large enough $C > 0$. Now, recalling our remarks in the beginning of the section and the first claim, it follows that

$$\begin{aligned} |\langle W^\varepsilon - \rho_1^\varepsilon, \phi \rangle| &\leq |\langle W^\varepsilon - \rho_1^\varepsilon, \phi_M \rangle| + |\langle W^\varepsilon - \rho_1^\varepsilon, \phi_M - \phi \rangle| \leq \\ (4.26) \quad &\leq F(\varepsilon) \|\phi_M\|_{L^2} + (1 + \|W_0^\varepsilon\|_{L^1}) \|\phi_M - \phi\|_{\mathcal{A}} \leq \\ &\leq F(\varepsilon) \frac{2^n \pi^{\frac{n}{2}}}{\sqrt{\Gamma(n+1)}} M^n + (1 + \|W_0^\varepsilon\|_{L^1}) \|\phi_M - \phi\|_{\mathcal{A}} \quad \forall \varepsilon, M. \end{aligned}$$

The proof is completed by selecting, for each value of ε a “small enough” M , so that $M = M(\varepsilon) \rightarrow \infty$, and

$$\lim_{\varepsilon \rightarrow 0} F(\varepsilon) \|\phi_{M(\varepsilon)}\|_{L^2} = 0.$$

In the statement of the Theorem, the calibration $M = F(\varepsilon)^{-\frac{1}{2n}}$ is used; it follows that $\|\phi_{M(\varepsilon)}\|_{L^2} \leq \frac{2^n \pi^{\frac{n}{2}}}{\sqrt{F(\varepsilon) \Gamma(n+1)}}$.

The proof is complete.

5. EXAMPLES

In this section we isolate a subset of the assumptions of Theorems 2.2, 2.3 and construct some non-trivial examples for which they are satisfied. Essentially these are “graceful degradation” properties for the flow. The remaining assumptions, which we don’t check explicitly, are much simpler to check (regularity of the potential and initial data, finite energy etc).

5.1. Examples for Theorem 2.2. Here we are concerned with Cauchy problems for the Liouville equation,

$$\begin{cases} \partial_t \rho_1^\varepsilon + 2\pi k \partial_x \rho_1^\varepsilon - \frac{1}{2\pi} \partial_x \widetilde{V}^\gamma \cdot \partial_x \rho_1^\varepsilon = 0, \\ \rho_1^\varepsilon(t=0) = W_0^\varepsilon, \end{cases}$$

which have the following

Property 1. *There exist $T > 0$, $\delta \in (0, \frac{\theta}{2+\theta})$ and $[W_0^\varepsilon] \in H^2(\mathbb{R}^{2n})$ such that*

$$(5.1) \quad \|[W_0^\varepsilon] - W_0^\varepsilon\|_{L^2} = o(1) \|W_0^\varepsilon\|_{L^2}$$

and the solution of

$$(5.2) \quad \begin{cases} \partial_t \rho_2^\varepsilon + 2\pi k \partial_x \rho_2^\varepsilon - \frac{1}{2\pi} \partial_x \widetilde{V}^\gamma \cdot \partial_x \rho_2^\varepsilon = 0, \\ \rho_2^\varepsilon(t=0) = [W_0^\varepsilon], \end{cases}$$

satisfies

$$(5.3) \quad \|\rho_2^\varepsilon(t)\|_{H^2} = O(\varepsilon^{-\delta} \|W_0^\varepsilon\|_{L^2}), \quad \text{uniformly for } t \in [0, T].$$

We treat κ, γ as given parameters; of course when checking the property in the context of Theorem 2.3 they are controlled by the statement of Theorem 2.2.

Lemma 5.1. *Let $\theta \in (0, 1)$, $\delta \in (0, \frac{\theta}{2+\theta})$, $n = 2$, $V(x) = -|x|^{1+\theta}$ with an appropriate smooth cutoff outside $\{|x| < 2\}$. Assume moreover that there exists a function of compact support $w \in H^2(\mathbb{R}^4) \cap L^\infty$, such that*

$$(5.4) \quad W_0^\varepsilon(x, k) = \delta_x^{-2} \delta_k^{-2} w\left(\frac{x - (z_1, z_2)}{\delta_x}, \frac{k - (z_3, z_4)}{\delta_k}\right),$$

with $(z_1, z_2) = -L(z_3, z_4)$ (i.e. the wavepacket is “shot towards zero”). $\|w\|_{H^2}$, $\|w\|_{L^\infty}$, $|z|$ have to be bounded uniformly in ε , $\|w\|_{H^2}$, $\|w\|_{L^\infty}$, $|z| = O(1)$; other than that w and z can be allowed to depend on ε .

The small parameters involved $\delta_x, \delta_k, R = o(1)$ are calibrated as follows:

$$R = \left(\log \left(\frac{1}{\varepsilon} \right) \right)^{-\frac{1}{3}},$$

as in equation (6.26), and

$$(5.5) \quad \begin{aligned} \delta_x^{-1} (R + \delta_k) &= o(1), \\ (\delta_x + \delta_k)^{-2} (\delta_k + R)^{-2} &= O(\varepsilon^{-\frac{\delta}{2}}). \end{aligned}$$

Then Property 1 is satisfied.

Remarks:

- In fact it follows from the lemma that property 1 holds for *any* $\delta \in (0, \frac{\theta}{2+\theta})$.
- The difficulties arise from the non-smoothness at zero, and the details of a smooth behaviour away from zero are irrelevant here. So we will work for a small enough time, before any trajectory starting in a neighbourhood of zero reaches the support of the cutoff function. Therefore, to keep the presentation simple, we will not introduce any explicit treatment of the cutoff function. This approach is followed in the sequel as well.
- It is obviously much easier to work if the wavepacket is not “shot towards zero”. However in that case it’s basically covered by the standard theory; the interesting cases are when in the limit a delta function passes over a set where the flow associated with the original potential $V(x)$ doesn’t exist.
- An example of a scaling satisfying the above constraints is $\delta_x = \sqrt{\delta_k} = \sqrt{R}$.

Proof: Assume without loss of generality that $z = (0, -L, 0, 1)$. Consider $\phi : \mathbb{R} \rightarrow [0, 1]$ to be a C^∞ function such that

$$(5.6) \quad \begin{aligned} \phi(x) &= 0, & |x| < \frac{1}{2}, \\ \phi(x) &= 1, & |x| > 1. \end{aligned}$$

The modified initial data $[W_0^\varepsilon]$ is selected as

$$(5.7) \quad [W_0^\varepsilon](x, k) = W_0^\varepsilon(x, k) \phi \left(\frac{|x_1|}{R + 2L\delta_k} \right).$$

The key claim is that ρ_2^ε never touches $\{|x| < R\}$. Indeed $[W_0^\varepsilon]$ has two disjointly supported components. The calibration of the parameters and the cut-off is such that, if $[W_0^\varepsilon]$ was propagated by a Liouville equation corresponding to $V(x) = 0$, each of the components would stay on either side of the strip $\{|x_1| < R\}$ (see Figure 2). The idea is that since there is a potential driving the flow *away* from $x = 0$, the claim follows. (In fact it is slightly more complicated for this case, since the potential depends on x_2 as well: one easily gets an $O(1)$ upper bound for the time it takes for the trajectories to reach $x_2 = 0$, and then checks that in this longer time, x_1 doesn’t have the time to change sign. The difference is an $O(1)$ factor which we absorb in C below).

Therefore, in this problem we can take $\tilde{V}_{eff}^\gamma(x) = \tilde{V}^\gamma(x) \phi \left(\frac{|x|}{R + CL\delta_k} \right)$. Now for condition (5.3), making use of observation 6.6 (enlarging the cut-off area in fact strengthens observation 6.6, i.e. substituting $R + 2L\delta_k$ for R is painless) and lemma 6.4 it follows that

$$(5.8) \quad \begin{aligned} \|\rho_2^\varepsilon(t)\|_{H^2} &\leq \| [W_0^\varepsilon] \|_{H^2} \varepsilon^{-\frac{\delta}{2}} \leq C \| W_0^\varepsilon \|_{H^2} \varepsilon^{-\frac{\delta}{2}} (\delta_k + R)^{-2} = \\ &= C \| W_0^\varepsilon \|_{L^2} (\delta_x + \delta_k)^{-2} (\delta_k + R)^{-2} \varepsilon^{-\frac{\delta}{2}}, \end{aligned}$$

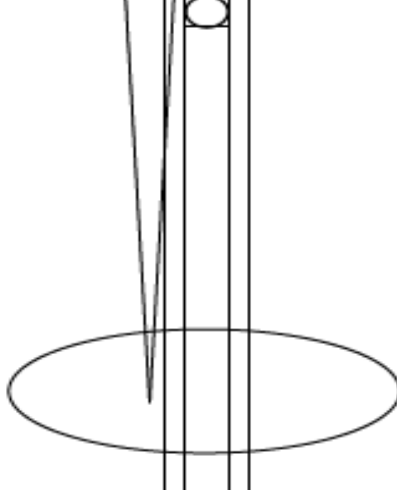


FIGURE 2. Any trajectory leaving the support of $[W_0^\varepsilon]$ has an initial velocity in a small cone around $k = (0, 1)$. If we were in free space, there wouldn't be enough space for sufficient movement in x_1 to reach $\{|x_1| < R\}$. Therefore the solution is the sum of two components, supported on either side of $\{|x_1| < R\} = 0$. The presence of a repulsive potential in many cases can be easily factored in this construction.

and therefore – using the scaling of equation (5.5) – $\|\rho_2^\varepsilon(t)\|_{H^2} = O(\varepsilon^{-\delta}\|W_0^\varepsilon\|_{L^2})$.

Now for $W_0^\varepsilon - [W_0^\varepsilon]$:

$$\begin{aligned}
 & \|W_0^\varepsilon - [W_0^\varepsilon]\|_{L^2}^2 \leq \\
 & \leq \delta_x^{-2n} \delta_k^{-2n} \int_{|x_1| < C(R+\delta_k)} |w(\frac{(x_1, x_2)}{\delta_x}, \frac{(k_1-1, k_2)}{\delta_k})|^2 dx dk = \\
 (5.9) \quad & = \delta_x^{-n} \delta_k^{-n} \int_{|x_1| < C\frac{R+\delta_k}{\delta_x}} |w(x_1, x_2, k_1 - 1, k_2)|^2 dx dk \leq \\
 & \leq C \|W_0^\varepsilon\|_{L^2}^2 \|w\|_{L^\infty}^2 \delta_x^{-1} (R + \delta_k)
 \end{aligned}$$

The same idea can be applied to different configurations:

Lemma 5.2. *Consider the setup of lemma 5.1 with $z = (0, -2, 0, 1)$ and the only difference that*

$$(5.10) \quad V(x) = -|x_1|^{1+\theta} \psi(x_1) \psi(x_2).$$

where ψ is a smooth cutoff function, $\psi = 1 - \phi \in \mathcal{S}(\mathbb{R})$ (ϕ was defined in equation (5.6)).

Then Property 1 holds.

Proof: The geometry is essentially the same as before, and it is clear that the obvious adaptation of observation 6.6, i.e. the one with

$$\widetilde{V}_{eff}^\gamma(x) = \widetilde{V}^\gamma(x) \phi\left(\frac{x_1}{R + C\delta_k}\right)$$

holds.

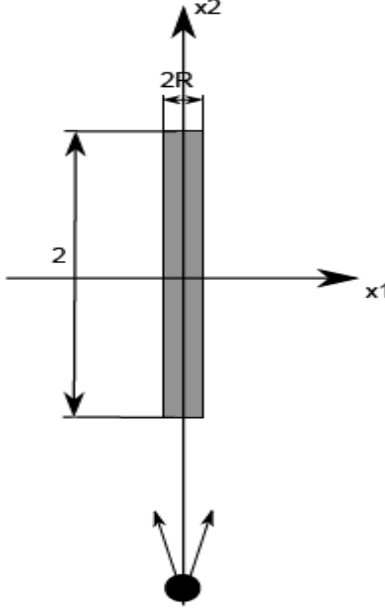


FIGURE 3. The construction of lemma 5.1 holds, with obvious adjustments, to the example of lemma 5.2.

5.2. Examples for Theorem 2.3. In relation to Theorem 2.3, we introduce

Property 2. *Given $V(x)$, W_0^c with $\|W_0^\varepsilon\|_{L^2} = o(\varepsilon^{-\kappa})$, there exist $T > 0$, $\delta \in (0, \frac{\theta}{2+\theta})$ and $[W_0^\varepsilon] \in H^2(\mathbb{R}^{2n})$ such that*

$$(5.11) \quad \|[W_0^\varepsilon] - W_0^\varepsilon\|_{L^2} = o(1)$$

and the solution of

$$(5.12) \quad \begin{cases} \partial_t \rho_2^\varepsilon + 2\pi k \partial_x \rho_2^\varepsilon - \frac{1}{2\pi} \partial_x \widetilde{V}^\gamma \cdot \partial_x \rho_2^\varepsilon = 0, \\ \rho_2^\varepsilon(t=0) = [W_0^\varepsilon], \end{cases}$$

satisfies

$$(5.13) \quad \|\rho_2^\varepsilon(t)\|_{H^2} = O(\varepsilon^{-\delta} \|W_0^\varepsilon\|_{L^2}), \quad \text{uniformly for } t \in [0, T].$$

As was already seen in section 4.1, $\|f_0^\varepsilon - f_0^\varepsilon * (\frac{2}{\varepsilon})^n e^{-2\pi\frac{x^2+k^2}{\varepsilon}}\|_{L^2} = o(1)$. So without loss of generality we can check Property 2 in the context of Theorem 2.1 considering initial data of the form f_0^ε , and not the smoothed version that appears there. (More generally, working with compactly supported initial data – and hence removing the smoothing – might be very helpful whenever we check Properties 1, 2. In any case, we expect that the smoothing can be removed without loss of generality, just like in this case, whenever the initial data decays rapidly and $\|W_0^\varepsilon\|_{H^1} = o(\varepsilon^{-\frac{1}{2}})$).

Lemma 5.3. *Let $n = 1$, $\theta \in (0, 1)$, $V(x) = -|x|^{1+\theta}$ with an appropriate smooth cutoff outside $\{|x| < 2\}$. Assume moreover that $w(x, k) \in H^2 \cap L^\infty \cap L^1$, $\text{supp } w \subseteq \{|x|, |k| < 1\}$, and*

$$(5.14) \quad f_0^\varepsilon = \delta_x^{-1} \delta_k^{-1} w\left(\frac{x}{\delta_x}, \frac{k}{\delta_k}\right).$$

Finally, set $R = (\log(\frac{1}{\varepsilon}))^{-\frac{1}{3}}$.

Then Property 2 is satisfied if $\delta_k = C'R^{\frac{1+\theta}{2}}$, $\delta_x = C''R^{\frac{1-\theta}{5}}$.

Proof: We will cutoff a strip of the form $\{|x| \leq CR\}$, and show that in fact this suffices.

As is illustrated in Figure 5.2, the preimage under the flow of $\{|x| < R \wedge |k| < \delta_k\}$ is contained between the level sets $\{2\pi^2 k^2 - \tilde{V}^\gamma(x) = \tilde{V}^\gamma(0)\}$ and $\{2\pi^2 k^2 + \tilde{V}^\gamma(x) = \tilde{V}^\gamma(R)\}$.

A big help with the algebra will be to approximate $\tilde{V}^\gamma(x) = -|x|^{1+\theta} + O(\varepsilon^{\frac{\gamma}{2}})$. (γ is as in the statement of Theorem 2.2). Since all the other small parameters are (negative) powers of $\log(\frac{1}{\varepsilon})$, $O(\varepsilon^{\frac{\gamma}{2}})$ is negligible everywhere. (The justification is that without loss of generality we can localize the problem on a compact set, and then $V(x) \in W^{1,\infty}$ uniformly in ε , see lemma 6.5. The conclusion follows by a standard observation on mollifiers, see lemma 6.2).

It is easily seen that the needed length is x_* , defined by

$$2\pi^2 \delta_k^2 + \tilde{V}^\gamma(x_*) = \tilde{V}^\gamma(R)$$

or

$$|x_*|^{1+\theta} = 2\pi^2 \delta_k^2 + R^{1+\theta} + O(\varepsilon^{\frac{\gamma}{2}}).$$

Here is where $\delta_k = C'R^{\frac{1+\theta}{2}}$ comes from; making that scaling we get $x_* = ((1 + 2\pi^2)R^{1+\theta} + O(\varepsilon^{\frac{\gamma}{2}}))^{\frac{1}{1+\theta}} = C'R$.

So far we have ensured by construction that, if $\delta_k = R^{\frac{1+\theta}{2}}$, (there is an $O(1)$ constant C so that) if

$$(5.15) \quad [W_0^\varepsilon](x, k) = f_0^\varepsilon(x, k) \phi\left(\frac{x}{CR}\right),$$

its propagation under equation (5.12) will never enter $\{|x| < R\}$.

Now for the approximation error:

$$\begin{aligned}
 (5.16) \quad \|f_0^\varepsilon - [W_0^\varepsilon]\|_{L^2}^2 &\leq C\delta_x^{-2}\delta_k^{-2} \int_{|x| < CR} |w(\frac{x}{\delta_x}, \frac{k}{\delta_k})|^2 dx dk = \\
 &= C\delta_x^{-1}\delta_k^{-1} \int_{|x| < C\frac{R}{\delta_x}} |w(x, k)|^2 dx dk \leq C\delta_x^{-2} R^{\frac{1-\theta}{2}}.
 \end{aligned}$$

This gives the constraint $R^{\frac{1-\theta}{4}} = o(\delta_x)$ for the error to be small, which is satisfied e.g. by our earlier selection $\delta_x = CR^{\frac{1-\theta}{5}}$.

Again, since all the small parameters are powers of $\log(\frac{1}{\varepsilon})$, $\|[W_0^\varepsilon]\|_{H^2} = o(\varepsilon^{-\frac{\delta}{2}})$ follows automatically for any $\delta \in (0, \frac{\theta}{2+\theta})$.

The proof is complete.

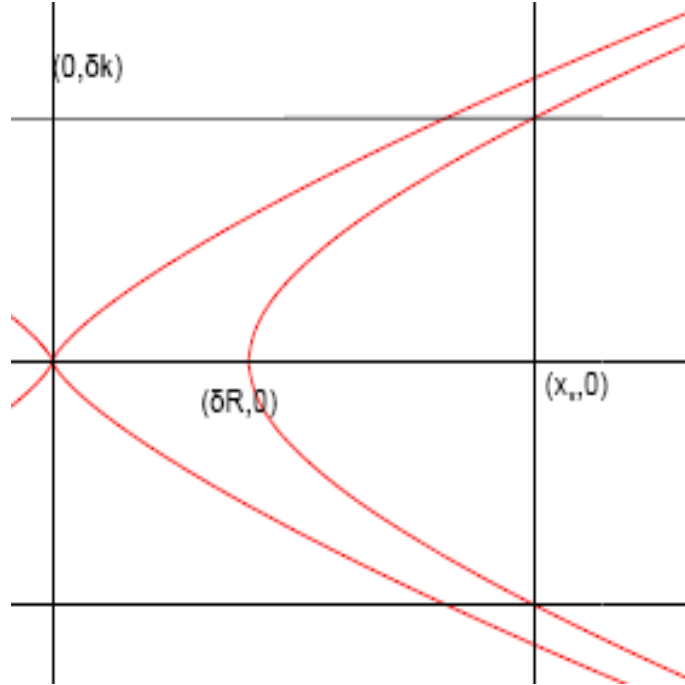


FIGURE 4. Schematic for lemma 5.3; cutting off a strip in x , $\{|x| < x_*\}$, suffices to cut off the preimage of $\{|x| < R\}$

The following is a somewhat artificial example, but it highlights an interesting behaviour.

Lemma 5.4. *Assume $n = 2$, V as in equation (5.10). Moreover, there is a function $f \in \mathcal{S}(\mathbb{R}^4)$, $\int f(x, k) dx dk = 1$, such that*

$$(5.17) \quad \text{supp } f \subseteq \{|x| < 1\} \times \{|k| < 1 \wedge k_1 > 0\}.$$

Denote by \bar{f}

$$(5.18) \quad \bar{f}(x_1, x_2, k_1, k_2) = f(-x_1, x_2, -k_1, k_2)$$

Now take

$$(5.19) \quad W_0^\varepsilon(x, k) = \frac{1}{\delta_x^2 \delta_k^2} \left(c_1 f\left(\frac{x_1 - 2R, x_2 + 2}{\delta_x}, \frac{k_1, k_2 + 1}{\delta_k}\right) + c_2 \bar{f}\left(\frac{x_1 - 2R, x_2 + 2}{\delta_x}, \frac{k_1, k_2 + 1}{\delta_k}\right) \right).$$

If $\delta_k = C' \delta_x = C'' \sqrt{R}$, this problem has Property 2.

Proof: Two things should be obvious by construction: that $W_0^\varepsilon \rightarrow \delta(x + (0, 2), k - (0, 1))$, and that the propagation of W_0^ε under equation (2.8), i.e. ρ_1^ε , is never supported inside $\{|x_1| < R\}$. In other words, for this specifically constructed data, $W_0^\varepsilon = [W_0^\varepsilon]$.

The scaling of δ_x, δ_k in this case controls simply the rate of concentration, and therefore $\|W_0^\varepsilon\|_{H^2}$. The result follows.

6. AUXILIARY RESULTS

Lemma 6.1 (2^{nd} order derivatives equations for the Liouville equation). *Consider the Cauchy problem for the Liouville equation with potential $V(x)$ on \mathbb{R}^n ,*

$$(6.1) \quad \begin{aligned} f_t + 2\pi k \nabla_x f - \frac{1}{2\pi} \nabla_x V(x) \nabla_k f &= 0, \\ f(t=0) &= f_0. \end{aligned}$$

There are constants $C_1, C_2 > 0$ depending only on n such that

$$\|f(t)\|_{H^2} \leq C_1 e^{C_2 \sup_{|a| \leq 3} \|\partial_x^a V(x)\|_{L^\infty}} \|f_0\|_{H^2}.$$

Proof: The proof follows readily with the method of characteristics.

It suffices to observe that if

$$(6.2) \quad \dot{x}_i(t) = 2\pi k_i(t), \quad \dot{k}_i(t) = -\frac{1}{2\pi} \partial_{x_i} V(x(t)),$$

$$(6.3) \quad \begin{aligned} z(t) &= f(x(t), k(t)), \\ z_{x_i}(t) &= \partial_{x_i} f(x(t), k(t)), \quad z_{x_i x_j}(t) = \partial_{x_i x_j} f(x(t), k(t)), \\ z_{k_i}(t) &= \partial_{k_i} f(x(t), k(t)), \quad z_{k_i k_j}(t) = \partial_{k_i k_j} f(x(t), k(t)), \\ z_{x_i k_j}(t) &= \partial_{x_i k_j} f(x(t), k(t)), \end{aligned}$$

it follows that

$$(6.4) \quad \dot{z} = 0$$

$$(6.5) \quad \dot{z}_{x_i}(t) = \frac{1}{2\pi} \sum_m \partial_{x_i x_m} V(x(t)) z_{x_i k_m}(t),$$

$$(6.6) \quad \begin{aligned} \dot{z}_{k_i}(t) &= -2\pi z_{x_i}(t), \\ \dot{z}_{x_i x_j}(t) &= \end{aligned}$$

$$(6.7) \quad \frac{1}{2\pi} \sum_m [\partial_{x_j x_m} V z_{x_i k_m}(t) + \partial_{x_i x_m} V z_{x_j k_m}(t) + \partial_{x_i x_j x_m} V z_{k_m}(t)]$$

$$(6.8) \quad \dot{z}_{k_i k_j}(t) = -2\pi(z_{x_j k_i} + z_{x_i k_j}),$$

$$(6.9) \quad \dot{z}_{k_i x_j}(t) = -2\pi z_{x_i x_j}(t) + \frac{1}{2\pi} \sum_m \partial_{x_m x_j} V(x(t)) z_{k_m k_i}(t).$$

The result now follows by the Gronwall inequality.

Lemma 6.2. Consider a function $f \in W^{1,\infty}$, i.e. $\sup_{|a| \leq 1} \|\partial_x^a f\|_{L^\infty} < \infty$.

Then, if $\tilde{f} = \left(\frac{2}{\eta}\right)^{\frac{n}{2}} \int e^{-2\pi \frac{|x-x'|^2}{\eta}} f(x') dx'$, we have

$$(6.10) \quad \|f - \tilde{f}\|_{L^\infty} = O(\|f\|_{W^{1,\infty}} \sqrt{\eta}).$$

Proof: Take any $\zeta \in (0, \frac{1}{2})$. Now we have

$$(6.11) \quad \begin{aligned} |f(x) - \tilde{f}(x)| &= \left| \left(\frac{2}{\eta}\right)^{\frac{n}{2}} \int e^{-2\pi \frac{|x-x'|^2}{\eta}} [f(x-x') - f(x)] dx' \right| = \\ &= \left(\frac{2}{\eta}\right)^{\frac{n}{2}} \left| \int_{|x'| < \eta^{\frac{1}{2}-\zeta}} e^{-2\pi \frac{|x-x'|^2}{\eta}} [f(x-x') - f(x)] dx' \right| + O(\eta^\infty) \leq \\ &\leq C \|f\|_{W^{1,\infty}} \left(\frac{2}{\eta}\right)^{\frac{n}{2}} \int_{|x'| < \eta^{\frac{1}{2}-\zeta}} e^{-2\pi \frac{|x-x'|^2}{\eta}} |x'| dx' + O(\|f\|_{L^\infty} \eta^\infty) = \\ &= O(\sqrt{\eta} 2^{\frac{n}{2}}) \|f\|_{W^{1,\infty}} \int_{|y| < \eta^{-\zeta}} e^{-2\pi |y|^2} |y| dy + O(\|f\|_{L^\infty} \eta^\infty) = \\ &= O(\|f\|_{W^{1,\infty}} \sqrt{\eta}). \end{aligned}$$

The proof is complete.

Remark: A sharper version is used in subsection 4.1, namely

$$|f(x) - \tilde{f}(x)| \leq C \left(\sup_{\substack{|a|=1 \\ |x-x'| < \eta^{\frac{1}{2}-\zeta}}} |\partial_x^a f| \right) \left(\frac{2}{\eta} \right)^{\frac{n}{2}} \int_{|x'| < \eta^{\frac{1}{2}-\zeta}} e^{-2\pi \frac{|x'|^2}{\eta}} |x'| dx' + \\ + O(\|f\|_{L^\infty} \eta^\infty).$$

The following observations are used in Section 5:

Observation 6.3 (Locality of the Liouville equation). *For a Liouville equation with initial data of compact support ρ_0 and a $C^{1,1}$ potential, interchanging the potential with any one that coincides with it on the “path” of the solution,*

$$(6.12) \quad \mathbb{S} = \bigcup_{t \in [0, T]} \phi_t(\text{supp} \rho_0),$$

does not change the solution.

Also,

Lemma 6.4 (An H^2 estimate). *Consider equation (2.8) with initial data $\rho_0 = [W_0^\varepsilon] \in H^2$. Assume that there is a function \tilde{V}_{eff}^γ such that*

$$(6.13) \quad \tilde{V}^\gamma = \tilde{V}_{eff}^\gamma \quad \text{on } \mathbb{S},$$

where \mathbb{S} is defined as in (6.12), and

$$(6.14) \quad \sup_{|A| \leq 3} \|\partial_x^A \tilde{V}_{eff}^\gamma(x)\|_{L^\infty} = O\left(\log\left(\varepsilon^{-\frac{\delta}{2}}\right)\right),$$

Then,

$$(6.15) \quad \|\rho_2^\varepsilon\|_{H^2} = O\left(\varepsilon^{-\frac{\delta}{2}} \|W_0^\varepsilon\|_{H^2}\right).$$

Proof: The proof consists of using \tilde{V}_{eff}^γ in place of \tilde{V}^γ , making use of observation 6.3, and then applying directly theorem 6.1.

We will also use the following

Lemma 6.5. *It is easy to observe that, if $\nabla V \in L^\infty$ and $\text{supp} W_0^\varepsilon$ is compact, it follows that*

$$(6.16) \quad \exists M > 0 : \forall t \in [0, T], \varepsilon > 0 : \bigcup_{t \in [0, T]} \text{supp} \rho_1^\varepsilon(t) \subseteq \{|(x, k)| < M\}.$$

Observation 6.6 (\tilde{V}_{eff}^γ and R). Let $V(x) = -|x|^{1+\theta}$. \tilde{V}^γ is a mollified version, according to equation (2.6).

Consider $\phi : \mathbb{R}^n \rightarrow [0, 1]$ to be a C^∞ function such that

$$(6.17) \quad \begin{aligned} \phi(x) &= 0, & |x| &< \frac{1}{2}, \\ \phi(x) &= 1, & |x| &> 1, \end{aligned}$$

and $\|\phi\|_{W^{3,\infty}} \leq 10$. It is clear that such a function exists; this is of course an arbitrary requirement, but one that allows us not to carry the cutoff function ϕ to other results.

Then, setting $R \geq (\log(\varepsilon^{-1}))^{-\frac{1}{3}}$, $R = o(1)$, it follows that

$$(6.18) \quad \tilde{V}_{eff}^\gamma(x) := \phi\left(\frac{x}{R}\right) \tilde{V}^\gamma(x),$$

satisfies

$$(6.19) \quad \sup_{|A| \leq 3} \|\partial_x^A \tilde{V}_{eff}^\gamma(x)\|_{L^\infty} = O\left(\log\left(\varepsilon^{-\frac{\delta}{2}}\right)\right),$$

while, of course,

$$(6.20) \quad \tilde{V}_{eff}^\gamma = \tilde{V}^\gamma \text{ on } \mathbb{R}^n \setminus \{|x| < R\}.$$

Proof: Observe that $1 - \phi(x) = \psi(x) \in \mathcal{S}(\mathbb{R}^n)$. Moreover, making use of observations 6.5 and 6.3, we can restrict \tilde{V}^γ to $\{|x| < M\}$ without loss of generality,

$$(6.21) \quad \tilde{V}^\gamma(x) \mapsto \tilde{V}^\gamma(x) \left(1 - \phi\left(\frac{x}{2M}\right)\right).$$

Denote

$$(6.22) \quad \begin{aligned} \tilde{V}_{eff}^\gamma(x) &= \tilde{V}^\gamma(x) \left(1 - \phi\left(\frac{x}{2M}\right)\right) \phi\left(\frac{x}{R}\right) = \\ &= \tilde{V}^\gamma(x) \left(\psi\left(\frac{x}{2M}\right) - \psi\left(\frac{x}{R}\right)\right). \end{aligned}$$

Since

$$(6.23) \quad \|\partial_x^A \tilde{f}\|_{L^\infty} \leq \|\partial_x^A f\|_{L^\infty},$$

it suffices to work with

$$(6.24) \quad \partial_x^A |x|^{1+\theta} \left(\psi\left(\frac{x}{2M}\right) - \psi\left(\frac{x}{R}\right)\right).$$

Set $x' = \frac{x}{R}$; then $\partial_x = R^{-1}\partial_{x'}$. Now we have

$$\begin{aligned}
(6.25) \quad & \|\partial_x^A |x|^{1+\theta} (\psi(\frac{x}{2M}) - \psi(\frac{x}{R}))\|_{L^\infty} = \\
& = R^{\theta-2} \|\partial_x^A |x|^{1+\theta} (\psi(\frac{R}{2M}x) - \psi(x))\|_{L^\infty} \leq \\
& \leq R^{\theta-2} \sup_{|A| \leq 3} \|\partial_x^A |x|^{1+\theta}\|_{L^\infty([\frac{1}{2}, \frac{2M}{R}])} \sup_{|A| \leq 3} \|\partial_x^A (\psi(\frac{R}{2M}x) - \psi(x))\|_{L^\infty(\mathbb{R}^n)} \leq \\
& \leq (2M)^{1+\theta} \|\phi\|_{W^{3,\infty}} R^{-3}.
\end{aligned}$$

Recall that the constant M is chosen so that any trajectory leaving the support of the initial data doesn't not escape $\{|x| < M\}$ for $t \in [0, T]$. That is, to properly quantify it, one needs to consider initial data of compact support associated with the Liouville equation, and a time-scale T . Assuming that the initial data is supported in $\{|(x, k)| < R_0\}$, it is easy to check that one can set $M = R_0 + 1 + R_0 T + \|\nabla V(x)\|_{L^\infty} T^2$. So now for (6.19) to hold it suffices that

$$\frac{2^{1+\theta} (1 + R_0 + R_0 T + \|\nabla V(x)\|_{L^\infty} T^2)^{1+\theta} 10}{C \frac{\delta}{2}} R^{-3} \leq \log(\varepsilon^{-1})$$

The constant C comes from the $O(\cdot)$ of equation (6.19); it is clear that it can be chosen so that the constraint finally becomes $R \geq (\log(\varepsilon^{-1}))^{-\frac{1}{3}}$, which is satisfied by choosing

$$(6.26) \quad R = (\log(\varepsilon^{-1}))^{-\frac{1}{3}}.$$

The following is contained in [13]; we include here a brief mention for completeness:

Lemma 6.7 (Density matrices). *Let μ be a probability measure on \mathbb{R}^{2n} . Then*

$$W_0^\varepsilon(x, k) = \left(\frac{2}{\varepsilon}\right)^n \int e^{-2\pi i \frac{(x-x')^2 + (k-k')^2}{\varepsilon}} d\mu(x', k')$$

is the Wigner function of a density matrix, i.e. the corresponding operator D^ε is a positive trace-class operator with $\text{tr}(D^\varepsilon) = 1$.

Proof: We know that $\text{tr}(D^\varepsilon) = \int W^\varepsilon dx dk = 1$. Let us now look at positivity. To that end, observe that the integral kernel

$$K^\varepsilon(x, y) = \left(\frac{2}{\varepsilon}\right)^{\frac{n}{2}} \int_{x_0, k_0} e^{2\pi i \frac{k_0}{\varepsilon} (x-y)} e^{-\frac{\pi}{\varepsilon} [(x-x_0)^2 + (y-x_0)^2]} d\mu(x_0, k_0)$$

is the kernel of a positive operator. Indeed:

$$\int K^\varepsilon(x, y) u(x) \bar{u}(y) dx dy = \left(\frac{2}{\varepsilon}\right)^{\frac{n}{2}} \int_{x_0, k_0} |\langle e^{-2\pi i \frac{k_0}{\varepsilon} x + \frac{\pi}{\varepsilon} (x-x_0)^2}, u \rangle|^2 d\mu(x_0, k_0) \geq 0.$$

The proof is complete by observing that the Wigner function corresponding to the kernel ρ^ε is

$$\int e^{-2\pi iky} K^\varepsilon\left(x + \frac{\varepsilon y}{2}, x - \frac{\varepsilon y}{2}\right) dy = W_0^\varepsilon.$$

REFERENCES

- [1] L. Ambrosio, “Transport equation and Cauchy problem for BV vector fields”, (2004) *Invent. Math.* **158** 227–260
- [2] L. Ambrosio, A. Figalli, G. Friesecke, J. Giannoulis & T. Paul, “Semiclassical limit of quantum dynamics with rough potentials and well posedness of transport equations with measure initial data”, arXiv:1006.5388v1
- [3] A. Athanassoulis, N. J. Mauser & T. Paul, “Coarse-scale representations and Smoothed Wigner transforms”, (2008) *J. Math. Pures Appl.* **91** no.3 296–338
- [4] A. Athanassoulis & T. Paul, “Strong phase-space semiclassical asymptotics”, arXiv:1002.1371
- [5] A. Athanassoulis, T. Paul, F. Pezzotti & M. Pulvirenti, “Strong Semiclassical Approximation of Wigner Functions for the Hartree Dynamics”, arXiv:1009.0470
- [6] L. Ambrosio, G. Friesecke & J. Giannoulis, “Passage from quantum to classical molecular dynamics in the presence of Coulomb interactions” (2010) *Comm. PDE.* **35** no. 8 1490–1515
- [7] R. DiPerna & P.L. Lions, “Ordinary differential equations, transport theory and Sobolev spaces”, (1989) *Invent. Math.* **98** 511–547
- [8] A. Figalli, M. Ligabò & T. Paul, preprint
- [9] P. Gérard, “Mesures semi-classiques et ondes de Bloch” (1991) *Seminaire sur les Équations aux Dérivées Partielles*, 1990–1991 Ecole Polytechnique, Palaiseau, Exp. No. XVI, 19 pp.
- [10] P. Gérard, P. A. Markowich, N.J. Mauser & F. Poupaud, “Homogenization limits and Wigner transforms” (1997) *Comm. Pure Appl. Math.* **50** 323–379
- [11] S. Keraani, “Wigner measures dynamics in a Coulomb potential” (2005) *J. Math. Phys.* **46** 063512
- [12] A. E. Mohr, E. A. Riskin & R. E. Ladner, “Unequal Loss Protection: Graceful Degradation of Image Quality over Packet Erasure Channels Through Forward Error Correction”, (2000) *IEEE Journal on selected areas in Communications* **18** No. 6
- [13] P.-L. Lions & T. Paul, “Sur les mesures de Wigner”, (1993) *Rev. Mat. Iberoamericana* **9** No. 3 553–618
- [14] F. Macia, “High-frequency propagation for the Schroedinger equation on the torus” (2010) *J. Funct. Anal.* **258** 933–955
- [15] T. Paul, “Échelles de temps pour l’évolution quantique à petite constante de Planck”, *Séminaire X-EDP 2007–2008*, Publications de l’École Polytechnique (2008).
- [16] M. Pulvirenti, “Semiclassical expansion of Wigner functions”, (2006) *J. Mat. Phys.* **47** 052103

(A. Athanassoulis) CMLS, ÉCOLE POLYTECHNIQUE, 91128 PALAISEAU CEDEX, FRANCE
E-mail address: `agis.athanasoulis@math.polytechnique.fr`

(T. Paul) CNRS AND CMLS, ÉCOLE POLYTECHNIQUE, 91128 PALAISEAU CEDEX, FRANCE
E-mail address: `thierry.paul@math.polytechnique.fr`